



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 01:49 AM UTC

PDB ID : 5GOA / pdb_00005goa
EMDB ID : EMD-9529
Title : Cryo-EM structure of RyR2 in open state
Authors : Peng, W.; Wu, J.P.; Yan, N.
Deposited on : 2016-07-26
Resolution : 4.20 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

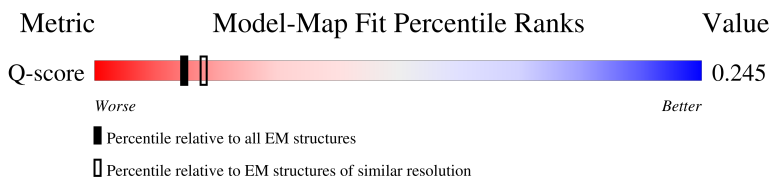
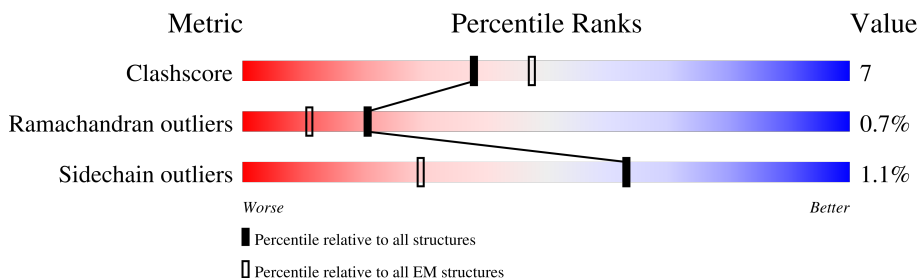
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	4968	14% 52% 15% • 31%
1	B	4968	14% 52% 15% • 31%
1	C	4968	14% 52% 15% • 31%
1	D	4968	14% 52% 16% • 31%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 105072 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called RyR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3423	Total	C	N	O	S	0	0
			26267	16741	4498	4874	154		
1	B	3423	Total	C	N	O	S	0	0
			26267	16741	4498	4874	154		
1	C	3423	Total	C	N	O	S	0	0
			26267	16741	4498	4874	154		
1	D	3423	Total	C	N	O	S	0	0
			26267	16741	4498	4874	154		

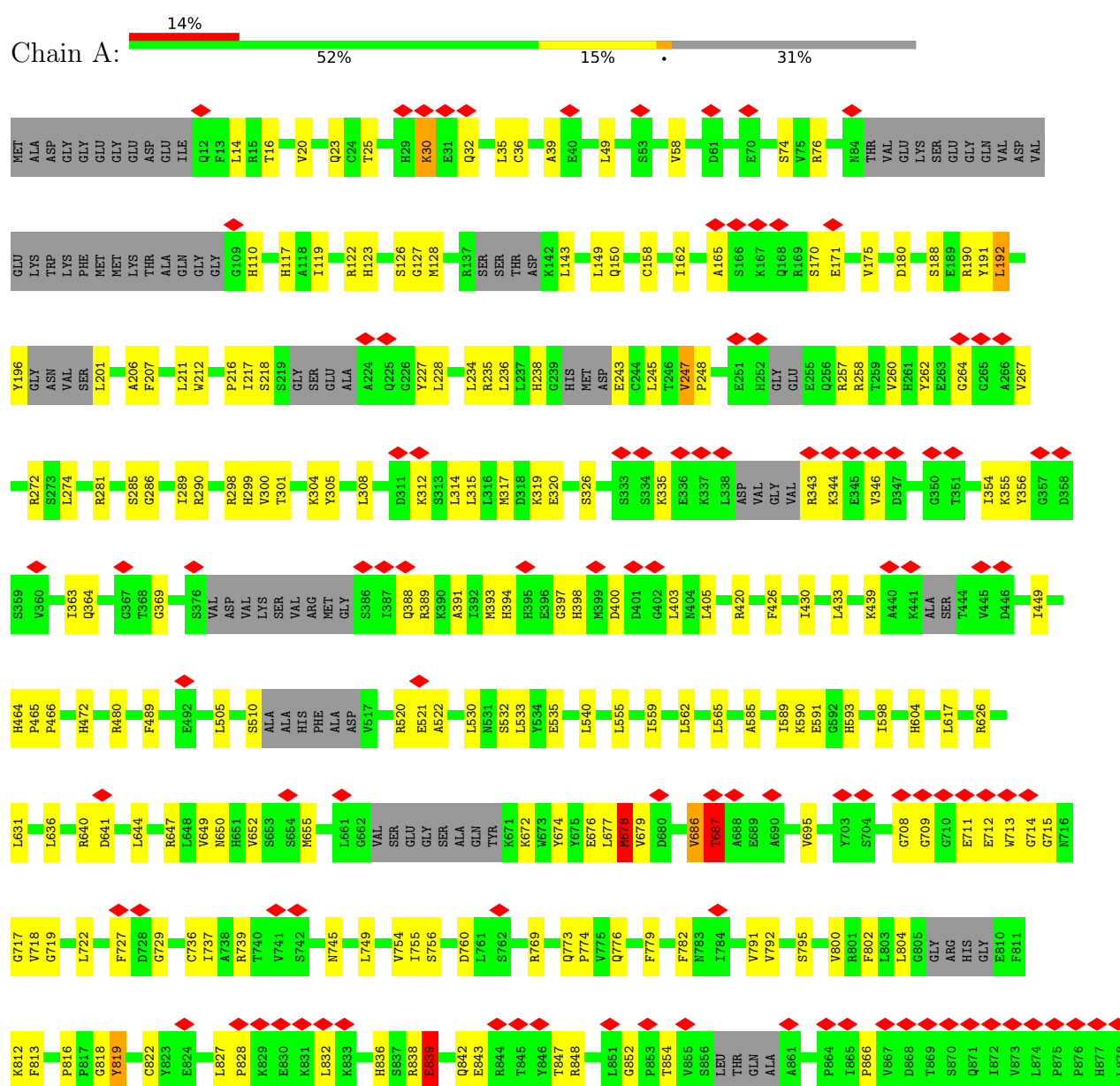
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

3 Residue-property plots

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

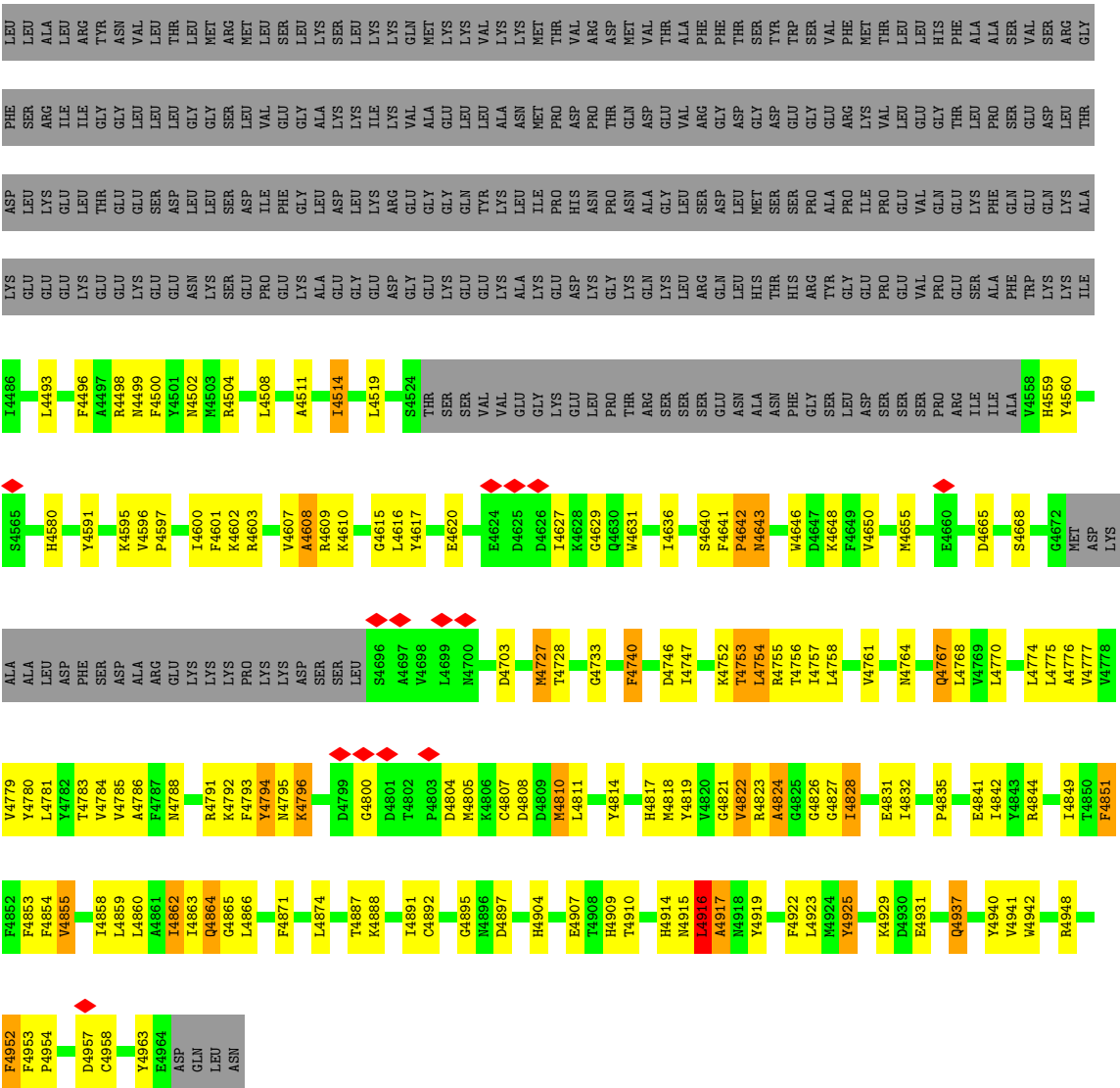
• Molecule 1: RyR2



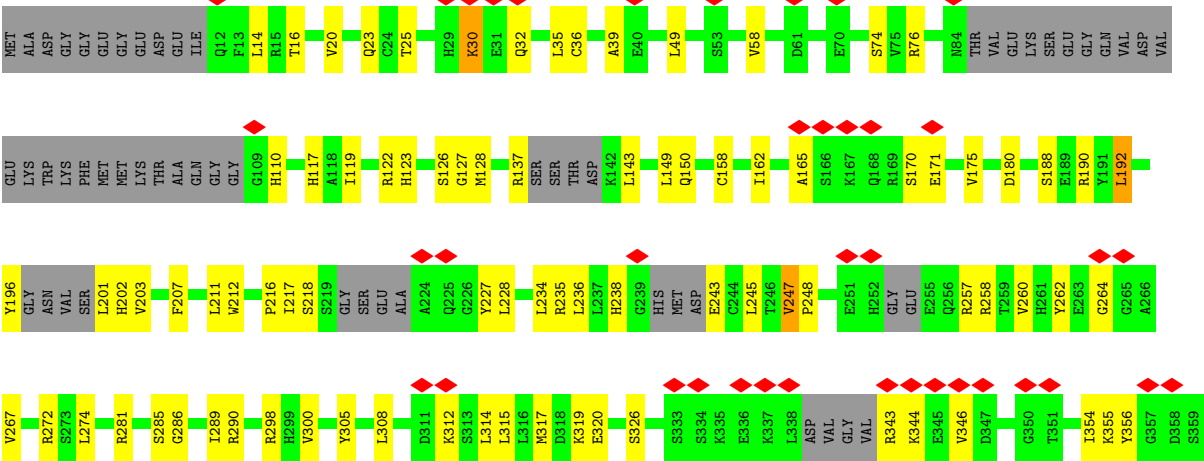
ALA	ALA	THR	E1763	V1664	Q1581	M1487	ASP	GLY	SER	S1186	GLU	GLY	E879
LEU	LEU	LEU	S1764	A1666	P1584	V1488	ASP	HIS	PRO	G1187	R1084	ILE	R880
THR	THR	LYS	S1767	A1665	R1585	C1489	ARG	LEU	CYS	S1188	R1085	GLN	I381
ALA	ALA	GLU	F1768	N1669	L1586	GLY	ASP	PRO	LYS	E1189	F1086	ASP	R882
ARG	ARG	PRO	V1769	N1669	H1587	SER	TYR	ASP	ARG	L1190	F1088	VAL	I389
LYS	LYS	CYS	S1770	V1672	V1588	MET	ASP	ARG	T1286	L1193	R1089	LYS	L892
THR	THR	ALA	ILE	D1681	Q1589	SER	ASP	VAL	Q1293	K1193	A1090	ASN	M395
LYS	LYS	SER	ASN	D1681	F1590	GLY	ASP	ASP	N1294	D1194	E1091	R1027	M396
GLU	GLU	ASP	ASN	I1689	H1593	GLY	THR	LYS	M1300	D1196	Y1094	L1032	V894
ARG	ARG	SER	GLU	N1690	R1598	GLN	ALA	GLY	M1300	E1197	A1098	V1033	M895
PRO	PRO	LEU	CYS	N1691	M1600	THR	THR	ALA	R1303	F1195	L1032	V1033	M896
PRO	PRO	LEU	TYR	K1692	M1600	THR	THR	ALA	R1303	E1195	L1032	V1033	K397
GLN	GLN	GLY	Y1693	Y1693	N1601	THR	THR	ALA	R1303	F1195	L1032	V1033	I898
GLU	GLU	PRO	Y1778	Y1778	N1601	THR	THR	ALA	R1303	E1195	L1032	V1033	E399
ALA	ALA	ALA	S1779	P1695	P1602	THR	THR	ALA	R1303	E1195	L1032	V1033	L900
GLU	GLU	GLU	L1787	R1699	K1605	GLY	GLY	ASN	E1309	S1206	G1121	ASN	G901
GLU	GLU	GLU	K1790	R1699	V1606	GLY	ASN	ALA	E1309	L1207	G1121	ASN	W902
LEU	LEU	SER	K1790	R1699	V1606	GLY	ASN	ALA	E1309	L1207	G1121	ASN	Q903
LYS	LYS	LYS	V1799	Y1703	D1607	GLY	HIS	VAL	E1309	L1207	G1121	ASN	Y904
GLY	GLY	GLY	Q1800	L1706	S1609	ASP	ASP	THR	E1309	L1207	G1121	ASN	G905
LYS	LYS	LYS	E1801	I1707	L1611	ALA	ALA	ALA	E1309	L1207	G1121	ASN	P906
LYS	LYS	LYS	G1802	L1711	S1612	SER	SER	GLY	E1309	L1207	G1121	ASN	V907
ARG	ARG	PRO	S1803	S1712	E1613	GLY	GLY	GLY	E1309	L1207	G1121	ASN	R908
LYS	LYS	LYS	L1804	T1716	R1614	GLY	GLY	GLY	E1309	L1207	G1121	ASN	D909
GLU	GLU	GLU	D1808	L1719	V1617	GLY	GLY	GLY	E1309	L1207	G1121	ASN	D910
CYS	CYS	CYS	V1810	M1720	L1618	GLY	GLY	GLY	E1309	L1207	G1121	ASN	N911
PRO	PRO	PRO	F1816	I1726	V1619	GLY	GLY	GLY	E1309	L1207	G1121	ASN	K912
GLU	GLU	GLU	L1817	V1727	Q1620	GLY	GLY	GLY	E1309	L1207	G1121	ASN	R913
GLU	GLU	GLU	F1818	V1727	Q1620	GLY	GLY	GLY	E1309	L1207	G1121	ASN	Q914
ILE	ILE	ILE	V1819	I1736	E1623	GLY	GLY	GLY	E1309	L1207	G1121	ASN	H915
ARG	ARG	ARG	P1820	T1737	E1623	GLY	GLY	GLY	E1309	L1207	G1121	ASN	L318
ASP	ASP	ASP	L1821	L1738	Q1626	GLY	GLY	GLY	E1309	L1207	G1121	ASN	V919
GLN	GLN	GLN	I1833	D1741	S1629	GLY	GLY	GLY	E1309	L1207	G1121	ASN	E920
LEU	LEU	LEU	F1834	GLU	Q1554	GLY	GLY	GLY	E1309	L1207	G1121	ASN	F921
LEU	LEU	LEU	H1835	ASN	F1555	GLY	GLY	GLY	E1309	L1207	G1121	ASN	S922
LEU	LEU	LEU	N1836	LYS	F1556	GLY	GLY	GLY	E1309	L1207	G1121	ASN	K923
LEU	LEU	LEU	E1847	LYS	LEU	GLY	GLY	GLY	E1309	L1207	G1121	ASN	L924
VAL	VAL	TYR	S1849	GLY	LEU	GLY	GLY	GLY	E1309	L1207	G1121	ASN	P925
PHE	PHE	ASN	VAL	GLY	LEU	GLY	GLY	GLY	E1309	L1207	G1121	ASN	E926
ASN	ASN	ASN	PHE	GLY	LEU	GLY	GLY	GLY	E1309	L1207	G1121	ASN	Q927
LEU	LEU	LEU	LYS	GLY	LEU	GLY	GLY	GLY	E1309	L1207	G1121	ASN	N930
ASP	ASP	GLU	GLY	GLY	LEU	GLY	GLY	GLY	E1309	L1207	G1121	ASN	Y931
GLY	GLY	VAL	GLU	GLY	LEU	GLY	GLY	GLY	E1309	L1207	G1121	ASN	N932
SER	SER	VAL	GLU	GLY	LEU	GLY	GLY	GLY	E1309	L1207	G1121	ASN	L933
LEU	LEU	ASN	ALA	GLY	LEU	GLY	GLY	GLY	E1309	L1207	G1121	ASN	Q934
ALA	ALA	GLN	ALA	GLY	LEU	GLY	GLY	GLY	E1309	L1207	G1121	ASN	M935
LEU	LEU	LEU	PRO	GLY	LEU	GLY	GLY	GLY	E1309	L1207	G1121	ASN	S936
ASN	ASN	ASN	PRO	GLY	LEU	GLY	GLY	GLY	E1309	L1207	G1121	ASN	L937
MET	MET	MET	GLU	GLY	LEU	GLY	GLY	GLY	E1309	L1207	G1121	ASN	E938
SER	SER	SER	GLU	GLY	LEU	GLY	GLY	GLY	E1309	L1207	G1121	ASN	T939
SER	SER	SER	GLU	GLY	LEU	GLY	GLY	GLY	E1309	L1207	G1121	ASN	K941
SER	SER	SER	GLU	GLY	LEU	GLY	GLY	GLY	E1309	L1207	G1121	ASN	T942
SER	SER	SER	GLU	GLY	LEU	GLY	GLY	GLY	E1309	L1207	G1121	ASN	L943
SER	SER	SER	GLU	GLY	LEU	GLY	GLY	GLY	E1309	L1207	G1121	ASN	L944
SER	SER	SER	GLU	GLY	LEU	GLY	GLY	GLY	E1309	L1207	G1121	ASN	A945
SER	SER	SER	GLU	GLY	LEU	GLY	GLY	GLY	E1309	L1207	G1121	ASN	L946

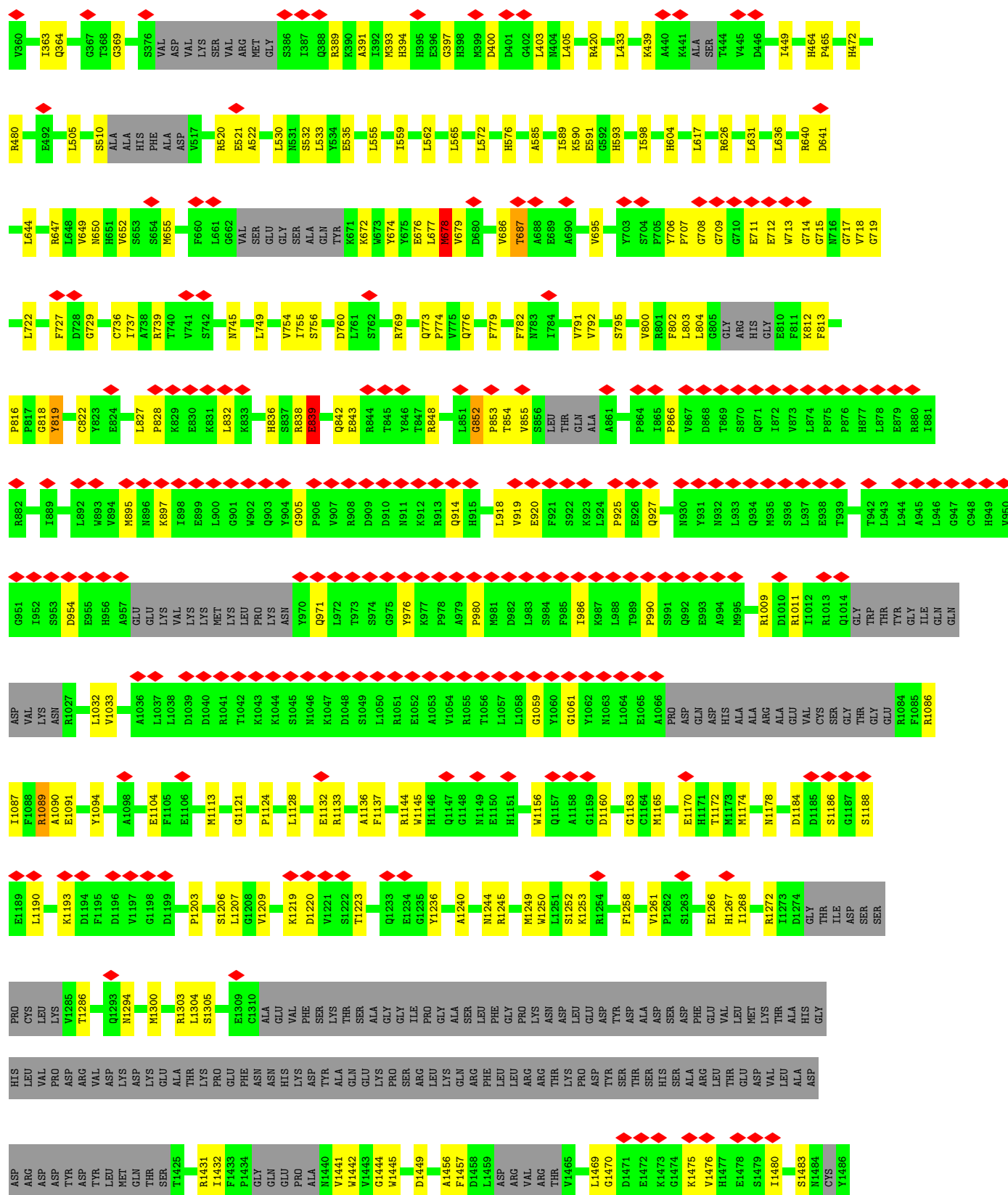


E4077	T4078	V3980	W3891	M3798	ASP	ARG	PRO	GLY	ASP	GLN	SER	TYR	E3125	A3065
V4078	V3981	V3980	Y3892	Q3799	ASP	MET	GLU	ASP	ASP	PRO	TYR	ASN	D3126	A3066
V4085	M3982	M3982	Y3893	S3800	GLY	ALA	LYS	LYS	ASP	LEU	MET	THR	E3067	E3067
K4086	L3983	L3983	K3896	S3802	GLU	PRO	THR	VAL	ASP	LEU	ASN	LYS	Q3127	D3068
V4087				S3803	GLU	TYR	GLU	VAL	GLY	LEU	SER	LYS	Q3128	D3069
E3988	E3988	E3988	T3899	L3804	GLU	ASN	ARG	ARG	TYR	ALA	TRP	SER	V3129	E3070
G3989	G3989	G3989		D3805	VAL	LEU	VAL	VAL	VAL	LEU	PHE	GLU	S3130	C3071
N3990	V3991	V3991	Q3904	R3811	ASP	R3613	ASP	ASP	GLY	LEU	GLY	ALA	C3131	T3072
V3992	V3992	V3992	N3906	R3812	ILE	R3614	ILE	ILE	ASN	THR	PRO	ALA	V3132	M3073
			N3907	R3813	ALA	Y3625	ALA	ALA	ARG	THR	GLU	LEU	R3133	E3074
V4101	V4101	V4101	A3910	M3814	VAL	H3635	VAL	VAL	SER	LYS	ASN	ASN	T3134	N3075
L4102	D4002	D4002	I3911	GLU	L3732	H3635	LEU	LEU	LEU	THR	PRO	PRO	L3135	L3076
M4110	M4003	M4003		GLY	H3733	I3642	PHE	PHE	LYS	PHE	GLY	THR	T3136	K3077
P4111			A3914	LEU	D3734	H3642	HIS	HIS	ASP	LEU	ARG	ASN	S3137	Q3078
M4112	E4006	E4006	K3915	GLY	R3735	L3645	LEU	LEU	THR	LYS	ALA	VAL	L3138	Q3079
D4113	V4011	V4011	Q3916	MET	G3736	P3648	GLU	GLU	GLY	ALA	MET	GLU	Y3139	Q3080
T4114			V3917	THR	A3737	GLY	VAL	VAL	ASP	VAL	TRP	CYS	A3140	F3081
R4115			N3919	GLU	E3738	ALA	SER	SER	VAL	LYS	LEU	CYS	L3141	T3082
L4116	L4014	L4014	T3920	GLU	M3740	VAL	THR	THR	VAL	LYS	GLY	THR	G3142	HIS
Q4117	L4016	L4016	L3921	GLY	V3741	PRO	CYS	ARG	ASP	GLN	ALA	ASN	T3143	THR
F4017	F4018	F4018	E3923	GLY	L3742	PRO	MET	ILE	ILE	GLU	LEU	ILE	S3144	ARG
D4019	D4019	D4019	Y3924	GLY	Q3743	GLU	ARG	ARG	ILE	LYS	ASN	SER	LYS	ASN
M4020	M4020	M4020	I3925	LYS	T3744	GLU	ARG	ARG	GLY	ALA	GLU	LEU	ILE	GLN
F4021	F4021	F4021	Q3926	VAL	I3745	ASP	TYR	TYR	ASP	GLY	ALA	GLY	Q3152	ILE
F4130					S3748	GLY	THR	THR	GLY	VAL	HIS	VAL	R3153	ASN
L4134	G4135	G4135	T3930	GLN	E3751	LYS	PRO	GLN	LEU	GLY	ILE	ASP	A3154	TYR
R4136	R4136	R4136	G3931	D3833	M3755	L3665	GLN	GLN	ASP	GLY	LEU	LEU	L3156	T3098
E4138	E4137	E4137	N3932	D3839	L3670	L3668	SER	SER	ASP	GLY	LEU	LEU	G3157	T3099
T4139	T4032	T4032	Q3933	L3840	L3769	I3669	GLY	GLY	TRP	TRP	ASN	ILE	V3100	V3100
M4140	Y4036	Y4036	L3936	F3841	L3760	L3670	VAL	VAL	GLN	THR	LYS	ALA	A3101	A3101
G4141					G3763	L3671	LYS	LYS	VAL	THR	PHE	ILE	L3102	L3102
S4142	S4045	S4045	S3939	L3846	L3766	R3674	ALA	ALA	ARG	SER	ILE	GLY	A3161	P3104
R4145	K4046	K4046	R3940	E3849	L3767	T3675	VAL	VAL	TRP	GLY	TYR	GLY	M3105	M3105
T4146	R4047	R4047	L3941	Q3850	G3769	T3675	TRP	TRP	GLN	GLY	ASN	ILE	L3106	L3106
E4147	D4048	D4048	W3942	D3854	G3770	A3676	HIS	HIS	GLN	VAL	ASP	VAL	A3164	A316



• Molecule 1: RyR2

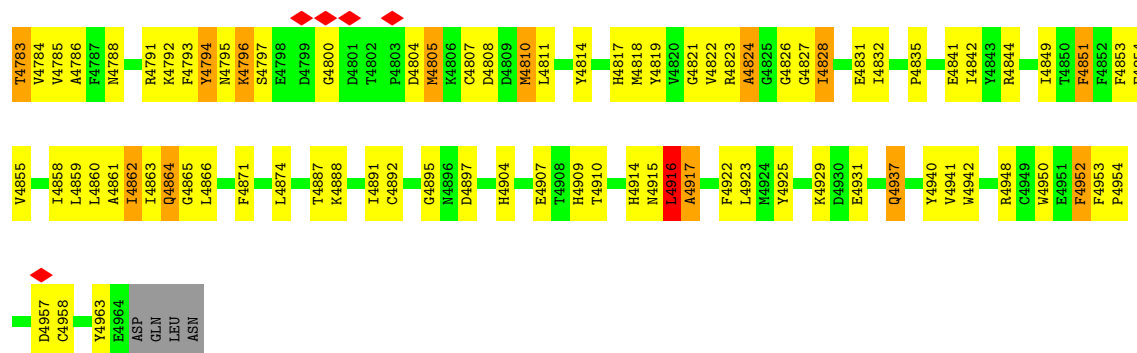




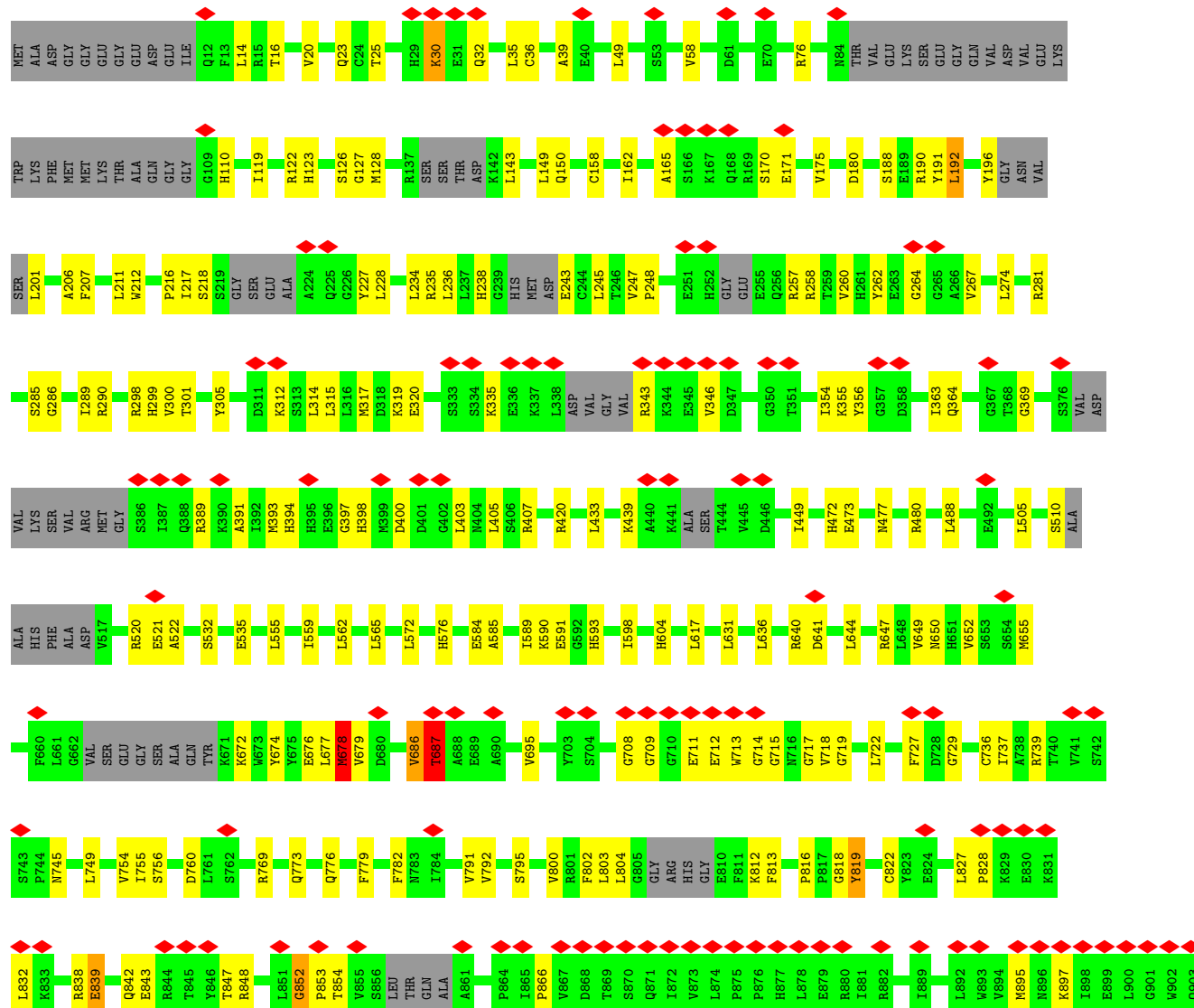








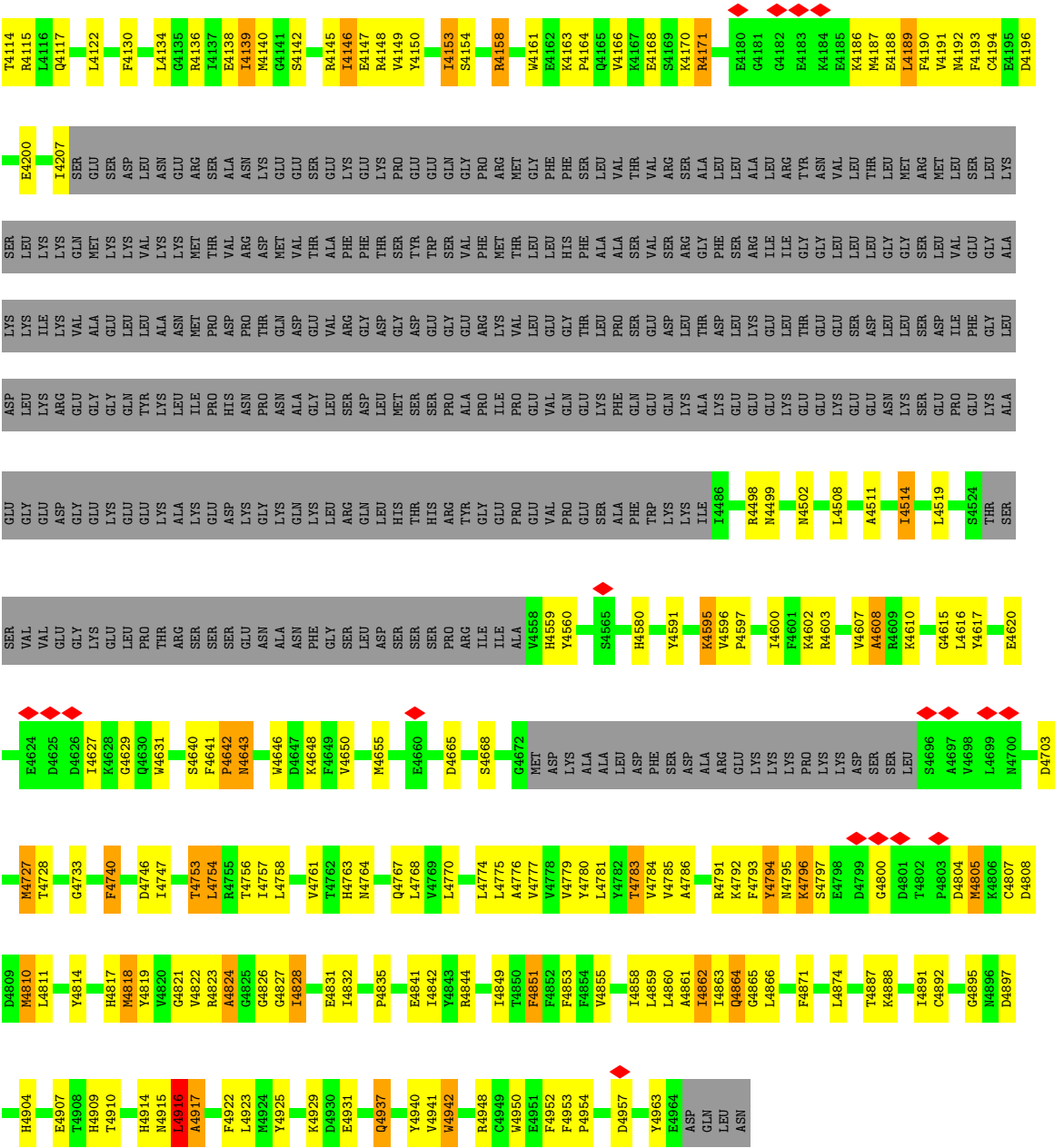
• Molecule 1: RyR2



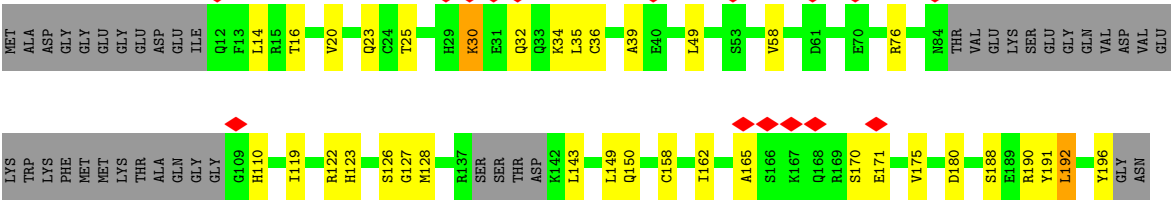


LEU	ASN	PHE	LYS	ASP	LYS	SER	CYS	PRO	CYS	PRO	GLU	GLU	ARG	ASP	GLN	LEU	D1999	T2239	D2013	GLU	ASP	SER	LEU	ASP	GLY	ASN	SER	ASP	D2024	V2039	LEU	LYS	LYS	GLN	ALA	GLU	LYS	VAL	GLU	SER	ASP	SER	LYS	THR	LYS	THR	LYS	PHE	SER	T2068	Q2071	Q2072	E2073						
S2074	V2075	I2076	E2077	D2078	P2079	E2080	L2081	R2083	A2084	M2085	L2103	I2109	L2121	A2122	S2123	L2130	V2133	ARG	MET	GLY	E2138	M2143	D2149	F2156	M2163	L2166	M2173	E2174	V2175	G2181	GLY	GLU	SER	LYS	GLN	ASP	GLY	GLU	SER	GLN	MET	LEU	VAL	SER	THR	LYS	PHE	P2191	K2192	M2193	V2194	F2204							
M2211	Q2212	K2213	D2217	L2222	S2226	S2227	V2228	GLY	ALA	SER	PRO	ALA	MET	ARG	GLY	SER	T2239	P2240	L2241	D2242	V2243	L2254	L2255	L2256	L2258	E2259	P2261	D2262	L2263	E2264	R2268	C2273	G2274	L2275	GLN	SER	CYS	GLN	LYS	MET	LEU	VAL	SER	THR	LYS	GLY	TYR	PRO	ASP	ILE	GLY								
TRP	ASN	P2293	D2301	R2304	F2305	A2306	L2326	R2327	R2328	E2330	CYS	PHE	GLY	PRO	ALA	ALA	GLY	ARG	LEU	ASN	G2343	M2348	E2349	L2354	ALA	GLU	ASP	PRO	ARG	ASP	GLY	PRO	THR	SER	GLY	SER	LYS	MET	PRO	ASP	PRO	THR	GLU	GLY	GLU	GLY	ASP												
THR	ILE	HIS	MET	G2386	M2390	C2403	A2404	PRO	GLU	MET	HIS	LEU	ILE	ALA	ALA	LYS	GLY	E2416	S2426	L2427	ILE	PRO	LEU	G2431	G2435	V2436	L2437	S2438	I2439	A2440	F2441	G2442	MET	PRO	THR	ILE	ALA	LYS	ASP	GLY	ASN	VAL	VAL	GLU	PRO	ASP	MET	ALA	F2461	C2462	D2463	D2464							
H2465	M2469	R2475	V2476	Y2477	GLY	ILE	GLU	V2481	Q2482	D2483	L2489	VAL	G2492	P2495	D2496	L2503	ASP	THR	ALA	ALA	LEU	SER	ILE	T2511	R2519	Y2520	L2521	C2522	T2523	L2528	L2529	THR	ARG	CYS	ALA	F2534	L2535	F2536	T2552	V2553	TYR	ARG	LEU	SER	K2558	A2565	D2568	S2569											
I2570	E2571	S2572	C2573	L2574	L2575	S2576	ILE	CYS	GLY	GLN	LEU	P2583	S2584	Q2587	R2591	V2597	P2598	L2599	L2600	N2601	HIS	ALA	K2605	M2606	P2607	H2614	C2618	C2623	L2624	P2625	G2626	G2627	TRP	GLY	ASN	PHE	GLY	ALA	A2634	S2635	E2636	E2637	K2644	I2649	F2650	D2651	A2652	L2653	SER										
GLN	LYS	LYS	Y2658	E2659	Q2660	E2661	L2662	L2665	A2666	L2667	P2668	C2669	V2673	A2674	G2675	A2676	L2677	P2678	P2679	ASP	TYR	MET	GLU	SER	ASN	VAL	THR	ARG	THR	ILE	SER	GLN	LYS	SER	GLN	SER	MET	ASP	GLY	N2701	F2702	N2703	P2704	Q2705	P2706	V2707	D2708	T2709	S2710	N2711	I2712	T2713	I2714	P2715	E2716	K2717			
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E2778	S2779	L2780	K2781	T2782	M2783	L2784	A2785	G2786	G2787	W2788	R2789	I2790	E2791	L2792	T2793	A2794	E2795	G2796	D2797	SER	MET	ALA	LEU	TYR	ASN	ARG	THR	ARG	ILE	SER	GLN	THR	SER	GLN	VAL	SER	V2816	D2817	A2818	H2820	G2821	Y2822	S2823	F2824	R2825	A2826	L2827	D2828	M2829	S2830	N2831	V2832	T2833	L2834	S2835	D2836	D2837		
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Q2898	I2899	N2900	G2901	Y2902	A2903	V2904	S2905	R2906	G2907	PHE	LYS	ASP	LEU	GLU	LEU	THR	PRO	SER	ILE	GLU	ARG	LYS	LYS	ARG	LEU	F2982	F2983	L2984	S2985	A2986	A2987	S2988	L2991	C2992	S2993	G2994	G2995	H2996	A2997	S2998	N2999	K3000	E3001	K3002	E3003	K3004	V3005	THR	SER	LEU	F3009	C3010	K3011	L3012	G3013	V3014	L3015	V3016	K3017

E4006	A3914	R3731	H5635	VAL	SER	SER	VAL	THR	ASN	LEU	L3138	Q3078	H3018
V4011	V3917	L3732	I3642	LEU	LEU	LEU	PHE	THR	PRO	PRO	Y3139	G3079	R3019
T4014	N3919	H3733	I3645	HIS	ASP	ASP	HIS	LEU	ARG	THR	A3140	Q3080	I3020
L4015	T3920	D3734	L3648	LEU	THR	THR	LEU	PRO	ALA	VAL	L3141	F3081	S3021
F4017	T3922	G3735	P3648	GLN	ASP	ASP	GLU	LEU	MET	ASP	T3143	HIS	T3022
D4019	E3923	A3736	GLY	LYS	VAL	VAL	VAL	THR	CYS	VAL	S3144	ARG	F3023
M4020	Y3924	E3737	ALA	THR	ASP	ASP	GLY	LEU	ALA	PRO	LYS	ASN	G3024
F4021	I3925	M3740	PRO	CYS	ASP	ASP	GLN	LYS	LEU	ILE	ILE	ASN	H3025
L4022	Q3926	V3741	ILE	ARG	ILE	ILE	GLU	LYS	ASN	PRO	TYR	PRO	D3026
S4030	T3930	G3742	ARG	ARG	ARG	ARG	LYS	LYS	SER	SER	V3149	GLY	D3027
D4031	G3931	T3743	THR	ARG	SER	SER	LYS	ALA	ALA	LEU	E3150	VAL	SER
T4032	N3932	I3744	LYS	ARG	THR	THR	GLY	VAL	HIS	GLU	R3151	THR	ILE
D4039	Q3933	S3748	THR	SER	HIS	HIS	ASP	VAL	ASN	LEU	Q3152	GLN	ASN
S4045	L3936	E3751	LYS	LEU	GLN	GLN	GLY	GLU	LEU	GLU	S3154	ILE	CYS
K4046	S3939	M3755	R3661	VAL	GLY	GLY	ASP	PHE	LEU	LEU	S3155	TYR	L3034
A4052	R3940	T3759	L3665	HIS	LEU	LEU	LYS	ARG	GLY	ILE	L3156	T3098	H3035
H4056	L3941	L3760	L3668	GLN	GLU	GLU	THR	VAL	ILE	VAL	E3157	T3099	I3036
T4060	V3945	G3763	L3670	ARG	PRO	PRO	ASP	VAL	LYS	ALA	E3158	V3100	L3037
Q4061	V3951	T3766	L3671	SER	LYS	LYS	ALA	THR	ILE	THR	L3159	A3101	G3038
S4062	F3952	N3767	R3674	VAL	LYS	LYS	THR	ILE	GLY	GLY	L3160	L3102	Q3039
E4063	A3953	G3769	T3675	ALA	THR	THR	TRP	TRP	ASN	ILE	A3161	L3103	T3040
L4067	H3954	Q3770	L3677	TRP	MET	MET	VAL	SER	ASP	ASP	A3162	P3104	L3041
L4068	N3955	S3772	E3684	HIS	ALA	ALA	ALA	LYS	LEU	LEU	F3163	M3105	D3042
A4071	M3956	T3773	E3685	LYS	LEU	LEU	LEU	ASP	GLY	GLU	A3164	L3106	A3043
E4072	L3957	V3774	L3688	SER	LYS	LYS	ARG	PHE	GLY	PRO	G3165	S3107	G3050
T4073	L3968	E3780	L3689	GLN	LEU	LEU	LEU	ARG	ALA	VAL	E3173	F3110	L3051
E4075	E3971	Y3781	K3696	ARG	PRO	PRO	ILE	GLU	MET	GLU	L3172	E3111	E3052
N4076	L3972	L3782	S3699	ALA	ARG	ARG	THR	ASN	THR	LEU	E3174	H3112	G3053
E4077	M3973	K3783	C3700	VAL	GLU	GLU	PHE	VAL	VAL	PRO	T3174	G3114	V3054
T4078	D3974	E3784	HIS	VAL	ASP	THR	ILE	VAL	VAL	MET	D3177	Q3115	K3055
V4085	M3982	L3794	ASP	ALA	THR	THR	CYS	VAL	PHE	LEU	K3178	H3116	SER
K4086	L3983	L3797	GLU	CYS	SER	SER	ALA	GLN	LEU	THR	H3179	Q3117	ALA
R4087	L3988	M3798	ASP	PHE	ASP	ASP	PRO	GLU	GLN	ASP	N3180	ILE	ARG
HIS	E3988	Q3799	ASP	ARG	PRO	PRO	MET	ASP	ILE	ILE	I3181	GLY	ALA
E4090	G3989	C3801	ASP	ALA	GLY	GLY	GLN	ILE	THR	THR	T3182	ASP	ALA
T4095	N3990	S3802	ASP	PRO	THR	THR	VAL	THR	ASN	ASN	I3182	ILE	F3061
V4101	V3991	L3803	GLY	LEU	VAL	VAL	ARG	PHE	VAL	TRP	E3124	L3124	L3062
L4102	V3992	D3805	VAL	ASN	VAL	VAL	ALA	ILE	LYS	LYS	D3126	E3125	D3063
M4110	K3998	R3811	L3813	LYS	VAL	VAL	LEU	THR	PRO	GLY	V3127	V3127	N3064
N4112	D4002	Q3812	R3614	ASP	ASP	ASP	THR	THR	LEU	GLU	Q3128	Q3128	A3065
D4113	M4003	N3813	Y3625	ILE	ALA	ALA	ARG	ARG	LEU	ASN	V3129	V3129	A3066
		K3814		ASN					LYS	THR	S3130	S3130	E3067
										LYS	C3131	C3131	D3068
										SER	Y3132	Y3132	E3070
										ARG	R3133	R3133	T3072
										GLU	I3134	I3134	K3073
										ARG	L3135	L3135	E3074
										ALA	T3136	T3136	N3075
										LEU	S3137	S3137	K3077



● Molecule 1: RyR2

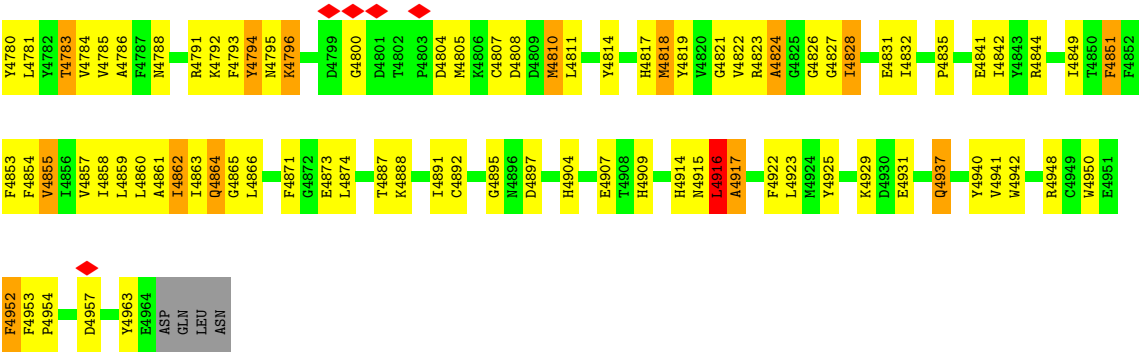


ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094	F1195	H1294	ASP	VAL	R281	S376	Q645	G729	Y823	W893	H956	L1032	Y1094
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	133196	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 ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.155	Depositor
Minimum map value	-0.067	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	546.0, 546.0, 546.0	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.41	210/26752 (0.8%)	1.10	88/36151 (0.2%)
1	B	1.41	203/26752 (0.8%)	1.10	89/36151 (0.2%)
1	C	1.41	202/26752 (0.8%)	1.10	88/36151 (0.2%)
1	D	1.41	210/26752 (0.8%)	1.11	93/36151 (0.3%)
All	All	1.41	825/107008 (0.8%)	1.10	358/144604 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	23
1	B	0	23
1	C	0	24
1	D	0	23
All	All	0	93

All (825) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4849	ILE	C-O	16.70	1.44	1.24
1	D	4849	ILE	C-O	16.67	1.44	1.24
1	C	4849	ILE	C-O	15.45	1.44	1.24
1	B	4849	ILE	C-O	15.28	1.43	1.24
1	C	4150	TYR	C-O	-10.51	1.11	1.23
1	B	4150	TYR	C-O	-10.50	1.11	1.23
1	D	4150	TYR	C-O	-10.50	1.11	1.23
1	A	4150	TYR	C-O	-10.44	1.11	1.23
1	A	3755	MET	N-CA	-10.37	1.34	1.46
1	B	3755	MET	N-CA	-9.99	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	3755	MET	N-CA	-9.91	1.34	1.46
1	C	4862	ILE	CA-CB	-9.88	1.42	1.54
1	A	4862	ILE	CA-CB	-9.84	1.42	1.54
1	D	4862	ILE	CA-CB	-9.82	1.42	1.54
1	B	2192	LYS	N-CA	9.78	1.59	1.46
1	B	4853	PHE	N-CA	9.66	1.57	1.46
1	A	4853	PHE	N-CA	9.62	1.57	1.46
1	A	2192	LYS	N-CA	9.62	1.58	1.46
1	C	3755	MET	N-CA	-9.62	1.35	1.46
1	C	4853	PHE	N-CA	9.50	1.57	1.46
1	D	2192	LYS	N-CA	9.36	1.58	1.46
1	C	4150	TYR	CA-C	-9.34	1.41	1.52
1	C	2192	LYS	N-CA	9.32	1.58	1.46
1	D	4853	PHE	N-CA	9.27	1.57	1.46
1	B	4150	TYR	CA-C	-9.14	1.42	1.52
1	D	4150	TYR	CA-C	-9.03	1.42	1.52
1	B	4862	ILE	CA-CB	-8.95	1.42	1.54
1	B	1819	VAL	CA-CB	8.88	1.59	1.54
1	A	4150	TYR	CA-C	-8.83	1.42	1.52
1	D	4136	ARG	C-O	-8.66	1.13	1.23
1	A	1819	VAL	CA-CB	8.61	1.59	1.54
1	A	4136	ARG	C-O	-8.58	1.13	1.23
1	C	4136	ARG	C-O	-8.49	1.14	1.23
1	C	1819	VAL	CA-CB	8.46	1.58	1.54
1	D	4818	MET	CG-SD	8.41	2.01	1.80
1	B	4136	ARG	C-O	-8.32	1.14	1.23
1	A	3860	ARG	CA-C	-8.31	1.42	1.52
1	C	4818	MET	CG-SD	8.30	2.01	1.80
1	D	3860	ARG	CA-C	-8.23	1.42	1.52
1	B	4941	VAL	N-CA	-8.21	1.36	1.46
1	C	3860	ARG	CA-C	-8.17	1.42	1.52
1	A	4818	MET	CG-SD	8.15	2.01	1.80
1	A	3759	THR	CA-C	-8.08	1.42	1.52
1	D	1819	VAL	CA-CB	8.06	1.58	1.54
1	D	3759	THR	CA-C	-8.02	1.42	1.52
1	B	3860	ARG	CA-C	-8.02	1.43	1.52
1	C	4941	VAL	N-CA	-8.01	1.36	1.46
1	B	3878	TYR	CG-CD1	-7.97	1.22	1.39
1	B	4818	MET	CG-SD	7.96	2.00	1.80
1	D	4941	VAL	N-CA	-7.96	1.37	1.46
1	A	4941	VAL	N-CA	-7.93	1.37	1.46
1	C	3759	THR	CA-C	-7.91	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2258	LEU	C-O	-7.87	1.13	1.23
1	C	4753	THR	C-O	-7.86	1.13	1.23
1	C	3878	TYR	CG-CD1	-7.83	1.22	1.39
1	A	4764	ASN	N-CA	-7.74	1.37	1.46
1	A	3878	TYR	CG-CD1	-7.73	1.23	1.39
1	D	4753	THR	C-O	-7.73	1.13	1.23
1	D	3878	TYR	CG-CD1	-7.73	1.23	1.39
1	B	3759	THR	CA-C	-7.69	1.42	1.52
1	C	4764	ASN	N-CA	-7.67	1.37	1.46
1	B	4819	TYR	CA-C	-7.67	1.43	1.52
1	C	4819	TYR	CA-C	-7.66	1.43	1.52
1	B	4753	THR	C-O	-7.65	1.13	1.23
1	A	4753	THR	C-O	-7.62	1.13	1.23
1	D	4764	ASN	N-CA	-7.57	1.37	1.46
1	A	4776	ALA	CA-C	-7.56	1.43	1.52
1	D	4819	TYR	CA-C	-7.53	1.43	1.52
1	B	4828	ILE	N-CA	-7.52	1.37	1.46
1	D	2258	LEU	C-O	-7.50	1.14	1.23
1	A	4828	ILE	N-CA	-7.49	1.37	1.46
1	D	4776	ALA	CA-C	-7.49	1.43	1.52
1	C	4828	ILE	N-CA	-7.49	1.37	1.46
1	B	4764	ASN	N-CA	-7.44	1.37	1.46
1	A	4819	TYR	CA-C	-7.43	1.43	1.52
1	B	4754	LEU	N-CA	-7.39	1.36	1.45
1	D	3766	ILE	CA-C	-7.36	1.43	1.52
1	B	4776	ALA	CA-C	-7.35	1.43	1.52
1	C	4824	ALA	CA-C	-7.33	1.43	1.52
1	C	4865	GLY	CA-C	-7.31	1.42	1.51
1	C	3766	ILE	CA-C	-7.28	1.43	1.52
1	B	2258	LEU	C-O	-7.27	1.14	1.23
1	A	3766	ILE	CA-C	-7.26	1.43	1.52
1	C	4754	LEU	N-CA	-7.25	1.36	1.45
1	B	3700	CYS	CB-SG	7.25	2.05	1.81
1	D	4860	LEU	CA-C	-7.24	1.43	1.52
1	D	3700	CYS	CB-SG	7.22	2.05	1.81
1	D	4828	ILE	N-CA	-7.22	1.37	1.46
1	B	3766	ILE	CA-C	-7.22	1.43	1.52
1	B	4865	GLY	CA-C	-7.20	1.43	1.51
1	A	3700	CYS	CB-SG	7.19	2.04	1.81
1	D	4865	GLY	CA-C	-7.18	1.43	1.51
1	C	4842	ILE	N-CA	-7.17	1.37	1.46
1	C	4776	ALA	CA-C	-7.17	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	4860	LEU	CA-C	-7.16	1.43	1.52
1	D	4824	ALA	CA-C	-7.16	1.43	1.52
1	A	4860	LEU	CA-C	-7.15	1.43	1.52
1	B	4860	LEU	CA-C	-7.15	1.43	1.52
1	A	4940	TYR	CA-C	-7.12	1.43	1.52
1	C	4940	TYR	CA-C	-7.11	1.44	1.52
1	D	4754	LEU	N-CA	-7.10	1.36	1.45
1	D	4842	ILE	N-CA	-7.07	1.37	1.46
1	A	4754	LEU	N-CA	-7.06	1.36	1.45
1	C	3700	CYS	CB-SG	7.04	2.04	1.81
1	A	4865	GLY	CA-C	-7.03	1.43	1.51
1	C	4887	THR	CA-C	-7.01	1.45	1.53
1	A	4887	THR	CA-C	-7.01	1.45	1.53
1	A	4824	ALA	CA-C	-7.00	1.43	1.52
1	D	4940	TYR	CA-C	-7.00	1.44	1.52
1	A	4842	ILE	N-CA	-6.98	1.38	1.46
1	C	3685	GLU	C-O	-6.98	1.15	1.24
1	A	2258	LEU	C-O	-6.97	1.15	1.23
1	D	4158	ARG	CA-C	-6.96	1.43	1.52
1	B	4794	TYR	C-O	-6.94	1.15	1.24
1	C	4779	VAL	N-CA	-6.94	1.38	1.46
1	A	4158	ARG	CA-C	-6.93	1.43	1.52
1	B	4842	ILE	N-CA	-6.93	1.38	1.46
1	A	4794	TYR	C-O	-6.93	1.15	1.24
1	B	4940	TYR	CA-C	-6.92	1.44	1.52
1	A	4862	ILE	CA-C	-6.91	1.44	1.52
1	B	4871	PHE	CA-C	-6.91	1.43	1.52
1	C	4158	ARG	CA-C	-6.90	1.44	1.52
1	D	4871	PHE	CA-C	-6.89	1.43	1.52
1	D	3876	VAL	N-CA	-6.88	1.38	1.46
1	A	3876	VAL	N-CA	-6.86	1.38	1.46
1	D	4862	ILE	CA-C	-6.85	1.44	1.52
1	C	3849	GLU	C-O	6.85	1.32	1.24
1	D	4887	THR	CA-C	-6.85	1.45	1.53
1	C	4871	PHE	CA-C	-6.85	1.43	1.52
1	C	3738	ALA	N-CA	-6.84	1.37	1.46
1	B	4779	VAL	N-CA	-6.84	1.38	1.46
1	C	813	PHE	C-O	-6.84	1.15	1.23
1	C	4102	LEU	CA-C	-6.82	1.44	1.52
1	D	3685	GLU	C-O	-6.82	1.16	1.24
1	A	3738	ALA	N-CA	-6.81	1.37	1.46
1	C	4161	TRP	CG-CD2	-6.80	1.31	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	4161	TRP	CG-CD2	-6.78	1.31	1.43
1	B	3876	VAL	N-CA	-6.78	1.38	1.46
1	B	3685	GLU	C-O	-6.78	1.16	1.24
1	B	4158	ARG	CA-C	-6.78	1.44	1.52
1	C	4189	LEU	CA-C	-6.77	1.43	1.52
1	D	3738	ALA	N-CA	-6.77	1.37	1.46
1	D	4779	VAL	N-CA	-6.76	1.38	1.46
1	A	3854	ASP	CG-OD1	-6.76	1.12	1.25
1	A	4871	PHE	CA-C	-6.76	1.43	1.52
1	C	3876	VAL	N-CA	-6.75	1.38	1.46
1	D	4161	TRP	CG-CD2	-6.75	1.31	1.43
1	D	3924	TYR	CA-C	-6.74	1.44	1.52
1	D	813	PHE	C-O	-6.74	1.16	1.23
1	D	4794	TYR	C-O	-6.73	1.15	1.24
1	A	2222	LEU	N-CA	-6.72	1.37	1.46
1	A	4161	TRP	CG-CD2	-6.71	1.31	1.43
1	D	4917	ALA	CA-C	-6.71	1.43	1.52
1	C	4862	ILE	CA-C	-6.70	1.44	1.52
1	A	4917	ALA	CA-C	-6.69	1.43	1.52
1	D	4923	LEU	N-CA	-6.69	1.37	1.46
1	A	3685	GLU	C-O	-6.69	1.16	1.24
1	D	3849	GLU	C-O	6.69	1.32	1.24
1	D	4189	LEU	CA-C	-6.68	1.43	1.52
1	B	3738	ALA	N-CA	-6.67	1.37	1.46
1	A	4818	MET	N-CA	-6.67	1.37	1.46
1	B	3854	ASP	CG-OD1	-6.66	1.12	1.25
1	B	4824	ALA	CA-C	-6.66	1.43	1.52
1	C	4917	ALA	CA-C	-6.66	1.43	1.52
1	D	4793	PHE	N-CA	-6.66	1.37	1.46
1	B	4189	LEU	CA-C	-6.65	1.43	1.52
1	B	4887	THR	CA-C	-6.65	1.46	1.53
1	A	4779	VAL	N-CA	-6.65	1.38	1.46
1	A	4937	GLN	N-CA	-6.64	1.38	1.46
1	D	3914	ALA	N-CA	-6.64	1.38	1.46
1	B	4608	ALA	N-CA	-6.64	1.37	1.46
1	C	3854	ASP	CG-OD1	-6.63	1.12	1.25
1	C	3924	TYR	CA-C	-6.62	1.44	1.52
1	D	4818	MET	N-CA	-6.61	1.37	1.46
1	B	4139	ILE	CB-CG1	-6.61	1.40	1.53
1	A	4102	LEU	CA-C	-6.60	1.44	1.52
1	C	2222	LEU	N-CA	-6.60	1.37	1.46
1	B	4153	ILE	C-O	-6.59	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	4794	TYR	C-O	-6.59	1.15	1.24
1	B	2222	LEU	N-CA	-6.58	1.37	1.46
1	A	3914	ALA	N-CA	-6.58	1.38	1.46
1	D	4954	PRO	CA-C	-6.57	1.45	1.52
1	C	4923	LEU	N-CA	-6.57	1.38	1.46
1	D	4102	LEU	CA-C	-6.56	1.44	1.52
1	A	3924	TYR	CA-C	-6.56	1.44	1.52
1	D	3773	THR	CA-C	-6.54	1.44	1.52
1	C	4793	PHE	N-CA	-6.53	1.37	1.46
1	A	4608	ALA	N-CA	-6.51	1.38	1.46
1	B	4937	GLN	N-CA	-6.50	1.38	1.46
1	C	4608	ALA	N-CA	-6.50	1.38	1.46
1	C	3914	ALA	N-CA	-6.50	1.38	1.46
1	A	4793	PHE	N-CA	-6.50	1.37	1.46
1	B	3914	ALA	N-CA	-6.50	1.38	1.46
1	A	4189	LEU	CA-C	-6.48	1.43	1.52
1	D	3854	ASP	CG-OD1	-6.48	1.13	1.25
1	B	4917	ALA	CA-C	-6.47	1.43	1.52
1	C	4153	ILE	C-O	-6.47	1.17	1.24
1	B	4954	PRO	CA-C	-6.47	1.45	1.52
1	A	4923	LEU	N-CA	-6.46	1.37	1.46
1	A	4139	ILE	CB-CG1	-6.44	1.40	1.53
1	D	4153	ILE	N-CA	-6.44	1.39	1.46
1	B	3924	TYR	CA-C	-6.43	1.44	1.52
1	B	4862	ILE	CA-C	-6.43	1.44	1.52
1	C	4785	VAL	CA-C	-6.42	1.44	1.52
1	D	2222	LEU	N-CA	-6.41	1.38	1.46
1	C	4139	ILE	CB-CG1	-6.41	1.40	1.53
1	B	3982	MET	N-CA	-6.40	1.38	1.46
1	D	4608	ALA	C-O	6.40	1.32	1.24
1	C	4954	PRO	CA-C	-6.40	1.45	1.52
1	D	4785	VAL	CA-C	-6.40	1.44	1.52
1	B	4923	LEU	N-CA	-6.40	1.38	1.46
1	A	3982	MET	N-CA	-6.38	1.38	1.46
1	D	4560	TYR	C-O	-6.38	1.16	1.23
1	D	4608	ALA	N-CA	-6.38	1.38	1.46
1	C	3770	GLY	C-O	-6.36	1.15	1.24
1	B	4793	PHE	N-CA	-6.36	1.37	1.46
1	B	4153	ILE	N-CA	-6.36	1.39	1.46
1	B	4853	PHE	CA-CB	6.35	1.63	1.53
1	A	4560	TYR	C-O	-6.34	1.16	1.23
1	B	4102	LEU	CA-C	-6.34	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4153	ILE	N-CA	-6.34	1.39	1.46
1	C	3794	LEU	CA-C	-6.30	1.44	1.52
1	A	4607	VAL	N-CA	-6.29	1.39	1.46
1	C	4853	PHE	CA-CB	6.29	1.63	1.53
1	B	3732	LEU	N-CA	-6.28	1.38	1.46
1	A	3773	THR	CA-C	-6.28	1.44	1.52
1	A	3849	GLU	C-O	6.27	1.31	1.24
1	B	4953	PHE	CG-CD1	-6.27	1.25	1.38
1	C	3850	GLY	N-CA	-6.27	1.37	1.45
1	B	3850	GLY	N-CA	-6.27	1.37	1.45
1	C	4607	VAL	N-CA	-6.26	1.39	1.46
1	D	4607	VAL	N-CA	-6.26	1.39	1.46
1	D	4139	ILE	CB-CG1	-6.25	1.41	1.53
1	B	3849	GLU	C-O	6.24	1.31	1.24
1	C	4818	MET	N-CA	-6.24	1.38	1.46
1	B	4646	TRP	CZ3-CH2	6.24	1.56	1.40
1	C	3982	MET	N-CA	-6.24	1.39	1.46
1	A	3920	THR	CA-C	-6.22	1.44	1.52
1	D	3982	MET	N-CA	-6.21	1.39	1.46
1	A	4646	TRP	CZ3-CH2	6.21	1.55	1.40
1	B	3951	VAL	CA-C	-6.21	1.45	1.52
1	A	4853	PHE	CA-CB	6.20	1.63	1.53
1	D	3770	GLY	C-O	-6.20	1.15	1.24
1	A	813	PHE	C-O	-6.19	1.16	1.23
1	B	813	PHE	C-O	-6.19	1.16	1.23
1	D	4937	GLN	N-CA	-6.18	1.38	1.46
1	B	4560	TYR	C-O	-6.18	1.16	1.23
1	B	1943	PHE	N-CA	6.18	1.53	1.46
1	C	4608	ALA	C-O	6.17	1.31	1.24
1	C	4153	ILE	N-CA	-6.17	1.39	1.46
1	D	4853	PHE	CA-CB	6.17	1.63	1.53
1	B	816	PRO	CA-C	6.16	1.57	1.52
1	C	4560	TYR	C-O	-6.16	1.16	1.23
1	A	4785	VAL	CA-C	-6.16	1.44	1.52
1	B	4136	ARG	N-CA	-6.15	1.39	1.46
1	D	3739	GLU	N-CA	-6.15	1.38	1.46
1	A	4608	ALA	C-O	6.15	1.31	1.24
1	C	4646	TRP	CZ3-CH2	6.15	1.55	1.40
1	D	3917	VAL	CA-CB	-6.14	1.46	1.54
1	A	3917	VAL	CA-CB	-6.14	1.46	1.54
1	A	4953	PHE	CG-CD1	-6.13	1.25	1.38
1	B	4607	VAL	N-CA	-6.13	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	4161	TRP	CA-C	-6.13	1.44	1.52
1	A	4146	ILE	N-CA	-6.13	1.38	1.46
1	B	3773	THR	CA-C	-6.13	1.44	1.52
1	B	2077	GLU	C-O	-6.13	1.15	1.24
1	A	4954	PRO	CA-C	-6.12	1.45	1.52
1	B	4818	MET	N-CA	-6.11	1.38	1.46
1	B	4785	VAL	CA-C	-6.11	1.45	1.52
1	C	4937	GLN	N-CA	-6.10	1.38	1.46
1	B	3770	GLY	C-O	-6.09	1.15	1.24
1	C	4161	TRP	CA-C	-6.09	1.45	1.52
1	A	3850	GLY	N-CA	-6.08	1.37	1.45
1	B	3858	TYR	CA-C	-6.08	1.44	1.52
1	C	816	PRO	CA-C	6.08	1.57	1.52
1	D	3794	LEU	CA-C	-6.08	1.44	1.52
1	A	4136	ARG	N-CA	-6.08	1.39	1.46
1	B	3668	LEU	CA-C	-6.07	1.45	1.52
1	B	3763	GLY	CA-C	-6.07	1.44	1.52
1	D	816	PRO	CA-C	6.07	1.57	1.52
1	D	4916	LEU	N-CA	-6.07	1.38	1.46
1	A	3770	GLY	C-O	-6.07	1.15	1.24
1	A	3936	LEU	N-CA	-6.06	1.38	1.46
1	A	3732	LEU	N-CA	-6.06	1.39	1.46
1	B	4863	ILE	N-CA	-6.06	1.39	1.46
1	D	3850	GLY	N-CA	-6.06	1.37	1.45
1	B	4608	ALA	C-O	6.06	1.31	1.24
1	B	3840	LEU	CA-C	-6.05	1.45	1.52
1	A	3951	VAL	CA-C	-6.05	1.45	1.52
1	B	3920	THR	CA-C	-6.04	1.45	1.52
1	D	4810	MET	C-O	-6.04	1.16	1.24
1	B	3737	ALA	CA-C	-6.04	1.44	1.52
1	A	816	PRO	CA-C	6.03	1.57	1.52
1	A	3763	GLY	CA-C	-6.02	1.44	1.52
1	B	4146	ILE	N-CA	-6.02	1.38	1.46
1	C	3951	VAL	CA-C	-6.02	1.45	1.52
1	C	3773	THR	CA-C	-6.02	1.45	1.52
1	D	3939	SER	CA-C	-6.01	1.45	1.53
1	C	3763	GLY	CA-C	-6.01	1.44	1.52
1	C	4136	ARG	N-CA	-6.01	1.39	1.46
1	C	3917	VAL	CA-CB	-6.00	1.46	1.54
1	A	1898	LYS	C-O	-6.00	1.16	1.23
1	B	3917	VAL	CA-CB	-6.00	1.46	1.54
1	D	4146	ILE	N-CA	-5.99	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	4953	PHE	CG-CD1	-5.99	1.26	1.38
1	C	3668	LEU	CA-C	-5.99	1.45	1.52
1	A	3867	THR	C-O	-5.98	1.16	1.24
1	D	3858	TYR	CA-C	-5.98	1.44	1.52
1	D	3936	LEU	N-CA	-5.98	1.38	1.46
1	D	4953	PHE	CG-CD1	-5.98	1.26	1.38
1	A	4863	ILE	N-CA	-5.98	1.39	1.46
1	B	3936	LEU	N-CA	-5.97	1.38	1.46
1	B	3794	LEU	CA-C	-5.97	1.44	1.52
1	D	3763	GLY	CA-C	-5.97	1.44	1.52
1	C	3920	THR	CA-C	-5.97	1.45	1.52
1	C	3732	LEU	N-CA	-5.96	1.39	1.46
1	C	4786	ALA	N-CA	-5.96	1.39	1.46
1	C	3739	GLU	N-CA	-5.96	1.38	1.46
1	B	4643	ASN	CA-C	-5.95	1.44	1.52
1	C	4810	MET	C-O	-5.95	1.16	1.24
1	D	3942	TRP	N-CA	-5.95	1.39	1.46
1	C	4146	ILE	N-CA	-5.95	1.39	1.46
1	D	4646	TRP	CZ3-CH2	5.95	1.55	1.40
1	A	3939	SER	CA-C	-5.94	1.45	1.53
1	D	3920	THR	CA-C	-5.94	1.45	1.52
1	A	3794	LEU	CA-C	-5.94	1.44	1.52
1	A	3942	TRP	N-CA	-5.94	1.39	1.46
1	A	3840	LEU	CA-C	-5.93	1.45	1.52
1	A	4922	PHE	CA-C	-5.92	1.45	1.52
1	C	3737	ALA	CA-C	-5.91	1.44	1.52
1	B	3676	ALA	N-CA	-5.91	1.38	1.46
1	A	4643	ASN	CA-C	-5.91	1.44	1.52
1	B	3867	THR	C-O	-5.91	1.16	1.24
1	D	4863	ILE	N-CA	-5.91	1.39	1.46
1	B	2403	CYS	C-O	-5.91	1.17	1.23
1	C	2403	CYS	C-O	-5.91	1.17	1.23
1	B	4728	THR	C-O	5.90	1.31	1.24
1	D	3732	LEU	N-CA	-5.90	1.39	1.46
1	D	4138	GLU	CA-C	-5.90	1.45	1.52
1	D	3951	VAL	CA-C	-5.89	1.45	1.52
1	B	3841	PHE	N-CA	-5.89	1.38	1.46
1	B	4810	MET	C-O	-5.89	1.16	1.24
1	C	3676	ALA	N-CA	-5.88	1.38	1.46
1	D	2077	GLU	C-O	-5.88	1.15	1.24
1	D	3668	LEU	CA-C	-5.88	1.45	1.52
1	B	3739	GLU	N-CA	-5.88	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	4728	THR	C-O	5.88	1.31	1.24
1	C	2077	GLU	C-O	-5.88	1.15	1.24
1	D	3841	PHE	N-CA	-5.88	1.38	1.46
1	A	3668	LEU	CA-C	-5.87	1.45	1.52
1	A	4810	MET	C-O	-5.87	1.16	1.24
1	B	4145	ARG	CA-C	-5.87	1.45	1.52
1	A	3858	TYR	CA-C	-5.86	1.44	1.52
1	B	4864	GLN	CA-C	-5.86	1.45	1.52
1	A	3739	GLU	N-CA	-5.86	1.38	1.46
1	D	3840	LEU	CA-C	-5.86	1.45	1.52
1	A	2077	GLU	C-O	-5.85	1.15	1.24
1	C	3936	LEU	N-CA	-5.85	1.38	1.46
1	C	3939	SER	CA-C	-5.85	1.45	1.53
1	A	4597	PRO	N-CA	-5.85	1.39	1.47
1	C	1943	PHE	N-CA	5.85	1.52	1.46
1	C	4863	ILE	N-CA	-5.84	1.39	1.46
1	C	3867	THR	C-O	-5.84	1.17	1.24
1	A	4161	TRP	CA-C	-5.83	1.44	1.52
1	A	3841	PHE	N-CA	-5.83	1.38	1.46
1	D	4153	ILE	C-O	-5.83	1.18	1.24
1	B	2078	ASP	CA-C	-5.82	1.45	1.52
1	B	4597	PRO	N-CA	-5.82	1.39	1.47
1	B	3932	ASN	C-O	-5.82	1.16	1.24
1	C	4761	VAL	N-CA	-5.82	1.39	1.46
1	D	3737	ALA	CA-C	-5.82	1.44	1.52
1	D	3760	LEU	N-CA	-5.82	1.38	1.46
1	B	4786	ALA	N-CA	-5.81	1.39	1.46
1	C	4922	PHE	CA-C	-5.81	1.45	1.52
1	D	4761	VAL	N-CA	-5.81	1.39	1.46
1	C	4138	GLU	CA-C	-5.80	1.45	1.52
1	C	4864	GLN	CA-C	-5.80	1.45	1.52
1	A	1943	PHE	N-CA	5.80	1.52	1.46
1	A	3760	LEU	N-CA	-5.80	1.38	1.46
1	C	3840	LEU	CA-C	-5.80	1.45	1.52
1	D	1943	PHE	N-CA	5.79	1.52	1.46
1	C	3922	THR	CA-C	-5.79	1.45	1.52
1	B	3774	VAL	N-CA	-5.79	1.39	1.46
1	D	4851	PHE	C-O	-5.79	1.16	1.24
1	C	4916	LEU	N-CA	-5.79	1.38	1.46
1	D	4786	ALA	N-CA	-5.78	1.39	1.46
1	C	3774	VAL	N-CA	-5.77	1.39	1.46
1	A	3676	ALA	N-CA	-5.77	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	4874	LEU	N-CA	-5.77	1.39	1.46
1	B	3759	THR	N-CA	-5.76	1.39	1.46
1	C	3841	PHE	N-CA	-5.76	1.38	1.46
1	A	4728	THR	C-O	5.76	1.31	1.24
1	B	4161	TRP	CA-C	-5.76	1.45	1.52
1	C	3760	LEU	N-CA	-5.75	1.39	1.46
1	D	4728	THR	C-O	5.75	1.31	1.24
1	D	4643	ASN	CA-C	-5.75	1.45	1.52
1	C	3942	TRP	N-CA	-5.75	1.39	1.46
1	A	4138	GLU	CA-C	-5.74	1.45	1.52
1	C	4851	PHE	C-O	-5.74	1.16	1.24
1	D	4154	SER	C-O	-5.74	1.16	1.23
1	D	3689	TYR	CA-C	-5.73	1.45	1.52
1	B	3939	SER	CA-C	-5.72	1.45	1.53
1	B	3760	LEU	N-CA	-5.72	1.39	1.46
1	B	3846	LEU	CA-C	-5.72	1.44	1.52
1	B	4148	ARG	C-O	-5.72	1.16	1.24
1	C	3772	SER	N-CA	-5.72	1.39	1.46
1	A	3700	CYS	CA-C	5.72	1.65	1.52
1	D	4597	PRO	N-CA	-5.72	1.39	1.47
1	A	3737	ALA	CA-C	-5.71	1.44	1.52
1	C	4597	PRO	N-CA	-5.71	1.39	1.47
1	B	4774	LEU	C-O	5.71	1.30	1.24
1	D	3676	ALA	N-CA	-5.71	1.38	1.46
1	D	4136	ARG	N-CA	-5.71	1.39	1.46
1	A	3759	THR	N-CA	-5.70	1.39	1.46
1	B	4761	VAL	N-CA	-5.70	1.39	1.46
1	C	3748	SER	CA-C	-5.70	1.45	1.52
1	D	1902	PRO	N-CA	-5.70	1.40	1.47
1	C	3858	TYR	CA-C	-5.69	1.45	1.52
1	B	4922	PHE	CA-C	-5.69	1.45	1.52
1	D	3748	SER	CA-C	-5.69	1.45	1.52
1	B	4851	PHE	C-O	-5.68	1.17	1.24
1	A	4774	LEU	C-O	5.68	1.30	1.24
1	C	4774	LEU	C-O	5.68	1.30	1.24
1	A	3774	VAL	N-CA	-5.68	1.39	1.46
1	C	4643	ASN	CA-C	-5.68	1.45	1.52
1	B	3922	THR	CA-C	-5.68	1.45	1.52
1	A	3689	TYR	CA-C	-5.67	1.45	1.52
1	B	3745	ILE	N-CA	-5.67	1.39	1.46
1	A	4916	LEU	N-CA	-5.67	1.38	1.46
1	A	4145	ARG	CA-C	-5.67	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	4775	LEU	CA-CB	-5.66	1.44	1.53
1	C	1726	ILE	C-O	-5.66	1.17	1.24
1	B	3731	ARG	CA-C	-5.66	1.45	1.52
1	D	3867	THR	C-O	-5.66	1.17	1.24
1	B	1536	SER	C-O	-5.66	1.18	1.24
1	B	3689	TYR	CA-C	-5.65	1.45	1.52
1	D	4775	LEU	CA-CB	-5.64	1.44	1.53
1	A	4153	ILE	C-O	-5.64	1.18	1.24
1	B	1651	LEU	C-O	-5.64	1.17	1.24
1	A	3772	SER	N-CA	-5.64	1.39	1.46
1	A	3846	LEU	CA-C	-5.63	1.45	1.52
1	B	4193	PHE	CA-C	-5.63	1.45	1.52
1	C	3689	TYR	CA-C	-5.63	1.45	1.52
1	A	4761	VAL	N-CA	-5.62	1.39	1.46
1	A	4851	PHE	C-O	-5.62	1.17	1.24
1	C	3846	LEU	CA-C	-5.62	1.45	1.52
1	B	3839	ASP	N-CA	-5.61	1.38	1.46
1	D	2080	GLU	N-CA	-5.61	1.39	1.46
1	D	3772	SER	N-CA	-5.61	1.39	1.46
1	B	4138	GLU	CA-C	-5.61	1.45	1.52
1	C	4874	LEU	N-CA	-5.61	1.39	1.46
1	C	4795	ASN	CA-C	-5.60	1.47	1.53
1	C	4154	SER	C-O	-5.60	1.16	1.23
1	A	3748	SER	CA-C	-5.60	1.45	1.52
1	A	4600	ILE	N-CA	-5.60	1.39	1.46
1	C	1902	PRO	N-CA	-5.59	1.40	1.47
1	C	3759	THR	N-CA	-5.59	1.39	1.46
1	D	3774	VAL	N-CA	-5.58	1.39	1.46
1	B	3869	VAL	CA-C	-5.58	1.46	1.52
1	D	1898	LYS	C-O	-5.58	1.17	1.23
1	C	3932	ASN	C-O	-5.57	1.17	1.24
1	D	4864	GLN	CA-C	-5.57	1.45	1.52
1	A	4514	ILE	C-O	-5.57	1.17	1.24
1	D	4142	SER	N-CA	-5.57	1.38	1.46
1	A	1726	ILE	C-O	-5.57	1.18	1.24
1	C	4148	ARG	C-O	-5.57	1.16	1.24
1	A	4874	LEU	N-CA	-5.56	1.39	1.46
1	C	4145	ARG	CA-C	-5.56	1.45	1.52
1	D	4922	PHE	CA-C	-5.56	1.45	1.52
1	A	3932	ASN	C-O	-5.56	1.17	1.24
1	A	4864	GLN	CA-C	-5.56	1.45	1.52
1	B	4811	LEU	CA-C	-5.56	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	4193	PHE	CA-C	-5.56	1.45	1.52
1	A	3745	ILE	N-CA	-5.55	1.39	1.46
1	C	4753	THR	C-N	-5.55	1.25	1.33
1	D	1726	ILE	C-O	-5.55	1.18	1.24
1	D	4763	HIS	CA-C	-5.55	1.45	1.52
1	D	4874	LEU	N-CA	-5.55	1.39	1.46
1	D	4600	ILE	N-CA	-5.55	1.40	1.46
1	C	4193	PHE	CA-C	-5.55	1.45	1.52
1	A	842	GLN	C-O	5.55	1.31	1.23
1	A	1902	PRO	N-CA	-5.55	1.40	1.47
1	B	3919	ASN	N-CA	-5.55	1.38	1.46
1	B	4753	THR	C-N	-5.55	1.25	1.33
1	C	1536	SER	C-O	-5.54	1.18	1.24
1	D	4774	LEU	C-O	5.54	1.30	1.24
1	A	4636	ILE	N-CA	-5.54	1.39	1.46
1	B	3748	SER	CA-C	-5.53	1.45	1.52
1	B	3744	THR	CA-C	-5.53	1.45	1.52
1	D	3759	THR	N-CA	-5.53	1.39	1.46
1	B	3772	SER	N-CA	-5.53	1.39	1.46
1	C	4186	LYS	C-O	-5.53	1.17	1.24
1	C	3731	ARG	CA-C	-5.53	1.45	1.52
1	D	3700	CYS	CA-CB	5.53	1.64	1.53
1	A	4101	VAL	N-CA	-5.52	1.40	1.46
1	B	1898	LYS	C-O	-5.52	1.17	1.23
1	B	4142	SER	N-CA	-5.52	1.38	1.46
1	D	4101	VAL	N-CA	-5.52	1.40	1.46
1	A	2080	GLU	N-CA	-5.52	1.39	1.46
1	C	3744	THR	CA-C	-5.52	1.45	1.52
1	C	1699	ARG	CA-C	-5.51	1.45	1.52
1	C	4775	LEU	CA-CB	-5.51	1.44	1.53
1	A	3731	ARG	CA-C	-5.51	1.45	1.52
1	B	4916	LEU	N-CA	-5.51	1.39	1.46
1	C	4792	LYS	CA-C	-5.50	1.45	1.52
1	A	3700	CYS	CA-CB	5.50	1.64	1.53
1	D	3700	CYS	CA-C	5.50	1.64	1.52
1	B	3942	TRP	N-CA	-5.50	1.39	1.46
1	D	3846	LEU	CA-C	-5.50	1.45	1.52
1	C	4808	ASP	C-O	-5.50	1.16	1.24
1	D	3922	THR	CA-C	-5.50	1.45	1.52
1	D	1536	SER	C-O	-5.49	1.18	1.24
1	D	2239	THR	CA-C	5.49	1.64	1.52
1	B	4514	ILE	C-O	-5.49	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	4753	THR	C-N	-5.49	1.25	1.33
1	A	4859	LEU	C-O	-5.48	1.16	1.24
1	D	4603	ARG	N-CA	-5.48	1.39	1.46
1	A	4193	PHE	CA-C	-5.48	1.45	1.52
1	A	4753	THR	C-N	-5.47	1.25	1.33
1	A	4786	ALA	N-CA	-5.47	1.39	1.46
1	B	3920	THR	CA-CB	-5.47	1.44	1.53
1	C	3745	ILE	N-CA	-5.47	1.39	1.46
1	D	3745	ILE	N-CA	-5.47	1.39	1.46
1	A	3839	ASP	N-CA	-5.47	1.39	1.46
1	B	4101	VAL	N-CA	-5.47	1.40	1.46
1	A	4768	LEU	CA-C	-5.46	1.45	1.52
1	A	4781	LEU	N-CA	-5.46	1.39	1.46
1	A	4811	LEU	CA-C	-5.46	1.46	1.52
1	B	1902	PRO	N-CA	-5.46	1.40	1.47
1	A	2226	SER	C-O	5.46	1.30	1.24
1	C	4805	MET	C-O	-5.46	1.17	1.24
1	D	3869	VAL	CA-C	-5.45	1.46	1.52
1	D	4148	ARG	C-O	-5.45	1.17	1.24
1	A	2306	ALA	N-CA	-5.45	1.39	1.46
1	A	3920	THR	CA-CB	-5.45	1.44	1.53
1	B	4149	VAL	C-O	5.45	1.29	1.24
1	A	4940	TYR	CG-CD2	-5.44	1.27	1.39
1	C	3839	ASP	N-CA	-5.44	1.39	1.46
1	D	4795	ASN	CA-C	-5.44	1.47	1.53
1	C	3919	ASN	N-CA	-5.44	1.39	1.46
1	C	4940	TYR	CG-CD2	-5.44	1.27	1.39
1	C	4149	VAL	C-O	5.44	1.29	1.24
1	C	4768	LEU	CA-C	-5.44	1.45	1.52
1	A	3919	ASN	N-CA	-5.43	1.39	1.46
1	B	4600	ILE	N-CA	-5.43	1.40	1.46
1	B	4603	ARG	N-CA	-5.43	1.39	1.46
1	C	4781	LEU	N-CA	-5.43	1.39	1.46
1	C	3869	VAL	CA-C	-5.43	1.46	1.52
1	A	4756	THR	N-CA	-5.43	1.39	1.46
1	C	1898	LYS	C-O	-5.43	1.17	1.23
1	A	4792	LYS	CA-C	-5.42	1.45	1.52
1	D	3732	LEU	CA-C	-5.42	1.46	1.53
1	C	4603	ARG	N-CA	-5.42	1.39	1.46
1	B	4953	PHE	CG-CD2	-5.42	1.27	1.38
1	C	4602	LYS	N-CA	-5.42	1.39	1.46
1	D	1483	SER	N-CA	5.42	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	4600	ILE	N-CA	-5.41	1.40	1.46
1	D	2403	CYS	C-O	-5.41	1.17	1.23
1	A	1666	ALA	CA-C	-5.41	1.46	1.53
1	A	2078	ASP	CA-C	-5.41	1.46	1.52
1	C	1483	SER	N-CA	5.41	1.53	1.45
1	A	4186	LYS	C-O	-5.41	1.17	1.24
1	C	3930	THR	N-CA	-5.41	1.39	1.46
1	D	4186	LYS	C-O	-5.41	1.17	1.24
1	A	3869	VAL	CA-C	-5.41	1.46	1.52
1	B	3700	CYS	CA-CB	5.41	1.64	1.53
1	D	3839	ASP	N-CA	-5.41	1.39	1.46
1	C	4101	VAL	N-CA	-5.40	1.40	1.46
1	B	842	GLN	C-O	5.40	1.30	1.23
1	B	4186	LYS	C-O	-5.40	1.17	1.24
1	B	4805	MET	C-O	-5.40	1.17	1.24
1	D	4849	ILE	N-CA	-5.40	1.39	1.46
1	A	4140	MET	C-O	-5.40	1.16	1.23
1	A	4142	SER	N-CA	-5.40	1.38	1.46
1	D	4810	MET	CA-C	-5.40	1.45	1.52
1	D	842	GLN	C-O	5.40	1.30	1.23
1	D	4145	ARG	CA-C	-5.40	1.46	1.52
1	C	4142	SER	N-CA	-5.39	1.38	1.46
1	C	4190	PHE	N-CA	-5.39	1.40	1.46
1	B	4746	ASP	C-N	-5.39	1.28	1.34
1	D	3731	ARG	CA-C	-5.38	1.45	1.52
1	D	4138	GLU	C-O	-5.38	1.17	1.23
1	C	4811	LEU	CA-C	-5.38	1.46	1.52
1	A	4810	MET	CA-C	-5.38	1.45	1.52
1	D	4149	VAL	C-O	5.38	1.29	1.24
1	D	3920	THR	CA-CB	-5.37	1.44	1.53
1	A	3744	THR	CA-C	-5.37	1.45	1.52
1	D	4940	TYR	CG-CD2	-5.37	1.28	1.39
1	A	4603	ARG	N-CA	-5.36	1.39	1.46
1	D	3919	ASN	N-CA	-5.36	1.39	1.46
1	C	2306	ALA	N-CA	-5.36	1.39	1.46
1	A	4190	PHE	N-CA	-5.36	1.40	1.46
1	A	4775	LEU	CA-CB	-5.36	1.44	1.53
1	A	4811	LEU	N-CA	-5.36	1.40	1.46
1	B	4147	GLU	CA-C	-5.36	1.46	1.52
1	D	4740	PHE	C-O	5.36	1.30	1.24
1	D	4792	LYS	CA-C	-5.35	1.45	1.52
1	A	4953	PHE	CG-CD2	-5.35	1.27	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	4140	MET	C-O	-5.35	1.16	1.23
1	B	4781	LEU	N-CA	-5.35	1.39	1.46
1	C	1694	MET	C-O	-5.35	1.17	1.24
1	C	4140	MET	C-O	-5.35	1.16	1.23
1	C	3920	THR	CA-CB	-5.35	1.44	1.53
1	C	4953	PHE	CG-CD2	-5.34	1.27	1.38
1	A	4166	VAL	N-CA	-5.34	1.40	1.46
1	C	3953	ALA	C-O	-5.34	1.18	1.24
1	B	4763	HIS	CA-C	-5.34	1.46	1.52
1	B	4190	PHE	N-CA	-5.34	1.40	1.46
1	B	4940	TYR	CG-CD2	-5.34	1.28	1.39
1	C	2078	ASP	CA-C	-5.34	1.46	1.52
1	B	4756	THR	N-CA	-5.33	1.39	1.46
1	B	4811	LEU	N-CA	-5.33	1.40	1.46
1	C	1651	LEU	C-O	-5.33	1.17	1.24
1	C	4596	VAL	CA-C	-5.33	1.47	1.52
1	C	2077	GLU	CA-C	-5.33	1.45	1.53
1	D	4514	ILE	C-O	-5.33	1.17	1.24
1	D	4855	VAL	N-CA	-5.33	1.39	1.46
1	A	2403	CYS	C-O	-5.32	1.17	1.23
1	A	4149	VAL	C-O	5.32	1.29	1.24
1	A	1536	SER	C-O	-5.32	1.18	1.24
1	A	4154	SER	C-O	-5.32	1.17	1.23
1	D	2306	ALA	N-CA	-5.32	1.39	1.46
1	D	4190	PHE	N-CA	-5.31	1.40	1.46
1	A	1651	LEU	C-O	-5.31	1.17	1.24
1	D	4937	GLN	CA-CB	-5.31	1.44	1.53
1	B	4814	TYR	C-O	-5.31	1.17	1.24
1	D	2228	VAL	N-CA	5.31	1.56	1.46
1	A	4808	ASP	C-O	-5.30	1.17	1.24
1	B	1694	MET	C-O	-5.30	1.17	1.24
1	D	3932	ASN	C-O	-5.30	1.17	1.24
1	D	2226	SER	C-O	5.30	1.30	1.24
1	A	4805	MET	C-O	-5.30	1.17	1.24
1	D	1666	ALA	CA-C	-5.30	1.46	1.53
1	B	4740	PHE	C-O	5.30	1.30	1.24
1	C	4740	PHE	C-O	5.30	1.30	1.24
1	A	1694	MET	C-O	-5.29	1.17	1.24
1	B	4819	TYR	C-O	-5.29	1.17	1.24
1	A	4148	ARG	C-O	-5.29	1.17	1.24
1	B	2306	ALA	N-CA	-5.28	1.39	1.46
1	C	4819	TYR	C-O	-5.28	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3922	THR	CA-C	-5.28	1.45	1.52
1	D	4953	PHE	CG-CD2	-5.28	1.27	1.38
1	B	4602	LYS	N-CA	-5.27	1.39	1.46
1	B	4851	PHE	C-N	-5.27	1.26	1.33
1	C	3811	ARG	CZ-NH1	5.27	1.40	1.32
1	D	1694	MET	C-O	-5.27	1.17	1.24
1	A	2243	VAL	N-CA	-5.27	1.40	1.46
1	B	1726	ILE	C-O	-5.26	1.18	1.24
1	B	4937	GLN	CA-CB	-5.26	1.45	1.53
1	C	4810	MET	CA-C	-5.26	1.45	1.52
1	C	842	GLN	C-O	5.26	1.30	1.23
1	D	4859	LEU	C-O	-5.26	1.17	1.24
1	A	4138	GLU	C-O	-5.25	1.17	1.23
1	A	4147	GLU	CA-C	-5.25	1.46	1.52
1	B	4792	LYS	CA-C	-5.25	1.45	1.52
1	A	2239	THR	CA-C	5.25	1.64	1.52
1	B	3732	LEU	CA-C	-5.25	1.46	1.53
1	B	1456	ALA	C-O	-5.24	1.17	1.23
1	D	2078	ASP	CA-C	-5.24	1.46	1.52
1	D	4596	VAL	CA-C	-5.24	1.47	1.52
1	D	4781	LEU	N-CA	-5.24	1.39	1.46
1	A	4849	ILE	N-CA	-5.24	1.40	1.46
1	A	4919	TYR	CA-C	-5.24	1.45	1.52
1	A	1599	MET	N-CA	5.23	1.52	1.46
1	B	3858	TYR	CG-CD2	-5.23	1.28	1.39
1	B	4154	SER	C-O	-5.23	1.17	1.23
1	B	4808	ASP	C-O	-5.23	1.17	1.24
1	D	4808	ASP	C-O	-5.23	1.17	1.24
1	A	3941	LEU	CA-C	-5.23	1.45	1.52
1	A	4740	PHE	C-O	5.22	1.30	1.24
1	D	39	ALA	C-O	-5.22	1.17	1.23
1	A	2258	LEU	CA-C	-5.22	1.46	1.52
1	C	3700	CYS	CA-CB	5.22	1.63	1.53
1	D	3744	THR	CA-C	-5.22	1.45	1.52
1	C	39	ALA	C-O	-5.22	1.17	1.23
1	B	4596	VAL	CA-C	-5.22	1.47	1.52
1	C	4937	GLN	CA-CB	-5.22	1.45	1.53
1	C	2239	THR	CA-C	5.21	1.63	1.52
1	D	3953	ALA	C-O	-5.21	1.18	1.24
1	A	4937	GLN	CA-CB	-5.21	1.45	1.53
1	D	4579	LEU	CA-C	-5.21	1.46	1.52
1	D	4602	LYS	N-CA	-5.21	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	3930	THR	N-CA	-5.20	1.39	1.46
1	A	1483	SER	N-CA	5.20	1.52	1.45
1	B	2194	VAL	CA-C	-5.20	1.46	1.52
1	A	3800	SER	CA-C	-5.20	1.45	1.52
1	A	4851	PHE	C-N	-5.20	1.26	1.33
1	C	1599	MET	N-CA	5.20	1.52	1.46
1	D	1033	VAL	CA-C	5.19	1.56	1.52
1	A	4952	PHE	CG-CD1	-5.19	1.27	1.38
1	D	1651	LEU	C-O	-5.19	1.18	1.24
1	C	4814	TYR	C-O	-5.19	1.18	1.24
1	A	4767	GLN	N-CA	-5.19	1.39	1.46
1	C	4138	GLU	C-O	-5.19	1.17	1.23
1	A	2077	GLU	CA-C	-5.18	1.45	1.53
1	A	4808	ASP	N-CA	5.18	1.52	1.45
1	B	4767	GLN	N-CA	-5.18	1.39	1.46
1	D	4756	THR	N-CA	-5.18	1.39	1.46
1	B	1699	ARG	CA-C	-5.18	1.46	1.52
1	C	2194	VAL	CA-C	-5.18	1.46	1.52
1	D	1599	MET	N-CA	5.18	1.52	1.46
1	A	3173	GLU	N-CA	5.17	1.52	1.46
1	D	2077	GLU	CA-C	-5.17	1.45	1.53
1	B	4166	VAL	N-CA	-5.17	1.40	1.46
1	D	4851	PHE	C-N	-5.17	1.26	1.33
1	B	4727	MET	CG-SD	5.17	1.93	1.80
1	C	4763	HIS	CA-C	-5.16	1.46	1.52
1	C	584	GLU	N-CA	-5.16	1.40	1.46
1	C	3921	LEU	CA-C	-5.16	1.45	1.52
1	C	4756	THR	N-CA	-5.16	1.39	1.46
1	A	4602	LYS	N-CA	-5.16	1.40	1.46
1	B	4601	PHE	CA-C	-5.15	1.45	1.52
1	B	4865	GLY	N-CA	-5.15	1.39	1.45
1	B	4795	ASN	CA-C	-5.15	1.47	1.53
1	B	3800	SER	CA-C	-5.15	1.45	1.52
1	B	3871	ILE	N-CA	-5.15	1.40	1.46
1	B	4777	VAL	CA-C	-5.15	1.45	1.52
1	C	1666	ALA	CA-C	-5.15	1.46	1.53
1	A	4788	ASN	N-CA	-5.14	1.39	1.46
1	B	1483	SER	N-CA	5.14	1.52	1.45
1	B	1691	ASN	CA-C	-5.14	1.46	1.52
1	D	4166	VAL	N-CA	-5.14	1.40	1.46
1	C	4777	VAL	CA-C	-5.14	1.45	1.52
1	D	4805	MET	C-O	-5.14	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	4851	PHE	C-N	-5.14	1.26	1.33
1	B	203	VAL	C-O	-5.14	1.18	1.24
1	A	4746	ASP	C-N	-5.13	1.28	1.34
1	C	4166	VAL	N-CA	-5.13	1.40	1.46
1	D	3800	SER	CA-C	-5.13	1.46	1.52
1	A	3930	THR	N-CA	-5.13	1.39	1.46
1	C	4783	THR	N-CA	-5.13	1.39	1.46
1	D	1716	THR	C-O	-5.13	1.17	1.24
1	A	4777	VAL	CA-C	-5.13	1.45	1.52
1	B	2243	VAL	N-CA	-5.13	1.40	1.46
1	A	1691	ASN	CA-C	-5.13	1.46	1.52
1	D	3690	MET	N-CA	-5.13	1.39	1.46
1	A	4159	THR	CA-C	-5.13	1.45	1.52
1	B	4952	PHE	CG-CD1	-5.13	1.28	1.38
1	C	3173	GLU	N-CA	5.13	1.52	1.46
1	C	3800	SER	CA-C	-5.13	1.46	1.52
1	B	2226	SER	C-O	5.12	1.30	1.24
1	A	4196	ASP	CA-C	-5.12	1.46	1.52
1	B	4574	ARG	NE-CZ	5.12	1.38	1.33
1	C	2243	VAL	N-CA	-5.12	1.40	1.46
1	D	4822	VAL	C-O	-5.12	1.18	1.24
1	A	3690	MET	N-CA	-5.12	1.39	1.46
1	C	4950	TRP	CD2-CE3	-5.12	1.32	1.40
1	B	1666	ALA	CA-C	-5.12	1.46	1.53
1	A	4814	TYR	C-O	-5.12	1.18	1.24
1	B	4768	LEU	CA-C	-5.12	1.46	1.52
1	D	3916	GLN	CA-C	-5.12	1.46	1.52
1	B	4950	TRP	CD2-CE3	-5.12	1.32	1.40
1	D	4865	GLY	N-CA	-5.12	1.39	1.45
1	A	4596	VAL	CA-C	-5.11	1.48	1.52
1	B	39	ALA	C-O	-5.11	1.18	1.23
1	C	4147	GLU	CA-C	-5.11	1.46	1.52
1	C	4514	ILE	C-O	-5.11	1.17	1.24
1	B	2213	LYS	CA-C	-5.11	1.45	1.52
1	D	3921	LEU	CA-C	-5.11	1.45	1.52
1	C	4853	PHE	CD1-CE1	5.11	1.53	1.38
1	D	4952	PHE	CG-CD1	-5.11	1.28	1.38
1	B	4859	LEU	C-O	-5.10	1.17	1.24
1	D	4636	ILE	N-CA	-5.10	1.39	1.46
1	B	4783	THR	N-CA	-5.10	1.39	1.46
1	B	4810	MET	CA-C	-5.10	1.45	1.52
1	D	3811	ARG	CZ-NH1	5.10	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	584	GLU	N-CA	-5.10	1.40	1.46
1	B	4808	ASP	N-CA	5.10	1.52	1.45
1	C	2080	GLU	N-CA	-5.10	1.39	1.46
1	A	39	ALA	C-O	-5.09	1.18	1.23
1	B	1599	MET	N-CA	5.09	1.52	1.46
1	B	3811	ARG	CZ-NH1	5.09	1.39	1.32
1	A	3871	ILE	N-CA	-5.09	1.40	1.46
1	A	1033	VAL	CA-C	5.09	1.56	1.52
1	D	4140	MET	C-O	-5.09	1.16	1.23
1	C	4822	VAL	C-O	-5.08	1.18	1.24
1	D	4811	LEU	N-CA	-5.08	1.40	1.46
1	A	4925	TYR	CA-C	-5.08	1.45	1.52
1	D	4811	LEU	CA-C	-5.08	1.46	1.52
1	B	2258	LEU	CA-C	-5.07	1.46	1.52
1	B	1261	VAL	N-CA	-5.07	1.42	1.46
1	A	4754	LEU	CA-C	-5.07	1.45	1.52
1	C	3941	LEU	CA-C	-5.07	1.45	1.52
1	D	3173	GLU	N-CA	5.07	1.52	1.46
1	A	3858	TYR	CG-CD2	-5.07	1.28	1.39
1	C	2226	SER	C-O	5.07	1.30	1.24
1	B	3930	THR	N-CA	-5.06	1.39	1.46
1	C	2258	LEU	CA-C	-5.06	1.46	1.52
1	C	4865	GLY	N-CA	-5.06	1.39	1.45
1	A	4855	VAL	N-CA	-5.06	1.40	1.46
1	D	4950	TRP	CD2-CE3	-5.06	1.32	1.40
1	A	3811	ARG	CZ-NH1	5.06	1.39	1.32
1	D	4777	VAL	CA-C	-5.05	1.45	1.52
1	D	4853	PHE	CD1-CE1	5.05	1.53	1.38
1	A	4819	TYR	C-O	-5.05	1.18	1.24
1	C	3841	PHE	CG-CD2	-5.05	1.28	1.38
1	A	1456	ALA	C-O	-5.05	1.17	1.23
1	A	4601	PHE	CA-C	-5.05	1.45	1.52
1	C	3684	GLU	N-CA	-5.04	1.39	1.45
1	D	4768	LEU	CA-C	-5.04	1.46	1.52
1	A	2213	LYS	CA-C	-5.04	1.46	1.52
1	A	3732	LEU	CA-C	-5.04	1.47	1.53
1	D	4147	GLU	CA-C	-5.04	1.46	1.52
1	A	3916	GLN	CA-C	-5.04	1.46	1.52
1	C	1691	ASN	CA-C	-5.04	1.46	1.52
1	C	3840	LEU	C-O	5.04	1.29	1.24
1	D	4727	MET	CG-SD	5.03	1.93	1.80
1	D	4814	TYR	C-O	-5.03	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	4942	TRP	N-CA	-5.03	1.40	1.46
1	D	4873	GLU	CA-C	-5.03	1.46	1.52
1	D	4788	ASN	N-CA	-5.03	1.39	1.46
1	B	4788	ASN	N-CA	-5.03	1.39	1.46
1	A	1716	THR	C-O	-5.03	1.17	1.24
1	A	1261	VAL	N-CA	-5.02	1.42	1.46
1	C	4746	ASP	C-N	-5.02	1.28	1.34
1	D	4601	PHE	CA-C	-5.02	1.45	1.52
1	D	2243	VAL	N-CA	-5.02	1.40	1.46
1	D	3858	TYR	CG-CD2	-5.01	1.28	1.39
1	D	4767	GLN	N-CA	-5.01	1.39	1.46
1	C	4727	MET	CG-SD	5.01	1.93	1.80
1	C	4859	LEU	C-O	-5.01	1.17	1.24
1	B	4138	GLU	C-O	-5.01	1.17	1.23
1	D	4783	THR	N-CA	-5.00	1.39	1.46
1	B	1033	VAL	CA-C	5.00	1.56	1.52
1	D	1691	ASN	CA-C	-5.00	1.46	1.52

All (358) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1847	GLU	CA-C-N	12.00	134.84	119.84
1	B	1847	GLU	C-N-CA	12.00	134.84	119.84
1	A	1847	GLU	CA-C-N	11.99	134.83	119.84
1	A	1847	GLU	C-N-CA	11.99	134.83	119.84
1	D	1847	GLU	CA-C-N	11.96	134.79	119.84
1	D	1847	GLU	C-N-CA	11.96	134.79	119.84
1	C	1847	GLU	CA-C-N	11.82	134.62	119.84
1	C	1847	GLU	C-N-CA	11.82	134.62	119.84
1	B	4853	PHE	N-CA-CB	11.78	127.06	109.98
1	D	4853	PHE	N-CA-CB	11.75	127.01	109.98
1	A	4853	PHE	N-CA-CB	11.73	126.99	109.98
1	C	4853	PHE	N-CA-CB	11.63	126.84	109.98
1	D	2239	THR	N-CA-CB	-9.80	94.85	111.50
1	C	2239	THR	N-CA-CB	-9.48	95.38	111.50
1	B	247	VAL	N-CA-C	-9.44	101.45	109.19
1	A	2239	THR	N-CA-CB	-9.42	95.49	111.50
1	D	247	VAL	N-CA-C	-9.40	101.48	109.19
1	A	247	VAL	N-CA-C	-9.21	101.63	109.19
1	B	4853	PHE	N-CA-C	-9.15	100.87	111.03
1	C	247	VAL	N-CA-C	-9.15	101.69	109.19
1	C	4853	PHE	N-CA-C	-9.14	100.89	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4853	PHE	N-CA-C	-9.09	100.94	111.03
1	D	4853	PHE	N-CA-C	-9.01	101.03	111.03
1	D	2495	PRO	N-CA-CB	8.98	113.04	103.52
1	A	2495	PRO	N-CA-CB	8.94	112.99	103.52
1	C	2495	PRO	N-CA-CB	8.91	112.96	103.52
1	B	2495	PRO	N-CA-CB	8.90	112.96	103.52
1	A	4948	ARG	NE-CZ-NH2	8.76	127.08	119.20
1	B	2239	THR	N-CA-CB	-8.74	96.65	111.50
1	D	1579	VAL	CA-C-N	-8.59	109.10	119.84
1	D	1579	VAL	C-N-CA	-8.59	109.10	119.84
1	D	4948	ARG	NE-CZ-NH2	8.58	126.92	119.20
1	A	1579	VAL	CA-C-N	-8.57	109.13	119.84
1	A	1579	VAL	C-N-CA	-8.57	109.13	119.84
1	B	1579	VAL	CA-C-N	-8.56	109.14	119.84
1	B	1579	VAL	C-N-CA	-8.56	109.14	119.84
1	C	1579	VAL	CA-C-N	-8.52	109.19	119.84
1	C	1579	VAL	C-N-CA	-8.52	109.19	119.84
1	B	4948	ARG	NE-CZ-NH2	8.49	126.84	119.20
1	B	2583	PRO	N-CA-CB	8.31	112.33	103.52
1	A	2583	PRO	N-CA-CB	8.21	112.22	103.52
1	D	267	VAL	N-CA-C	-8.15	105.96	113.71
1	A	2678	PRO	N-CA-CB	8.14	110.98	103.08
1	A	267	VAL	N-CA-C	-8.11	106.00	113.71
1	C	2678	PRO	N-CA-CB	8.10	110.93	103.08
1	D	2678	PRO	N-CA-CB	8.09	110.93	103.08
1	C	267	VAL	N-CA-C	-8.09	106.02	113.71
1	B	2678	PRO	N-CA-CB	8.08	110.92	103.08
1	C	4948	ARG	NE-CZ-NH2	8.05	126.44	119.20
1	C	2583	PRO	N-CA-CB	8.02	112.02	103.52
1	B	267	VAL	N-CA-C	-8.01	106.10	113.71
1	D	816	PRO	N-CA-C	7.93	120.37	110.70
1	B	816	PRO	N-CA-C	7.91	120.35	110.70
1	A	816	PRO	N-CA-C	7.90	120.33	110.70
1	D	2583	PRO	N-CA-CB	7.90	111.89	103.52
1	C	816	PRO	N-CA-C	7.86	120.29	110.70
1	A	2156	PHE	N-CA-C	-7.69	105.06	114.75
1	B	2156	PHE	N-CA-C	-7.67	105.08	114.75
1	C	2607	PRO	N-CA-CB	7.63	111.99	103.44
1	B	2625	PRO	N-CA-CB	7.60	111.58	103.52
1	A	2625	PRO	N-CA-CB	7.60	111.58	103.52
1	D	2598	PRO	N-CA-CB	7.59	111.95	103.44
1	D	2156	PHE	N-CA-C	-7.59	105.19	114.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2156	PHE	N-CA-C	-7.59	105.19	114.75
1	A	2607	PRO	N-CA-CB	7.57	111.92	103.44
1	D	2625	PRO	N-CA-CB	7.56	111.53	103.52
1	B	2598	PRO	N-CA-CB	7.55	111.90	103.44
1	B	2607	PRO	N-CA-CB	7.55	111.90	103.44
1	D	2607	PRO	N-CA-CB	7.52	111.86	103.44
1	A	2598	PRO	N-CA-CB	7.50	111.84	103.44
1	C	2598	PRO	N-CA-CB	7.50	111.84	103.44
1	B	3104	PRO	N-CA-CB	7.44	111.41	103.52
1	A	3104	PRO	N-CA-CB	7.44	111.41	103.52
1	C	2625	PRO	N-CA-CB	7.43	111.40	103.52
1	D	4596	VAL	CA-C-N	-7.28	112.21	119.56
1	D	4596	VAL	C-N-CA	-7.28	112.21	119.56
1	C	3104	PRO	N-CA-CB	7.28	111.23	103.52
1	B	1819	VAL	CA-C-N	-7.27	112.19	120.04
1	B	1819	VAL	C-N-CA	-7.27	112.19	120.04
1	A	4596	VAL	CA-C-N	-7.26	112.23	119.56
1	A	4596	VAL	C-N-CA	-7.26	112.23	119.56
1	D	2679	PRO	N-CA-CB	7.25	110.98	103.00
1	D	3104	PRO	N-CA-CB	7.20	111.15	103.52
1	C	1819	VAL	CA-C-N	-7.18	112.29	120.04
1	C	1819	VAL	C-N-CA	-7.18	112.29	120.04
1	C	2679	PRO	N-CA-CB	7.18	110.90	103.00
1	C	4596	VAL	CA-C-N	-7.18	112.31	119.56
1	C	4596	VAL	C-N-CA	-7.18	112.31	119.56
1	D	1819	VAL	CA-C-N	-7.16	112.30	120.04
1	D	1819	VAL	C-N-CA	-7.16	112.30	120.04
1	A	2679	PRO	N-CA-CB	7.16	110.87	103.00
1	A	1819	VAL	CA-C-N	-7.15	112.32	120.04
1	A	1819	VAL	C-N-CA	-7.15	112.32	120.04
1	B	4596	VAL	CA-C-N	-7.10	112.39	119.56
1	B	4596	VAL	C-N-CA	-7.10	112.39	119.56
1	B	2679	PRO	N-CA-CB	7.03	110.73	103.00
1	C	2668	PRO	N-CA-CB	6.95	111.23	103.44
1	D	2668	PRO	N-CA-CB	6.93	111.21	103.44
1	A	2668	PRO	N-CA-CB	6.89	111.16	103.44
1	D	4818	MET	CA-CB-CG	6.82	127.73	114.10
1	D	3700	CYS	N-CA-CB	-6.80	98.94	110.50
1	B	2668	PRO	N-CA-CB	6.78	111.03	103.44
1	D	2990	PRO	N-CA-CB	6.67	110.91	103.44
1	C	4818	MET	CA-CB-CG	6.67	127.44	114.10
1	A	2990	PRO	N-CA-CB	6.63	110.86	103.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2990	PRO	N-CA-CB	6.62	110.86	103.44
1	C	3700	CYS	N-CA-CB	-6.60	99.29	110.50
1	B	3700	CYS	N-CA-CB	-6.58	99.31	110.50
1	B	2990	PRO	N-CA-CB	6.56	110.79	103.44
1	C	2329	PRO	N-CA-C	6.53	122.03	113.86
1	A	4818	MET	CA-CB-CG	6.50	127.10	114.10
1	B	2329	PRO	N-CA-C	6.47	121.95	113.86
1	B	4853	PHE	CA-C-O	-6.46	114.25	120.90
1	C	4853	PHE	CA-C-O	-6.44	114.26	120.90
1	A	3700	CYS	N-CA-CB	-6.44	99.56	110.50
1	A	1636	ASN	N-CA-C	6.43	119.94	110.30
1	C	3700	CYS	CB-CA-C	6.39	122.25	110.10
1	B	1636	ASN	N-CA-C	6.38	119.87	110.30
1	A	3941	LEU	N-CA-C	6.37	119.90	111.75
1	C	1636	ASN	N-CA-C	6.35	119.83	110.30
1	D	2329	PRO	N-CA-C	6.35	121.80	113.86
1	A	4818	MET	CG-SD-CE	6.34	114.86	100.90
1	C	3941	LEU	N-CA-C	6.34	119.87	111.75
1	A	2329	PRO	N-CA-C	6.34	121.78	113.86
1	D	1636	ASN	N-CA-C	6.32	119.77	110.30
1	B	3700	CYS	CB-CA-C	6.30	122.07	110.10
1	D	3941	LEU	N-CA-C	6.29	119.80	111.75
1	D	3700	CYS	CB-CA-C	6.28	122.03	110.10
1	B	4818	MET	CA-CB-CG	6.28	126.65	114.10
1	D	4853	PHE	CA-C-O	-6.27	114.44	120.90
1	D	3991	VAL	N-CA-C	-6.26	103.22	110.05
1	C	3991	VAL	N-CA-C	-6.26	103.23	110.05
1	A	3700	CYS	CB-CA-C	6.25	121.98	110.10
1	A	4853	PHE	CA-C-O	-6.25	114.47	120.90
1	A	3991	VAL	N-CA-C	-6.24	103.25	110.05
1	C	4596	VAL	O-C-N	6.22	124.49	120.07
1	A	4596	VAL	O-C-N	6.21	124.48	120.07
1	B	4596	VAL	O-C-N	6.21	124.48	120.07
1	B	3941	LEU	N-CA-C	6.19	119.67	111.75
1	D	4596	VAL	O-C-N	6.15	124.44	120.07
1	B	3991	VAL	N-CA-C	-6.09	103.41	110.05
1	D	4818	MET	CG-SD-CE	6.07	114.25	100.90
1	B	4818	MET	CG-SD-CE	6.05	114.21	100.90
1	C	4818	MET	CG-SD-CE	6.05	114.21	100.90
1	D	3803	VAL	N-CA-CB	-6.04	101.27	111.23
1	C	2534	PRO	N-CA-CB	6.02	109.62	103.00
1	C	3803	VAL	N-CA-CB	-5.97	101.38	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4764	ASN	CA-C-N	5.96	127.59	120.14
1	D	4764	ASN	C-N-CA	5.96	127.59	120.14
1	A	3803	VAL	N-CA-CB	-5.95	101.41	111.23
1	D	2534	PRO	N-CA-CB	5.94	109.53	103.00
1	C	521	GLU	N-CA-C	-5.93	105.96	113.43
1	D	521	GLU	N-CA-C	-5.92	105.98	113.43
1	A	2534	PRO	N-CA-CB	5.87	109.46	103.00
1	B	2534	PRO	N-CA-CB	5.86	109.45	103.00
1	A	4897	ASP	N-CA-C	5.86	117.66	111.28
1	B	4831	GLU	N-CA-C	5.85	118.82	110.68
1	A	4795	ASN	CB-CA-C	-5.84	103.77	111.42
1	D	1712	SER	N-CA-C	5.84	117.64	111.28
1	C	1712	SER	N-CA-C	5.84	117.64	111.28
1	C	4795	ASN	CB-CA-C	-5.82	103.80	111.42
1	D	919	VAL	CB-CA-C	5.81	117.96	111.45
1	D	4795	ASN	CB-CA-C	-5.80	103.82	111.42
1	C	919	VAL	CB-CA-C	5.80	117.94	111.45
1	B	3803	VAL	N-CA-CB	-5.79	101.67	111.23
1	A	4831	GLU	N-CA-C	5.76	118.68	110.68
1	C	2074	SER	CA-C-O	-5.75	115.34	121.78
1	D	4897	ASP	N-CA-C	5.72	117.52	111.28
1	C	4831	GLU	N-CA-C	5.72	118.64	110.68
1	B	919	VAL	CB-CA-C	5.72	117.85	111.45
1	C	4764	ASN	CA-C-N	5.70	127.26	120.14
1	C	4764	ASN	C-N-CA	5.70	127.26	120.14
1	B	4727	MET	CG-SD-CE	5.67	113.39	100.90
1	A	919	VAL	CB-CA-C	5.67	117.80	111.45
1	B	4795	ASN	CB-CA-C	-5.67	104.00	111.42
1	D	4831	GLU	N-CA-C	5.67	118.56	110.68
1	C	4727	MET	CG-SD-CE	5.67	113.36	100.90
1	D	3803	VAL	O-C-N	-5.66	115.50	122.57
1	D	4948	ARG	NE-CZ-NH1	-5.66	115.84	121.50
1	B	4764	ASN	CA-C-N	5.65	127.20	120.14
1	B	4764	ASN	C-N-CA	5.65	127.20	120.14
1	A	1712	SER	N-CA-C	5.65	117.44	111.28
1	B	2074	SER	CA-C-O	-5.65	115.45	121.78
1	D	2074	SER	CA-C-O	-5.65	115.45	121.78
1	C	2260	GLU	CA-C-N	-5.65	113.94	119.64
1	C	2260	GLU	C-N-CA	-5.65	113.94	119.64
1	A	687	THR	N-CA-C	-5.64	98.78	110.80
1	D	687	THR	N-CA-C	-5.64	98.78	110.80
1	A	4764	ASN	CA-C-N	5.64	127.19	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4764	ASN	C-N-CA	5.64	127.19	120.14
1	C	4897	ASP	N-CA-C	5.64	117.43	111.28
1	C	1756	SER	N-CA-C	5.63	122.79	110.80
1	B	687	THR	N-CA-C	-5.63	98.82	110.80
1	B	1456	ALA	N-CA-C	5.61	117.32	108.96
1	D	2260	GLU	CA-C-N	-5.60	113.99	119.64
1	D	2260	GLU	C-N-CA	-5.60	113.99	119.64
1	B	4897	ASP	N-CA-C	5.58	117.37	111.28
1	B	3804	LEU	CA-C-N	5.58	132.19	121.54
1	B	3804	LEU	C-N-CA	5.58	132.19	121.54
1	C	687	THR	N-CA-C	-5.57	98.94	110.80
1	D	1756	SER	N-CA-C	5.56	122.65	110.80
1	D	4727	MET	CG-SD-CE	5.56	113.14	100.90
1	D	1759	PRO	N-CA-C	5.55	119.94	111.11
1	A	4948	ARG	NE-CZ-NH1	-5.54	115.96	121.50
1	A	2083	ARG	CG-CD-NE	-5.53	99.83	112.00
1	C	927	GLN	N-CA-C	-5.53	107.78	114.75
1	B	678	MET	CB-CG-SD	5.53	129.29	112.70
1	C	812	LYS	N-CA-C	-5.53	108.32	114.62
1	C	678	MET	CB-CG-SD	5.53	129.28	112.70
1	A	1456	ALA	N-CA-C	5.51	117.17	108.96
1	A	30	LYS	CA-CB-CG	5.51	125.12	114.10
1	A	1756	SER	N-CA-C	5.51	122.54	110.80
1	D	927	GLN	N-CA-C	-5.50	107.82	114.75
1	B	4740	PHE	CA-C-N	-5.50	113.88	122.73
1	B	4740	PHE	C-N-CA	-5.50	113.88	122.73
1	C	3804	LEU	CA-C-N	5.50	132.04	121.54
1	C	3804	LEU	C-N-CA	5.50	132.04	121.54
1	D	4862	ILE	CA-CB-CG1	-5.50	101.05	110.40
1	C	1759	PRO	N-CA-C	5.49	119.84	111.11
1	D	812	LYS	N-CA-C	-5.48	108.37	114.62
1	A	4740	PHE	CA-C-N	-5.48	113.91	122.73
1	A	4740	PHE	C-N-CA	-5.48	113.91	122.73
1	A	1759	PRO	N-CA-C	5.48	119.82	111.11
1	A	3804	LEU	CA-C-N	5.48	132.00	121.54
1	A	3804	LEU	C-N-CA	5.48	132.00	121.54
1	B	1759	PRO	N-CA-C	5.48	119.82	111.11
1	B	521	GLU	N-CA-C	-5.46	105.91	113.18
1	A	678	MET	CB-CG-SD	5.46	129.08	112.70
1	A	2074	SER	CA-C-O	-5.46	115.67	121.78
1	D	678	MET	CB-CG-SD	5.46	129.07	112.70
1	B	1712	SER	N-CA-C	5.46	117.23	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	30	LYS	CA-CB-CG	5.46	125.01	114.10
1	B	30	LYS	CA-CB-CG	5.45	125.00	114.10
1	A	3803	VAL	O-C-N	-5.45	115.75	122.57
1	A	4862	ILE	CA-CB-CG1	-5.45	101.13	110.40
1	A	521	GLU	N-CA-C	-5.44	105.95	113.18
1	C	3803	VAL	O-C-N	-5.44	115.78	122.57
1	D	3804	LEU	CA-C-N	5.43	131.91	121.54
1	D	3804	LEU	C-N-CA	5.43	131.91	121.54
1	C	4595	LYS	CA-C-N	5.43	123.66	120.24
1	C	4595	LYS	C-N-CA	5.43	123.66	120.24
1	A	927	GLN	N-CA-C	-5.42	107.92	114.75
1	C	1456	ALA	N-CA-C	5.42	117.04	108.96
1	D	2083	ARG	CG-CD-NE	-5.42	100.09	112.00
1	D	3803	VAL	N-CA-C	-5.40	98.11	109.34
1	B	1818	PHE	CA-C-N	5.38	124.64	120.33
1	B	1818	PHE	C-N-CA	5.38	124.64	120.33
1	B	927	GLN	N-CA-C	-5.37	107.98	114.75
1	C	3803	VAL	N-CA-C	-5.37	98.17	109.34
1	B	1754	SER	N-CA-C	5.36	118.83	111.54
1	A	812	LYS	N-CA-C	-5.36	108.51	114.62
1	B	2260	GLU	CA-C-N	-5.36	114.15	119.56
1	B	2260	GLU	C-N-CA	-5.36	114.15	119.56
1	C	30	LYS	CA-CB-CG	5.36	124.82	114.10
1	B	2083	ARG	CG-CD-NE	-5.35	100.22	112.00
1	D	1013	ARG	CB-CG-CD	5.35	123.61	111.30
1	C	4740	PHE	CA-C-N	-5.35	114.12	122.73
1	C	4740	PHE	C-N-CA	-5.35	114.12	122.73
1	B	1756	SER	N-CA-C	5.34	122.18	110.80
1	C	1013	ARG	CB-CG-CD	5.34	123.59	111.30
1	B	812	LYS	N-CA-C	-5.34	108.54	114.62
1	A	4822	VAL	CA-CB-CG1	5.33	119.47	110.40
1	D	4854	PHE	N-CA-C	5.33	117.09	111.28
1	D	2173	MET	CG-SD-CE	-5.33	89.17	100.90
1	C	1818	PHE	CA-C-N	5.33	124.59	120.33
1	C	1818	PHE	C-N-CA	5.33	124.59	120.33
1	B	3803	VAL	N-CA-C	-5.32	98.27	109.34
1	D	1456	ALA	N-CA-C	5.32	116.89	108.96
1	D	4822	VAL	CA-CB-CG1	5.32	119.44	110.40
1	A	4727	MET	CG-SD-CE	5.31	112.58	100.90
1	B	2103	LEU	CA-C-N	-5.31	114.31	120.04
1	B	2103	LEU	C-N-CA	-5.31	114.31	120.04
1	A	2260	GLU	CA-C-N	-5.30	114.20	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2260	GLU	C-N-CA	-5.30	114.20	119.56
1	A	1818	PHE	CA-C-N	5.30	124.57	120.33
1	A	1818	PHE	C-N-CA	5.30	124.57	120.33
1	A	3803	VAL	N-CA-C	-5.30	98.31	109.34
1	C	4948	ARG	NE-CZ-NH1	-5.30	116.20	121.50
1	D	4740	PHE	CA-C-N	-5.30	114.20	122.73
1	D	4740	PHE	C-N-CA	-5.30	114.20	122.73
1	C	4758	LEU	N-CA-C	-5.29	106.33	112.89
1	C	4822	VAL	CA-CB-CG1	5.28	119.37	110.40
1	A	1013	ARG	CB-CG-CD	5.27	123.43	111.30
1	B	3803	VAL	O-C-N	-5.27	115.98	122.57
1	B	4822	VAL	CA-CB-CG1	5.27	119.36	110.40
1	B	4595	LYS	CA-C-N	5.27	123.56	120.24
1	B	4595	LYS	C-N-CA	5.27	123.56	120.24
1	C	2083	ARG	CG-CD-NE	-5.26	100.42	112.00
1	D	1754	SER	N-CA-C	5.26	118.70	111.54
1	D	4753	THR	CA-C-O	5.26	125.51	119.35
1	B	640	ARG	CA-C-O	5.26	124.26	119.00
1	B	1305	SER	N-CA-C	5.26	117.92	111.82
1	C	1305	SER	N-CA-C	5.26	117.92	111.82
1	C	2103	LEU	CA-C-N	-5.26	114.36	120.04
1	C	2103	LEU	C-N-CA	-5.26	114.36	120.04
1	A	4854	PHE	N-CA-C	5.25	117.01	111.28
1	C	1754	SER	N-CA-C	5.24	118.67	111.54
1	A	1754	SER	N-CA-C	5.24	118.67	111.54
1	D	1818	PHE	CA-C-N	5.24	124.52	120.33
1	D	1818	PHE	C-N-CA	5.24	124.52	120.33
1	D	4758	LEU	N-CA-C	-5.23	106.40	112.89
1	D	1305	SER	N-CA-C	5.23	117.89	111.82
1	A	4758	LEU	N-CA-C	-5.23	106.41	112.89
1	A	2103	LEU	CA-C-N	-5.23	114.40	120.04
1	A	2103	LEU	C-N-CA	-5.23	114.40	120.04
1	C	4862	ILE	CA-CB-CG1	-5.22	101.53	110.40
1	D	4853	PHE	CE1-CZ-CE2	-5.21	110.61	120.00
1	A	2173	MET	CG-SD-CE	-5.21	89.43	100.90
1	B	4753	THR	CA-C-O	5.20	125.43	119.35
1	B	4727	MET	CB-CG-SD	5.19	128.28	112.70
1	D	640	ARG	CA-C-O	5.19	124.19	119.00
1	B	4862	ILE	CA-CB-CG1	-5.19	101.58	110.40
1	C	4753	THR	CA-C-O	5.18	125.42	119.35
1	A	1305	SER	N-CA-C	5.18	117.83	111.82
1	A	3896	LYS	CD-CE-NZ	5.17	128.45	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4641	PHE	N-CA-C	5.17	120.59	113.77
1	C	4853	PHE	CE1-CZ-CE2	-5.16	110.71	120.00
1	D	2103	LEU	CA-C-N	-5.15	114.48	120.04
1	D	2103	LEU	C-N-CA	-5.15	114.48	120.04
1	B	2173	MET	CG-SD-CE	-5.15	89.58	100.90
1	B	4948	ARG	NE-CZ-NH1	-5.14	116.36	121.50
1	C	4963	TYR	N-CA-C	5.13	115.15	108.07
1	C	4818	MET	N-CA-CB	5.13	118.23	110.28
1	D	4963	TYR	N-CA-C	5.13	115.15	108.07
1	A	640	ARG	CA-C-O	5.13	124.13	119.00
1	D	3992	VAL	N-CA-C	5.12	115.55	110.23
1	B	839	GLU	N-CA-C	5.10	121.67	110.80
1	A	839	GLU	N-CA-C	5.10	121.66	110.80
1	D	2173	MET	CB-CG-SD	5.10	127.99	112.70
1	C	4641	PHE	N-CA-C	5.09	120.49	113.77
1	D	4595	LYS	CA-C-N	5.09	123.45	120.24
1	D	4595	LYS	C-N-CA	5.09	123.45	120.24
1	B	3992	VAL	N-CA-C	5.09	115.52	110.23
1	D	3896	LYS	CD-CE-NZ	5.09	128.18	111.90
1	A	1720	MET	CA-C-O	5.08	125.81	120.42
1	C	2173	MET	CG-SD-CE	-5.08	89.72	100.90
1	D	1473	LYS	N-CA-C	-5.08	108.83	114.62
1	D	839	GLU	N-CA-C	5.08	121.61	110.80
1	B	4758	LEU	N-CA-C	-5.07	106.60	112.89
1	B	4854	PHE	CB-CA-C	-5.07	102.37	110.79
1	A	4963	TYR	N-CA-C	5.07	115.07	108.07
1	A	3992	VAL	N-CA-C	5.05	115.49	110.23
1	A	4753	THR	CA-C-O	5.05	125.26	119.35
1	D	4561	VAL	CB-CA-C	-5.05	104.72	110.73
1	B	1778	TYR	N-CA-CB	5.05	119.09	110.50
1	B	4963	TYR	N-CA-C	5.05	115.04	108.07
1	C	1720	MET	CA-C-O	5.04	125.77	120.42
1	B	1758	ARG	NE-CZ-NH1	-5.04	116.46	121.50
1	C	3992	VAL	N-CA-C	5.04	115.47	110.23
1	D	388	GLN	N-CA-C	-5.04	102.64	109.54
1	B	3896	LYS	CD-CE-NZ	5.03	128.00	111.90
1	A	4641	PHE	N-CA-C	5.02	120.40	113.77
1	A	1778	TYR	N-CA-CB	5.01	119.02	110.50
1	C	839	GLU	N-CA-C	5.01	121.48	110.80
1	A	388	GLN	N-CA-C	-5.01	102.68	109.54
1	D	4854	PHE	CB-CA-C	-5.01	102.48	110.79
1	C	640	ARG	CA-C-O	5.00	124.00	119.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1720	MET	CA-C-O	5.00	125.72	120.42

There are no chirality outliers.

All (93) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1475	LYS	Peptide
1	A	1579	VAL	Peptide
1	A	1635	GLU	Peptide
1	A	1736	ILE	Peptide
1	A	1755	THR	Peptide
1	A	1808	ASP	Peptide
1	A	1835	HIS	Peptide
1	A	1847	GLU	Peptide
1	A	2075	VAL	Peptide
1	A	2329	PRO	Peptide,Mainchain
1	A	3800	SER	Peptide
1	A	4163	LYS	Peptide
1	A	4952	PHE	Sidechain
1	A	641	ASP	Peptide
1	A	686	VAL	Peptide
1	A	791	VAL	Peptide
1	A	818	GLY	Peptide
1	A	819	TYR	Peptide
1	A	827	LEU	Peptide
1	A	838	ARG	Peptide
1	A	852	GLY	Peptide,Mainchain
1	B	1475	LYS	Peptide
1	B	1579	VAL	Peptide
1	B	1635	GLU	Peptide
1	B	1736	ILE	Peptide
1	B	1755	THR	Peptide
1	B	1808	ASP	Peptide
1	B	1835	HIS	Peptide
1	B	1847	GLU	Peptide
1	B	2075	VAL	Peptide
1	B	2329	PRO	Peptide,Mainchain
1	B	3800	SER	Peptide
1	B	4163	LYS	Peptide
1	B	4952	PHE	Sidechain
1	B	641	ASP	Peptide
1	B	686	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	B	791	VAL	Peptide
1	B	818	GLY	Peptide
1	B	819	TYR	Peptide
1	B	827	LEU	Peptide
1	B	838	ARG	Peptide
1	B	852	GLY	Peptide,Mainchain
1	C	1475	LYS	Peptide
1	C	1579	VAL	Peptide
1	C	1635	GLU	Peptide
1	C	1736	ILE	Peptide
1	C	1755	THR	Peptide
1	C	1756	SER	Peptide
1	C	1808	ASP	Peptide
1	C	1835	HIS	Peptide
1	C	1847	GLU	Peptide
1	C	2075	VAL	Peptide
1	C	2329	PRO	Peptide,Mainchain
1	C	3800	SER	Peptide
1	C	4163	LYS	Peptide
1	C	4952	PHE	Sidechain
1	C	641	ASP	Peptide
1	C	686	VAL	Peptide
1	C	791	VAL	Peptide
1	C	818	GLY	Peptide
1	C	819	TYR	Peptide
1	C	827	LEU	Peptide
1	C	838	ARG	Peptide
1	C	852	GLY	Peptide,Mainchain
1	D	1475	LYS	Peptide
1	D	1579	VAL	Peptide
1	D	1635	GLU	Peptide
1	D	1736	ILE	Peptide
1	D	1755	THR	Peptide
1	D	1808	ASP	Peptide
1	D	1835	HIS	Peptide
1	D	1847	GLU	Peptide
1	D	2075	VAL	Peptide
1	D	2329	PRO	Peptide,Mainchain
1	D	3800	SER	Peptide
1	D	4163	LYS	Peptide
1	D	4952	PHE	Sidechain
1	D	641	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	D	686	VAL	Peptide
1	D	791	VAL	Peptide
1	D	818	GLY	Peptide
1	D	819	TYR	Peptide
1	D	827	LEU	Peptide
1	D	838	ARG	Peptide
1	D	852	GLY	Peptide,Mainchain

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	26267	0	24896	399	0
1	B	26267	0	24897	389	0
1	C	26267	0	24897	388	0
1	D	26267	0	24896	396	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
All	All	105072	0	99586	1519	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 (1519) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4818:MET:CG	1:D:4818:MET:SD	2.01	1.49
1:C:4818:MET:CG	1:C:4818:MET:SD	2.01	1.48
1:C:3700:CYS:CB	1:C:3700:CYS:SG	2.04	1.45
1:B:3700:CYS:CB	1:B:3700:CYS:SG	2.05	1.43
1:D:3700:CYS:SG	1:D:3700:CYS:CB	2.05	1.43
1:A:3700:CYS:CB	1:A:3700:CYS:SG	2.05	1.43
1:A:4171:ARG:NH1	1:A:4752:LYS:HD3	1.63	1.12
1:D:4171:ARG:NH1	1:D:4752:LYS:HE3	1.76	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4171:ARG:HH12	1:A:4752:LYS:HD3	1.28	0.94
1:A:4767:GLN:HE22	1:B:4753:THR:HB	1.29	0.94
1:B:4767:GLN:HE22	1:C:4753:THR:HB	1.31	0.93
1:A:4767:GLN:NE2	1:B:4753:THR:HB	1.84	0.93
1:C:4767:GLN:HE22	1:D:4753:THR:HB	1.32	0.93
1:D:4171:ARG:HH11	1:D:4752:LYS:HE3	1.30	0.93
1:B:4767:GLN:NE2	1:C:4753:THR:HB	1.84	0.92
1:A:4753:THR:HB	1:D:4767:GLN:HE22	1.32	0.92
1:A:4753:THR:HB	1:D:4767:GLN:NE2	1.85	0.91
1:C:4767:GLN:NE2	1:D:4753:THR:HB	1.85	0.91
1:A:76:ARG:HD2	1:B:3891:TRP:HB3	1.54	0.89
1:C:76:ARG:HD2	1:D:3891:TRP:HB3	1.54	0.89
1:A:3891:TRP:HB3	1:D:76:ARG:HD2	1.52	0.88
1:B:76:ARG:HD2	1:C:3891:TRP:HB3	1.53	0.87
1:A:4754:LEU:HD11	1:D:4770:LEU:HB3	1.66	0.78
1:C:4770:LEU:HB3	1:D:4754:LEU:HD11	1.67	0.77
1:B:4791:ARG:HH12	1:C:4559:HIS:CE1	2.04	0.76
1:C:4791:ARG:HH12	1:D:4559:HIS:CE1	2.04	0.75
1:A:4791:ARG:HH12	1:B:4559:HIS:CE1	2.04	0.75
1:B:4770:LEU:HB3	1:C:4754:LEU:HD11	1.68	0.75
1:C:4171:ARG:HG3	1:C:4171:ARG:HH21	1.50	0.74
1:A:4770:LEU:HB3	1:B:4754:LEU:HD11	1.69	0.74
1:A:4559:HIS:CE1	1:D:4791:ARG:HH12	2.05	0.73
1:A:4171:ARG:NH1	1:A:4752:LYS:CD	2.49	0.71
1:D:2349:GLU:HG2	1:D:2439:ILE:HD11	1.72	0.71
1:C:2349:GLU:HG2	1:C:2439:ILE:HD11	1.72	0.71
1:C:1011:ARG:HB3	1:C:1032:LEU:HD21	1.73	0.71
1:D:1011:ARG:HB3	1:D:1032:LEU:HD21	1.72	0.70
1:A:2349:GLU:HG2	1:A:2439:ILE:HD11	1.72	0.70
1:B:2349:GLU:HG2	1:B:2439:ILE:HD11	1.72	0.70
1:B:4832:ILE:HG21	1:B:4844:ARG:HH21	1.57	0.69
1:A:4832:ILE:HG21	1:A:4844:ARG:HH21	1.58	0.69
1:B:1011:ARG:HB3	1:B:1032:LEU:HD21	1.74	0.69
1:B:986:ILE:HD12	1:B:1059:GLY:HA2	1.74	0.69
1:B:1645:THR:HG22	1:B:1695:PRO:HG3	1.73	0.69
1:C:4817:HIS:HE1	1:C:4828:ILE:HD12	1.57	0.68
1:C:4832:ILE:HG21	1:C:4844:ARG:HH21	1.58	0.68
1:A:1011:ARG:HB3	1:A:1032:LEU:HD21	1.75	0.68
1:B:4817:HIS:HE1	1:B:4828:ILE:HD12	1.57	0.68
1:C:1645:THR:HG22	1:C:1695:PRO:HG3	1.73	0.68
1:A:4817:HIS:HE1	1:A:4828:ILE:HD12	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4642:PRO:HG2	1:A:4648:LYS:HD2	1.76	0.68
1:B:4642:PRO:HG2	1:B:4648:LYS:HD2	1.76	0.68
1:D:4832:ILE:HG21	1:D:4844:ARG:HH21	1.57	0.68
1:B:4511:ALA:HA	1:B:4514:ILE:HD12	1.77	0.67
1:D:1645:THR:HG22	1:D:1695:PRO:HG3	1.75	0.67
1:A:4511:ALA:HA	1:A:4514:ILE:HD12	1.77	0.67
1:C:1620:GLN:HE21	1:C:1622:LEU:HD21	1.60	0.67
1:D:4817:HIS:HE1	1:D:4828:ILE:HD12	1.58	0.67
1:A:143:LEU:HD23	1:B:2426:SER:HB3	1.77	0.67
1:B:2463:PRO:HB2	1:B:2519:ARG:HD2	1.76	0.67
1:D:644:LEU:HB2	1:D:1654:HIS:HD2	1.60	0.67
1:A:1645:THR:HG22	1:A:1695:PRO:HG3	1.75	0.66
1:C:4642:PRO:HG2	1:C:4648:LYS:HD2	1.77	0.66
1:D:2463:PRO:HB2	1:D:2519:ARG:HD2	1.77	0.66
1:B:1620:GLN:HE21	1:B:1622:LEU:HD21	1.60	0.66
1:D:4642:PRO:HG2	1:D:4648:LYS:HD2	1.77	0.66
1:C:644:LEU:HB2	1:C:1654:HIS:HD2	1.60	0.66
1:D:4511:ALA:HA	1:D:4514:ILE:HD12	1.78	0.66
1:A:1620:GLN:HE21	1:A:1622:LEU:HD21	1.60	0.66
1:A:986:ILE:HD12	1:A:1059:GLY:HA2	1.78	0.65
1:C:4511:ALA:HA	1:C:4514:ILE:HD12	1.78	0.65
1:D:3802:SER:OG	1:D:3833:ASP:O	2.14	0.65
1:D:1620:GLN:HE21	1:D:1622:LEU:HD21	1.60	0.65
1:B:1304:LEU:HB3	1:B:1541:PRO:HG2	1.79	0.65
1:B:1258:PHE:HB2	1:B:1593:HIS:HB3	1.79	0.65
1:B:3802:SER:OG	1:B:3833:ASP:O	2.15	0.65
1:A:2463:PRO:HB2	1:A:2519:ARG:HD2	1.76	0.65
1:A:3802:SER:OG	1:A:3833:ASP:O	2.14	0.65
1:B:644:LEU:HB2	1:B:1654:HIS:HD2	1.60	0.65
1:C:143:LEU:HD23	1:D:2426:SER:HB3	1.79	0.64
1:C:2463:PRO:HB2	1:C:2519:ARG:HD2	1.77	0.64
1:C:3802:SER:OG	1:C:3833:ASP:O	2.15	0.64
1:A:644:LEU:HB2	1:A:1654:HIS:HD2	1.61	0.64
1:A:1304:LEU:HB3	1:A:1541:PRO:HG2	1.79	0.64
1:A:4171:ARG:HH11	1:A:4752:LYS:HD3	1.59	0.64
1:D:1602:GLN:HE22	1:D:1642:LEU:HB3	1.63	0.64
1:B:3911:ILE:HG21	1:B:3971:GLU:HB3	1.80	0.64
1:C:986:ILE:HD12	1:C:1059:GLY:HA2	1.79	0.63
1:D:1258:PHE:HB2	1:D:1593:HIS:HB3	1.80	0.63
1:A:1602:GLN:HE22	1:A:1642:LEU:HB3	1.63	0.63
1:B:143:LEU:HD23	1:C:2426:SER:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:986:ILE:HD12	1:D:1059:GLY:HA2	1.79	0.63
1:A:1258:PHE:HB2	1:A:1593:HIS:HB3	1.80	0.63
1:C:1258:PHE:HB2	1:C:1593:HIS:HB3	1.79	0.63
1:C:4002:ASP:HA	1:C:4115:ARG:HH22	1.63	0.63
1:C:647:ARG:NH1	1:C:1681:ASP:OD2	2.32	0.63
1:D:1286:THR:HA	1:D:1586:LEU:HD11	1.80	0.63
1:D:1304:LEU:HB3	1:D:1541:PRO:HG2	1.80	0.63
1:C:1304:LEU:HB3	1:C:1541:PRO:HG2	1.79	0.62
1:C:1602:GLN:HE22	1:C:1642:LEU:HB3	1.63	0.62
1:A:3911:ILE:HG21	1:A:3971:GLU:HB3	1.81	0.62
1:A:3925:ILE:HG23	1:A:3933:GLN:HG2	1.82	0.62
1:B:1602:GLN:HE22	1:B:1642:LEU:HB3	1.63	0.62
1:A:1286:THR:HA	1:A:1586:LEU:HD11	1.80	0.62
1:A:4002:ASP:HA	1:A:4115:ARG:HH22	1.64	0.62
1:C:2256:LEU:O	1:C:3811:ARG:NH1	2.32	0.62
1:A:238:HIS:HE1	1:A:400:ASP:HB3	1.65	0.62
1:B:1286:THR:HA	1:B:1586:LEU:HD11	1.80	0.62
1:D:647:ARG:NH1	1:D:1681:ASP:OD2	2.33	0.62
1:D:1605:LYS:HD3	1:D:1606:VAL:HG23	1.81	0.62
1:D:3925:ILE:HG23	1:D:3933:GLN:HG2	1.82	0.62
1:B:2256:LEU:O	1:B:3811:ARG:NH1	2.32	0.62
1:D:228:LEU:HB3	1:D:289:ILE:HD12	1.82	0.62
1:A:228:LEU:HB3	1:A:289:ILE:HD12	1.82	0.62
1:A:647:ARG:NH1	1:A:1681:ASP:OD2	2.33	0.62
1:A:708:GLY:HA2	1:A:714:GLY:HA3	1.82	0.62
1:C:228:LEU:HB3	1:C:289:ILE:HD12	1.82	0.62
1:C:3911:ILE:HG21	1:C:3971:GLU:HB3	1.82	0.62
1:B:228:LEU:HB3	1:B:289:ILE:HD12	1.82	0.61
1:B:647:ARG:NH1	1:B:1681:ASP:OD2	2.32	0.61
1:D:238:HIS:HE1	1:D:400:ASP:HB3	1.65	0.61
1:A:1605:LYS:HD3	1:A:1606:VAL:HG23	1.82	0.61
1:B:4002:ASP:HA	1:B:4115:ARG:HH22	1.64	0.61
1:A:2426:SER:HB3	1:D:143:LEU:HD23	1.81	0.61
1:C:1286:THR:HA	1:C:1586:LEU:HD11	1.80	0.61
1:C:1605:LYS:HD3	1:C:1606:VAL:HG23	1.81	0.61
1:D:4002:ASP:HA	1:D:4115:ARG:HH22	1.63	0.61
1:A:2256:LEU:O	1:A:3811:ARG:NH1	2.32	0.61
1:B:3925:ILE:HG23	1:B:3933:GLN:HG2	1.83	0.61
1:C:238:HIS:HE1	1:C:400:ASP:HB3	1.66	0.61
1:B:238:HIS:HE1	1:B:400:ASP:HB3	1.66	0.61
1:B:708:GLY:HA2	1:B:714:GLY:HA3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:LEU:O	1:C:212:TRP:NE1	2.33	0.61
1:D:3922:THR:O	1:D:3926:GLN:N	2.34	0.61
1:B:1605:LYS:HD3	1:B:1606:VAL:HG23	1.82	0.61
1:C:3922:THR:O	1:C:3926:GLN:N	2.34	0.61
1:C:3925:ILE:HG23	1:C:3933:GLN:HG2	1.83	0.61
1:D:192:LEU:O	1:D:212:TRP:NE1	2.33	0.61
1:A:4170:LYS:HE2	1:A:4916:LEU:HD23	1.82	0.60
1:B:1445:TRP:HE1	1:B:1508:GLY:HA3	1.66	0.60
1:D:3911:ILE:HG21	1:D:3971:GLU:HB3	1.82	0.60
1:D:644:LEU:HD22	1:D:1632:ILE:HG22	1.83	0.60
1:D:2256:LEU:O	1:D:3811:ARG:NH1	2.32	0.60
1:A:4085:VAL:HG12	1:A:4090:GLU:HG3	1.84	0.60
1:C:3914:ALA:HB3	1:C:3975:LEU:HD11	1.82	0.60
1:C:4171:ARG:HH21	1:C:4171:ARG:CG	2.14	0.60
1:D:708:GLY:HA2	1:D:714:GLY:HA3	1.83	0.60
1:D:3914:ALA:HB3	1:D:3975:LEU:HD11	1.83	0.60
1:A:192:LEU:O	1:A:212:TRP:NE1	2.33	0.60
1:A:644:LEU:HD22	1:A:1632:ILE:HG22	1.83	0.60
1:A:3914:ALA:HB3	1:A:3975:LEU:HD11	1.84	0.60
1:C:708:GLY:HA2	1:C:714:GLY:HA3	1.83	0.60
1:A:4170:LYS:HE2	1:A:4916:LEU:CD2	2.32	0.60
1:B:300:VAL:HG13	1:B:420:ARG:HH21	1.67	0.60
1:C:300:VAL:HG13	1:C:420:ARG:HH21	1.66	0.60
1:D:4085:VAL:HG12	1:D:4090:GLU:HG3	1.84	0.60
1:C:4085:VAL:HG12	1:C:4090:GLU:HG3	1.84	0.60
1:B:188:SER:HB2	1:B:190:ARG:HH21	1.67	0.59
1:C:779:PHE:HB3	1:C:782:PHE:HE2	1.67	0.59
1:A:1445:TRP:HE1	1:A:1508:GLY:HA3	1.67	0.59
1:B:3914:ALA:HB3	1:B:3975:LEU:HD11	1.84	0.59
1:A:188:SER:HB2	1:A:190:ARG:HH21	1.67	0.59
1:B:779:PHE:HB3	1:B:782:PHE:HE2	1.67	0.59
1:B:1444:GLY:HA2	1:B:1487:MET:HB2	1.83	0.59
1:B:192:LEU:O	1:B:212:TRP:NE1	2.33	0.59
1:C:644:LEU:HD22	1:C:1632:ILE:HG22	1.83	0.59
1:C:711:GLU:HG3	1:C:1449:ASP:HB3	1.85	0.59
1:D:1272:ARG:NH1	1:D:1587:HIS:O	2.36	0.59
1:A:779:PHE:HB3	1:A:782:PHE:HE2	1.67	0.59
1:A:1444:GLY:HA2	1:A:1487:MET:HB2	1.83	0.59
1:D:779:PHE:HB3	1:D:782:PHE:HE2	1.67	0.59
1:D:1762:GLN:O	1:D:1779:SER:OG	2.21	0.59
1:A:650:ASN:HA	1:A:1626:GLN:HG2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4170:LYS:HE3	1:C:4916:LEU:HD23	1.85	0.59
1:D:300:VAL:HG13	1:D:420:ARG:HH21	1.67	0.59
1:D:2204:PHE:O	1:D:2211:ASN:ND2	2.36	0.59
1:A:300:VAL:HG13	1:A:420:ARG:HH21	1.67	0.59
1:B:644:LEU:HD22	1:B:1632:ILE:HG22	1.84	0.59
1:C:227:TYR:HE1	1:C:355:LYS:HG2	1.68	0.59
1:C:1445:TRP:HE1	1:C:1508:GLY:HA3	1.67	0.59
1:A:677:LEU:HB2	1:A:755:ILE:HB	1.85	0.59
1:C:1272:ARG:NH1	1:C:1587:HIS:O	2.36	0.58
1:C:1762:GLN:O	1:C:1779:SER:OG	2.21	0.58
1:C:2204:PHE:O	1:C:2211:ASN:ND2	2.36	0.58
1:A:1272:ARG:NH1	1:A:1587:HIS:O	2.36	0.58
1:B:3922:THR:O	1:B:3926:GLN:N	2.34	0.58
1:A:35:LEU:HD13	1:A:49:LEU:HD22	1.85	0.58
1:D:1444:GLY:HA2	1:D:1487:MET:HB2	1.84	0.58
1:D:1445:TRP:HE1	1:D:1508:GLY:HA3	1.68	0.58
1:B:711:GLU:HG3	1:B:1449:ASP:HB3	1.85	0.58
1:A:711:GLU:HG3	1:A:1449:ASP:HB3	1.84	0.58
1:A:2204:PHE:O	1:A:2211:ASN:ND2	2.36	0.58
1:A:1086:ARG:HB2	1:A:1207:LEU:HB2	1.86	0.58
1:B:4085:VAL:HG12	1:B:4090:GLU:HG3	1.84	0.58
1:C:677:LEU:HB2	1:C:755:ILE:HB	1.86	0.58
1:C:1444:GLY:HA2	1:C:1487:MET:HB2	1.84	0.58
1:B:58:VAL:HG22	1:B:320:GLU:HA	1.86	0.58
1:D:188:SER:HB2	1:D:190:ARG:HH21	1.68	0.58
1:D:650:ASN:HA	1:D:1626:GLN:HG2	1.86	0.58
1:D:1726:ILE:HD11	1:D:2121:LEU:HD11	1.86	0.58
1:B:2204:PHE:O	1:B:2211:ASN:ND2	2.37	0.58
1:A:1762:GLN:O	1:A:1779:SER:OG	2.22	0.58
1:C:3879:LEU:HD12	1:C:3917:VAL:HG13	1.86	0.58
1:D:35:LEU:HD13	1:D:49:LEU:HD22	1.85	0.58
1:B:3879:LEU:HD12	1:B:3917:VAL:HG13	1.85	0.57
1:C:58:VAL:HG22	1:C:320:GLU:HA	1.86	0.57
1:C:188:SER:HB2	1:C:190:ARG:HH21	1.69	0.57
1:B:1086:ARG:HB2	1:B:1207:LEU:HB2	1.85	0.57
1:D:227:TYR:HE1	1:D:355:LYS:HG2	1.68	0.57
1:D:711:GLU:HG3	1:D:1449:ASP:HB3	1.84	0.57
1:B:1272:ARG:NH1	1:B:1587:HIS:O	2.36	0.57
1:C:35:LEU:HD13	1:C:49:LEU:HD22	1.86	0.57
1:A:1726:ILE:HD11	1:A:2121:LEU:HD11	1.87	0.57
1:C:4617:TYR:OH	1:C:4629:GLY:O	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3922:THR:O	1:A:3926:GLN:N	2.34	0.57
1:C:1086:ARG:HB2	1:C:1207:LEU:HB2	1.86	0.57
1:B:672:LYS:HA	1:B:760:ASP:HA	1.87	0.57
1:B:897:LYS:HD3	1:B:918:LEU:HD21	1.86	0.57
1:C:897:LYS:HD3	1:C:918:LEU:HD21	1.86	0.57
1:D:58:VAL:HG22	1:D:320:GLU:HA	1.86	0.57
1:A:58:VAL:HG22	1:A:320:GLU:HA	1.87	0.57
1:B:650:ASN:HA	1:B:1626:GLN:HG2	1.85	0.57
1:B:677:LEU:HB2	1:B:755:ILE:HB	1.85	0.57
1:A:3879:LEU:HD12	1:A:3917:VAL:HG13	1.87	0.57
1:B:227:TYR:HE1	1:B:355:LYS:HG2	1.70	0.57
1:B:4617:TYR:OH	1:B:4629:GLY:O	2.23	0.57
1:C:672:LYS:HA	1:C:760:ASP:HA	1.87	0.57
1:D:672:LYS:HA	1:D:760:ASP:HA	1.87	0.57
1:A:895:MET:HE1	1:A:971:GLN:HB2	1.87	0.57
1:A:672:LYS:HA	1:A:760:ASP:HA	1.87	0.56
1:B:3914:ALA:HA	1:B:3917:VAL:HG12	1.87	0.56
1:D:1086:ARG:HB2	1:D:1207:LEU:HB2	1.86	0.56
1:C:650:ASN:HA	1:C:1626:GLN:HG2	1.86	0.56
1:D:4800:GLY:HA2	1:D:4804:ASP:HB3	1.87	0.56
1:A:2737:LYS:HB3	1:A:2742:TRP:HB2	1.88	0.56
1:B:756:SER:HB3	1:B:769:ARG:HB2	1.87	0.56
1:C:1726:ILE:HD11	1:C:2121:LEU:HD11	1.87	0.56
1:C:4045:SER:HA	1:C:4078:THR:HA	1.87	0.56
1:D:258:ARG:NH1	1:D:317:MET:SD	2.79	0.56
1:D:677:LEU:HB2	1:D:755:ILE:HB	1.86	0.56
1:D:2071:ALA:HA	1:D:2076:ILE:HD11	1.87	0.56
1:B:1762:GLN:O	1:B:1779:SER:OG	2.22	0.56
1:B:2737:LYS:HB3	1:B:2742:TRP:HB2	1.88	0.56
1:C:905:GLY:HA3	1:C:914:GLN:HB3	1.88	0.56
1:C:4888:LYS:HA	1:C:4895:GLY:HA2	1.88	0.56
1:D:4617:TYR:OH	1:D:4629:GLY:O	2.23	0.56
1:A:364:GLN:HE21	1:A:369:GLY:HA2	1.71	0.56
1:B:905:GLY:HA3	1:B:914:GLN:HB3	1.87	0.56
1:D:897:LYS:HD3	1:D:918:LEU:HD21	1.87	0.56
1:B:35:LEU:HD13	1:B:49:LEU:HD22	1.87	0.56
1:B:258:ARG:NH1	1:B:317:MET:SD	2.78	0.56
1:B:4888:LYS:HA	1:B:4895:GLY:HA2	1.87	0.56
1:A:258:ARG:NH1	1:A:317:MET:SD	2.79	0.56
1:A:897:LYS:HD3	1:A:918:LEU:HD21	1.87	0.56
1:A:905:GLY:HA3	1:A:914:GLN:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3804:LEU:HD13	1:A:3910:ALA:HB2	1.88	0.56
1:B:3804:LEU:HD13	1:B:3910:ALA:HB2	1.88	0.56
1:C:258:ARG:NH1	1:C:317:MET:SD	2.78	0.56
1:C:4800:GLY:HA2	1:C:4804:ASP:HB3	1.88	0.56
1:D:3879:LEU:HD12	1:D:3917:VAL:HG13	1.87	0.56
1:D:905:GLY:HA3	1:D:914:GLN:HB3	1.88	0.56
1:D:4045:SER:HA	1:D:4078:THR:HA	1.87	0.56
1:B:364:GLN:HE21	1:B:369:GLY:HA2	1.71	0.56
1:C:4835:PRO:HB2	1:C:4841:GLU:HG3	1.87	0.56
1:D:364:GLN:HE21	1:D:369:GLY:HA2	1.71	0.56
1:D:1137:PHE:HA	1:D:1144:ARG:HA	1.88	0.55
1:A:227:TYR:HE1	1:A:355:LYS:HG2	1.70	0.55
1:A:228:LEU:HD12	1:A:354:ILE:HB	1.89	0.55
1:A:4045:SER:HA	1:A:4078:THR:HA	1.87	0.55
1:A:4617:TYR:OH	1:A:4629:GLY:O	2.23	0.55
1:C:1137:PHE:HA	1:C:1144:ARG:HA	1.89	0.55
1:C:2737:LYS:HB3	1:C:2742:TRP:HB2	1.88	0.55
1:D:559:ILE:HD13	1:D:593:HIS:HB3	1.88	0.55
1:D:756:SER:HB3	1:D:769:ARG:HB2	1.87	0.55
1:A:756:SER:HB3	1:A:769:ARG:HB2	1.87	0.55
1:B:4780:TYR:HA	1:B:4783:THR:HG22	1.89	0.55
1:C:756:SER:HB3	1:C:769:ARG:HB2	1.88	0.55
1:C:4791:ARG:HH12	1:D:4559:HIS:HE1	1.53	0.55
1:D:3804:LEU:HD13	1:D:3910:ALA:HB2	1.88	0.55
1:A:1137:PHE:HA	1:A:1144:ARG:HA	1.88	0.55
1:B:4045:SER:HA	1:B:4078:THR:HA	1.88	0.55
1:D:3914:ALA:HA	1:D:3917:VAL:HG12	1.88	0.55
1:C:364:GLN:HE21	1:C:369:GLY:HA2	1.71	0.55
1:D:4817:HIS:CE1	1:D:4828:ILE:HD12	2.40	0.55
1:A:1245:ARG:HE	1:A:1692:LYS:HG2	1.72	0.55
1:D:776:GLN:HB3	1:D:1470:GLY:HA3	1.89	0.55
1:D:2737:LYS:HB3	1:D:2742:TRP:HB2	1.88	0.55
1:A:2404:ALA:HB3	1:A:2475:ARG:HH21	1.72	0.54
1:A:4888:LYS:HA	1:A:4895:GLY:HA2	1.89	0.54
1:B:895:MET:HE1	1:B:971:GLN:HB2	1.88	0.54
1:B:1726:ILE:HD11	1:B:2121:LEU:HD11	1.88	0.54
1:B:4835:PRO:HB2	1:B:4841:GLU:HG3	1.88	0.54
1:C:4817:HIS:CE1	1:C:4828:ILE:HD12	2.40	0.54
1:C:4915:ASN:O	1:C:4917:ALA:N	2.41	0.54
1:D:895:MET:HE1	1:D:971:GLN:HB2	1.88	0.54
1:A:1607:ASP:HB3	1:A:1608:VAL:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4817:HIS:CE1	1:B:4828:ILE:HD12	2.39	0.54
1:C:3804:LEU:HD13	1:C:3910:ALA:HB2	1.88	0.54
1:A:559:ILE:HD13	1:A:593:HIS:HB3	1.88	0.54
1:B:1137:PHE:HA	1:B:1144:ARG:HA	1.89	0.54
1:B:1245:ARG:HE	1:B:1692:LYS:HG2	1.72	0.54
1:B:4915:ASN:O	1:B:4917:ALA:N	2.40	0.54
1:C:3914:ALA:HA	1:C:3917:VAL:HG12	1.88	0.54
1:A:123:HIS:HD2	1:A:126:SER:H	1.55	0.54
1:A:1601:ASN:ND2	1:A:1643:GLU:OE2	2.41	0.54
1:A:3914:ALA:HA	1:A:3917:VAL:HG12	1.88	0.54
1:A:4754:LEU:CD1	1:D:4770:LEU:HB3	2.36	0.54
1:A:4791:ARG:HH12	1:B:4559:HIS:HE1	1.54	0.54
1:B:1607:ASP:HB3	1:B:1608:VAL:HG23	1.88	0.54
1:C:559:ILE:HD13	1:C:593:HIS:HB3	1.89	0.54
1:C:4780:TYR:HA	1:C:4783:THR:HG22	1.89	0.54
1:D:4835:PRO:HB2	1:D:4841:GLU:HG3	1.89	0.54
1:A:4817:HIS:CE1	1:A:4828:ILE:HD12	2.40	0.54
1:B:123:HIS:HD2	1:B:126:SER:H	1.56	0.54
1:B:1510:VAL:HG12	1:B:1511:VAL:HG23	1.90	0.54
1:A:1629:SER:HA	1:A:1640:ASP:HA	1.90	0.54
1:A:4915:ASN:O	1:A:4917:ALA:N	2.41	0.54
1:C:1252:SER:HB2	1:C:1598:ARG:HB2	1.90	0.54
1:C:1607:ASP:HB3	1:C:1608:VAL:HG23	1.89	0.54
1:C:2071:ALA:HA	1:C:2076:ILE:HD11	1.88	0.54
1:B:228:LEU:HD12	1:B:354:ILE:HB	1.90	0.54
1:C:2404:ALA:HB3	1:C:2475:ARG:HH21	1.73	0.54
1:A:3670:LEU:HD22	1:A:3674:ARG:HH21	1.73	0.54
1:B:281:ARG:NH1	1:B:346:VAL:O	2.41	0.54
1:C:652:VAL:HG11	1:C:715:GLY:HA2	1.90	0.54
1:C:1601:ASN:ND2	1:C:1643:GLU:OE2	2.41	0.54
1:C:2489:LEU:O	1:C:2492:GLY:N	2.41	0.54
1:D:228:LEU:HD12	1:D:354:ILE:HB	1.89	0.54
1:D:4915:ASN:O	1:D:4917:ALA:N	2.41	0.54
1:A:4835:PRO:HB2	1:A:4841:GLU:HG3	1.89	0.54
1:B:1601:ASN:ND2	1:B:1643:GLU:OE2	2.41	0.54
1:B:4800:GLY:HA2	1:B:4804:ASP:HB3	1.90	0.54
1:D:2404:ALA:HB3	1:D:2475:ARG:HH21	1.73	0.54
1:A:2489:LEU:O	1:A:2492:GLY:N	2.41	0.54
1:A:4823:ARG:NH1	1:D:4826:GLY:O	2.41	0.54
1:B:1267:HIS:HB3	1:B:1294:ASN:HD21	1.73	0.54
1:C:123:HIS:HD2	1:C:126:SER:H	1.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1267:HIS:HB3	1:C:1294:ASN:HD21	1.73	0.54
1:C:1629:SER:HA	1:C:1640:ASP:HA	1.90	0.54
1:D:1601:ASN:ND2	1:D:1643:GLU:OE2	2.41	0.54
1:D:1629:SER:HA	1:D:1640:ASP:HA	1.90	0.54
1:A:243:GLU:HA	1:A:264:GLY:HA2	1.89	0.53
1:A:776:GLN:HB3	1:A:1470:GLY:HA3	1.89	0.53
1:B:1431:ARG:HB3	1:B:1554:GLN:HB2	1.90	0.53
1:B:2489:LEU:O	1:B:2492:GLY:N	2.41	0.53
1:B:4171:ARG:HH21	1:B:4171:ARG:HG3	1.72	0.53
1:D:1267:HIS:HB3	1:D:1294:ASN:HD21	1.73	0.53
1:A:800:VAL:HG23	1:A:1619:VAL:HG13	1.90	0.53
1:A:1510:VAL:HG12	1:A:1511:VAL:HG23	1.90	0.53
1:A:2071:ALA:HA	1:A:2076:ILE:HD11	1.90	0.53
1:B:3670:LEU:HD22	1:B:3674:ARG:HH21	1.73	0.53
1:B:4810:MET:HB3	1:C:4519:LEU:O	2.08	0.53
1:A:4780:TYR:HA	1:A:4783:THR:HG22	1.89	0.53
1:B:800:VAL:HG23	1:B:1619:VAL:HG13	1.90	0.53
1:C:1510:VAL:HG12	1:C:1511:VAL:HG23	1.90	0.53
1:D:123:HIS:HD2	1:D:126:SER:H	1.55	0.53
1:D:1690:GLU:OE2	1:D:1790:LYS:NZ	2.39	0.53
1:A:1690:GLU:OE2	1:A:1790:LYS:NZ	2.39	0.53
1:B:1252:SER:HB2	1:B:1598:ARG:HB2	1.90	0.53
1:B:4191:VAL:HA	1:B:4194:CYS:HB2	1.91	0.53
1:D:3670:LEU:HD22	1:D:3674:ARG:HH21	1.74	0.53
1:A:4800:GLY:HA2	1:A:4804:ASP:HB3	1.90	0.53
1:B:1629:SER:HA	1:B:1640:ASP:HA	1.90	0.53
1:B:4188:GLU:O	1:B:4192:ASN:ND2	2.42	0.53
1:A:1442:TRP:HD1	1:A:1488:VAL:HG13	1.74	0.53
1:A:4826:GLY:O	1:B:4823:ARG:NH1	2.42	0.53
1:D:800:VAL:HG23	1:D:1619:VAL:HG13	1.91	0.53
1:A:1267:HIS:HB3	1:A:1294:ASN:HD21	1.74	0.53
1:B:1128:LEU:HD13	1:B:1206:SER:HB2	1.90	0.53
1:C:1128:LEU:HD13	1:C:1206:SER:HB2	1.91	0.53
1:D:2489:LEU:O	1:D:2492:GLY:N	2.41	0.53
1:D:4888:LYS:HA	1:D:4895:GLY:HA2	1.90	0.53
1:B:559:ILE:HD13	1:B:593:HIS:HB3	1.89	0.53
1:B:4752:LYS:HG3	1:B:4755:ARG:HE	1.74	0.53
1:B:4791:ARG:HH12	1:C:4559:HIS:HE1	1.53	0.53
1:C:228:LEU:HD12	1:C:354:ILE:HB	1.89	0.53
1:C:243:GLU:HA	1:C:264:GLY:HA2	1.90	0.53
1:D:243:GLU:HA	1:D:264:GLY:HA2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1607:ASP:HB3	1:D:1608:VAL:HG23	1.90	0.53
1:A:1128:LEU:HD13	1:A:1206:SER:HB2	1.90	0.53
1:A:1431:ARG:HB3	1:A:1554:GLN:HB2	1.90	0.53
1:C:3670:LEU:HD22	1:C:3674:ARG:HH21	1.72	0.53
1:D:1442:TRP:HB2	1:D:1544:PHE:HB2	1.91	0.53
1:A:1442:TRP:HB2	1:A:1544:PHE:HB2	1.91	0.53
1:C:895:MET:HE1	1:C:971:GLN:HB2	1.90	0.53
1:D:1245:ARG:HE	1:D:1692:LYS:HG2	1.74	0.53
1:D:4780:TYR:HA	1:D:4783:THR:HG22	1.90	0.53
1:C:800:VAL:HG23	1:C:1619:VAL:HG13	1.91	0.52
1:C:1431:ARG:HB3	1:C:1554:GLN:HB2	1.91	0.52
1:D:1510:VAL:HG12	1:D:1511:VAL:HG23	1.91	0.52
1:B:652:VAL:HG11	1:B:715:GLY:HA2	1.90	0.52
1:C:3645:LEU:HB2	1:C:3665:LEU:HD12	1.91	0.52
1:C:4810:MET:HB3	1:D:4519:LEU:O	2.09	0.52
1:D:1431:ARG:HB3	1:D:1554:GLN:HB2	1.91	0.52
1:B:243:GLU:HA	1:B:264:GLY:HA2	1.90	0.52
1:B:776:GLN:HB3	1:B:1470:GLY:HA3	1.90	0.52
1:C:712:GLU:OE2	1:C:1636:ASN:ND2	2.43	0.52
1:C:4014:ILE:HA	1:C:4017:PHE:HB3	1.92	0.52
1:D:1128:LEU:HD13	1:D:1206:SER:HB2	1.91	0.52
1:D:1266:GLU:O	1:D:1294:ASN:ND2	2.43	0.52
1:D:4014:ILE:HA	1:D:4017:PHE:HB3	1.92	0.52
1:D:4188:GLU:O	1:D:4192:ASN:ND2	2.43	0.52
1:A:4519:LEU:O	1:D:4810:MET:HB3	2.09	0.52
1:C:4191:VAL:HA	1:C:4194:CYS:HB2	1.92	0.52
1:B:2794:ARG:HB2	1:B:2901:GLY:HA3	1.92	0.52
1:B:3645:LEU:HB2	1:B:3665:LEU:HD12	1.92	0.52
1:C:1442:TRP:HB2	1:C:1544:PHE:HB2	1.91	0.52
1:B:227:TYR:CE1	1:B:355:LYS:HG2	2.45	0.52
1:B:1442:TRP:HB2	1:B:1544:PHE:HB2	1.92	0.52
1:B:2130:LEU:HD12	1:B:2133:VAL:HG21	1.92	0.52
1:B:2404:ALA:HB3	1:B:2475:ARG:HH21	1.74	0.52
1:C:2130:LEU:HD12	1:C:2133:VAL:HG21	1.92	0.52
1:D:3924:TYR:O	1:D:3932:ASN:ND2	2.43	0.52
1:A:4188:GLU:O	1:A:4192:ASN:ND2	2.42	0.52
1:A:4810:MET:HB3	1:B:4519:LEU:O	2.09	0.52
1:C:776:GLN:HB3	1:C:1470:GLY:HA3	1.90	0.52
1:D:281:ARG:NH1	1:D:346:VAL:O	2.42	0.52
1:A:4559:HIS:HE1	1:D:4791:ARG:HH12	1.54	0.52
1:C:2794:ARG:HB2	1:C:2901:GLY:HA3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4817:HIS:HA	1:C:4821:GLY:H	1.75	0.52
1:D:1252:SER:HB2	1:D:1598:ARG:HB2	1.91	0.52
1:D:3730:ALA:HA	1:D:3733:HIS:CE1	2.45	0.52
1:A:3665:LEU:HD22	1:A:3735:ARG:HH11	1.75	0.52
1:A:4608:ALA:HB1	1:A:4650:VAL:HG11	1.92	0.52
1:C:4770:LEU:HB3	1:D:4754:LEU:CD1	2.37	0.52
1:D:652:VAL:HG11	1:D:715:GLY:HA2	1.92	0.52
1:D:1272:ARG:NH2	1:D:1590:PHE:O	2.43	0.52
1:D:3645:LEU:HB2	1:D:3665:LEU:HD12	1.92	0.52
1:D:4817:HIS:HA	1:D:4821:GLY:H	1.74	0.52
1:A:2794:ARG:HB2	1:A:2901:GLY:HA3	1.92	0.52
1:B:1442:TRP:HD1	1:B:1488:VAL:HG13	1.75	0.52
1:C:227:TYR:CE1	1:C:355:LYS:HG2	2.44	0.52
1:C:3665:LEU:HD22	1:C:3735:ARG:HH11	1.75	0.52
1:C:4188:GLU:O	1:C:4192:ASN:ND2	2.42	0.52
1:D:598:ILE:HG23	1:D:636:LEU:HD12	1.92	0.52
1:A:3730:ALA:HA	1:A:3733:HIS:CE1	2.45	0.51
1:B:2071:ALA:HA	1:B:2076:ILE:HD11	1.91	0.51
1:D:1442:TRP:HD1	1:D:1488:VAL:HG13	1.75	0.51
1:D:1703:TYR:HD2	1:D:1820:PRO:HB2	1.75	0.51
1:D:2076:ILE:HG21	1:D:2081:LEU:HD22	1.92	0.51
1:D:4170:LYS:HE2	1:D:4916:LEU:HD23	1.91	0.51
1:A:227:TYR:CE1	1:A:355:LYS:HG2	2.45	0.51
1:A:4752:LYS:HG3	1:A:4755:ARG:HE	1.76	0.51
1:B:3665:LEU:HD22	1:B:3735:ARG:HH11	1.75	0.51
1:B:3730:ALA:HA	1:B:3733:HIS:CE1	2.46	0.51
1:C:2076:ILE:HG21	1:C:2081:LEU:HD22	1.92	0.51
1:C:2083:ARG:HG3	1:C:3688:LEU:HD22	1.92	0.51
1:D:3665:LEU:HD22	1:D:3735:ARG:HH11	1.76	0.51
1:D:4608:ALA:HB1	1:D:4650:VAL:HG11	1.91	0.51
1:A:2130:LEU:HD12	1:A:2133:VAL:HG21	1.93	0.51
1:A:3645:LEU:HB2	1:A:3665:LEU:HD12	1.93	0.51
1:A:4014:ILE:HA	1:A:4017:PHE:HB3	1.91	0.51
1:A:4191:VAL:HA	1:A:4194:CYS:HB2	1.93	0.51
1:B:3742:LEU:HD23	1:B:3781:TYR:HB3	1.92	0.51
1:D:227:TYR:CE1	1:D:355:LYS:HG2	2.45	0.51
1:A:1266:GLU:O	1:A:1294:ASN:ND2	2.43	0.51
1:B:4824:ALA:HB3	1:B:4827:GLY:H	1.75	0.51
1:C:1124:PRO:HB2	1:C:1252:SER:HB3	1.93	0.51
1:C:1272:ARG:NH2	1:C:1590:PHE:O	2.44	0.51
1:D:866:PRO:HD2	1:D:1009:ARG:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2083:ARG:HG3	1:D:3688:LEU:HD22	1.92	0.51
1:D:2794:ARG:HB2	1:D:2901:GLY:HA3	1.92	0.51
1:A:1252:SER:HB2	1:A:1598:ARG:HB2	1.91	0.51
1:A:1272:ARG:NH2	1:A:1590:PHE:O	2.44	0.51
1:C:866:PRO:HD2	1:C:1009:ARG:HD2	1.92	0.51
1:C:1266:GLU:O	1:C:1294:ASN:ND2	2.43	0.51
1:C:3730:ALA:HA	1:C:3733:HIS:CE1	2.45	0.51
1:C:3924:TYR:O	1:C:3932:ASN:ND2	2.43	0.51
1:A:281:ARG:NH1	1:A:346:VAL:O	2.42	0.51
1:A:4817:HIS:HA	1:A:4821:GLY:H	1.74	0.51
1:D:1124:PRO:HB2	1:D:1252:SER:HB3	1.93	0.51
1:A:866:PRO:HD2	1:A:1009:ARG:HD2	1.92	0.51
1:B:1272:ARG:NH2	1:B:1590:PHE:O	2.44	0.51
1:B:2076:ILE:HG21	1:B:2081:LEU:HD22	1.91	0.51
1:C:598:ILE:HG23	1:C:636:LEU:HD12	1.93	0.51
1:A:1124:PRO:HB2	1:A:1252:SER:HB3	1.93	0.51
1:B:1124:PRO:HB2	1:B:1252:SER:HB3	1.93	0.51
1:C:1245:ARG:HE	1:C:1692:LYS:HG2	1.75	0.51
1:C:1442:TRP:HD1	1:C:1488:VAL:HG13	1.75	0.51
1:D:712:GLU:OE2	1:D:1636:ASN:ND2	2.43	0.51
1:A:677:LEU:HD23	1:A:802:PHE:HA	1.93	0.51
1:B:598:ILE:HG23	1:B:636:LEU:HD12	1.93	0.51
1:B:866:PRO:HD2	1:B:1009:ARG:HD2	1.93	0.51
1:B:4817:HIS:HA	1:B:4821:GLY:H	1.75	0.51
1:D:2226:SER:HB2	1:D:2241:LEU:HB2	1.93	0.51
1:D:3945:VAL:HG12	1:D:4003:MET:HE1	1.93	0.51
1:A:394:HIS:HD2	1:A:397:GLY:H	1.59	0.51
1:A:1184:ASP:OD2	1:A:1188:SER:OG	2.29	0.51
1:A:3924:TYR:O	1:A:3932:ASN:ND2	2.44	0.51
1:D:2130:LEU:HD12	1:D:2133:VAL:HG21	1.92	0.51
1:D:3973:MET:HE3	1:D:4095:ILE:HD13	1.92	0.51
1:A:1703:TYR:HD2	1:A:1820:PRO:HB2	1.76	0.50
1:A:2076:ILE:HG21	1:A:2081:LEU:HD22	1.92	0.50
1:A:2083:ARG:HG3	1:A:3688:LEU:HD22	1.93	0.50
1:B:394:HIS:HD2	1:B:397:GLY:H	1.59	0.50
1:B:2163:MET:HA	1:B:2166:LEU:HD12	1.93	0.50
1:B:4014:ILE:HA	1:B:4017:PHE:HB3	1.91	0.50
1:B:4170:LYS:HE2	1:B:4174:ILE:HD11	1.93	0.50
1:C:1690:GLU:OE2	1:C:1790:LYS:NZ	2.39	0.50
1:C:2226:SER:HB2	1:C:2241:LEU:HB2	1.94	0.50
1:C:4891:ILE:HD13	1:C:4914:HIS:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2226:SER:HB2	1:A:2241:LEU:HB2	1.93	0.50
1:B:1703:TYR:HD2	1:B:1820:PRO:HB2	1.76	0.50
1:B:3924:TYR:O	1:B:3932:ASN:ND2	2.44	0.50
1:A:598:ILE:HG23	1:A:636:LEU:HD12	1.92	0.50
1:B:1266:GLU:O	1:B:1294:ASN:ND2	2.44	0.50
1:B:2083:ARG:HG3	1:B:3688:LEU:HD22	1.93	0.50
1:C:598:ILE:HD13	1:C:636:LEU:HB2	1.94	0.50
1:D:2163:MET:HA	1:D:2166:LEU:HD12	1.93	0.50
1:B:712:GLU:OE2	1:B:1636:ASN:ND2	2.44	0.50
1:C:3973:MET:HE3	1:C:4095:ILE:HD13	1.93	0.50
1:A:3779:LEU:HD11	1:A:3783:LYS:HE2	1.94	0.50
1:A:4780:TYR:O	1:A:4784:VAL:HG23	2.12	0.50
1:C:281:ARG:NH1	1:C:346:VAL:O	2.41	0.50
1:C:1703:TYR:HD2	1:C:1820:PRO:HB2	1.76	0.50
1:C:2163:MET:HA	1:C:2166:LEU:HD12	1.94	0.50
1:D:677:LEU:HD23	1:D:802:PHE:HA	1.93	0.50
1:D:4191:VAL:HA	1:D:4194:CYS:HB2	1.93	0.50
1:A:652:VAL:HG11	1:A:715:GLY:HA2	1.92	0.50
1:B:4608:ALA:HB1	1:B:4650:VAL:HG11	1.93	0.50
1:C:3945:VAL:HG12	1:C:4003:MET:HE1	1.93	0.50
1:D:394:HIS:HD2	1:D:397:GLY:H	1.60	0.50
1:A:3945:VAL:HG12	1:A:4003:MET:HE1	1.94	0.50
1:D:3779:LEU:HD11	1:D:3783:LYS:HE2	1.94	0.50
1:D:4891:ILE:HD13	1:D:4914:HIS:HB3	1.93	0.50
1:A:2521:LEU:HD22	1:A:2565:ALA:HB2	1.94	0.50
1:B:3779:LEU:HD11	1:B:3783:LYS:HE2	1.94	0.50
1:C:2723:ASN:OD1	1:C:2773:ARG:NH2	2.45	0.50
1:D:1706:LEU:HD21	1:D:1787:LEU:HD21	1.94	0.50
1:A:2163:MET:HA	1:A:2166:LEU:HD12	1.92	0.50
1:A:4824:ALA:HB3	1:A:4827:GLY:H	1.77	0.50
1:C:3742:LEU:HD23	1:C:3781:TYR:HB3	1.93	0.50
1:A:3879:LEU:HD13	1:A:3921:LEU:HD12	1.94	0.49
1:A:3973:MET:HE3	1:A:4095:ILE:HD13	1.93	0.49
1:B:1690:GLU:OE2	1:B:1790:LYS:NZ	2.39	0.49
1:C:677:LEU:HD23	1:C:802:PHE:HA	1.93	0.49
1:C:3779:LEU:HD11	1:C:3783:LYS:HE2	1.94	0.49
1:C:4060:THR:OG1	1:C:4063:GLU:OE1	2.26	0.49
1:C:4780:TYR:O	1:C:4784:VAL:HG23	2.12	0.49
1:D:1184:ASP:HB3	1:D:1186:SER:H	1.77	0.49
1:D:2723:ASN:OD1	1:D:2773:ARG:NH2	2.45	0.49
1:B:677:LEU:HD23	1:B:802:PHE:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1160:ASP:OD1	1:B:1178:ASN:ND2	2.43	0.49
1:C:3990:ASN:ND2	1:C:3991:VAL:O	2.45	0.49
1:A:4627:ILE:O	1:A:4631:TRP:N	2.46	0.49
1:A:4640:SER:OG	1:A:4703:ASP:OD2	2.29	0.49
1:A:4891:ILE:HD13	1:A:4914:HIS:HB3	1.93	0.49
1:C:1184:ASP:OD2	1:C:1188:SER:OG	2.29	0.49
1:C:1706:LEU:HD21	1:C:1787:LEU:HD21	1.95	0.49
1:D:598:ILE:HD13	1:D:636:LEU:HB2	1.94	0.49
1:D:4114:THR:HA	1:D:4117:GLN:HB2	1.95	0.49
1:D:4780:TYR:O	1:D:4784:VAL:HG23	2.11	0.49
1:D:4824:ALA:HB3	1:D:4827:GLY:H	1.77	0.49
1:A:235:ARG:HE	1:A:274:LEU:HD21	1.77	0.49
1:A:2222:LEU:HD21	1:A:2243:VAL:HB	1.94	0.49
1:B:2226:SER:HB2	1:B:2241:LEU:HB2	1.94	0.49
1:B:2723:ASN:OD1	1:B:2773:ARG:NH2	2.45	0.49
1:B:4780:TYR:O	1:B:4784:VAL:HG23	2.13	0.49
1:C:4824:ALA:HB3	1:C:4827:GLY:H	1.77	0.49
1:D:2521:LEU:HD22	1:D:2565:ALA:HB2	1.94	0.49
1:A:1899:LEU:O	1:A:1904:LYS:NZ	2.38	0.49
1:A:4114:THR:HA	1:A:4117:GLN:HB2	1.95	0.49
1:A:4189:LEU:HA	1:A:4192:ASN:HD22	1.77	0.49
1:B:3945:VAL:HG12	1:B:4003:MET:HE1	1.94	0.49
1:B:4060:THR:OG1	1:B:4063:GLU:OE1	2.26	0.49
1:D:3879:LEU:HD13	1:D:3921:LEU:HD12	1.95	0.49
1:A:712:GLU:OE2	1:A:1636:ASN:ND2	2.44	0.49
1:A:1706:LEU:HD21	1:A:1787:LEU:HD21	1.93	0.49
1:C:1184:ASP:HB3	1:C:1186:SER:H	1.77	0.49
1:D:335:LYS:NZ	1:D:398:HIS:O	2.38	0.49
1:D:2222:LEU:HD21	1:D:2243:VAL:HB	1.94	0.49
1:A:1716:THR:HA	1:A:1719:LEU:HD12	1.95	0.49
1:B:218:SER:HB3	1:B:286:GLY:HA3	1.94	0.49
1:B:1268:ILE:HG21	1:B:1300:MET:HE2	1.94	0.49
1:B:2222:LEU:HD21	1:B:2243:VAL:HB	1.94	0.49
1:B:4627:ILE:O	1:B:4631:TRP:N	2.46	0.49
1:C:1938:GLN:HE22	1:C:3614:ARG:HA	1.77	0.49
1:B:298:ARG:HA	1:B:305:TYR:HA	1.94	0.49
1:C:843:GLU:HA	1:C:848:ARG:HG2	1.95	0.49
1:C:1244:ASN:HD22	1:C:1801:GLU:HG2	1.78	0.49
1:C:4608:ALA:HB1	1:C:4650:VAL:HG11	1.93	0.49
1:D:1692:LYS:HA	1:D:1810:VAL:HG13	1.95	0.49
1:D:4189:LEU:HA	1:D:4192:ASN:HD22	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1160:ASP:OD1	1:A:1178:ASN:ND2	2.43	0.49
1:A:1654:HIS:O	1:A:1657:THR:OG1	2.27	0.49
1:A:2723:ASN:OD1	1:A:2773:ARG:NH2	2.45	0.49
1:B:843:GLU:HA	1:B:848:ARG:HG2	1.94	0.49
1:B:4189:LEU:HA	1:B:4192:ASN:HD22	1.78	0.49
1:C:2213:LYS:HA	1:C:2254:LEU:HD21	1.94	0.49
1:C:4627:ILE:O	1:C:4631:TRP:N	2.45	0.49
1:A:218:SER:HB3	1:A:286:GLY:HA3	1.95	0.49
1:A:3990:ASN:ND2	1:A:3991:VAL:O	2.46	0.49
1:B:3973:MET:HE3	1:B:4095:ILE:HD13	1.94	0.49
1:B:4891:ILE:HD13	1:B:4914:HIS:HB3	1.94	0.49
1:C:2222:LEU:HD21	1:C:2243:VAL:HB	1.95	0.49
1:C:4171:ARG:CG	1:C:4171:ARG:NH2	2.73	0.49
1:D:2857:LYS:HE3	1:D:2861:LEU:HD11	1.95	0.49
1:D:3742:LEU:HD23	1:D:3781:TYR:HB3	1.95	0.49
1:A:3729:GLN:NE2	1:A:3767:LEU:O	2.47	0.48
1:A:4796:LYS:NZ	1:A:4807:CYS:SG	2.82	0.48
1:B:598:ILE:HD13	1:B:636:LEU:HB2	1.95	0.48
1:B:678:MET:HG3	1:B:754:VAL:HG22	1.94	0.48
1:B:1121:GLY:O	1:B:1133:ARG:NH1	2.43	0.48
1:B:1184:ASP:OD2	1:B:1188:SER:OG	2.29	0.48
1:B:3990:ASN:ND2	1:B:3991:VAL:O	2.46	0.48
1:C:218:SER:HB3	1:C:286:GLY:HA3	1.95	0.48
1:C:1121:GLY:O	1:C:1133:ARG:NH1	2.43	0.48
1:C:1692:LYS:HA	1:C:1810:VAL:HG13	1.95	0.48
1:C:2435:GLY:O	1:C:2438:SER:OG	2.29	0.48
1:A:843:GLU:HA	1:A:848:ARG:HG2	1.94	0.48
1:B:290:ARG:HH22	1:B:343:ARG:HG3	1.78	0.48
1:B:4114:THR:HA	1:B:4117:GLN:HB2	1.95	0.48
1:D:128:MET:HB3	1:D:149:LEU:HB3	1.95	0.48
1:D:1160:ASP:OD1	1:D:1178:ASN:ND2	2.42	0.48
1:A:4770:LEU:HB3	1:B:4754:LEU:CD1	2.40	0.48
1:C:4826:GLY:O	1:D:4823:ARG:NH1	2.46	0.48
1:D:1184:ASP:OD2	1:D:1188:SER:OG	2.29	0.48
1:D:1931:ASP:O	1:D:3614:ARG:NH1	2.42	0.48
1:D:3990:ASN:ND2	1:D:3991:VAL:O	2.46	0.48
1:D:4060:THR:OG1	1:D:4063:GLU:OE1	2.26	0.48
1:D:4627:ILE:O	1:D:4631:TRP:N	2.45	0.48
1:D:4796:LYS:NZ	1:D:4807:CYS:SG	2.82	0.48
1:A:1184:ASP:HB3	1:A:1186:SER:H	1.78	0.48
1:C:128:MET:HB3	1:C:149:LEU:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:678:MET:HG3	1:C:754:VAL:HG22	1.96	0.48
1:C:1160:ASP:OD1	1:C:1178:ASN:ND2	2.43	0.48
1:D:1268:ILE:HG21	1:D:1300:MET:HE2	1.96	0.48
1:D:2213:LYS:HA	1:D:2254:LEU:HD21	1.95	0.48
1:A:2857:LYS:HE3	1:A:2861:LEU:HD11	1.95	0.48
1:B:3998:LYS:HG2	1:B:4110:MET:HE1	1.94	0.48
1:B:4826:GLY:O	1:C:4823:ARG:NH1	2.46	0.48
1:C:394:HIS:HD2	1:C:397:GLY:H	1.60	0.48
1:C:1268:ILE:HG21	1:C:1300:MET:HE2	1.95	0.48
1:D:218:SER:HB3	1:D:286:GLY:HA3	1.96	0.48
1:D:843:GLU:HA	1:D:848:ARG:HG2	1.94	0.48
1:B:1184:ASP:HB3	1:B:1186:SER:H	1.77	0.48
1:D:235:ARG:HE	1:D:274:LEU:HD21	1.78	0.48
1:D:4794:TYR:HB3	1:D:4807:CYS:HB2	1.95	0.48
1:A:4931:GLU:OE2	1:A:4942:TRP:NE1	2.46	0.48
1:B:4770:LEU:HB3	1:C:4754:LEU:CD1	2.39	0.48
1:C:2521:LEU:HD22	1:C:2565:ALA:HB2	1.95	0.48
1:A:2843:GLU:OE1	1:A:2887:ARG:NH2	2.47	0.48
1:B:1706:LEU:HD21	1:B:1787:LEU:HD21	1.94	0.48
1:D:1716:THR:HA	1:D:1719:LEU:HD12	1.95	0.48
1:D:3729:GLN:NE2	1:D:3767:LEU:O	2.47	0.48
1:D:4610:LYS:O	1:D:4615:GLY:N	2.46	0.48
1:A:678:MET:HG3	1:A:754:VAL:HG22	1.95	0.48
1:A:4794:TYR:HB3	1:A:4807:CYS:HB2	1.96	0.48
1:B:235:ARG:HE	1:B:274:LEU:HD21	1.79	0.48
1:B:1654:HIS:O	1:B:1657:THR:OG1	2.28	0.48
1:B:1716:THR:HA	1:B:1719:LEU:HD12	1.96	0.48
1:B:3729:GLN:NE2	1:B:3767:LEU:O	2.47	0.48
1:C:2857:LYS:HE3	1:C:2861:LEU:HD11	1.95	0.48
1:D:2528:LEU:HD11	1:D:2568:ASP:HA	1.96	0.48
1:B:1611:ILE:N	1:B:1620:GLN:O	2.43	0.48
1:B:1664:VAL:HG12	1:B:1672:VAL:HG11	1.96	0.48
1:C:235:ARG:HE	1:C:274:LEU:HD21	1.79	0.48
1:C:4114:THR:HA	1:C:4117:GLN:HB2	1.96	0.48
1:C:4610:LYS:O	1:C:4615:GLY:N	2.46	0.48
1:A:128:MET:HB3	1:A:149:LEU:HB3	1.96	0.47
1:B:1726:ILE:HB	1:B:2109:ILE:HD11	1.96	0.47
1:B:2521:LEU:HD22	1:B:2565:ALA:HB2	1.95	0.47
1:C:650:ASN:ND2	1:C:795:SER:O	2.47	0.47
1:C:2843:GLU:OE1	1:C:2887:ARG:NH2	2.47	0.47
1:C:3729:GLN:NE2	1:C:3767:LEU:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2843:GLU:OE1	1:D:2887:ARG:NH2	2.47	0.47
1:A:298:ARG:HA	1:A:305:TYR:HA	1.95	0.47
1:A:804:LEU:HD22	1:A:822:CYS:HB3	1.96	0.47
1:A:3696:MET:O	1:A:3699:SER:OG	2.32	0.47
1:A:3748:SER:HB2	1:A:3751:GLU:HB2	1.96	0.47
1:B:165:ALA:HB3	1:B:211:LEU:HD21	1.96	0.47
1:B:1899:LEU:O	1:B:1904:LYS:NZ	2.38	0.47
1:D:678:MET:HG3	1:D:754:VAL:HG22	1.96	0.47
1:B:2857:LYS:HE3	1:B:2861:LEU:HD11	1.95	0.47
1:B:3875:THR:HG21	1:B:3924:TYR:HE2	1.79	0.47
1:C:1716:THR:HA	1:C:1719:LEU:HD12	1.95	0.47
1:C:1931:ASP:O	1:C:3614:ARG:NH1	2.42	0.47
1:C:3952:PHE:HZ	1:C:3975:LEU:HD22	1.78	0.47
1:C:4931:GLU:OE2	1:C:4942:TRP:NE1	2.47	0.47
1:A:2435:GLY:O	1:A:2438:SER:OG	2.29	0.47
1:B:4046:LYS:HG3	1:B:4068:LEU:HD22	1.96	0.47
1:C:3875:THR:HG21	1:C:3924:TYR:HE2	1.79	0.47
1:D:718:VAL:HA	1:D:736:CYS:HB2	1.96	0.47
1:D:3748:SER:HB2	1:D:3751:GLU:HB2	1.96	0.47
1:D:4931:GLU:OE2	1:D:4942:TRP:NE1	2.46	0.47
1:A:718:VAL:HA	1:A:736:CYS:HB2	1.96	0.47
1:A:3742:LEU:HD23	1:A:3781:TYR:HB3	1.95	0.47
1:B:128:MET:HB3	1:B:149:LEU:HB3	1.96	0.47
1:B:4733:GLY:HA3	1:B:4740:PHE:CD1	2.50	0.47
1:C:165:ALA:HB3	1:C:211:LEU:HD21	1.96	0.47
1:C:3879:LEU:HD13	1:C:3921:LEU:HD12	1.96	0.47
1:C:4189:LEU:HA	1:C:4192:ASN:HD22	1.79	0.47
1:D:298:ARG:HA	1:D:305:TYR:HA	1.95	0.47
1:B:718:VAL:HA	1:B:736:CYS:HB2	1.97	0.47
1:B:2843:GLU:OE1	1:B:2887:ARG:NH2	2.47	0.47
1:C:25:THR:HB	1:C:32:GLN:HB3	1.97	0.47
1:C:1654:HIS:O	1:C:1657:THR:OG1	2.28	0.47
1:C:1707:ILE:HA	1:C:1711:LEU:HB2	1.96	0.47
1:C:2528:LEU:HD11	1:C:2568:ASP:HA	1.97	0.47
1:D:674:TYR:OH	1:D:676:GLU:OE2	2.31	0.47
1:D:1121:GLY:O	1:D:1133:ARG:NH1	2.43	0.47
1:A:260:VAL:HG12	1:A:391:ALA:HB3	1.97	0.47
1:A:290:ARG:HH22	1:A:343:ARG:HG3	1.79	0.47
1:A:598:ILE:HD13	1:A:636:LEU:HB2	1.96	0.47
1:A:1132:GLU:HG2	1:A:1133:ARG:HG3	1.97	0.47
1:A:1268:ILE:HG21	1:A:1300:MET:HE2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1611:ILE:N	1:A:1620:GLN:O	2.43	0.47
1:A:1664:VAL:HG12	1:A:1672:VAL:HG11	1.97	0.47
1:C:4796:LYS:NZ	1:C:4807:CYS:SG	2.82	0.47
1:D:25:THR:HB	1:D:32:GLN:HB3	1.97	0.47
1:D:260:VAL:HG12	1:D:391:ALA:HB3	1.97	0.47
1:B:1244:ASN:HD22	1:B:1801:GLU:HG2	1.79	0.47
1:B:2213:LYS:HA	1:B:2254:LEU:HD21	1.96	0.47
1:C:298:ARG:HA	1:C:305:TYR:HA	1.95	0.47
1:C:718:VAL:HA	1:C:736:CYS:HB2	1.97	0.47
1:C:804:LEU:HD22	1:C:822:CYS:HB3	1.97	0.47
1:C:4046:LYS:HG3	1:C:4068:LEU:HD22	1.96	0.47
1:D:165:ALA:HB3	1:D:211:LEU:HD21	1.96	0.47
1:D:3797:LEU:O	1:D:3800:SER:OG	2.32	0.47
1:A:674:TYR:OH	1:A:676:GLU:OE2	2.32	0.47
1:B:207:PHE:CE2	1:C:2326:ILE:HG21	2.50	0.47
1:B:2348:MET:HE1	1:B:2436:VAL:HG22	1.97	0.47
1:B:4931:GLU:OE2	1:B:4942:TRP:NE1	2.46	0.47
1:C:1726:ILE:HB	1:C:2109:ILE:HD11	1.97	0.47
1:C:1833:ILE:HG22	1:C:1834:PHE:H	1.79	0.47
1:D:1132:GLU:HG2	1:D:1133:ARG:HG3	1.97	0.47
1:D:1432:ILE:HD13	1:D:1441:VAL:HG21	1.97	0.47
1:D:1611:ILE:N	1:D:1620:GLN:O	2.43	0.47
1:D:1899:LEU:O	1:D:1904:LYS:NZ	2.38	0.47
1:D:3952:PHE:HZ	1:D:3975:LEU:HD22	1.80	0.47
1:D:4733:GLY:HA3	1:D:4740:PHE:CD1	2.50	0.47
1:A:1692:LYS:HA	1:A:1810:VAL:HG13	1.98	0.47
1:A:1707:ILE:HA	1:A:1711:LEU:HB2	1.96	0.47
1:A:2213:LYS:HA	1:A:2254:LEU:HD21	1.96	0.47
1:A:2390:MET:HG3	1:A:2465:HIS:CE1	2.50	0.47
1:A:4046:LYS:HG3	1:A:4068:LEU:HD22	1.96	0.47
1:B:260:VAL:HG12	1:B:391:ALA:HB3	1.96	0.47
1:B:559:ILE:HA	1:B:562:LEU:HB2	1.98	0.47
1:C:260:VAL:HG12	1:C:391:ALA:HB3	1.97	0.47
1:D:650:ASN:ND2	1:D:795:SER:O	2.47	0.47
1:D:1172:THR:HG21	1:D:1190:LEU:HD13	1.97	0.47
1:D:1833:ILE:HG22	1:D:1834:PHE:H	1.79	0.47
1:D:2264:GLU:OE2	1:D:2268:ARG:NH2	2.47	0.47
1:D:4046:LYS:HG3	1:D:4068:LEU:HD22	1.96	0.47
1:A:207:PHE:CE2	1:B:2326:ILE:HG21	2.51	0.46
1:A:335:LYS:NZ	1:A:398:HIS:O	2.38	0.46
1:A:1833:ILE:HG22	1:A:1834:PHE:H	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2528:LEU:HD11	1:A:2568:ASP:HA	1.97	0.46
1:A:4610:LYS:O	1:A:4615:GLY:N	2.46	0.46
1:B:802:PHE:HB2	1:B:1617:TRP:HB2	1.97	0.46
1:B:804:LEU:HD22	1:B:822:CYS:HB3	1.96	0.46
1:B:1707:ILE:HA	1:B:1711:LEU:HB2	1.96	0.46
1:B:3879:LEU:HD13	1:B:3921:LEU:HD12	1.96	0.46
1:D:170:SER:OG	1:D:171:GLU:N	2.49	0.46
1:D:1244:ASN:HD22	1:D:1801:GLU:HG2	1.79	0.46
1:D:4170:LYS:HE2	1:D:4916:LEU:CD2	2.45	0.46
1:A:314:LEU:HB2	1:A:393:MET:HG2	1.98	0.46
1:A:1219:LYS:NZ	1:A:1244:ASN:O	2.49	0.46
1:A:4733:GLY:HA3	1:A:4740:PHE:CD1	2.50	0.46
1:B:4794:TYR:HB3	1:B:4807:CYS:HB2	1.97	0.46
1:C:2390:MET:HG3	1:C:2465:HIS:CE1	2.50	0.46
1:C:3748:SER:HB2	1:C:3751:GLU:HB2	1.97	0.46
1:B:25:THR:HB	1:B:32:GLN:HB3	1.97	0.46
1:B:1833:ILE:HG22	1:B:1834:PHE:H	1.79	0.46
1:B:2773:ARG:HA	1:B:2776:ILE:HD12	1.97	0.46
1:C:1132:GLU:HG2	1:C:1133:ARG:HG3	1.97	0.46
1:C:4018:PHE:O	1:C:4022:LEU:N	2.40	0.46
1:C:4733:GLY:HA3	1:C:4740:PHE:CD1	2.50	0.46
1:A:25:THR:HB	1:A:32:GLN:HB3	1.97	0.46
1:A:2773:ARG:HA	1:A:2776:ILE:HD12	1.97	0.46
1:B:1172:THR:HG21	1:B:1190:LEU:HD13	1.96	0.46
1:B:2390:MET:HG3	1:B:2465:HIS:CE1	2.51	0.46
1:C:180:ASP:HB3	1:C:211:LEU:HD22	1.98	0.46
1:C:1172:THR:HG21	1:C:1190:LEU:HD13	1.96	0.46
1:D:14:LEU:HD12	1:D:175:VAL:HG12	1.97	0.46
1:D:1707:ILE:HA	1:D:1711:LEU:HB2	1.96	0.46
1:D:2390:MET:HG3	1:D:2465:HIS:CE1	2.50	0.46
1:A:165:ALA:HB3	1:A:211:LEU:HD21	1.97	0.46
1:A:2348:MET:HE1	1:A:2436:VAL:HG22	1.97	0.46
1:A:3904:GLN:NE2	1:A:3965:GLN:OE1	2.47	0.46
1:A:4018:PHE:O	1:A:4022:LEU:N	2.40	0.46
1:B:1692:LYS:HA	1:B:1810:VAL:HG13	1.98	0.46
1:C:20:VAL:HG12	1:C:216:PRO:HA	1.97	0.46
1:C:170:SER:OG	1:C:171:GLU:N	2.48	0.46
1:C:2264:GLU:OE2	1:C:2268:ARG:NH2	2.48	0.46
1:C:3998:LYS:HG2	1:C:4110:MET:HE1	1.96	0.46
1:D:649:VAL:HG21	1:D:713:TRP:HB3	1.98	0.46
1:D:2773:ARG:HA	1:D:2776:ILE:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4640:SER:OG	1:D:4703:ASP:OD2	2.29	0.46
1:A:1172:THR:HG21	1:A:1190:LEU:HD13	1.97	0.46
1:B:1165:MET:HB2	1:B:1174:MET:HB2	1.98	0.46
1:B:1219:LYS:H	1:B:1240:ALA:HB3	1.80	0.46
1:B:2264:GLU:OE2	1:B:2268:ARG:NH2	2.47	0.46
1:B:2897:LEU:HB3	1:B:2904:VAL:HG21	1.98	0.46
1:B:4052:ALA:O	1:B:4056:HIS:ND1	2.48	0.46
1:B:4640:SER:OG	1:B:4703:ASP:OD2	2.30	0.46
1:B:4796:LYS:NZ	1:B:4807:CYS:SG	2.82	0.46
1:C:290:ARG:HH22	1:C:343:ARG:HG3	1.81	0.46
1:D:686:VAL:O	1:D:687:THR:OG1	2.33	0.46
1:D:804:LEU:HD22	1:D:822:CYS:HB3	1.97	0.46
1:A:3875:THR:HG21	1:A:3924:TYR:HE2	1.81	0.46
1:B:1432:ILE:HD13	1:B:1441:VAL:HG21	1.98	0.46
1:B:1449:ASP:N	1:B:1449:ASP:OD1	2.49	0.46
1:B:1689:ILE:HA	1:B:1703:TYR:HE1	1.81	0.46
1:C:695:VAL:HG21	1:C:755:ILE:HD13	1.98	0.46
1:C:4616:LEU:HA	1:C:4620:GLU:HB2	1.98	0.46
1:D:695:VAL:HG21	1:D:755:ILE:HD13	1.98	0.46
1:D:717:GLY:O	1:D:736:CYS:N	2.45	0.46
1:A:650:ASN:ND2	1:A:795:SER:O	2.48	0.46
1:A:1165:MET:HB2	1:A:1174:MET:HB2	1.97	0.46
1:A:1258:PHE:HB3	1:A:1303:ARG:NH2	2.31	0.46
1:A:4171:ARG:HH11	1:A:4752:LYS:CD	2.23	0.46
1:B:14:LEU:HD12	1:B:175:VAL:HG12	1.98	0.46
1:B:20:VAL:HG12	1:B:216:PRO:HA	1.97	0.46
1:B:1938:GLN:HE22	1:B:3614:ARG:HA	1.81	0.46
1:B:2528:LEU:HD11	1:B:2568:ASP:HA	1.97	0.46
1:C:3904:GLN:NE2	1:C:3965:GLN:OE1	2.48	0.46
1:D:20:VAL:HG12	1:D:216:PRO:HA	1.98	0.46
1:A:2897:LEU:HB3	1:A:2904:VAL:HG21	1.98	0.46
1:B:650:ASN:ND2	1:B:795:SER:O	2.48	0.46
1:B:3794:LEU:HA	1:B:3797:LEU:HD12	1.97	0.46
1:C:1091:GLU:HA	1:C:1250:TRP:CZ3	2.51	0.46
1:D:238:HIS:HB3	1:D:243:GLU:HB3	1.98	0.46
1:D:1219:LYS:NZ	1:D:1244:ASN:O	2.49	0.46
1:D:3919:ASN:O	1:D:3922:THR:OG1	2.32	0.46
1:D:4018:PHE:O	1:D:4022:LEU:N	2.40	0.46
1:A:1219:LYS:H	1:A:1240:ALA:HB3	1.81	0.46
1:A:3952:PHE:HZ	1:A:3975:LEU:HD22	1.81	0.46
1:B:1132:GLU:HG2	1:B:1133:ARG:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4018:PHE:O	1:B:4022:LEU:N	2.40	0.46
1:C:1219:LYS:H	1:C:1240:ALA:HB3	1.81	0.46
1:C:1449:ASP:OD1	1:C:1449:ASP:N	2.49	0.46
1:C:1664:VAL:HG12	1:C:1672:VAL:HG11	1.97	0.46
1:C:2348:MET:HE1	1:C:2436:VAL:HG22	1.97	0.46
1:C:4794:TYR:HB3	1:C:4807:CYS:HB2	1.97	0.46
1:D:1219:LYS:H	1:D:1240:ALA:HB3	1.81	0.46
1:D:2897:LEU:HB3	1:D:2904:VAL:HG21	1.98	0.46
1:A:14:LEU:HD12	1:A:175:VAL:HG12	1.97	0.45
1:A:649:VAL:HG21	1:A:713:TRP:HB3	1.98	0.45
1:A:686:VAL:O	1:A:687:THR:OG1	2.33	0.45
1:B:449:ILE:HG13	1:B:522:ALA:HB1	1.98	0.45
1:B:1091:GLU:HA	1:B:1250:TRP:CZ3	2.51	0.45
1:B:3748:SER:HB2	1:B:3751:GLU:HB2	1.97	0.45
1:B:3952:PHE:HZ	1:B:3975:LEU:HD22	1.81	0.45
1:B:4610:LYS:O	1:B:4615:GLY:N	2.46	0.45
1:C:3794:LEU:HA	1:C:3797:LEU:HD12	1.98	0.45
1:D:954:ASP:HB3	1:D:1061:GLY:HA3	1.98	0.45
1:D:1258:PHE:HB3	1:D:1303:ARG:NH2	2.32	0.45
1:D:1938:GLN:HE22	1:D:3614:ARG:HA	1.81	0.45
1:D:2348:MET:HE1	1:D:2436:VAL:HG22	1.98	0.45
1:A:1432:ILE:HD13	1:A:1441:VAL:HG21	1.98	0.45
1:A:4616:LEU:HA	1:A:4620:GLU:HB2	1.99	0.45
1:B:1611:ILE:HB	1:B:1620:GLN:HB3	1.98	0.45
1:C:23:GLN:HA	1:C:36:CYS:HA	1.99	0.45
1:C:1570:LEU:HD13	1:C:1584:PRO:HG3	1.98	0.45
1:C:1611:ILE:N	1:C:1620:GLN:O	2.44	0.45
1:C:4130:PHE:O	1:C:4134:LEU:N	2.50	0.45
1:D:3875:THR:HG21	1:D:3924:TYR:HE2	1.81	0.45
1:A:1570:LEU:HD13	1:A:1584:PRO:HG3	1.98	0.45
1:A:4757:ILE:HG21	1:A:4757:ILE:HD13	1.71	0.45
1:B:180:ASP:HB3	1:B:211:LEU:HD22	1.98	0.45
1:B:480:ARG:NH2	1:B:3677:LEU:O	2.50	0.45
1:C:14:LEU:HD12	1:C:175:VAL:HG12	1.97	0.45
1:C:234:LEU:HD13	1:C:405:LEU:HD22	1.98	0.45
1:C:238:HIS:HB3	1:C:243:GLU:HB3	1.98	0.45
1:C:954:ASP:HB3	1:C:1061:GLY:HA3	1.99	0.45
1:C:1089:ARG:HH21	1:C:1600:PRO:HG3	1.81	0.45
1:C:1219:LYS:NZ	1:C:1244:ASN:O	2.49	0.45
1:C:1689:ILE:HA	1:C:1703:TYR:HE1	1.81	0.45
1:A:954:ASP:HB3	1:A:1061:GLY:HA3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3794:LEU:HA	1:A:3797:LEU:HD12	1.98	0.45
1:C:207:PHE:CE2	1:D:2326:ILE:HG21	2.51	0.45
1:C:433:LEU:HD21	1:C:505:LEU:HG	1.99	0.45
1:C:2773:ARG:HA	1:C:2776:ILE:HD12	1.98	0.45
1:D:472:HIS:CE1	1:D:3674:ARG:HB2	2.52	0.45
1:A:20:VAL:HG12	1:A:216:PRO:HA	1.97	0.45
1:A:472:HIS:CE1	1:A:3674:ARG:HB2	2.52	0.45
1:A:802:PHE:HB2	1:A:1617:TRP:HB2	1.97	0.45
1:A:1611:ILE:HB	1:A:1620:GLN:HB3	1.99	0.45
1:B:3798:MET:HE1	1:B:3871:ILE:HG23	1.98	0.45
1:C:1432:ILE:HD13	1:C:1441:VAL:HG21	1.97	0.45
1:C:1899:LEU:O	1:C:1904:LYS:NZ	2.37	0.45
1:D:1664:VAL:HG12	1:D:1672:VAL:HG11	1.98	0.45
1:A:23:GLN:HA	1:A:36:CYS:HA	1.98	0.45
1:A:1244:ASN:HD22	1:A:1801:GLU:HG2	1.79	0.45
1:A:2264:GLU:OE2	1:A:2268:ARG:NH2	2.48	0.45
1:A:3919:ASN:O	1:A:3922:THR:OG1	2.32	0.45
1:B:170:SER:OG	1:B:171:GLU:N	2.48	0.45
1:B:472:HIS:CE1	1:B:3674:ARG:HB2	2.51	0.45
1:B:1219:LYS:NZ	1:B:1244:ASN:O	2.49	0.45
1:B:1258:PHE:HB3	1:B:1303:ARG:NH2	2.32	0.45
1:B:1570:LEU:HD13	1:B:1584:PRO:HG3	1.98	0.45
1:B:1931:ASP:O	1:B:3614:ARG:NH1	2.41	0.45
1:C:248:PRO:HG2	1:C:257:ARG:HA	1.98	0.45
1:C:472:HIS:CE1	1:C:3674:ARG:HB2	2.51	0.45
1:C:1165:MET:HB2	1:C:1174:MET:HB2	1.98	0.45
1:C:3696:MET:O	1:C:3699:SER:OG	2.32	0.45
1:D:23:GLN:HA	1:D:36:CYS:HA	1.99	0.45
1:D:737:ILE:HG22	1:D:739:ARG:HG3	1.99	0.45
1:D:1091:GLU:HA	1:D:1250:TRP:CZ3	2.52	0.45
1:D:1689:ILE:HA	1:D:1703:TYR:HE1	1.81	0.45
1:D:3794:LEU:HA	1:D:3797:LEU:HD12	1.99	0.45
1:D:3798:MET:HE1	1:D:3871:ILE:HG23	1.98	0.45
1:D:4196:ASP:O	1:D:4200:GLU:N	2.49	0.45
1:A:1938:GLN:HE22	1:A:3614:ARG:HA	1.82	0.45
1:B:23:GLN:HA	1:B:36:CYS:HA	1.98	0.45
1:B:262:TYR:N	1:B:389:ARG:O	2.49	0.45
1:C:2897:LEU:HB3	1:C:2904:VAL:HG21	1.98	0.45
1:C:3729:GLN:O	1:C:3733:HIS:ND1	2.47	0.45
1:D:480:ARG:NH2	1:D:3677:LEU:O	2.49	0.45
1:D:655:MET:HE3	1:D:1610:ARG:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1174:MET:SD	1:D:1236:TYR:OH	2.74	0.45
1:D:1469:LEU:HG	1:D:1480:ILE:HD11	1.98	0.45
1:D:1726:ILE:HB	1:D:2109:ILE:HD11	1.99	0.45
1:D:3729:GLN:O	1:D:3733:HIS:ND1	2.47	0.45
1:B:248:PRO:HG2	1:B:257:ARG:HA	1.99	0.45
1:B:3919:ASN:O	1:B:3922:THR:OG1	2.32	0.45
1:C:559:ILE:HA	1:C:562:LEU:HB2	1.99	0.45
1:D:1449:ASP:N	1:D:1449:ASP:OD1	2.49	0.45
1:D:4616:LEU:HA	1:D:4620:GLU:HB2	1.99	0.45
1:D:4851:PHE:O	1:D:4855:VAL:HB	2.17	0.45
1:A:1091:GLU:HA	1:A:1250:TRP:CZ3	2.52	0.45
1:A:1689:ILE:HA	1:A:1703:TYR:HE1	1.81	0.45
1:A:1726:ILE:HB	1:A:2109:ILE:HD11	1.99	0.45
1:A:3737:ALA:O	1:A:3740:MET:HG2	2.17	0.45
1:A:3798:MET:HE1	1:A:3871:ILE:HG23	1.98	0.45
1:A:4904:HIS:NE2	1:A:4907:GLU:OE1	2.50	0.45
1:B:4616:LEU:HA	1:B:4620:GLU:HB2	1.99	0.45
1:C:480:ARG:NH2	1:C:3677:LEU:O	2.49	0.45
1:C:1699:ARG:NH1	1:C:1816:PHE:O	2.48	0.45
1:C:3737:ALA:O	1:C:3740:MET:HG2	2.17	0.45
1:C:3798:MET:HE1	1:C:3871:ILE:HG23	1.98	0.45
1:D:2436:VAL:HG21	1:D:2469:MET:HE3	1.99	0.45
1:D:3998:LYS:HG2	1:D:4110:MET:HE1	1.98	0.45
1:A:217:ILE:HG23	1:A:285:SER:HB3	1.99	0.45
1:A:480:ARG:NH2	1:A:3677:LEU:O	2.49	0.45
1:A:559:ILE:HA	1:A:562:LEU:HB2	1.99	0.45
1:A:1087:ILE:HG23	1:A:1128:LEU:HD12	1.98	0.45
1:A:1640:ASP:OD1	1:A:1640:ASP:N	2.49	0.45
1:A:4060:THR:OG1	1:A:4063:GLU:OE1	2.26	0.45
1:B:532:SER:HA	1:B:535:GLU:HB2	1.99	0.45
1:B:3904:GLN:NE2	1:B:3965:GLN:OE1	2.48	0.45
1:B:4904:HIS:NE2	1:B:4907:GLU:OE1	2.50	0.45
1:C:314:LEU:HB2	1:C:393:MET:HG2	1.98	0.45
1:C:649:VAL:HG21	1:C:713:TRP:HB3	1.98	0.45
1:C:655:MET:HE3	1:C:1610:ARG:HD2	1.99	0.45
1:C:1258:PHE:HB3	1:C:1303:ARG:NH2	2.32	0.45
1:C:1736:ILE:HG23	1:C:1753:LEU:HD12	1.99	0.45
1:D:290:ARG:HH22	1:D:343:ARG:HG3	1.81	0.45
1:D:709:GLY:O	1:D:1253:LYS:NZ	2.50	0.45
1:D:802:PHE:HB2	1:D:1617:TRP:HB2	1.98	0.45
1:D:1165:MET:HB2	1:D:1174:MET:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1570:LEU:HD13	1:D:1584:PRO:HG3	1.98	0.45
1:A:433:LEU:HD21	1:A:505:LEU:HG	1.98	0.44
1:A:449:ILE:HG13	1:A:522:ALA:HB1	1.98	0.44
1:A:2326:ILE:HG21	1:D:207:PHE:CE2	2.52	0.44
1:B:16:THR:HB	1:B:110:HIS:HA	1.99	0.44
1:C:4640:SER:OG	1:C:4703:ASP:OD2	2.29	0.44
1:D:1699:ARG:NH1	1:D:1816:PHE:O	2.48	0.44
1:D:1926:ILE:HD11	1:D:3625:TYR:CE2	2.53	0.44
1:D:3737:ALA:O	1:D:3740:MET:HG2	2.17	0.44
1:A:248:PRO:HG2	1:A:257:ARG:HA	1.98	0.44
1:A:4052:ALA:O	1:A:4056:HIS:ND1	2.48	0.44
1:A:4832:ILE:HG21	1:A:4844:ARG:NH2	2.30	0.44
1:B:4892:CYS:SG	1:B:4909:HIS:NE2	2.80	0.44
1:C:510:SER:O	1:C:520:ARG:NH2	2.51	0.44
1:C:802:PHE:HB2	1:C:1617:TRP:HB2	1.99	0.44
1:C:1613:GLU:HB2	1:C:1618:LEU:H	1.82	0.44
1:C:2071:ALA:HB2	1:C:2085:MET:HE1	2.00	0.44
1:C:4196:ASP:O	1:C:4200:GLU:N	2.49	0.44
1:C:4904:HIS:NE2	1:C:4907:GLU:OE1	2.50	0.44
1:D:234:LEU:HD13	1:D:405:LEU:HD22	1.98	0.44
1:D:248:PRO:HG2	1:D:257:ARG:HA	1.98	0.44
1:D:532:SER:HA	1:D:535:GLU:HB2	1.99	0.44
1:A:238:HIS:HB3	1:A:243:GLU:HB3	1.98	0.44
1:A:299:HIS:CD2	1:A:301:THR:HG1	2.34	0.44
1:A:1174:MET:SD	1:A:1236:TYR:OH	2.75	0.44
1:A:4153:ILE:HD13	1:A:4158:ARG:HH11	1.82	0.44
1:A:4196:ASP:O	1:A:4200:GLU:N	2.49	0.44
1:B:234:LEU:HD13	1:B:405:LEU:HD22	2.00	0.44
1:B:954:ASP:HB3	1:B:1061:GLY:HA3	1.99	0.44
1:C:16:THR:HB	1:C:110:HIS:HA	2.00	0.44
1:C:737:ILE:HG22	1:C:739:ARG:HG3	2.00	0.44
1:C:1611:ILE:HB	1:C:1620:GLN:HB3	1.99	0.44
1:C:3919:ASN:O	1:C:3922:THR:OG1	2.32	0.44
1:D:449:ILE:HG13	1:D:522:ALA:HB1	1.99	0.44
1:D:4153:ILE:HD13	1:D:4158:ARG:HH11	1.83	0.44
1:D:4904:HIS:NE2	1:D:4907:GLU:OE1	2.50	0.44
1:A:262:TYR:N	1:A:389:ARG:O	2.49	0.44
1:A:555:LEU:HD13	1:A:585:ALA:HB1	1.99	0.44
1:A:655:MET:HE3	1:A:1610:ARG:HD2	1.99	0.44
1:A:1736:ILE:HG23	1:A:1753:LEU:HD12	1.99	0.44
1:A:1931:ASP:O	1:A:3614:ARG:NH1	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3729:GLN:O	1:A:3733:HIS:ND1	2.48	0.44
1:A:3998:LYS:HG2	1:A:4110:MET:HE1	1.98	0.44
1:B:305:TYR:HE1	1:B:319:LYS:HG2	1.83	0.44
1:B:590:LYS:HB2	1:B:593:HIS:HD2	1.82	0.44
1:B:1089:ARG:HH21	1:B:1600:PRO:HG3	1.83	0.44
1:B:4130:PHE:O	1:B:4134:LEU:N	2.50	0.44
1:B:4153:ILE:HD13	1:B:4158:ARG:HH11	1.82	0.44
1:C:262:TYR:N	1:C:389:ARG:O	2.49	0.44
1:C:591:GLU:HA	1:C:631:LEU:HD21	1.99	0.44
1:C:3797:LEU:O	1:C:3800:SER:OG	2.32	0.44
1:D:555:LEU:HD13	1:D:585:ALA:HB1	1.99	0.44
1:D:3904:GLN:NE2	1:D:3965:GLN:OE1	2.48	0.44
1:D:4130:PHE:O	1:D:4134:LEU:N	2.50	0.44
1:A:695:VAL:HG21	1:A:755:ILE:HD13	1.99	0.44
1:A:1469:LEU:HG	1:A:1480:ILE:HD11	1.98	0.44
1:A:3893:TYR:CE2	1:A:3899:ILE:HG23	2.53	0.44
1:A:4130:PHE:O	1:A:4134:LEU:N	2.50	0.44
1:A:4817:HIS:O	1:A:4822:VAL:N	2.45	0.44
1:B:150:GLN:NE2	1:B:158:CYS:SG	2.72	0.44
1:B:314:LEU:HB2	1:B:393:MET:HG2	1.98	0.44
1:B:510:SER:O	1:B:520:ARG:NH2	2.50	0.44
1:D:217:ILE:HG23	1:D:285:SER:HB3	1.99	0.44
1:A:510:SER:O	1:A:520:ARG:NH2	2.51	0.44
1:A:1219:LYS:N	1:A:1240:ALA:HB3	2.33	0.44
1:A:3642:ILE:HD12	1:A:3642:ILE:HG23	1.79	0.44
1:B:433:LEU:HD21	1:B:505:LEU:HG	1.98	0.44
1:B:565:LEU:HG	1:B:604:HIS:CE1	2.53	0.44
1:B:3696:MET:O	1:B:3699:SER:OG	2.32	0.44
1:B:3936:LEU:HD21	1:B:3941:LEU:HD13	1.99	0.44
1:B:4752:LYS:HG2	1:B:4755:ARG:HH21	1.83	0.44
1:C:1174:MET:SD	1:C:1236:TYR:OH	2.74	0.44
1:D:30:LYS:HB2	1:D:30:LYS:HE3	1.82	0.44
1:A:16:THR:HB	1:A:110:HIS:HA	1.99	0.44
1:A:565:LEU:HD23	1:A:1588:VAL:HG23	1.99	0.44
1:A:1272:ARG:HH12	1:A:1588:VAL:HA	1.83	0.44
1:A:3921:LEU:HD23	1:A:3921:LEU:HA	1.78	0.44
1:B:236:LEU:HD23	1:B:245:LEU:HD22	2.00	0.44
1:B:238:HIS:HB3	1:B:243:GLU:HB3	1.99	0.44
1:B:695:VAL:HG21	1:B:755:ILE:HD13	1.99	0.44
1:B:1753:LEU:HD23	1:B:1753:LEU:HA	1.84	0.44
1:B:3737:ALA:O	1:B:3740:MET:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:TYR:HE1	1:C:319:LYS:HG2	1.83	0.44
1:D:433:LEU:HD21	1:D:505:LEU:HG	1.99	0.44
1:A:4804:ASP:N	1:A:4804:ASP:OD1	2.50	0.44
1:B:1219:LYS:N	1:B:1240:ALA:HB3	2.33	0.44
1:B:4862:ILE:O	1:B:4866:LEU:N	2.50	0.44
1:C:1899:LEU:HD23	1:C:1903:VAL:HG12	2.00	0.44
1:C:4052:ALA:O	1:C:4056:HIS:ND1	2.48	0.44
1:C:4851:PHE:O	1:C:4855:VAL:HB	2.18	0.44
1:D:180:ASP:HB3	1:D:211:LEU:HD22	1.98	0.44
1:D:510:SER:O	1:D:520:ARG:NH2	2.51	0.44
1:D:1219:LYS:N	1:D:1240:ALA:HB3	2.33	0.44
1:D:3893:TYR:CE2	1:D:3899:ILE:HG23	2.53	0.44
1:A:1926:ILE:HD11	1:A:3625:TYR:CE2	2.52	0.44
1:B:464:HIS:HA	1:B:465:PRO:HD3	1.86	0.44
1:B:591:GLU:HA	1:B:631:LEU:HD21	1.99	0.44
1:B:655:MET:HE3	1:B:1610:ARG:HD2	1.99	0.44
1:B:709:GLY:O	1:B:1253:LYS:NZ	2.51	0.44
1:B:1613:GLU:HB2	1:B:1618:LEU:H	1.82	0.44
1:B:2301:ASP:OD1	1:B:2304:ARG:NH2	2.51	0.44
1:B:3642:ILE:HD12	1:B:3642:ILE:HG23	1.78	0.44
1:C:709:GLY:O	1:C:1253:LYS:NZ	2.50	0.44
1:C:1087:ILE:HG23	1:C:1128:LEU:HD12	1.98	0.44
1:C:2770:GLU:HA	1:C:2773:ARG:HB2	2.00	0.44
1:C:4153:ILE:HD13	1:C:4158:ARG:HH11	1.82	0.44
1:C:4862:ILE:O	1:C:4866:LEU:N	2.50	0.44
1:D:314:LEU:HB2	1:D:393:MET:HG2	1.99	0.44
1:D:1087:ILE:HG23	1:D:1128:LEU:HD12	1.99	0.44
1:D:2071:ALA:HB2	1:D:2085:MET:HE1	2.00	0.44
1:A:1089:ARG:HH21	1:A:1600:PRO:HG3	1.83	0.43
1:A:1613:GLU:HB2	1:A:1618:LEU:H	1.82	0.43
1:B:649:VAL:HG21	1:B:713:TRP:HB3	1.98	0.43
1:B:1736:ILE:HG23	1:B:1753:LEU:HD12	1.99	0.43
1:C:565:LEU:HG	1:C:604:HIS:CE1	2.53	0.43
1:C:565:LEU:HD23	1:C:1588:VAL:HG23	2.00	0.43
1:D:1611:ILE:HB	1:D:1620:GLN:HB3	1.99	0.43
1:D:2738:LEU:HD22	1:D:2819:ALA:HB3	2.00	0.43
1:A:305:TYR:HE1	1:A:319:LYS:HG2	1.83	0.43
1:A:2770:GLU:HA	1:A:2773:ARG:HB2	2.00	0.43
1:B:565:LEU:HD23	1:B:1588:VAL:HG23	1.99	0.43
1:B:1170:GLU:O	1:B:1172:THR:N	2.51	0.43
1:B:1699:ARG:HH22	1:B:1821:LEU:HD11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4187:MET:SD	1:B:4187:MET:N	2.91	0.43
1:C:1219:LYS:N	1:C:1240:ALA:HB3	2.33	0.43
1:C:2738:LEU:HD22	1:C:2819:ALA:HB3	2.00	0.43
1:C:2887:ARG:O	1:C:2891:GLN:N	2.49	0.43
1:D:305:TYR:HE1	1:D:319:LYS:HG2	1.83	0.43
1:D:1089:ARG:HH21	1:D:1600:PRO:HG3	1.82	0.43
1:D:1736:ILE:HG23	1:D:1753:LEU:HD12	1.99	0.43
1:A:234:LEU:HD13	1:A:405:LEU:HD22	1.99	0.43
1:A:3936:LEU:HD21	1:A:3941:LEU:HD13	1.99	0.43
1:B:1899:LEU:HD23	1:B:1903:VAL:HG12	2.00	0.43
1:B:2071:ALA:HB2	1:B:2085:MET:HE1	2.00	0.43
1:C:1469:LEU:HG	1:C:1480:ILE:HD11	1.99	0.43
1:D:1613:GLU:HB2	1:D:1618:LEU:H	1.83	0.43
1:A:532:SER:HA	1:A:535:GLU:HB2	1.99	0.43
1:A:565:LEU:HG	1:A:604:HIS:CE1	2.53	0.43
1:B:4925:TYR:CZ	1:B:4929:LYS:HD2	2.54	0.43
1:C:674:TYR:OH	1:C:676:GLU:OE2	2.31	0.43
1:C:4187:MET:SD	1:C:4187:MET:N	2.91	0.43
1:D:559:ILE:HA	1:D:562:LEU:HB2	2.00	0.43
1:D:1445:TRP:H	1:D:1487:MET:HB2	1.83	0.43
1:D:2435:GLY:O	1:D:2438:SER:OG	2.29	0.43
1:D:4804:ASP:OD1	1:D:4804:ASP:N	2.50	0.43
1:A:122:ARG:HE	1:A:127:GLY:HA2	1.83	0.43
1:A:180:ASP:HB3	1:A:211:LEU:HD22	2.00	0.43
1:A:1647:GLN:O	1:A:1651:LEU:N	2.52	0.43
1:A:2071:ALA:HB2	1:A:2085:MET:HE1	2.01	0.43
1:A:2301:ASP:OD1	1:A:2304:ARG:NH2	2.51	0.43
1:A:4851:PHE:O	1:A:4855:VAL:HB	2.18	0.43
1:B:572:LEU:O	1:B:576:HIS:N	2.51	0.43
1:C:532:SER:HA	1:C:535:GLU:HB2	1.99	0.43
1:C:2436:VAL:HG21	1:C:2469:MET:HE3	2.00	0.43
1:C:4892:CYS:SG	1:C:4909:HIS:NE2	2.79	0.43
1:D:16:THR:HB	1:D:110:HIS:HA	2.00	0.43
1:D:4665:ASP:HA	1:D:4668:SER:HB2	2.00	0.43
1:A:464:HIS:HA	1:A:465:PRO:HD3	1.87	0.43
1:A:4862:ILE:O	1:A:4866:LEU:N	2.50	0.43
1:A:4925:TYR:CZ	1:A:4929:LYS:HD2	2.53	0.43
1:B:1104:GLU:HA	1:B:1163:GLY:HA2	2.00	0.43
1:B:1136:ALA:HB3	1:B:1145:TRP:HB2	2.01	0.43
1:B:1272:ARG:HH12	1:B:1588:VAL:HA	1.83	0.43
1:C:217:ILE:HG23	1:C:285:SER:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:679:VAL:HA	1:C:800:VAL:HG12	2.00	0.43
1:C:920:GLU:HG2	1:C:976:TYR:CE1	2.54	0.43
1:C:2301:ASP:OD1	1:C:2304:ARG:NH2	2.51	0.43
1:D:565:LEU:HD23	1:D:1588:VAL:HG23	2.00	0.43
1:D:679:VAL:HA	1:D:800:VAL:HG12	2.00	0.43
1:D:1899:LEU:HD23	1:D:1903:VAL:HG12	2.00	0.43
1:D:4862:ILE:O	1:D:4866:LEU:N	2.50	0.43
1:A:170:SER:OG	1:A:171:GLU:N	2.49	0.43
1:A:1699:ARG:HH22	1:A:1821:LEU:HD11	1.82	0.43
1:A:3891:TRP:CB	1:D:76:ARG:HD2	2.37	0.43
1:A:4892:CYS:SG	1:A:4909:HIS:NE2	2.80	0.43
1:B:119:ILE:HD13	1:B:162:ILE:HD11	2.01	0.43
1:C:590:LYS:HB2	1:C:593:HIS:HD2	1.83	0.43
1:C:1640:ASP:OD1	1:C:1640:ASP:N	2.49	0.43
1:C:1764:SER:N	1:C:1779:SER:O	2.51	0.43
1:C:1926:ILE:HD11	1:C:3625:TYR:CE2	2.54	0.43
1:C:4655:MET:HE2	1:C:4668:SER:HA	2.01	0.43
1:D:1699:ARG:HH22	1:D:1821:LEU:HD11	1.83	0.43
1:A:590:LYS:HB2	1:A:593:HIS:HD2	1.83	0.43
1:A:717:GLY:O	1:A:736:CYS:N	2.45	0.43
1:A:1104:GLU:HA	1:A:1163:GLY:HA2	1.99	0.43
1:A:1753:LEU:HD23	1:A:1753:LEU:HA	1.85	0.43
1:A:4508:LEU:HD11	1:A:4747:ILE:HD12	2.00	0.43
1:B:217:ILE:HG23	1:B:285:SER:HB3	2.00	0.43
1:B:737:ILE:HG22	1:B:739:ARG:HG3	2.00	0.43
1:B:2770:GLU:HA	1:B:2773:ARG:HB2	2.00	0.43
1:B:3729:GLN:O	1:B:3733:HIS:ND1	2.48	0.43
1:B:4851:PHE:O	1:B:4855:VAL:HB	2.18	0.43
1:C:449:ILE:HG13	1:C:522:ALA:HB1	1.99	0.43
1:C:473:GLU:OE2	1:C:477:ASN:ND2	2.50	0.43
1:C:1104:GLU:HA	1:C:1163:GLY:HA2	2.00	0.43
1:C:4072:GLU:HB3	1:C:4074:ASP:HB2	2.01	0.43
1:C:4591:TYR:HE1	1:C:4595:LYS:HD2	1.84	0.43
1:C:4804:ASP:OD1	1:C:4804:ASP:N	2.51	0.43
1:D:565:LEU:HG	1:D:604:HIS:CE1	2.53	0.43
1:D:4187:MET:SD	1:D:4187:MET:N	2.91	0.43
1:A:1121:GLY:O	1:A:1133:ARG:NH1	2.43	0.43
1:B:1172:THR:HG22	1:B:1193:LYS:HG3	2.01	0.43
1:B:4804:ASP:OD1	1:B:4804:ASP:N	2.51	0.43
1:C:119:ILE:HD13	1:C:162:ILE:HD11	2.01	0.43
1:C:1647:GLN:O	1:C:1651:LEU:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:920:GLU:HG2	1:D:976:TYR:CE1	2.54	0.43
1:D:2301:ASP:OD1	1:D:2304:ARG:NH2	2.51	0.43
1:A:591:GLU:HA	1:A:631:LEU:HD21	2.00	0.43
1:B:1087:ILE:HG23	1:B:1128:LEU:HD12	1.99	0.43
1:B:1174:MET:SD	1:B:1236:TYR:OH	2.74	0.43
1:B:1727:VAL:HG11	1:B:1927:VAL:HG21	2.00	0.43
1:C:719:GLY:H	1:C:722:LEU:HD12	1.84	0.43
1:C:1170:GLU:O	1:C:1172:THR:N	2.52	0.43
1:C:1172:THR:HG22	1:C:1193:LYS:HG3	2.01	0.43
1:C:3893:TYR:CE2	1:C:3899:ILE:HG23	2.54	0.43
1:D:1272:ARG:HH12	1:D:1588:VAL:HA	1.83	0.43
1:D:3936:LEU:HD21	1:D:3941:LEU:HD13	2.00	0.43
1:D:4508:LEU:HD11	1:D:4747:ILE:HD12	2.01	0.43
1:A:832:LEU:HG	1:A:1617:TRP:HE1	1.83	0.42
1:A:1449:ASP:OD1	1:A:1449:ASP:N	2.49	0.42
1:A:4011:VAL:HG12	1:A:4015:LEU:HG	2.01	0.42
1:B:3893:TYR:CE2	1:B:3899:ILE:HG23	2.54	0.42
1:C:3988:GLU:HB2	1:C:4937:GLN:NE2	2.34	0.42
1:A:2738:LEU:HD22	1:A:2819:ALA:HB3	2.00	0.42
1:A:4187:MET:SD	1:A:4187:MET:N	2.92	0.42
1:B:247:VAL:O	1:B:272:ARG:NH1	2.46	0.42
1:B:717:GLY:O	1:B:736:CYS:N	2.45	0.42
1:B:1469:LEU:HG	1:B:1480:ILE:HD11	2.01	0.42
1:C:1272:ARG:HH12	1:C:1588:VAL:HA	1.83	0.42
1:C:1445:TRP:H	1:C:1487:MET:HB2	1.83	0.42
1:C:4665:ASP:HA	1:C:4668:SER:HB2	2.00	0.42
1:D:676:GLU:HB2	1:D:803:LEU:HB2	2.01	0.42
1:A:119:ILE:HD13	1:A:162:ILE:HD11	2.02	0.42
1:A:1136:ALA:HB3	1:A:1145:TRP:HB2	2.01	0.42
1:A:1300:MET:O	1:A:1545:ALA:N	2.44	0.42
1:A:2436:VAL:HG21	1:A:2469:MET:HE3	2.01	0.42
1:B:122:ARG:HE	1:B:127:GLY:HA2	1.84	0.42
1:B:555:LEU:HD13	1:B:585:ALA:HB1	2.02	0.42
1:B:719:GLY:H	1:B:722:LEU:HD12	1.84	0.42
1:B:920:GLU:HG2	1:B:976:TYR:CE1	2.54	0.42
1:B:1094:TYR:OH	1:B:1808:ASP:OD1	2.37	0.42
1:B:2738:LEU:HD22	1:B:2819:ALA:HB3	2.01	0.42
1:B:3642:ILE:HG22	1:B:3731:ARG:HD3	2.01	0.42
1:B:4508:LEU:HD11	1:B:4747:ILE:HD12	2.01	0.42
1:C:1457:PHE:HD1	1:C:1488:VAL:HG21	1.84	0.42
1:C:1699:ARG:HH22	1:C:1821:LEU:HD11	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:832:LEU:HG	1:D:1617:TRP:HE1	1.84	0.42
1:D:2035:GLU:O	1:D:2038:THR:OG1	2.32	0.42
1:D:3907:PHE:HD2	1:D:3968:LEU:HD11	1.85	0.42
1:A:150:GLN:NE2	1:A:158:CYS:SG	2.73	0.42
1:A:1727:VAL:HG11	1:A:1927:VAL:HG21	2.01	0.42
1:A:3955:MET:O	1:A:3959:LEU:N	2.48	0.42
1:A:4655:MET:HE2	1:A:4668:SER:HA	2.02	0.42
1:B:308:LEU:N	1:B:326:SER:O	2.49	0.42
1:B:1926:ILE:HD11	1:B:3625:TYR:CE2	2.54	0.42
1:C:3642:ILE:HG22	1:C:3731:ARG:HD3	2.02	0.42
1:D:119:ILE:HD13	1:D:162:ILE:HD11	2.01	0.42
1:D:1647:GLN:O	1:D:1651:LEU:N	2.52	0.42
1:D:4655:MET:HE2	1:D:4668:SER:HA	2.02	0.42
1:A:709:GLY:O	1:A:1253:LYS:NZ	2.51	0.42
1:A:1094:TYR:OH	1:A:1808:ASP:OD1	2.38	0.42
1:B:679:VAL:HA	1:B:800:VAL:HG12	2.01	0.42
1:B:3718:LYS:O	1:B:3722:LYS:N	2.50	0.42
1:C:1136:ALA:HB3	1:C:1145:TRP:HB2	2.01	0.42
1:D:122:ARG:HE	1:D:127:GLY:HA2	1.84	0.42
1:D:4580:HIS:HB3	1:D:4740:PHE:HZ	1.84	0.42
1:D:4861:ALA:HA	1:D:4864:GLN:HB3	2.02	0.42
1:D:4925:TYR:CZ	1:D:4929:LYS:HD2	2.54	0.42
1:A:236:LEU:HD23	1:A:245:LEU:HD22	2.01	0.42
1:A:530:LEU:HD23	1:A:533:LEU:HD12	2.02	0.42
1:A:679:VAL:HA	1:A:800:VAL:HG12	2.01	0.42
1:A:1445:TRP:H	1:A:1487:MET:HB2	1.84	0.42
1:A:1899:LEU:HD23	1:A:1903:VAL:HG12	2.01	0.42
1:A:4864:GLN:HG3	1:D:4857:VAL:HG13	2.01	0.42
1:B:196:TYR:O	1:B:201:LEU:N	2.52	0.42
1:B:2884:ALA:HA	1:B:2887:ARG:HB3	2.02	0.42
1:B:4665:ASP:HA	1:B:4668:SER:HB2	2.00	0.42
1:C:555:LEU:HD13	1:C:585:ALA:HB1	2.00	0.42
1:C:1753:LEU:HD23	1:C:1753:LEU:HA	1.84	0.42
1:D:262:TYR:N	1:D:389:ARG:O	2.49	0.42
1:D:1104:GLU:HA	1:D:1163:GLY:HA2	1.99	0.42
1:D:1764:SER:N	1:D:1779:SER:O	2.52	0.42
1:D:4000:MET:HE3	1:D:4000:MET:HB2	1.87	0.42
1:A:30:LYS:HB2	1:A:30:LYS:HE3	1.83	0.42
1:A:737:ILE:HG22	1:A:739:ARG:HG3	2.01	0.42
1:B:1699:ARG:NH1	1:B:1816:PHE:O	2.48	0.42
1:B:2587:GLN:O	1:B:2591:ARG:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4146:ILE:HD12	1:B:4957:ASP:C	2.45	0.42
1:B:4207:ILE:O	1:B:4498:ARG:NH1	2.53	0.42
1:B:4580:HIS:HB3	1:B:4740:PHE:HZ	1.85	0.42
1:C:143:LEU:CD2	1:D:2426:SER:HB3	2.48	0.42
1:C:236:LEU:HD23	1:C:245:LEU:HD22	2.01	0.42
1:C:335:LYS:NZ	1:C:398:HIS:O	2.38	0.42
1:C:3921:LEU:HD23	1:C:3921:LEU:HA	1.79	0.42
1:C:4580:HIS:HB3	1:C:4740:PHE:HZ	1.85	0.42
1:D:196:TYR:O	1:D:201:LEU:N	2.53	0.42
1:D:238:HIS:N	1:D:243:GLU:O	2.53	0.42
1:D:591:GLU:HA	1:D:631:LEU:HD21	2.00	0.42
1:D:1505:LEU:HB2	1:D:1523:ASN:HA	2.02	0.42
1:D:4591:TYR:HE1	1:D:4595:LYS:HD2	1.85	0.42
1:A:4580:HIS:HB3	1:A:4740:PHE:HZ	1.84	0.42
1:A:4665:ASP:HA	1:A:4668:SER:HB2	2.01	0.42
1:B:674:TYR:OH	1:B:676:GLU:OE2	2.32	0.42
1:B:4591:TYR:HE1	1:B:4595:LYS:HD2	1.84	0.42
1:B:4655:MET:HE2	1:B:4668:SER:HA	2.02	0.42
1:C:4207:ILE:O	1:C:4498:ARG:NH1	2.53	0.42
1:D:1137:PHE:HD1	1:D:1144:ARG:HB3	1.85	0.42
1:A:191:TYR:N	1:A:206:ALA:O	2.48	0.42
1:A:1172:THR:HG22	1:A:1193:LYS:HG3	2.01	0.42
1:A:2587:GLN:O	1:A:2591:ARG:N	2.53	0.42
1:A:4161:TRP:CZ2	1:A:4917:ALA:HB2	2.55	0.42
1:A:4591:TYR:CE1	1:A:4595:LYS:HB2	2.55	0.42
1:B:76:ARG:HD2	1:C:3891:TRP:CB	2.38	0.42
1:B:832:LEU:HG	1:B:1617:TRP:HE1	1.84	0.42
1:B:2143:MET:SD	1:B:2175:VAL:HG11	2.60	0.42
1:B:2796:GLY:HA2	1:B:2900:ASN:HA	2.02	0.42
1:B:4072:GLU:HB3	1:B:4074:ASP:HB2	2.02	0.42
1:C:717:GLY:O	1:C:736:CYS:N	2.45	0.42
1:C:2143:MET:SD	1:C:2175:VAL:HG11	2.60	0.42
1:D:727:PHE:N	1:D:749:LEU:HD13	2.35	0.42
1:D:2770:GLU:HA	1:D:2773:ARG:HB2	2.00	0.42
1:D:4052:ALA:O	1:D:4056:HIS:ND1	2.48	0.42
1:D:4072:GLU:HB3	1:D:4074:ASP:HB2	2.02	0.42
1:D:4640:SER:HB3	1:D:4643:ASN:HD21	1.85	0.42
1:A:626:ARG:HG2	1:A:1669:ASN:HD21	1.84	0.42
1:A:920:GLU:HG2	1:A:976:TYR:CE1	2.54	0.42
1:A:1799:VAL:HG22	1:A:1894:LEU:HD13	2.02	0.42
1:B:238:HIS:CE1	1:B:400:ASP:HB3	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1799:VAL:HG22	1:B:1894:LEU:HD13	2.02	0.42
1:B:4196:ASP:O	1:B:4200:GLU:N	2.49	0.42
1:B:4591:TYR:CE1	1:B:4595:LYS:HB2	2.55	0.42
1:C:196:TYR:O	1:C:201:LEU:N	2.52	0.42
1:C:299:HIS:NE2	1:C:301:THR:OG1	2.47	0.42
1:C:3936:LEU:HD21	1:C:3941:LEU:HD13	2.00	0.42
1:C:4146:ILE:HD12	1:C:4957:ASP:C	2.45	0.42
1:D:465:PRO:HA	1:D:466:PRO:HD3	1.87	0.42
1:D:590:LYS:HB2	1:D:593:HIS:HD2	1.83	0.42
1:D:4146:ILE:HD12	1:D:4957:ASP:C	2.45	0.42
1:A:1090:ALA:HA	1:A:1249:MET:HG2	2.01	0.41
1:A:2162:LEU:HB3	1:A:2163:MET:HE2	2.02	0.41
1:B:30:LYS:HE3	1:B:30:LYS:HB2	1.82	0.41
1:B:1764:SER:N	1:B:1779:SER:O	2.52	0.41
1:B:2162:LEU:HB3	1:B:2163:MET:HE2	2.01	0.41
1:C:150:GLN:NE2	1:C:158:CYS:SG	2.72	0.41
1:C:644:LEU:HB2	1:C:1654:HIS:CD2	2.48	0.41
1:C:852:GLY:HA2	1:C:853:PRO:HA	1.82	0.41
1:C:3955:MET:O	1:C:3959:LEU:N	2.48	0.41
1:D:2162:LEU:HB3	1:D:2163:MET:HE2	2.02	0.41
1:D:3718:LYS:O	1:D:3722:LYS:N	2.50	0.41
1:D:3988:GLU:HB2	1:D:4937:GLN:NE2	2.35	0.41
1:A:238:HIS:CE1	1:A:400:ASP:HB3	2.51	0.41
1:A:1137:PHE:HD1	1:A:1144:ARG:HB3	1.85	0.41
1:A:1752:GLY:HA3	1:A:1836:ASN:ND2	2.35	0.41
1:A:1764:SER:N	1:A:1779:SER:O	2.52	0.41
1:A:3988:GLU:HB2	1:A:4937:GLN:NE2	2.35	0.41
1:A:4640:SER:HB3	1:A:4643:ASN:HD21	1.85	0.41
1:B:2436:VAL:HG21	1:B:2469:MET:HE3	2.01	0.41
1:C:191:TYR:N	1:C:206:ALA:O	2.48	0.41
1:C:1090:ALA:HB3	1:C:1203:PRO:HD2	2.03	0.41
1:C:3907:PHE:HD2	1:C:3968:LEU:HD11	1.84	0.41
1:D:488:LEU:HD23	1:D:488:LEU:HA	1.93	0.41
1:D:4161:TRP:CZ2	1:D:4917:ALA:HB2	2.55	0.41
1:A:238:HIS:N	1:A:243:GLU:O	2.53	0.41
1:A:719:GLY:H	1:A:722:LEU:HD12	1.84	0.41
1:A:727:PHE:N	1:A:749:LEU:HD13	2.36	0.41
1:A:1505:LEU:HB2	1:A:1523:ASN:HA	2.03	0.41
1:A:4146:ILE:HD12	1:A:4957:ASP:C	2.44	0.41
1:A:4591:TYR:HE1	1:A:4595:LYS:HD2	1.85	0.41
1:B:1445:TRP:H	1:B:1487:MET:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2435:GLY:O	1:B:2438:SER:OG	2.29	0.41
1:B:2436:VAL:HG11	1:B:2469:MET:HE3	2.02	0.41
1:C:572:LEU:O	1:C:576:HIS:N	2.52	0.41
1:C:4861:ALA:HA	1:C:4864:GLN:HB3	2.02	0.41
1:D:191:TYR:N	1:D:206:ALA:O	2.48	0.41
1:D:1136:ALA:HB3	1:D:1145:TRP:HB2	2.01	0.41
1:A:773:GLN:HA	1:A:774:PRO:HD3	1.93	0.41
1:A:2123:SER:OG	1:A:2149:ASP:OD2	2.39	0.41
1:A:3907:PHE:HD2	1:A:3968:LEU:HD11	1.86	0.41
1:A:4011:VAL:HA	1:A:4014:ILE:HG12	2.03	0.41
1:A:4207:ILE:O	1:A:4498:ARG:NH1	2.53	0.41
1:B:855:VAL:HG22	1:B:1209:VAL:HG12	2.02	0.41
1:B:4011:VAL:HG12	1:B:4015:LEU:HG	2.02	0.41
1:C:122:ARG:HE	1:C:127:GLY:HA2	1.84	0.41
1:C:1752:GLY:HA3	1:C:1836:ASN:ND2	2.36	0.41
1:C:4170:LYS:HE3	1:C:4916:LEU:CD2	2.49	0.41
1:C:4757:ILE:HD13	1:C:4757:ILE:HG21	1.69	0.41
1:D:236:LEU:HD23	1:D:245:LEU:HD22	2.01	0.41
1:D:719:GLY:H	1:D:722:LEU:HD12	1.84	0.41
1:D:1727:VAL:HG11	1:D:1927:VAL:HG21	2.01	0.41
1:D:4583:ILE:HD13	1:D:4583:ILE:HG21	1.81	0.41
1:A:196:TYR:O	1:A:201:LEU:N	2.53	0.41
1:A:3919:ASN:C	1:A:3922:THR:HG1	2.28	0.41
1:A:4500:PHE:O	1:A:4504:ARG:N	2.52	0.41
1:B:717:GLY:H	1:B:722:LEU:HD13	1.85	0.41
1:B:727:PHE:N	1:B:749:LEU:HD13	2.36	0.41
1:B:1647:GLN:O	1:B:1651:LEU:N	2.52	0.41
1:B:1752:GLY:HA3	1:B:1836:ASN:ND2	2.35	0.41
1:C:727:PHE:N	1:C:749:LEU:HD13	2.36	0.41
1:D:473:GLU:OE2	1:D:477:ASN:ND2	2.50	0.41
1:D:626:ARG:HG2	1:D:1669:ASN:HD21	1.85	0.41
1:D:847:THR:HG22	1:D:848:ARG:H	1.86	0.41
1:D:4011:VAL:HG12	1:D:4015:LEU:HG	2.01	0.41
1:A:247:VAL:O	1:A:272:ARG:NH1	2.46	0.41
1:A:2436:VAL:HG11	1:A:2469:MET:HE3	2.03	0.41
1:A:4609:ARG:HH11	1:A:4609:ARG:HD3	1.71	0.41
1:B:3907:PHE:HD2	1:B:3968:LEU:HD11	1.86	0.41
1:B:4499:ASN:ND2	1:B:4502:ASN:HB3	2.36	0.41
1:C:832:LEU:HG	1:C:1617:TRP:HE1	1.85	0.41
1:C:1137:PHE:HD1	1:C:1144:ARG:HB3	1.85	0.41
1:C:2436:VAL:HG11	1:C:2469:MET:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2587:GLN:O	1:C:2591:ARG:N	2.53	0.41
1:C:4020:MET:HB3	1:C:4067:LEU:HD11	2.02	0.41
1:D:1094:TYR:OH	1:D:1808:ASP:OD1	2.38	0.41
1:D:4193:PHE:O	1:D:4197:THR:OG1	2.34	0.41
1:A:74:SER:HA	1:A:117:HIS:HA	2.03	0.41
1:A:2426:SER:HB3	1:D:143:LEU:CD2	2.47	0.41
1:A:3891:TRP:CG	1:D:76:ARG:CG	3.03	0.41
1:B:626:ARG:HG2	1:B:1669:ASN:HD21	1.85	0.41
1:B:852:GLY:HA2	1:B:853:PRO:HA	1.82	0.41
1:B:4020:MET:HB3	1:B:4067:LEU:HD11	2.01	0.41
1:C:676:GLU:HB2	1:C:803:LEU:HB2	2.01	0.41
1:C:745:ASN:ND2	1:C:773:GLN:OE1	2.54	0.41
1:C:847:THR:HG22	1:C:848:ARG:H	1.86	0.41
1:C:1090:ALA:HA	1:C:1249:MET:HG2	2.02	0.41
1:C:1094:TYR:OH	1:C:1808:ASP:OD1	2.38	0.41
1:C:1228:THR:HA	1:C:1232:LEU:HD12	2.03	0.41
1:D:589:ILE:HG21	1:D:617:LEU:HD22	2.02	0.41
1:D:3642:ILE:HG22	1:D:3731:ARG:HD3	2.03	0.41
1:A:308:LEU:N	1:A:326:SER:O	2.50	0.41
1:A:465:PRO:HA	1:A:466:PRO:HD3	1.89	0.41
1:B:312:LYS:HD2	1:B:315:LEU:HD11	2.02	0.41
1:B:706:TYR:HA	1:B:707:PRO:HD3	1.91	0.41
1:B:1090:ALA:HA	1:B:1249:MET:HG2	2.02	0.41
1:B:1137:PHE:HD1	1:B:1144:ARG:HB3	1.85	0.41
1:B:4161:TRP:CZ2	1:B:4917:ALA:HB2	2.56	0.41
1:C:589:ILE:HG21	1:C:617:LEU:HD22	2.02	0.41
1:C:1727:VAL:HG11	1:C:1927:VAL:HG21	2.02	0.41
1:C:2273:CYS:HB3	1:C:2293:PRO:HD2	2.02	0.41
1:C:2884:ALA:HA	1:C:2887:ARG:HB3	2.02	0.41
1:C:4925:TYR:CZ	1:C:4929:LYS:HD2	2.55	0.41
1:D:530:LEU:HD23	1:D:533:LEU:HD12	2.02	0.41
1:D:1090:ALA:HB3	1:D:1203:PRO:HD2	2.03	0.41
1:D:1090:ALA:HA	1:D:1249:MET:HG2	2.02	0.41
1:D:2587:GLN:O	1:D:2591:ARG:N	2.53	0.41
1:D:4500:PHE:O	1:D:4504:ARG:N	2.52	0.41
1:D:4892:CYS:SG	1:D:4909:HIS:NE2	2.79	0.41
1:A:76:ARG:CG	1:B:3891:TRP:CG	3.04	0.41
1:A:363:ILE:HD12	1:A:403:LEU:HD12	2.03	0.41
1:A:745:ASN:ND2	1:A:773:GLN:OE1	2.54	0.41
1:A:1137:PHE:CE2	1:A:1139:GLY:HA2	2.56	0.41
1:A:1170:GLU:O	1:A:1172:THR:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1184:ASP:HB2	1:A:1188:SER:H	1.86	0.41
1:A:3642:ILE:HG22	1:A:3731:ARG:HD3	2.03	0.41
1:A:4072:GLU:HB3	1:A:4074:ASP:HB2	2.03	0.41
1:B:76:ARG:CG	1:C:3891:TRP:CG	3.04	0.41
1:B:137:ARG:HE	1:B:202:HIS:HB3	1.86	0.41
1:B:238:HIS:N	1:B:243:GLU:O	2.53	0.41
1:B:363:ILE:HD12	1:B:403:LEU:HD12	2.03	0.41
1:B:530:LEU:HD23	1:B:533:LEU:HD12	2.02	0.41
1:B:676:GLU:HB2	1:B:803:LEU:HB2	2.02	0.41
1:B:1694:MET:HE3	1:B:1699:ARG:HA	2.02	0.41
1:B:2857:LYS:HE2	1:B:2869:HIS:CD2	2.56	0.41
1:C:363:ILE:HD12	1:C:403:LEU:HD12	2.03	0.41
1:C:1505:LEU:HB2	1:C:1523:ASN:HA	2.03	0.41
1:C:1799:VAL:HG22	1:C:1894:LEU:HD13	2.02	0.41
1:C:4011:VAL:HG12	1:C:4015:LEU:HG	2.02	0.41
1:C:4508:LEU:HD11	1:C:4747:ILE:HD12	2.03	0.41
1:C:4832:ILE:HG21	1:C:4844:ARG:NH2	2.30	0.41
1:D:150:GLN:NE2	1:D:158:CYS:SG	2.73	0.41
1:D:228:LEU:HD23	1:D:356:TYR:CE1	2.56	0.41
1:D:312:LYS:HD2	1:D:315:LEU:HD11	2.02	0.41
1:D:646:THR:OG1	1:D:1684:GLN:NE2	2.51	0.41
1:D:745:ASN:ND2	1:D:773:GLN:OE1	2.54	0.41
1:D:855:VAL:HG22	1:D:1209:VAL:HG12	2.03	0.41
1:D:1654:HIS:O	1:D:1657:THR:OG1	2.28	0.41
1:D:3841:PHE:HB3	1:D:3920:THR:HG21	2.02	0.41
1:D:4020:MET:HB3	1:D:4067:LEU:HD11	2.03	0.41
1:A:717:GLY:H	1:A:722:LEU:HD13	1.85	0.41
1:A:836:HIS:HB2	1:A:839:GLU:CD	2.46	0.41
1:A:1699:ARG:NH1	1:A:1816:PHE:O	2.48	0.41
1:A:4499:ASN:ND2	1:A:4502:ASN:HB3	2.36	0.41
1:B:745:ASN:ND2	1:B:773:GLN:OE1	2.54	0.41
1:B:1113:MET:HG3	1:B:1156:TRP:HZ2	1.86	0.41
1:B:1457:PHE:CD1	1:B:1488:VAL:HG21	2.56	0.41
1:B:3988:GLU:HB2	1:B:4937:GLN:NE2	2.35	0.41
1:B:4170:LYS:HE2	1:B:4916:LEU:CD2	2.51	0.41
1:B:4493:LEU:HA	1:B:4496:PHE:HD2	1.86	0.41
1:B:4861:ALA:HA	1:B:4864:GLN:HB3	2.03	0.41
1:C:76:ARG:CG	1:D:3891:TRP:CG	3.04	0.41
1:C:1457:PHE:CD1	1:C:1488:VAL:HG21	2.55	0.41
1:C:2796:GLY:HA2	1:C:2900:ASN:HA	2.03	0.41
1:D:23:GLN:HE21	1:D:34:LYS:HB3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1172:THR:HG22	1:D:1193:LYS:HG3	2.02	0.41
1:D:1457:PHE:CD1	1:D:1488:VAL:HG21	2.56	0.41
1:D:2143:MET:SD	1:D:2175:VAL:HG11	2.61	0.41
1:D:4011:VAL:HA	1:D:4014:ILE:HG12	2.03	0.41
1:D:4171:ARG:HH11	1:D:4752:LYS:CE	2.17	0.41
1:D:4591:TYR:CE1	1:D:4595:LYS:HB2	2.56	0.41
1:A:312:LYS:HD2	1:A:315:LEU:HD11	2.02	0.40
1:A:589:ILE:HG21	1:A:617:LEU:HD22	2.03	0.40
1:A:3760:LEU:HD13	1:A:3840:LEU:HA	2.02	0.40
1:A:4020:MET:HB3	1:A:4067:LEU:HD11	2.03	0.40
1:A:4036:TYR:HE2	1:A:4048:ASP:HB3	1.87	0.40
1:B:773:GLN:HA	1:B:774:PRO:HD3	1.94	0.40
1:B:2424:LEU:HD23	1:B:2476:VAL:HG22	2.02	0.40
1:B:3768:ASN:H	1:B:3846:LEU:HD23	1.86	0.40
1:B:4640:SER:HB3	1:B:4643:ASN:HD21	1.85	0.40
1:D:1170:GLU:O	1:D:1172:THR:N	2.52	0.40
1:D:1300:MET:O	1:D:1545:ALA:N	2.45	0.40
1:D:2520:TYR:HA	1:D:2523:THR:HB	2.03	0.40
1:A:228:LEU:HD23	1:A:356:TYR:CE1	2.56	0.40
1:A:426:PHE:O	1:A:430:ILE:N	2.54	0.40
1:A:847:THR:HG22	1:A:848:ARG:H	1.86	0.40
1:B:1505:LEU:HB2	1:B:1523:ASN:HA	2.03	0.40
1:B:4797:SER:HB3	1:B:4805:MET:H	1.85	0.40
1:C:1455:THR:HB	1:C:1546:GLN:NE2	2.36	0.40
1:C:2123:SER:OG	1:C:2149:ASP:OD2	2.39	0.40
1:C:3920:THR:O	1:C:3924:TYR:N	2.52	0.40
1:C:4640:SER:HB3	1:C:4643:ASN:HD21	1.85	0.40
1:C:4797:SER:HB3	1:C:4805:MET:H	1.86	0.40
1:D:836:HIS:HB2	1:D:839:GLU:CD	2.46	0.40
1:D:1752:GLY:HA3	1:D:1836:ASN:ND2	2.36	0.40
1:D:3983:LEU:HD23	1:D:3983:LEU:H	1.86	0.40
1:D:4207:ILE:O	1:D:4498:ARG:NH1	2.54	0.40
1:A:2884:ALA:HA	1:A:2887:ARG:HB3	2.03	0.40
1:B:1090:ALA:HB3	1:B:1203:PRO:HD2	2.03	0.40
1:B:1220:ASP:O	1:B:1223:THR:N	2.36	0.40
1:C:2520:TYR:HA	1:C:2523:THR:HB	2.03	0.40
1:C:2857:LYS:HE2	1:C:2869:HIS:CD2	2.57	0.40
1:C:3841:PHE:HB3	1:C:3920:THR:HG21	2.03	0.40
1:C:3983:LEU:HD23	1:C:3983:LEU:H	1.86	0.40
1:C:4499:ASN:ND2	1:C:4502:ASN:HB3	2.36	0.40
1:D:644:LEU:HD12	1:D:1654:HIS:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:832:LEU:HB3	1:D:1614:ARG:NH1	2.37	0.40
1:D:1799:VAL:HG22	1:D:1894:LEU:HD13	2.03	0.40
1:A:299:HIS:N	1:A:304:LYS:O	2.50	0.40
1:A:1228:THR:HA	1:A:1232:LEU:HD12	2.03	0.40
1:A:1761:MET:SD	1:A:1761:MET:N	2.92	0.40
1:A:4493:LEU:HA	1:A:4496:PHE:HD2	1.86	0.40
1:B:74:SER:HA	1:B:117:HIS:HA	2.03	0.40
1:B:228:LEU:HD23	1:B:356:TYR:CE1	2.57	0.40
1:B:836:HIS:HB2	1:B:839:GLU:CD	2.46	0.40
1:B:3797:LEU:O	1:B:3800:SER:OG	2.32	0.40
1:C:30:LYS:HB2	1:C:30:LYS:HE3	1.82	0.40
1:C:686:VAL:O	1:C:687:THR:OG1	2.34	0.40
1:D:572:LEU:O	1:D:576:HIS:N	2.51	0.40
1:D:844:ARG:HD2	1:D:849:ASP:OD2	2.22	0.40
1:D:1457:PHE:HD1	1:D:1488:VAL:HG21	1.86	0.40
1:D:1506:GLU:HA	1:D:1522:ALA:HA	2.03	0.40
1:D:2857:LYS:HE2	1:D:2869:HIS:CD2	2.57	0.40
1:D:3955:MET:O	1:D:3959:LEU:N	2.48	0.40
1:D:4182:GLY:O	1:D:4186:LYS:N	2.55	0.40
1:A:489:PHE:HD2	1:A:540:LEU:HD21	1.87	0.40
1:A:3980:VAL:HA	1:A:3983:LEU:HD23	2.04	0.40
1:B:589:ILE:HG21	1:B:617:LEU:HD22	2.03	0.40
1:B:1184:ASP:HB2	1:B:1188:SER:H	1.86	0.40
1:B:4054:GLU:HG3	1:B:4061:GLN:HG2	2.03	0.40
1:B:4182:GLY:O	1:B:4186:LYS:N	2.54	0.40
1:C:312:LYS:HD2	1:C:315:LEU:HD11	2.03	0.40
1:C:356:TYR:CE1	1:C:407:ARG:HB3	2.57	0.40
1:C:488:LEU:HD23	1:C:488:LEU:HA	1.94	0.40
1:C:1138:ASP:HB2	1:C:1145:TRP:HE1	1.87	0.40
1:C:4591:TYR:CE1	1:C:4595:LYS:HB2	2.56	0.40
1:D:299:HIS:NE2	1:D:301:THR:OG1	2.47	0.40
1:D:363:ILE:HD12	1:D:403:LEU:HD12	2.04	0.40
1:D:426:PHE:O	1:D:430:ILE:N	2.54	0.40
1:D:1113:MET:HG3	1:D:1156:TRP:HZ2	1.86	0.40
1:D:1306:MET:HB3	1:D:1575:HIS:CE1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3289/4968 (66%)	2988 (91%)	279 (8%)	22 (1%)	18	54
1	B	3289/4968 (66%)	2994 (91%)	273 (8%)	22 (1%)	18	54
1	C	3289/4968 (66%)	2988 (91%)	280 (8%)	21 (1%)	21	58
1	D	3289/4968 (66%)	2986 (91%)	282 (9%)	21 (1%)	21	58
All	All	13156/19872 (66%)	11956 (91%)	1114 (8%)	86 (1%)	20	54

All (86) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1737	THR
1	A	1756	SER
1	A	4071	ALA
1	B	1737	THR
1	B	1756	SER
1	B	4071	ALA
1	C	1737	THR
1	C	1756	SER
1	C	4071	ALA
1	D	1737	THR
1	D	1756	SER
1	D	4071	ALA
1	A	1580	PRO
1	A	3805	ASP
1	A	4916	LEU
1	B	1580	PRO
1	B	3805	ASP
1	B	4916	LEU
1	C	1580	PRO
1	C	3805	ASP
1	C	4916	LEU
1	D	1580	PRO

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Mol	Chain	Res	Type
1	D	3805	ASP
1	D	4916	LEU
1	A	819	TYR
1	A	4164	PRO
1	B	819	TYR
1	B	4164	PRO
1	C	819	TYR
1	C	4164	PRO
1	D	819	TYR
1	D	4164	PRO
1	A	1738	LEU
1	A	3804	LEU
1	A	4030	SER
1	B	1738	LEU
1	B	2075	VAL
1	B	3804	LEU
1	B	4030	SER
1	C	1738	LEU
1	C	2075	VAL
1	C	3804	LEU
1	C	4030	SER
1	D	1738	LEU
1	D	3804	LEU
1	D	4030	SER
1	A	792	VAL
1	A	839	GLU
1	A	1581	GLN
1	B	792	VAL
1	B	839	GLU
1	B	1581	GLN
1	C	792	VAL
1	C	839	GLU
1	D	792	VAL
1	D	839	GLU
1	D	2075	VAL
1	A	980	PRO
1	A	2075	VAL
1	A	4642	PRO
1	A	4958	CYS
1	B	980	PRO
1	B	4642	PRO
1	B	4958	CYS

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Mol	Chain	Res	Type
1	C	980	PRO
1	C	1581	GLN
1	C	3769	GLY
1	C	4642	PRO
1	D	980	PRO
1	D	1581	GLN
1	D	4642	PRO
1	A	729	GLY
1	A	3769	GLY
1	B	729	GLY
1	B	3769	GLY
1	C	729	GLY
1	D	729	GLY
1	D	3769	GLY
1	A	1476	VAL
1	B	828	PRO
1	B	1476	VAL
1	C	1476	VAL
1	D	1476	VAL
1	A	828	PRO
1	C	828	PRO
1	D	828	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2660/4355 (61%)	2629 (99%)	31 (1%)	63	73
1	B	2657/4355 (61%)	2631 (99%)	26 (1%)	68	75
1	C	2658/4355 (61%)	2629 (99%)	29 (1%)	65	73
1	D	2660/4355 (61%)	2629 (99%)	31 (1%)	63	73
All	All	10635/17420 (61%)	10518 (99%)	117 (1%)	63	73

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	192	LEU
1	A	344	LYS
1	A	439	LYS
1	A	678	MET
1	A	687	THR
1	A	854	THR
1	A	925	PRO
1	A	950	VAL
1	A	986	ILE
1	A	990	PRO
1	A	1054	VAL
1	A	1089	ARG
1	A	1619	VAL
1	A	1632	ILE
1	A	1748	LEU
1	A	2080	GLU
1	A	2211	ASN
1	A	2293	PRO
1	A	3670	LEU
1	A	3671	LEU
1	A	3813	ASN
1	A	3906	ASN
1	A	3975	LEU
1	A	4032	THR
1	A	4122	LEU
1	A	4139	ILE
1	A	4170	LYS
1	A	4727	MET
1	A	4796	LYS
1	A	4858	ILE
1	A	4910	THR
1	B	192	LEU
1	B	344	LYS
1	B	439	LYS
1	B	678	MET
1	B	687	THR
1	B	854	THR
1	B	925	PRO
1	B	990	PRO
1	B	1089	ARG
1	B	1619	VAL
1	B	1632	ILE
1	B	1748	LEU

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Mol	Chain	Res	Type
1	B	2211	ASN
1	B	2293	PRO
1	B	3670	LEU
1	B	3671	LEU
1	B	3813	ASN
1	B	3906	ASN
1	B	3975	LEU
1	B	4032	THR
1	B	4122	LEU
1	B	4139	ILE
1	B	4727	MET
1	B	4796	LYS
1	B	4858	ILE
1	B	4910	THR
1	C	192	LEU
1	C	439	LYS
1	C	678	MET
1	C	687	THR
1	C	854	THR
1	C	925	PRO
1	C	986	ILE
1	C	990	PRO
1	C	1054	VAL
1	C	1089	ARG
1	C	1619	VAL
1	C	1632	ILE
1	C	1748	LEU
1	C	2211	ASN
1	C	2293	PRO
1	C	3670	LEU
1	C	3671	LEU
1	C	3813	ASN
1	C	3906	ASN
1	C	3975	LEU
1	C	4032	THR
1	C	4122	LEU
1	C	4139	ILE
1	C	4168	GLU
1	C	4171	ARG
1	C	4727	MET
1	C	4796	LYS
1	C	4858	ILE

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Mol	Chain	Res	Type
1	C	4910	THR
1	D	192	LEU
1	D	344	LYS
1	D	439	LYS
1	D	678	MET
1	D	687	THR
1	D	854	THR
1	D	925	PRO
1	D	950	VAL
1	D	986	ILE
1	D	990	PRO
1	D	1054	VAL
1	D	1089	ARG
1	D	1619	VAL
1	D	1632	ILE
1	D	1748	LEU
1	D	2080	GLU
1	D	2211	ASN
1	D	2293	PRO
1	D	3670	LEU
1	D	3671	LEU
1	D	3813	ASN
1	D	3906	ASN
1	D	3975	LEU
1	D	4032	THR
1	D	4122	LEU
1	D	4139	ILE
1	D	4170	LYS
1	D	4171	ARG
1	D	4727	MET
1	D	4796	LYS
1	D	4858	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (264) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	23	GLN
1	A	44	ASN
1	A	71	GLN
1	A	84	ASN
1	A	123	HIS

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Mol	Chain	Res	Type
1	A	238	HIS
1	A	252	HIS
1	A	293	GLN
1	A	364	GLN
1	A	394	HIS
1	A	427	ASN
1	A	490	GLN
1	A	531	ASN
1	A	547	ASN
1	A	593	HIS
1	A	604	HIS
1	A	628	ASN
1	A	630	HIS
1	A	681	HIS
1	A	745	ASN
1	A	776	GLN
1	A	1149	ASN
1	A	1244	ASN
1	A	1294	ASN
1	A	1452	GLN
1	A	1503	ASN
1	A	1602	GLN
1	A	1620	GLN
1	A	1654	HIS
1	A	1912	GLN
1	A	1938	GLN
1	A	2090	HIS
1	A	2152	ASN
1	A	2210	GLN
1	A	2211	ASN
1	A	2212	GLN
1	A	2225	ASN
1	A	2310	ASN
1	A	2387	ASN
1	A	2728	HIS
1	A	3666	HIS
1	A	3729	GLN
1	A	3743	GLN
1	A	3852	ASN
1	A	3862	GLN
1	A	3906	ASN
1	A	3919	ASN

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Mol	Chain	Res	Type
1	A	3933	GLN
1	A	3954	HIS
1	A	3956	GLN
1	A	3990	ASN
1	A	4179	ASN
1	A	4192	ASN
1	A	4499	ASN
1	A	4559	HIS
1	A	4737	ASN
1	A	4767	GLN
1	A	4817	HIS
1	A	4880	GLN
1	A	4896	ASN
1	A	4914	HIS
1	A	4946	GLN
1	B	12	GLN
1	B	23	GLN
1	B	44	ASN
1	B	71	GLN
1	B	84	ASN
1	B	123	HIS
1	B	238	HIS
1	B	252	HIS
1	B	293	GLN
1	B	364	GLN
1	B	394	HIS
1	B	427	ASN
1	B	464	HIS
1	B	490	GLN
1	B	531	ASN
1	B	547	ASN
1	B	593	HIS
1	B	604	HIS
1	B	628	ASN
1	B	681	HIS
1	B	745	ASN
1	B	776	GLN
1	B	1005	ASN
1	B	1149	ASN
1	B	1244	ASN
1	B	1294	ASN
1	B	1440	ASN

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Mol	Chain	Res	Type
1	B	1452	GLN
1	B	1503	ASN
1	B	1546	GLN
1	B	1602	GLN
1	B	1620	GLN
1	B	1654	HIS
1	B	1938	GLN
1	B	2090	HIS
1	B	2152	ASN
1	B	2211	ASN
1	B	2212	GLN
1	B	2225	ASN
1	B	2310	ASN
1	B	2319	ASN
1	B	2387	ASN
1	B	2728	HIS
1	B	3666	HIS
1	B	3729	GLN
1	B	3743	GLN
1	B	3862	GLN
1	B	3906	ASN
1	B	3916	GLN
1	B	3919	ASN
1	B	3933	GLN
1	B	3954	HIS
1	B	3956	GLN
1	B	3990	ASN
1	B	4050	HIS
1	B	4160	GLN
1	B	4179	ASN
1	B	4192	ASN
1	B	4499	ASN
1	B	4559	HIS
1	B	4700	ASN
1	B	4707	GLN
1	B	4737	ASN
1	B	4767	GLN
1	B	4817	HIS
1	B	4880	GLN
1	B	4896	ASN
1	B	4914	HIS
1	B	4946	GLN

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Mol	Chain	Res	Type
1	C	12	GLN
1	C	23	GLN
1	C	44	ASN
1	C	71	GLN
1	C	84	ASN
1	C	123	HIS
1	C	238	HIS
1	C	252	HIS
1	C	293	GLN
1	C	364	GLN
1	C	394	HIS
1	C	427	ASN
1	C	464	HIS
1	C	490	GLN
1	C	531	ASN
1	C	547	ASN
1	C	593	HIS
1	C	604	HIS
1	C	628	ASN
1	C	681	HIS
1	C	745	ASN
1	C	776	GLN
1	C	1005	ASN
1	C	1149	ASN
1	C	1244	ASN
1	C	1294	ASN
1	C	1452	GLN
1	C	1503	ASN
1	C	1602	GLN
1	C	1620	GLN
1	C	1654	HIS
1	C	1912	GLN
1	C	1938	GLN
1	C	2090	HIS
1	C	2152	ASN
1	C	2211	ASN
1	C	2212	GLN
1	C	2225	ASN
1	C	2310	ASN
1	C	2728	HIS
1	C	2831	ASN
1	C	3666	HIS

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Mol	Chain	Res	Type
1	C	3729	GLN
1	C	3862	GLN
1	C	3906	ASN
1	C	3916	GLN
1	C	3919	ASN
1	C	3933	GLN
1	C	3954	HIS
1	C	3956	GLN
1	C	3990	ASN
1	C	4179	ASN
1	C	4192	ASN
1	C	4499	ASN
1	C	4559	HIS
1	C	4700	ASN
1	C	4707	GLN
1	C	4737	ASN
1	C	4767	GLN
1	C	4817	HIS
1	C	4880	GLN
1	C	4896	ASN
1	C	4914	HIS
1	C	4946	GLN
1	D	12	GLN
1	D	23	GLN
1	D	44	ASN
1	D	71	GLN
1	D	84	ASN
1	D	123	HIS
1	D	238	HIS
1	D	252	HIS
1	D	293	GLN
1	D	364	GLN
1	D	394	HIS
1	D	427	ASN
1	D	464	HIS
1	D	486	GLN
1	D	490	GLN
1	D	531	ASN
1	D	544	ASN
1	D	593	HIS
1	D	604	HIS
1	D	628	ASN

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Mol	Chain	Res	Type
1	D	630	HIS
1	D	681	HIS
1	D	745	ASN
1	D	776	GLN
1	D	1005	ASN
1	D	1149	ASN
1	D	1244	ASN
1	D	1294	ASN
1	D	1452	GLN
1	D	1503	ASN
1	D	1587	HIS
1	D	1602	GLN
1	D	1620	GLN
1	D	1654	HIS
1	D	1912	GLN
1	D	1938	GLN
1	D	2090	HIS
1	D	2152	ASN
1	D	2211	ASN
1	D	2212	GLN
1	D	2225	ASN
1	D	2310	ASN
1	D	2387	ASN
1	D	2728	HIS
1	D	2831	ASN
1	D	3666	HIS
1	D	3729	GLN
1	D	3862	GLN
1	D	3906	ASN
1	D	3916	GLN
1	D	3919	ASN
1	D	3933	GLN
1	D	3954	HIS
1	D	3956	GLN
1	D	3990	ASN
1	D	4179	ASN
1	D	4192	ASN
1	D	4499	ASN
1	D	4559	HIS
1	D	4700	ASN
1	D	4707	GLN
1	D	4737	ASN

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Mol	Chain	Res	Type
1	D	4767	GLN
1	D	4817	HIS
1	D	4880	GLN
1	D	4896	ASN
1	D	4914	HIS
1	D	4946	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

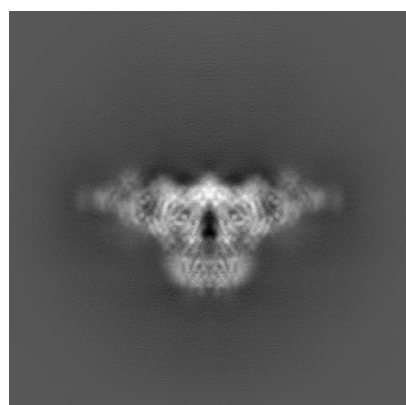
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9529. These allow visual inspection of the internal detail of the map and identification of artifacts.

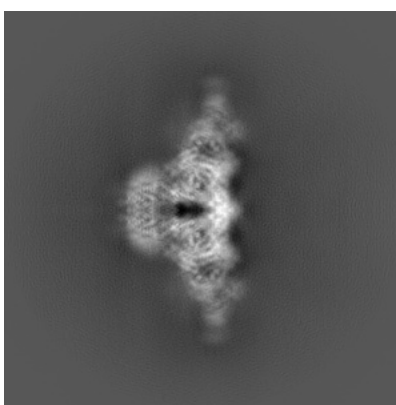
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

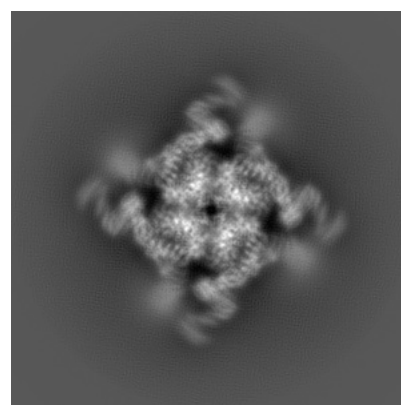
6.1.1 Primary map



X



Y

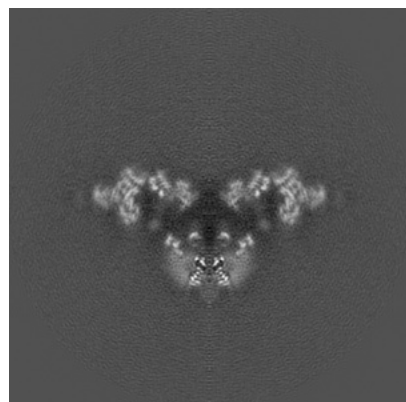


Z

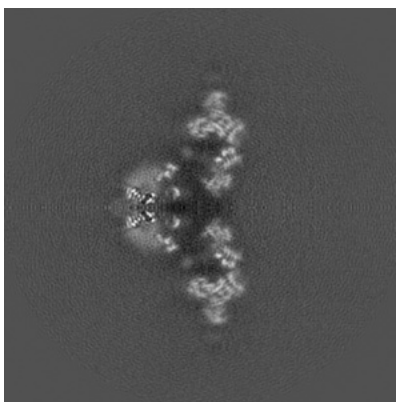
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

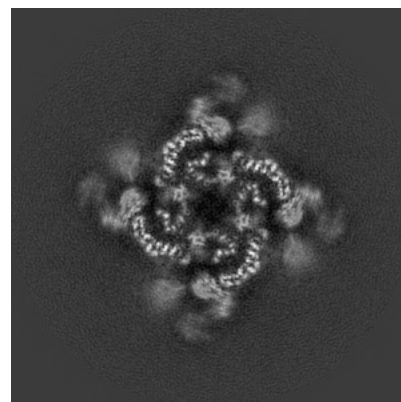
6.2.1 Primary map



X Index: 260



Y Index: 260

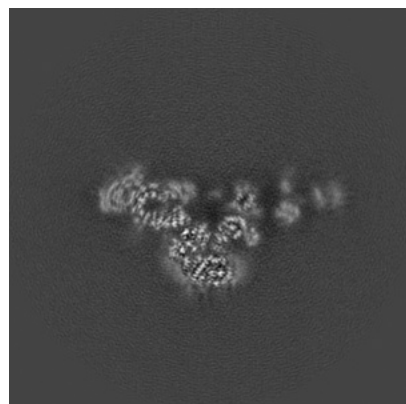


Z Index: 260

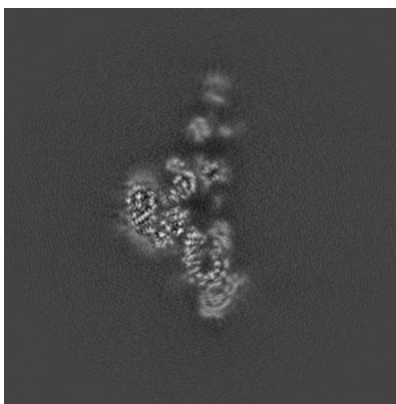
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

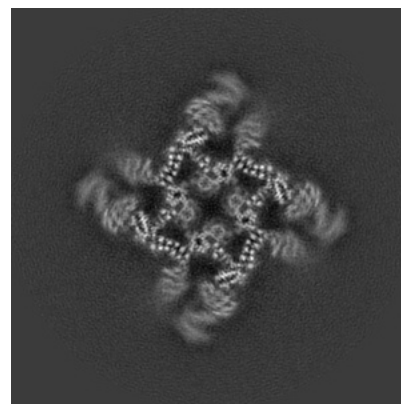
6.3.1 Primary map



X Index: 276



Y Index: 244

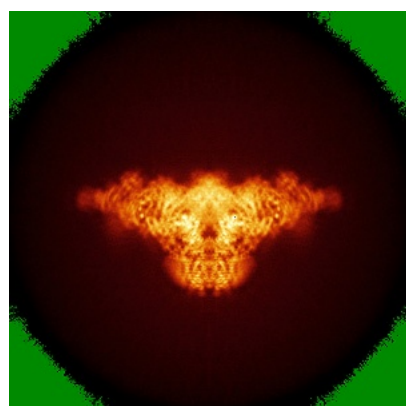


Z Index: 271

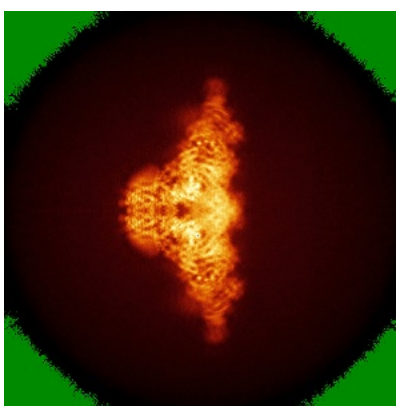
The images above show the largest variance slices of the map in three orthogonal directions.

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

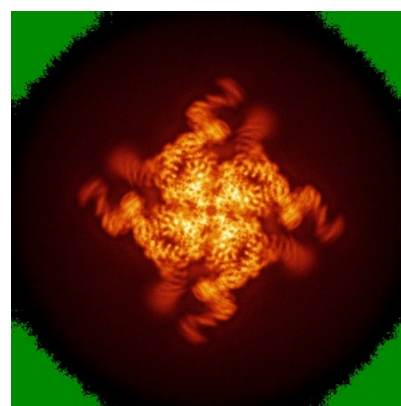
6.4.1 Primary map



X



Y

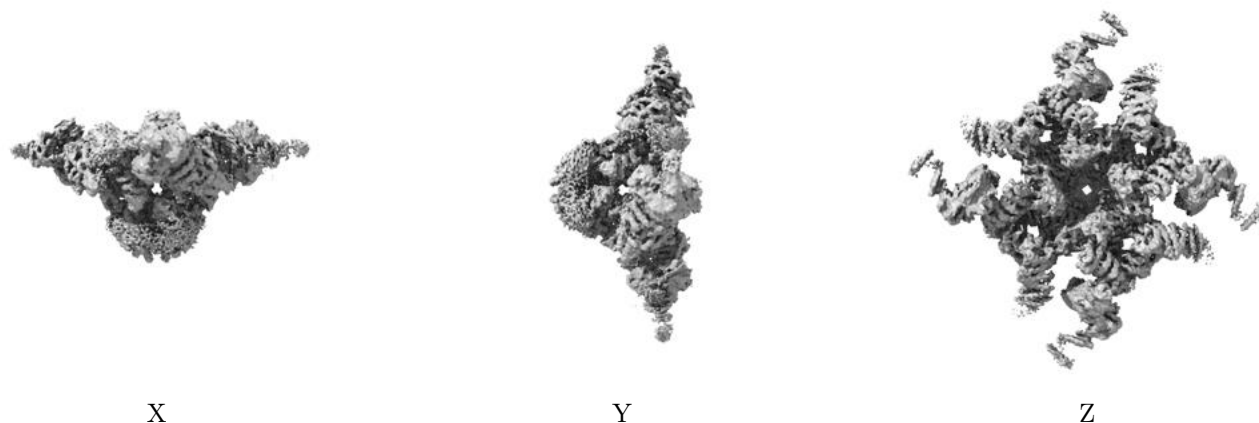


Z

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 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

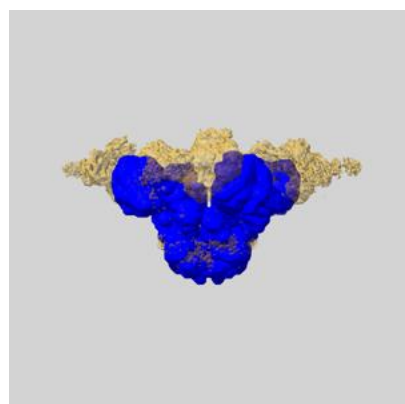
6.6 Mask visualisation [i](#)

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

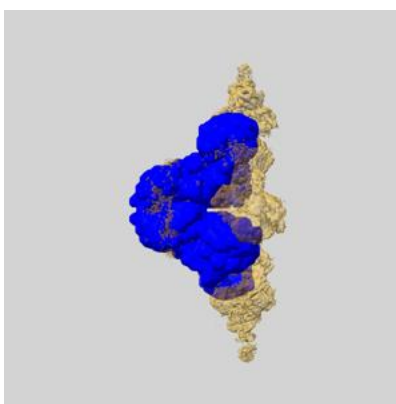
A mask typically either:

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

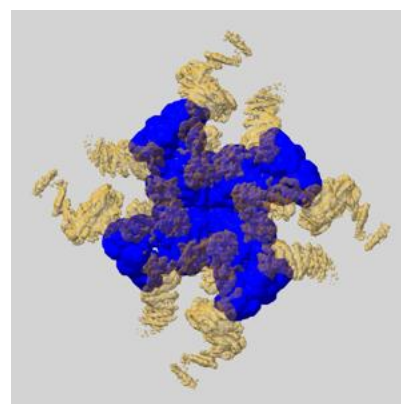
6.6.1 emd_9529_msk_1.map [i](#)



X



Y

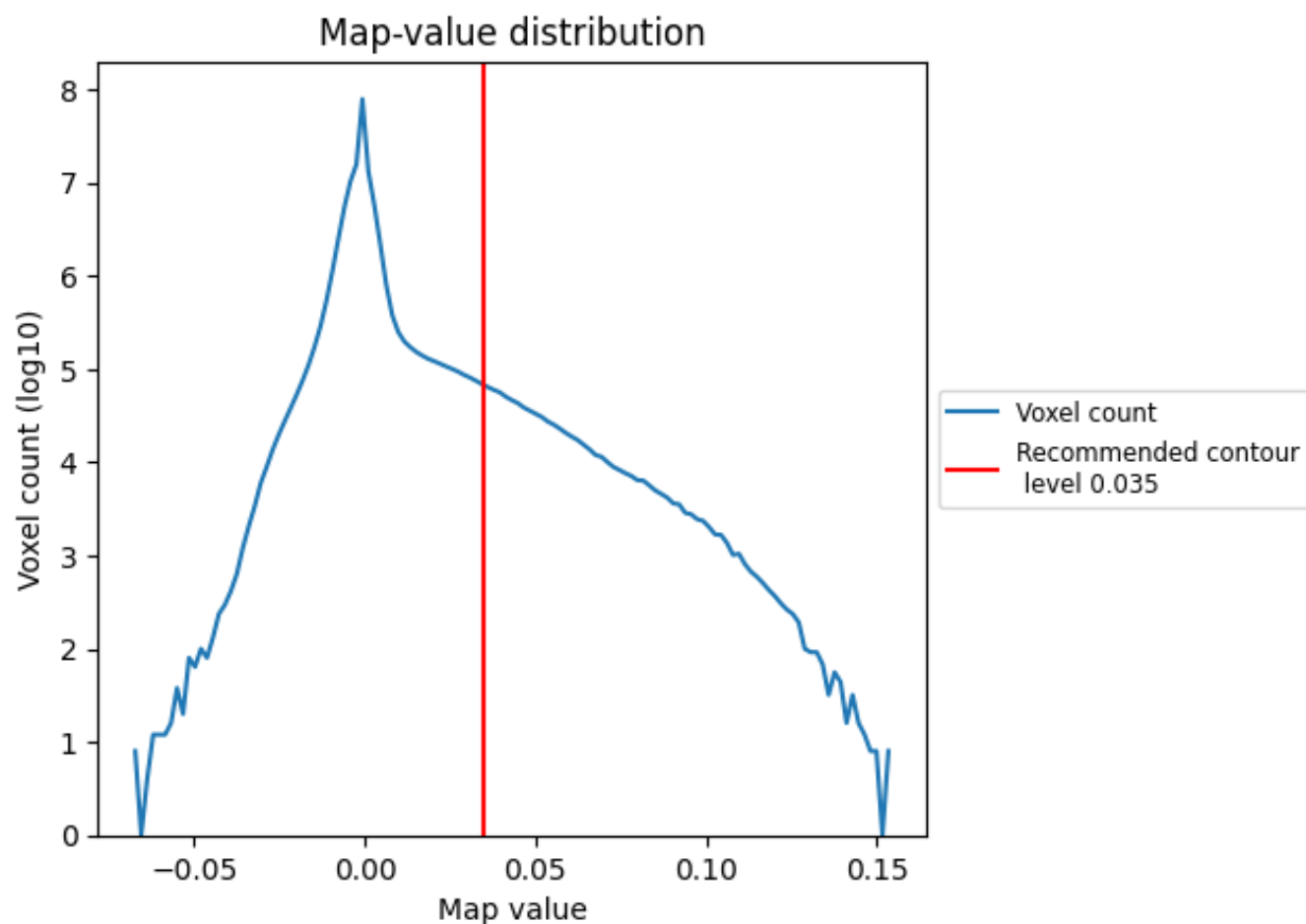


Z

7 Map analysis [i](#)

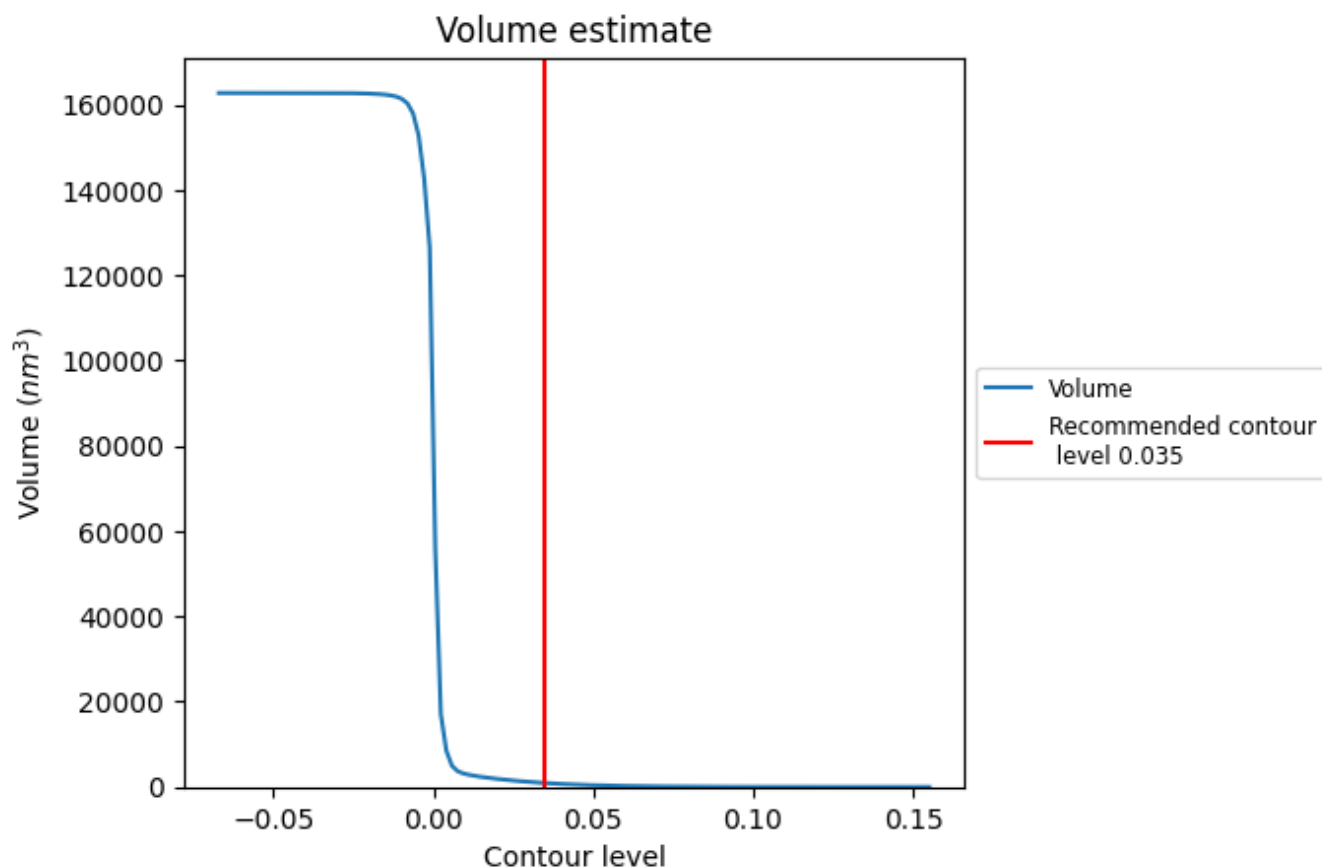
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

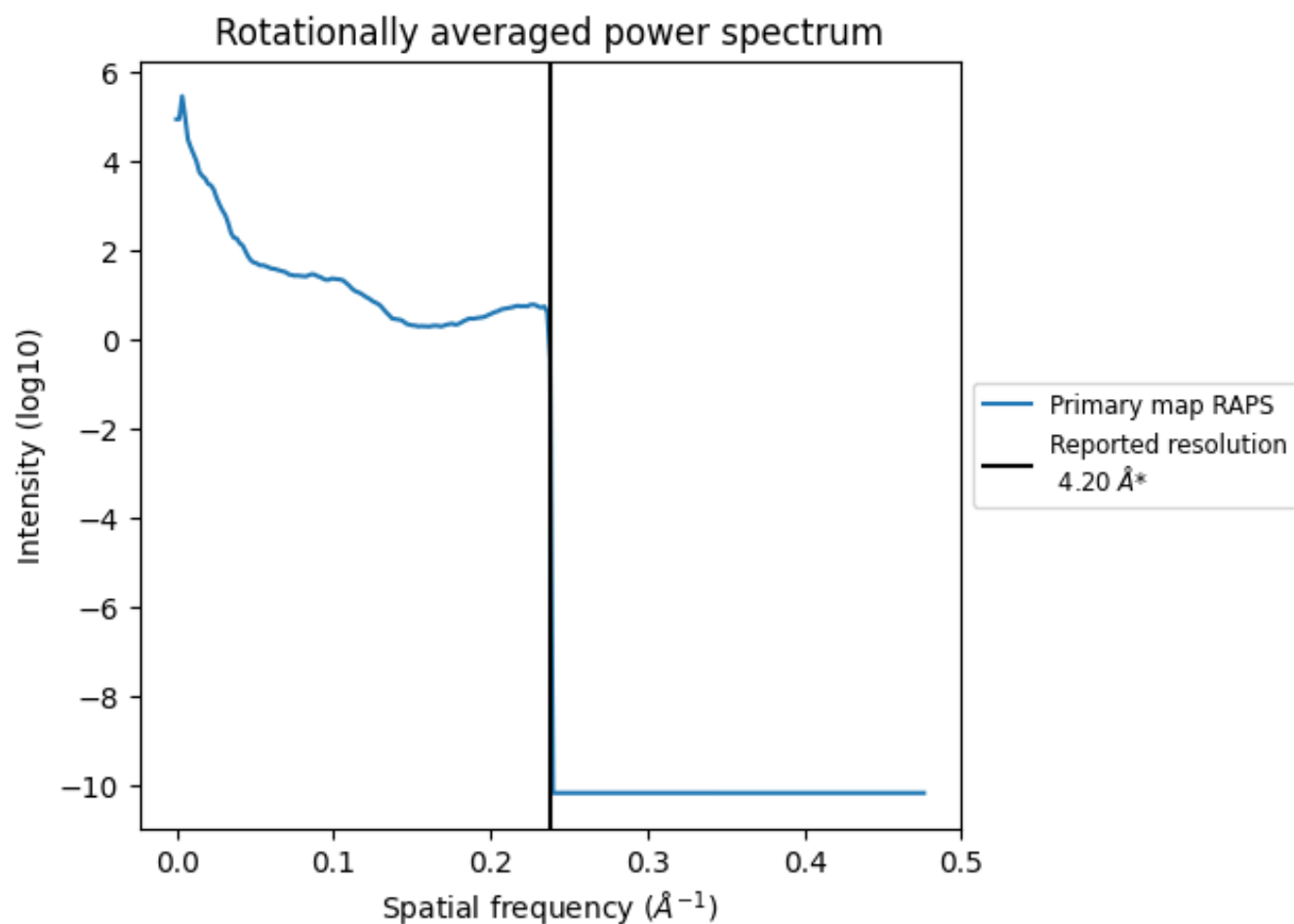
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 919 nm³; this corresponds to an approximate mass of 830 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



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

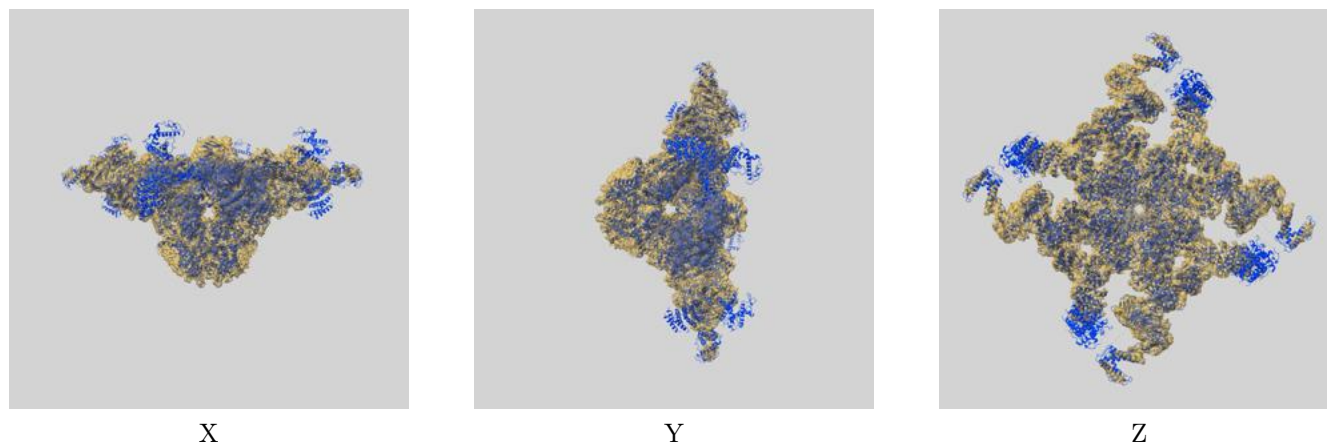
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

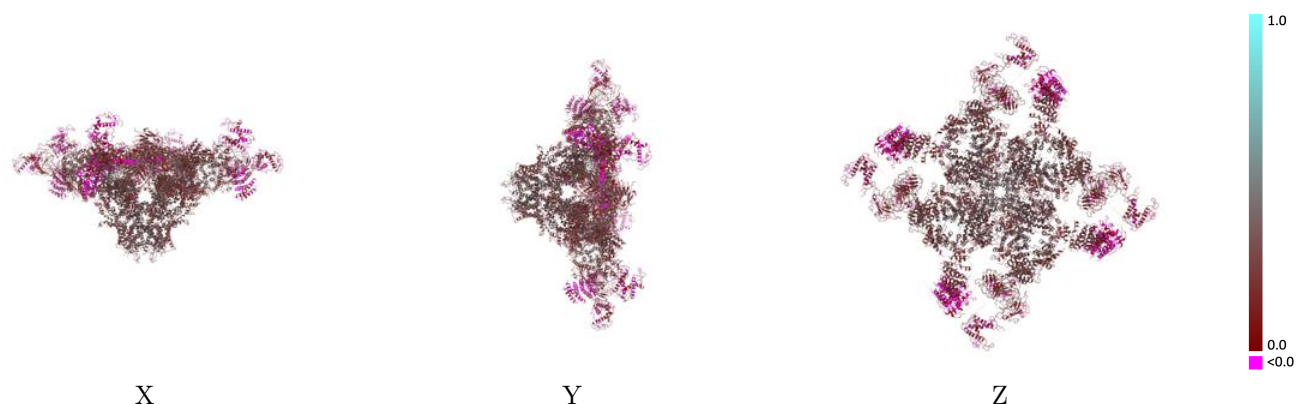
This section contains information regarding the fit between EMDB map EMD-9529 and PDB model 5GOA. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



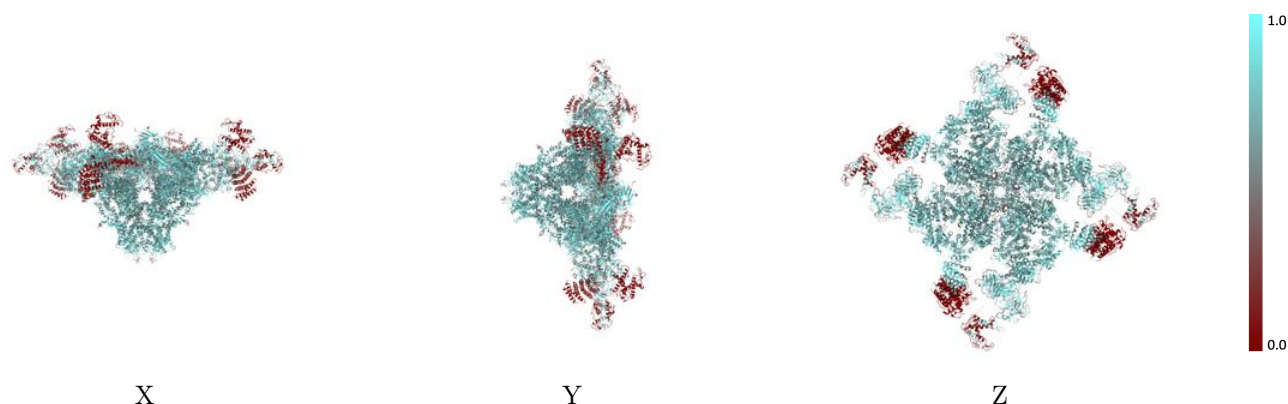
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



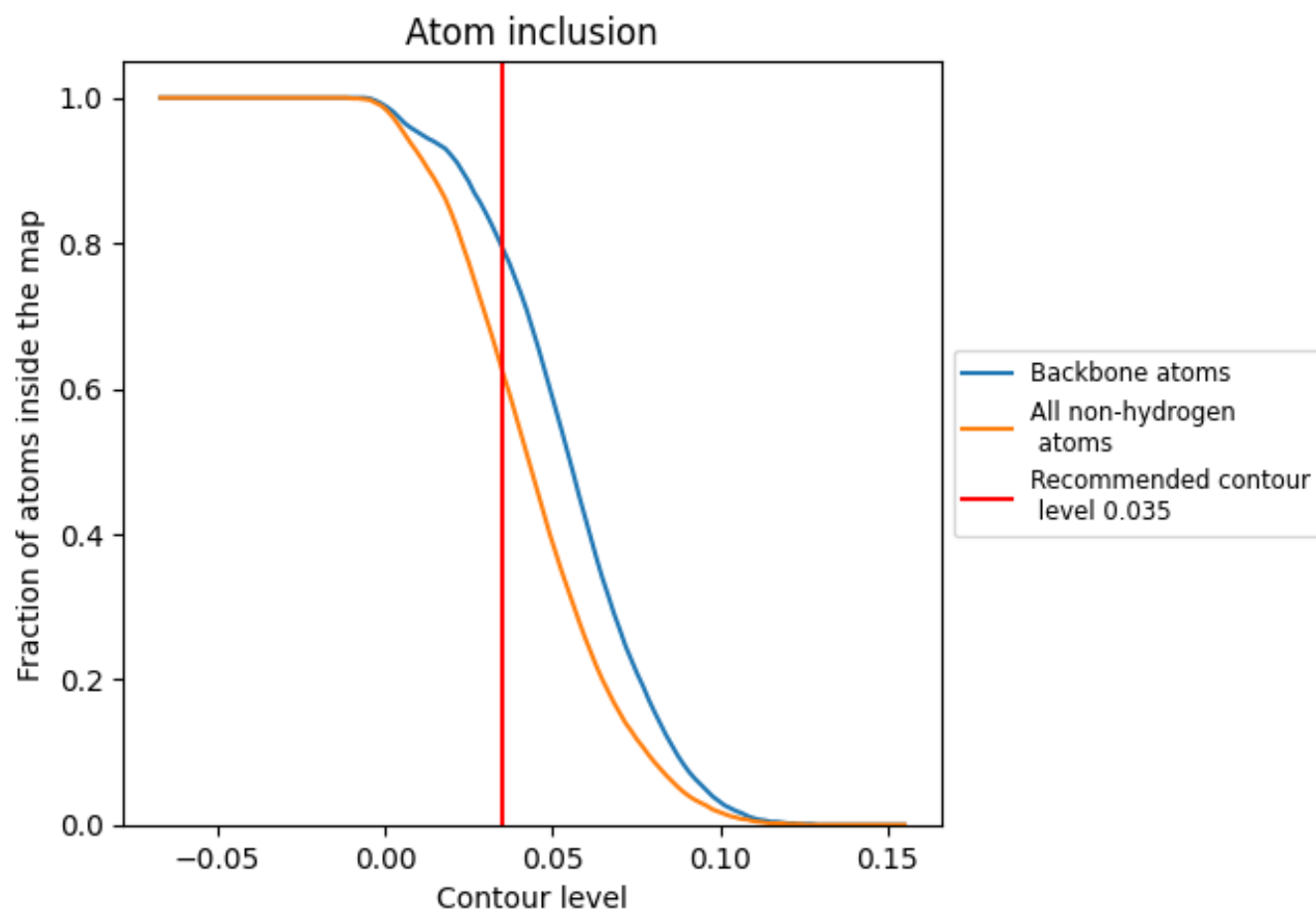
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.035).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 62% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6230	0.2450
A	0.6230	0.2450
B	0.6240	0.2440
C	0.6230	0.2440
D	0.6230	0.2440

