



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 05:46 PM UTC

PDB ID : 6FG3 / pdb_00006fg3
EMDB ID : EMD-4258
Title : Structure of Ryanodine receptor 1 in nanodiscs in the presence of calcium, ATP and ryanodine
Authors : Willegems, K.; Efremov, R.G.
Deposited on : 2018-01-09
Resolution : 7.30 Å(reported)

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

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

A user guide is available at

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

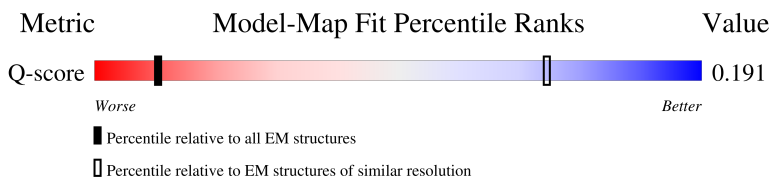
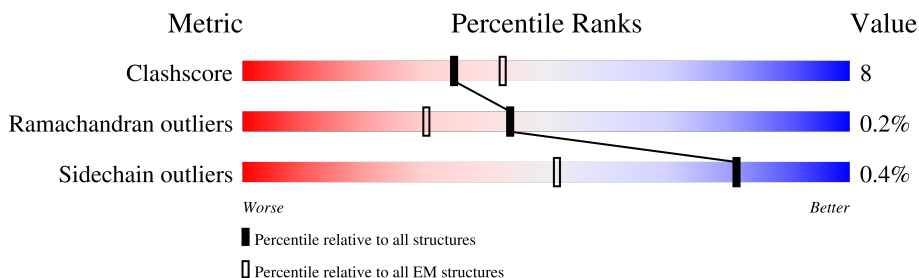
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.30 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	436 (6.80 - 7.80)

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	5037	14% 68% 14% 17%
1	B	5037	14% 68% 14% 17%
1	C	5037	14% 68% 14% 17%
1	D	5037	14% 68% 14% 17%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 117484 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
1	B	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
1	C	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
1	D	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		

- 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	

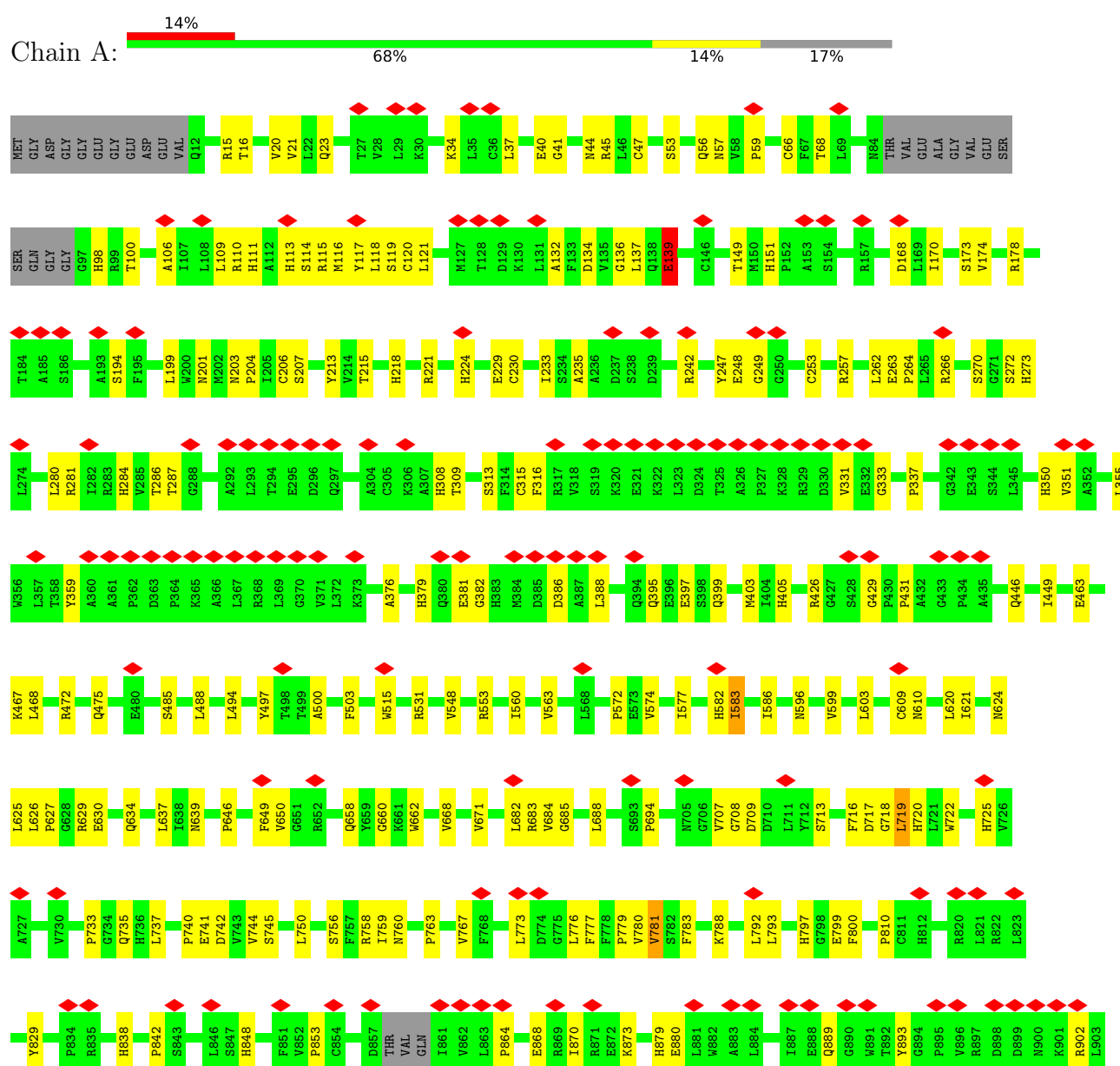
- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

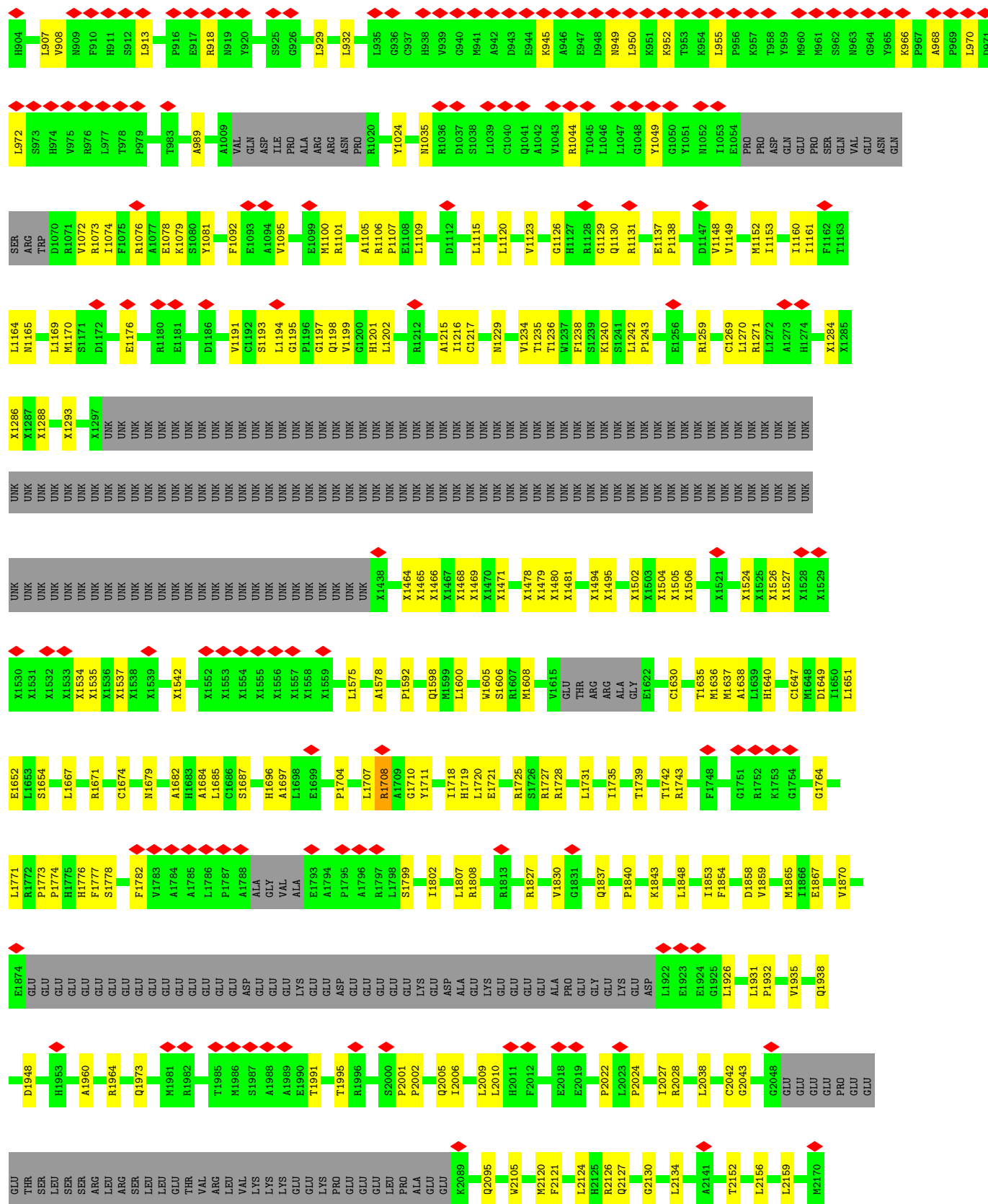
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Ca	0
			1	1	
3	B	1	Total	Ca	0
			1	1	
3	C	1	Total	Ca	0
			1	1	
3	D	1	Total	Ca	0
			1	1	

3 Residue-property plots [i](#)

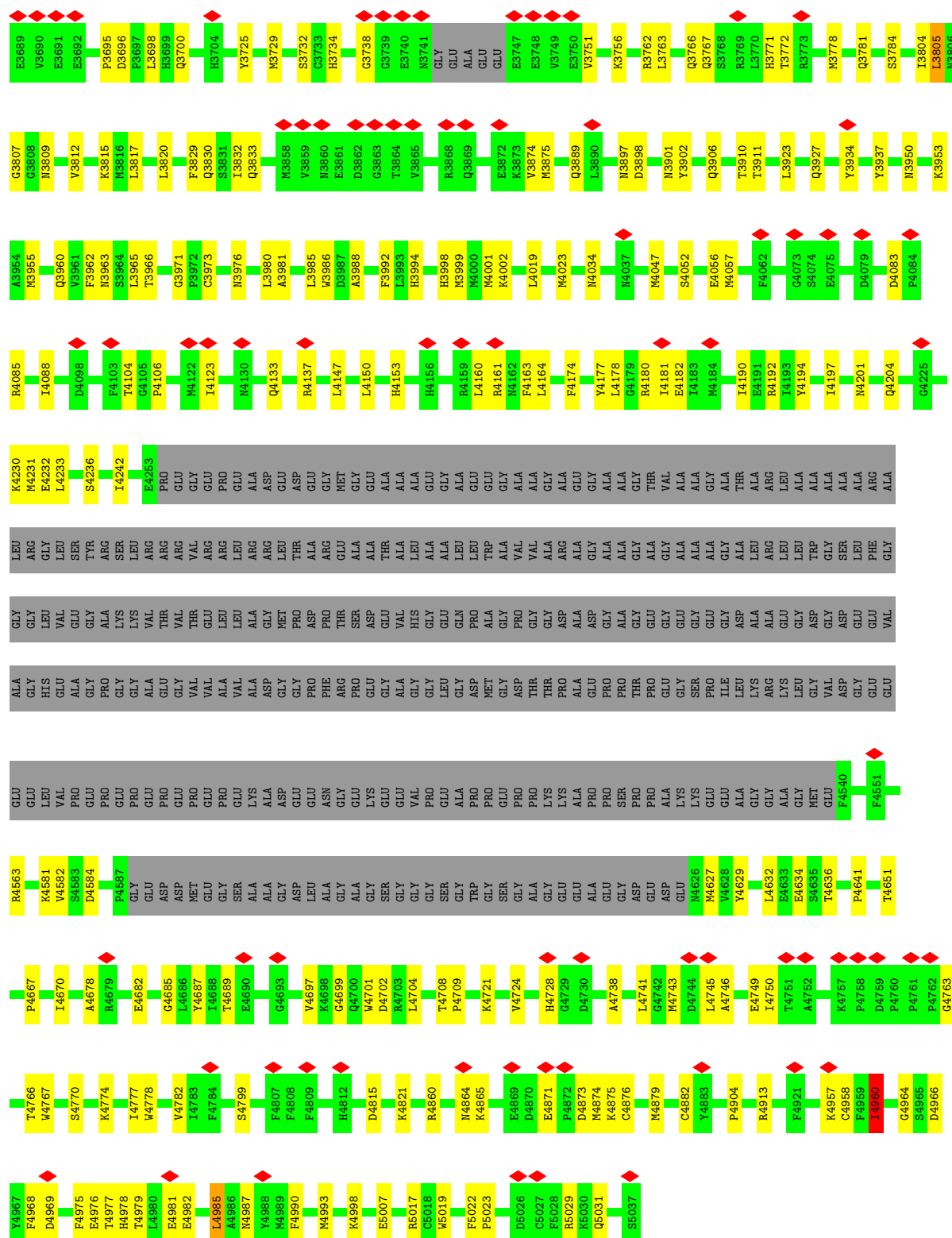
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Ryanodine receptor 1

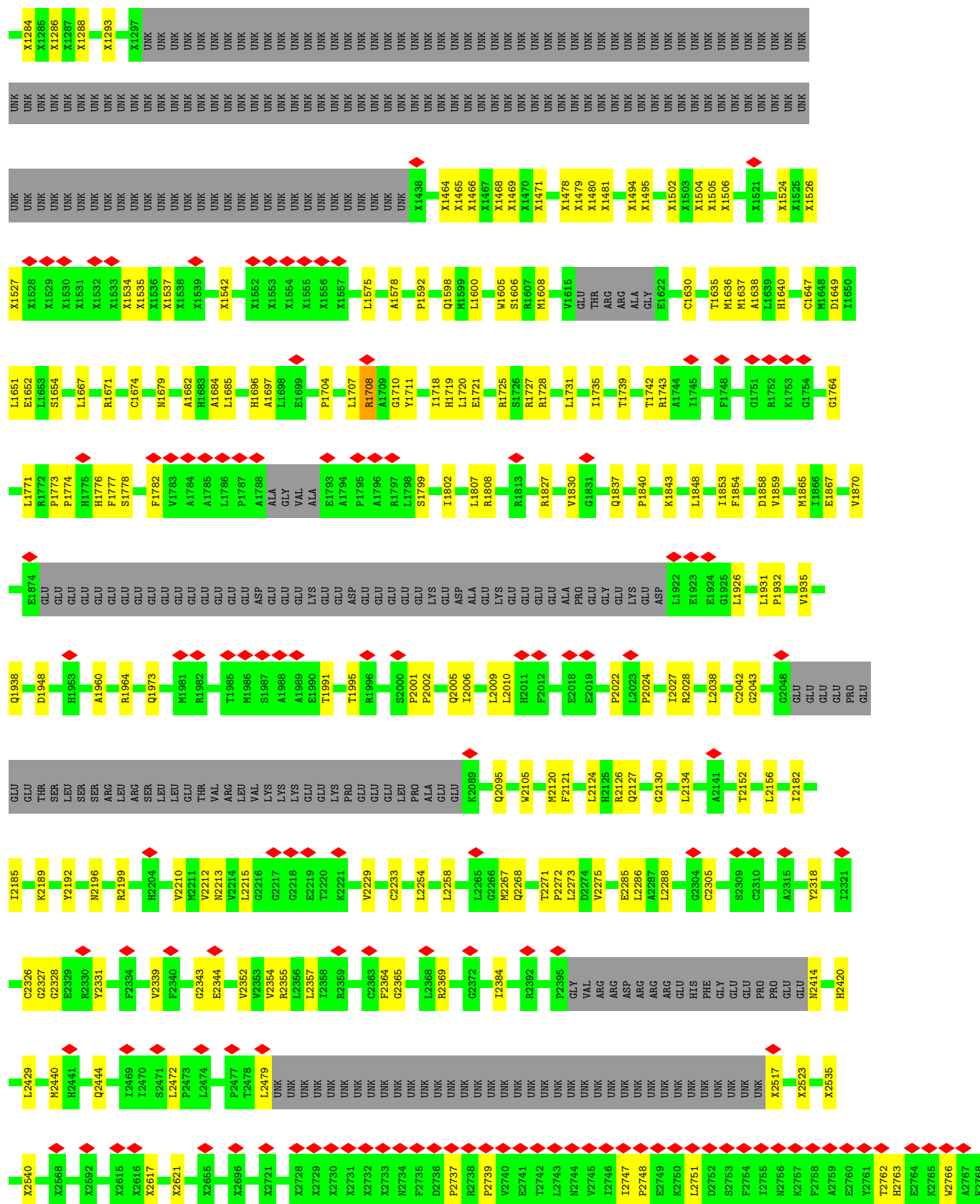


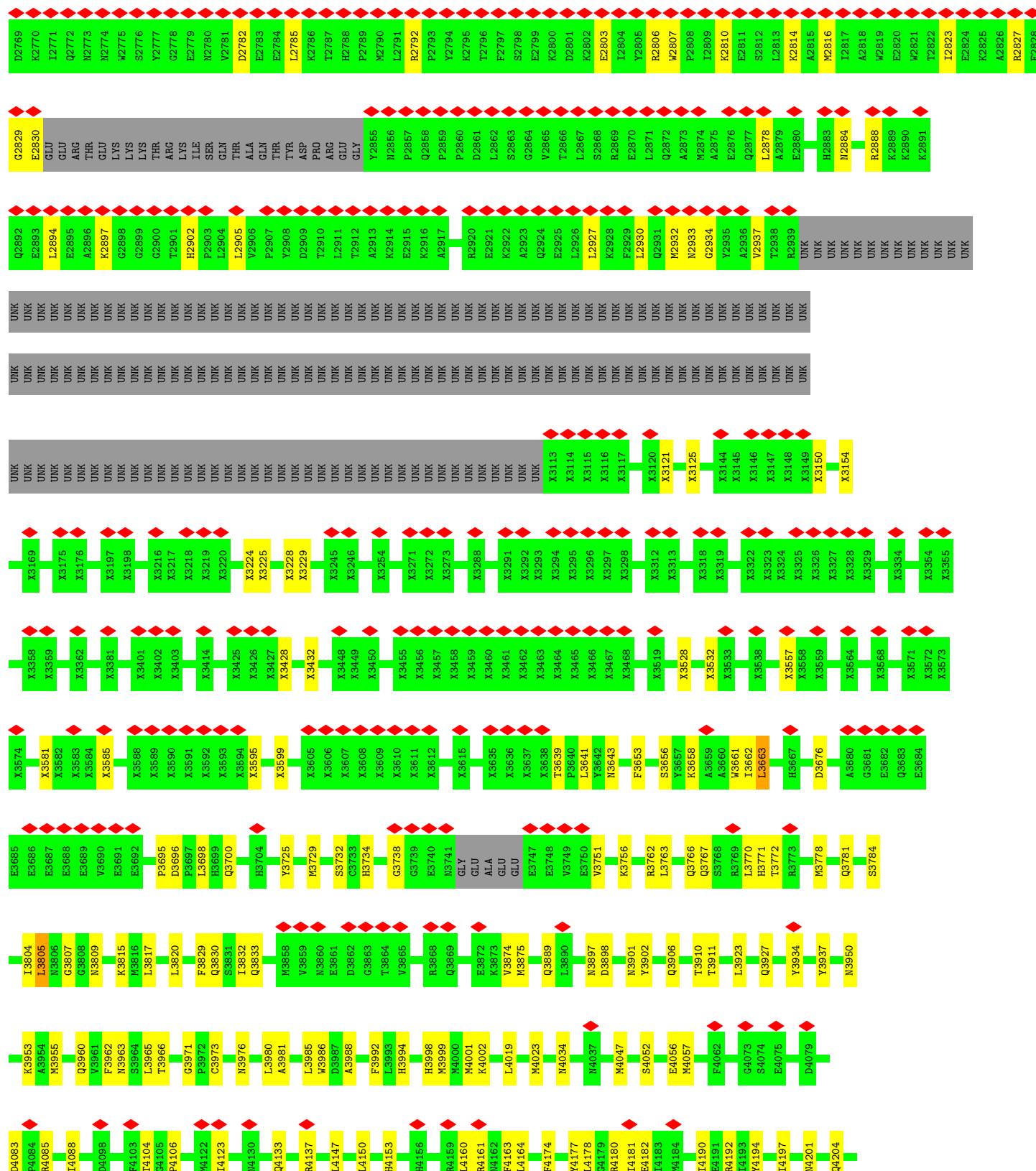




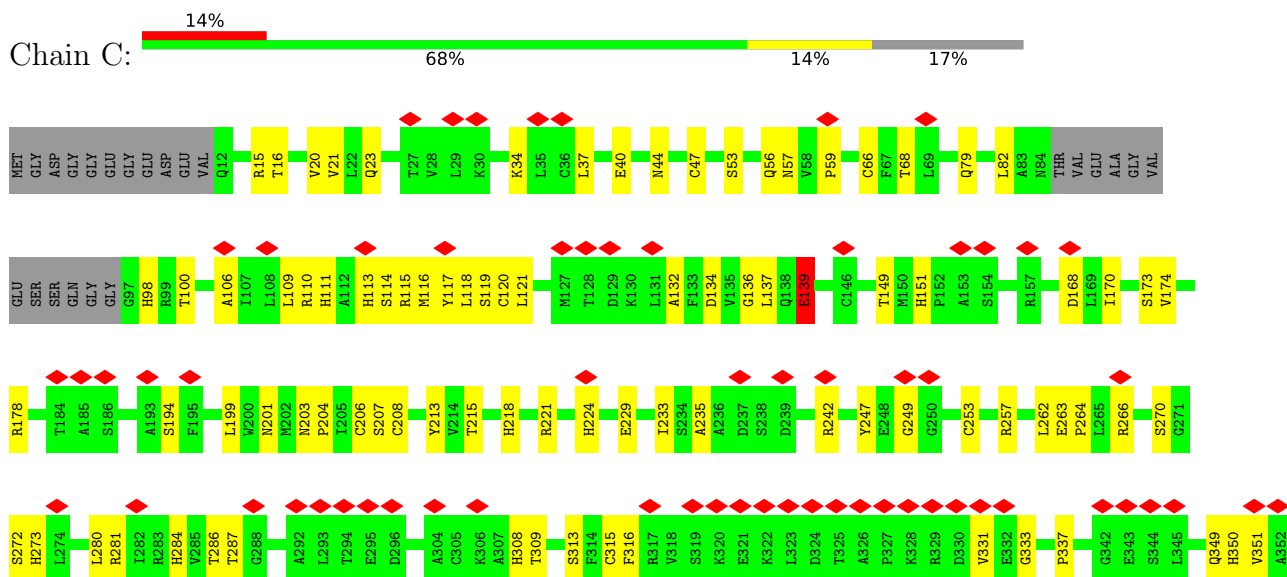


I1161	F1162	T1163	L1164	M1165	L1169	M1170	S1171	D1172	E1176	R1180	D1186	V1191	S1193	L1194	G1195	P1196	G1197	Q1198	V1199	G1200	H1201	R1212	A1215	I1216	C1217	F1223	N1229	V1234	T1235	T1236	V1237	F1238	S1239	K1240	S1241	L1242	P1243	E1256	R1259	C1269	L1270	R1271	L1272	A1273	H1274								
ASN	GLN	SER	ARG	TRP	D1070	R1071	V1072	R1073	H1074	F1075	R1076	A1077	E1078	K1079	S1080	Y1081	F1092	E1093	GLN	ASP	I1094	V1095	E1099	M1100	R1101	A1105	R1106	P1107	E1108	L1109	R1110	P1111	D1112	L1115	L1120	V1123	G1126	H1127	R1128	G1129	Q1130	R1131	E1137	P1138	D1147	V1148	V1149	M1152	I1153	L1156			
D971	L972	S973	H974	R975	R976	L977	T978	R979	A980	T983	A989	A1009	VAL	GLN	ASP	I1010	ALA	ARG	ARG	ASN	PRO	R1020	Y1024	N1035	R1036	D1037	S1038	E1039	C1040	Q1041	A1042	V1043	R1044	T1045	L1046	L1047	G1048	Y1049	G1050	Y1051	N1052	I1053	E1054	PRO	PRO	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU
H722	H725	V730	P733	G734	Q735	H736	L737	P740	E741	D742	V743	V744	S745	L750	S756	F757	R758	I759	K661	V662	V668	V671	L675	T676	A677	L682	R683	V684	L688	V707	G708	D709	D710	L711	S713	F716	D717	G718	L719	H720	L721												
R822	L823	Y829	P834	R835	H838	G841	P842	S843	L846	S847	H848	P853	C854	D857	THR	VAL	GLN	T861	V862	L863	P864	E868	R869	I870	R871	L876	F777	F778	P779	V780	S781	S782	F783	K788	L792	L793	H797	G798	E799	F800	P810	C811	H812	R820	L821								
L903	H904	L907	V908	N909	F910	H911	S912	L913	F916	E917	R918	N919	Y920	S925	G926	L929	L932	L935	Q936	C937	H938	V939	Q940	M941	A942	D943	E944	K945	A946	E947	D948	N949	L950	K951	K952	T953	K954	L955	P956	K957	T958	Y959	M960	H961	S962	N963	G964	R965	K966	P967	A968	P969	L970
D971	L972	S973	H974	R975	R976	L977	T978	R979	A980	T983	A989	A1009	VAL	GLN	ASP	I1010	ALA	ARG	ARG	ASN	PRO	R1020	Y1024	N1035	R1036	D1037	S1038	E1039	C1040	Q1041	A1042	V1043	R1044	T1045	L1046	L1047	G1048	Y1049	G1050	Y1051	N1052	I1053	E1054	PRO	PRO	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU
ASN	GLN	SER	ARG	TRP	D1070	R1071	V1072	R1073	H1074	F1075	R1076	A1077	E1078	K1079	S1080	Y1081	F1092	E1093	GLN	ASP	I1094	V1095	E1099	M1100	R1101	A1105	R1106	P1107	E1108	L1109	R1110	P1111	D1112	L1115	L1120	V1123	G1126	H1127	R1128	G1129	Q1130	R1131	E1137	P1138	D1147	V1148	V1149	M1152	I1153	L1156			
I1161	F1162	T1163	L1164	M1165	L1169	M1170	S1171	D1172	E1176	R1180	D1186	V1191	S1193	L1194	G1195	P1196	G1197	Q1198	V1199	G1200	H1201	R1212	A1215	I1216	C1217	F1223	N1229	V1234	T1235	T1236	V1237	F1238	S1239	K1240	S1241	L1242	P1243	E1256	R1259	C1269	L1270	R1271	L1272	A1273	H1274								
GLN	GLY	GLY	G97	H98	R99	T100	A106	L107	L108	L109	R110	H111	A112	I1205	S114	R115	M116	Y117	L118	S119	C120	L121	M127	T128	D129	K130	L131	A132	F133	D134	V135	G136	L137	Q138	E139	C146	T149	R150	H151	P152	A153	S154	R157	D168	L169	I170	S173	L174	R178	T184			
A185	S186	A193	S194	F195	L199	N200	W201	W202	W203	P204	C206	S207	Y213	W214	T215	H218	R221	H224	E229	I233	S234	A235	A236	D237	S238	L239	D239	R242	Y247	E248	C249	G250	A251	V252	C253	T254	H255	A256	R257	L262	E263	P264	L265	R266	S270	G271	S272						
H273	L274	L280	R281	I282	R283	H284	W285	T286	T287	G288	A292	L293	T294	E295	D296	A304	C305	K306	A307	H308	T309	S313	F314	C315	F316	R317	V318	S319	K320	E321	K322	L323	D324	T325	A326	P327	K328	R329	D330	V331	E332	G333	P337	G342	E343	S344	L345	H350	V351	A352	L355		
W356	L357	T358	Y359	A360	A361	P362	D363	P364	K365	A366	L367	R368	L369	G370	V371	L372	K373	A376	H379	Q380	E381	H382	K384	D385	D386	A387	L388	F389	Q394	Q395	E396	E397	S398	Q399	M403	I404	H405	R426	G427	S428	G429	P430	A431	A432	G433	P434	A435	Q446	L449	E463			
K467	L468	R472	Q475	E480	L484	S485	L488	L494	Y497	T498	T499	A500	A501	H502	F503	W515	R531	V548	R553	L560	V563	L568	V574	S577	H582	L583	L586	N596	V599	L603	C609	N610	L620	L621																			

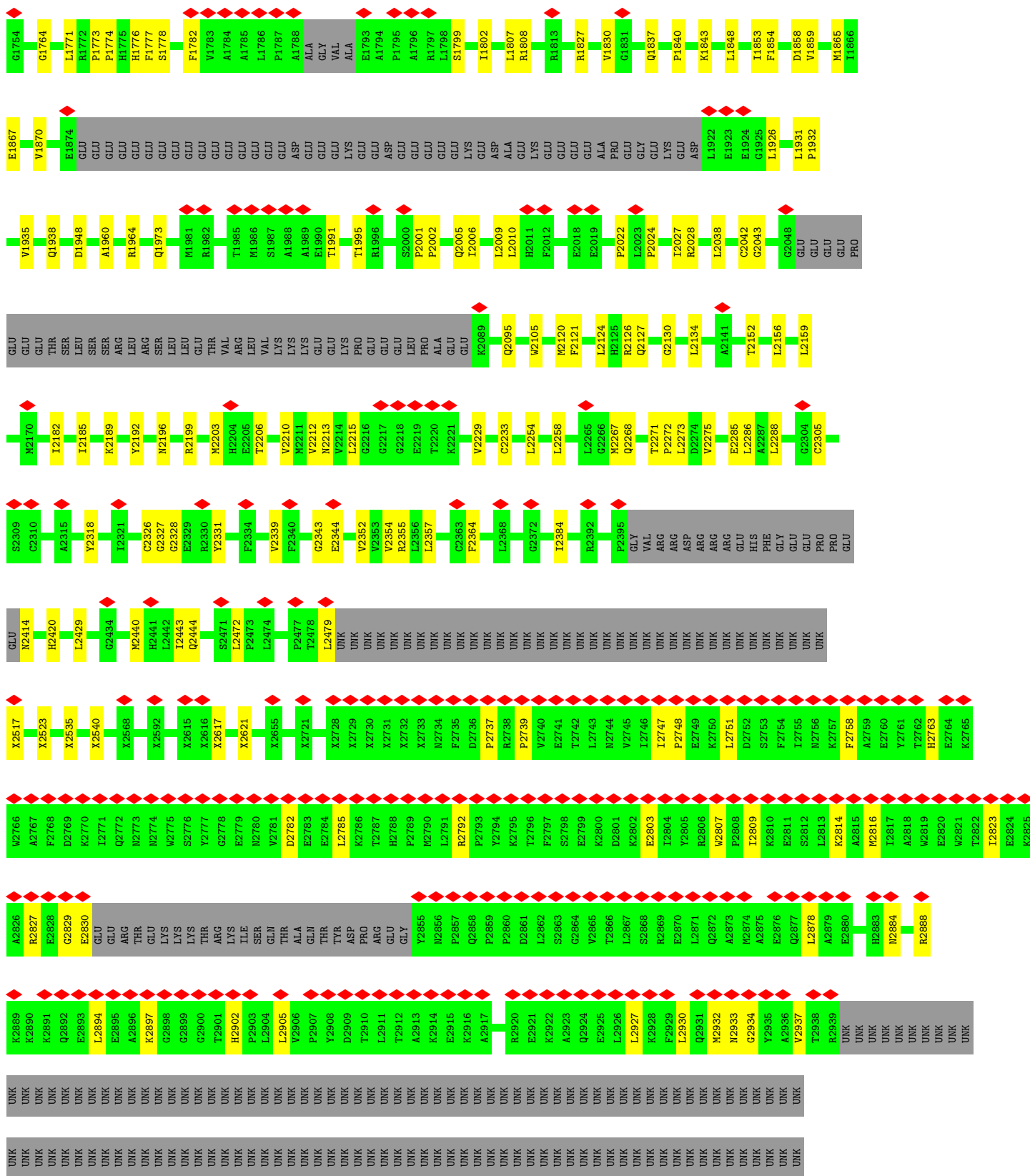




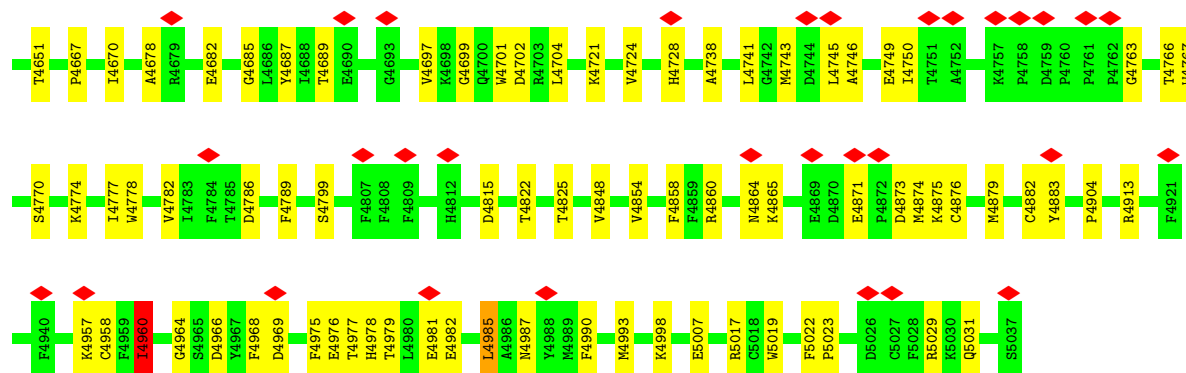
- Molecule 1: Ryanodine receptor 1



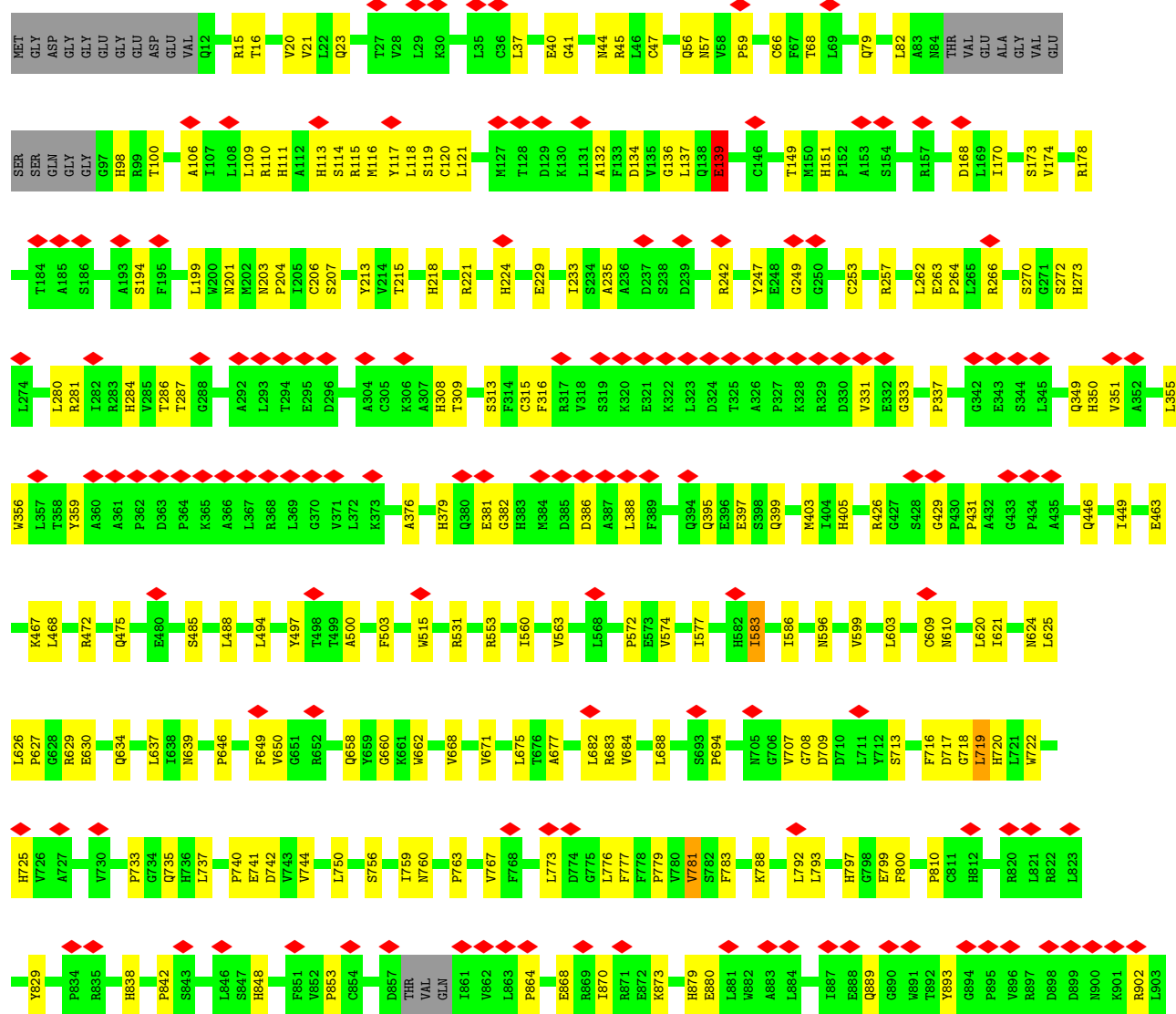




GLU	R4563	GLY	HIS	M4231	F3962	X3815	E3688	X3582	X3355	X3168	UNK
LEU	Y4580	VAL	GLU	E4232	M3963	X3816	E3689	X3583	X3356	UNK	UNK
PRO	Y4581	ALA	GLU	L4233	L3965	L3817	V3690	X3584	X3357	UNK	UNK
PRO	Y4582	PRO	GLY	S4236	T3966	L3820	E3691	X3585	X3358	UNK	UNK
GLU	S4583	ALA	PRO	I4242	G3971	F3829	E3692	X3588	X3359	UNK	UNK
PRO	D4584	GLY	GLY	E4253	C3972	Q3831	P3695	X3589	X3360	UNK	UNK
PRO	P4587	VAL	ARG	PRU	F3973	S3832	P3696	X3590	X3361	UNK	UNK
GLU	GLY	GLU	ARG	GLU	N3976	L3833	P3697	X3591	X3362	UNK	UNK
GLU	GLY	VAL	VAL	GLY	N3976	Q3833	L3698	X3592	X3363	UNK	UNK
GLU	GLY	THR	THR	GLY	L3980	X3858	H3699	X3593	X3364	UNK	UNK
GLU	GLY	ARG	ARG	PRO	A3981	V3859	Q3700	X3594	X3365	UNK	UNK
GLU	GLY	ARG	ARG	GLU	Q4133	V3860	H3704	X3595	X3366	UNK	UNK
GLU	GLY	ARG	ARG	ALA	L3985	N3861	Y3725	X3599	X3367	UNK	UNK
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GLU	GLY	THR	THR	ALA	F3992	Q3863	G3738	X3608	X3371	UNK	UNK
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GLU	GLY	THR	THR	ALA	H3994	V3865	E3740	X3610	X3373	UNK	UNK
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GLU	GLY	THR	THR	ALA	M4001	X3873	ALA	X3635	X3377	UNK	UNK
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GLU	GLY	THR	THR	ALA	L4003	V3875	GLU	X3637	X3379	UNK	UNK
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GLU	GLY	THR	THR	ALA	Q4225	V3961	L3805	E3684	X3401	UNK	UNK
GLU	GLY	THR	THR	ALA	K4230	Q3961	N3806	E3685	X3402	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	G3807	E3686	X3403	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	G3808	E3687	X3404	UNK	UNK
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GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3691	X3408	UNK	UNK
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GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3693	X3410	UNK	UNK
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GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3695	X3412	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3696	X3413	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3697	X3414	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3698	X3415	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3699	X3416	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3700	X3417	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3701	X3418	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3702	X3419	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3703	X3420	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3704	X3421	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3705	X3422	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3706	X3423	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3707	X3424	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3708	X3425	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3709	X3426	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3710	X3427	UNK	UNK
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GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3712	X3429	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3713	X3430	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3714	X3431	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3715	X3432	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3716	X3433	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3717	X3434	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3718	X3435	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3719	X3436	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3720	X3437	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3721	X3438	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3722	X3439	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3723	X3440	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3724	X3441	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3725	X3442	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3726	X3443	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3727	X3444	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3728	X3445	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3729	X3446	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3730	X3447	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3731	X3448	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3732	X3449	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3733	X3450	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3734	X3451	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3735	X3452	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3736	X3453	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3737	X3454	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3738	X3455	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3739	X3456	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3740	X3457	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3741	X3458	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3742	X3459	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3743	X3460	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3744	X3461	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3745	X3462	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3746	X3463	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3747	X3464	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3748	X3465	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3749	X3466	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3750	X3467	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3751	X3468	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3752	X3469	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3753	X3470	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3754	X3471	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3755	X3472	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3756	X3473	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3757	X3474	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3758	X3475	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3759	X3476	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3760	X3477	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3761	X3478	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3762	X3479	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3763	X3480	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3764	X3481	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3765	X3482	UNK	UNK
GLU	GLY	THR	THR	ALA	Q4230	Q3961	N3809	E3766	X3483	UNK	UNK
GLU	GLY	THR	THR	ALA							



• Molecule 1: Ryanodine receptor 1









4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	61773	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 ($e^-/\text{\AA}^2$)	28	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.217	Depositor
Minimum map value	-0.087	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	514.9, 514.9, 514.9	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.355, 1.355, 1.355	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.25	0/25428	0.59	4/34534 (0.0%)
1	B	0.25	0/25428	0.59	4/34534 (0.0%)
1	C	0.25	0/25428	0.59	4/34534 (0.0%)
1	D	0.25	0/25428	0.59	4/34534 (0.0%)
All	All	0.25	0/101712	0.59	16/138136 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	10
1	B	0	10
1	C	0	10
1	D	0	10
All	All	0	40

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	139	GLU	N-CA-C	-6.33	104.80	114.16
1	A	139	GLU	N-CA-C	-6.32	104.81	114.16
1	B	139	GLU	N-CA-C	-6.31	104.82	114.16
1	C	139	GLU	N-CA-C	-6.26	104.89	114.16
1	B	4153	HIS	CA-C-N	-5.49	118.08	122.85
1	B	4153	HIS	C-N-CA	-5.49	118.08	122.85
1	C	4153	HIS	CA-C-N	-5.47	118.09	122.85
1	C	4153	HIS	C-N-CA	-5.47	118.09	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4153	HIS	CA-C-N	-5.47	118.09	122.85
1	A	4153	HIS	C-N-CA	-5.47	118.09	122.85
1	D	4153	HIS	CA-C-N	-5.43	118.13	122.85
1	D	4153	HIS	C-N-CA	-5.43	118.13	122.85
1	C	4960	ILE	N-CA-C	-5.22	107.50	111.62
1	A	4960	ILE	N-CA-C	-5.20	107.51	111.62
1	B	4960	ILE	N-CA-C	-5.18	107.53	111.62
1	D	4960	ILE	N-CA-C	-5.18	107.53	111.62

There are no chirality outliers.

All (40) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	GLU	Peptide
1	A	1720	LEU	Peptide
1	A	1840	PRO	Peptide
1	A	2001	PRO	Peptide
1	A	2343	GLY	Peptide
1	A	3557	UNK	Peptide
1	A	3971	GLY	Peptide
1	A	4960	ILE	Peptide
1	A	5029	ARG	Peptide
1	A	694	PRO	Peptide
1	B	139	GLU	Peptide
1	B	1720	LEU	Peptide
1	B	1840	PRO	Peptide
1	B	2001	PRO	Peptide
1	B	2343	GLY	Peptide
1	B	3557	UNK	Peptide
1	B	3971	GLY	Peptide
1	B	4960	ILE	Peptide
1	B	5029	ARG	Peptide
1	B	694	PRO	Peptide
1	C	139	GLU	Peptide
1	C	1720	LEU	Peptide
1	C	1840	PRO	Peptide
1	C	2001	PRO	Peptide
1	C	2343	GLY	Peptide
1	C	3557	UNK	Peptide
1	C	3971	GLY	Peptide
1	C	4960	ILE	Peptide
1	C	5029	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	C	694	PRO	Peptide
1	D	139	GLU	Peptide
1	D	1720	LEU	Peptide
1	D	1840	PRO	Peptide
1	D	2001	PRO	Peptide
1	D	2343	GLY	Peptide
1	D	3557	UNK	Peptide
1	D	3971	GLY	Peptide
1	D	4960	ILE	Peptide
1	D	5029	ARG	Peptide
1	D	694	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	29369	0	24692	433	0
1	B	29369	0	24692	429	0
1	C	29369	0	24692	440	0
1	D	29369	0	24692	436	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	117484	0	98768	1731	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (1731) 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:B:4958:CYS:HG	1:B:4978:HIS:HE2	1.36	0.73
1:C:4958:CYS:HG	1:C:4978:HIS:HE2	1.35	0.73
1:A:4958:CYS:HG	1:A:4978:HIS:HE2	1.36	0.71
1:C:4678:ALA:O	1:C:4682:GLU:HB2	1.91	0.71
1:B:4678:ALA:O	1:B:4682:GLU:HB2	1.91	0.70
1:D:4678:ALA:O	1:D:4682:GLU:HB2	1.91	0.70
1:A:4678:ALA:O	1:A:4682:GLU:HB2	1.91	0.70
1:D:4958:CYS:HG	1:D:4978:HIS:HE2	1.37	0.70
1:C:4741:LEU:HB2	1:C:4743:MET:HE2	1.75	0.69
1:B:4741:LEU:HB2	1:B:4743:MET:HE2	1.75	0.69
1:C:4958:CYS:SG	1:C:4978:HIS:NE2	2.65	0.69
1:A:4741:LEU:HB2	1:A:4743:MET:HE2	1.75	0.68
1:D:4741:LEU:HB2	1:D:4743:MET:HE2	1.75	0.68
1:B:639:ASN:HA	1:B:1635:THR:HA	1.77	0.67
1:B:1671:ARG:NH2	1:B:1710:GLY:O	2.29	0.66
1:C:1671:ARG:NH2	1:C:1710:GLY:O	2.29	0.66
1:D:1671:ARG:NH2	1:D:1710:GLY:O	2.29	0.66
1:C:639:ASN:HA	1:C:1635:THR:HA	1.77	0.66
1:A:264:PRO:HG2	1:A:270:SER:HB2	1.78	0.66
1:D:639:ASN:HA	1:D:1635:THR:HA	1.77	0.65
1:A:1671:ARG:NH2	1:A:1710:GLY:O	2.29	0.65
1:B:264:PRO:HG2	1:B:270:SER:HB2	1.78	0.65
1:B:3805:LEU:HA	1:B:3809:ASN:HD22	1.62	0.65
1:A:3994:HIS:O	1:A:3998:HIS:ND1	2.30	0.65
1:B:4958:CYS:SG	1:B:4978:HIS:NE2	2.65	0.65
1:C:3805:LEU:HA	1:C:3809:ASN:HD22	1.62	0.65
1:D:1079:LYS:NZ	1:D:1107:PRO:O	2.30	0.65
1:D:3973:CYS:SG	1:D:3976:ASN:ND2	2.70	0.65
1:D:3994:HIS:O	1:D:3998:HIS:ND1	2.30	0.65
1:A:639:ASN:HA	1:A:1635:THR:HA	1.77	0.65
1:B:1079:LYS:NZ	1:B:1107:PRO:O	2.30	0.65
1:D:264:PRO:HG2	1:D:270:SER:HB2	1.78	0.64
1:C:3973:CYS:SG	1:C:3976:ASN:ND2	2.70	0.64
1:A:3973:CYS:SG	1:A:3976:ASN:ND2	2.70	0.64
1:C:1079:LYS:NZ	1:C:1107:PRO:O	2.30	0.64
1:B:263:GLU:HB2	1:B:281:ARG:HB2	1.80	0.64
1:B:3973:CYS:SG	1:B:3976:ASN:ND2	2.70	0.64
1:C:263:GLU:HB2	1:C:281:ARG:HB2	1.80	0.64
1:A:3805:LEU:HA	1:A:3809:ASN:HD22	1.62	0.64
1:A:1079:LYS:NZ	1:A:1107:PRO:O	2.30	0.63
1:C:264:PRO:HG2	1:C:270:SER:HB2	1.78	0.63
1:C:2748:PRO:HD2	1:C:2751:LEU:HD12	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:650:VAL:HB	1:D:777:PHE:HB2	1.81	0.63
1:D:3805:LEU:HA	1:D:3809:ASN:HD22	1.62	0.63
1:A:379:HIS:HD2	1:A:382:GLY:H	1.47	0.63
1:A:650:VAL:HB	1:A:777:PHE:HB2	1.81	0.63
1:A:3889:GLN:OE1	1:A:3960:GLN:NE2	2.32	0.63
1:A:2748:PRO:HD2	1:A:2751:LEU:HD12	1.79	0.63
1:C:3889:GLN:OE1	1:C:3960:GLN:NE2	2.32	0.63
1:C:650:VAL:HB	1:C:777:PHE:HB2	1.81	0.63
1:B:3889:GLN:OE1	1:B:3960:GLN:NE2	2.32	0.63
1:D:497:TYR:HB3	1:D:500:ALA:HB2	1.81	0.63
1:D:2748:PRO:HD2	1:D:2751:LEU:HD12	1.79	0.63
1:A:629:ARG:O	1:A:634:GLN:NE2	2.32	0.63
1:A:718:GLY:HA3	1:A:737:LEU:HA	1.81	0.63
1:B:2748:PRO:HD2	1:B:2751:LEU:HD12	1.79	0.63
1:D:792:LEU:HD22	1:D:799:GLU:H	1.63	0.62
1:B:650:VAL:HB	1:B:777:PHE:HB2	1.81	0.62
1:C:3994:HIS:O	1:C:3998:HIS:ND1	2.30	0.62
1:D:3889:GLN:OE1	1:D:3960:GLN:NE2	2.32	0.62
1:A:263:GLU:HB2	1:A:281:ARG:HB2	1.80	0.62
1:B:379:HIS:HD2	1:B:382:GLY:H	1.47	0.62
1:D:629:ARG:O	1:D:634:GLN:NE2	2.32	0.62
1:A:497:TYR:HB3	1:A:500:ALA:HB2	1.81	0.62
1:B:792:LEU:HD22	1:B:799:GLU:H	1.63	0.62
1:C:792:LEU:HD22	1:C:799:GLU:H	1.63	0.62
1:B:718:GLY:HA3	1:B:737:LEU:HA	1.81	0.62
1:B:497:TYR:HB3	1:B:500:ALA:HB2	1.81	0.62
1:D:263:GLU:HB2	1:D:281:ARG:HB2	1.80	0.62
1:C:629:ARG:O	1:C:634:GLN:NE2	2.32	0.62
1:A:792:LEU:HD22	1:A:799:GLU:H	1.63	0.62
1:C:497:TYR:HB3	1:C:500:ALA:HB2	1.80	0.62
1:D:718:GLY:HA3	1:D:737:LEU:HA	1.81	0.62
1:D:733:PRO:HG2	1:D:763:PRO:HD2	1.82	0.62
1:B:3910:THR:HG23	1:B:3911:THR:HG23	1.82	0.62
1:D:379:HIS:HD2	1:D:382:GLY:H	1.47	0.62
1:D:3910:THR:HG23	1:D:3911:THR:HG23	1.82	0.62
1:A:4582:VAL:HG23	1:A:4629:TYR:HA	1.81	0.62
1:D:4083:ASP:HA	1:D:4085:ARG:HH11	1.65	0.62
1:B:4582:VAL:HG23	1:B:4629:TYR:HA	1.81	0.61
1:A:4083:ASP:HA	1:A:4085:ARG:HH11	1.65	0.61
1:B:629:ARG:O	1:B:634:GLN:NE2	2.32	0.61
1:A:494:LEU:HD22	1:A:515:TRP:HE1	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2318:TYR:HH	1:B:2414:ASN:N	1.99	0.61
1:B:3994:HIS:O	1:B:3998:HIS:ND1	2.30	0.61
1:D:494:LEU:HD22	1:D:515:TRP:HE1	1.65	0.61
1:A:733:PRO:HG2	1:A:763:PRO:HD2	1.82	0.61
1:B:733:PRO:HG2	1:B:763:PRO:HD2	1.82	0.61
1:C:718:GLY:HA3	1:C:737:LEU:HA	1.81	0.61
1:C:2318:TYR:HH	1:C:2414:ASN:N	1.99	0.61
1:C:4960:ILE:HD11	1:C:4985:LEU:HD23	1.83	0.61
1:D:4582:VAL:HG23	1:D:4629:TYR:HA	1.80	0.61
1:A:2318:TYR:HH	1:A:2414:ASN:N	1.99	0.61
1:C:4083:ASP:HA	1:C:4085:ARG:HH11	1.65	0.61
1:A:110:ARG:HH21	1:A:115:ARG:HB3	1.65	0.61
1:B:110:ARG:HH21	1:B:115:ARG:HB3	1.65	0.61
1:C:3910:THR:HG23	1:C:3911:THR:HG23	1.82	0.61
1:C:3751:VAL:O	1:C:3756:LYS:NZ	2.34	0.61
1:D:4960:ILE:HD11	1:D:4985:LEU:HD23	1.83	0.61
1:A:3910:THR:HG23	1:A:3911:THR:HG23	1.82	0.61
1:B:1808:ARG:NH1	1:B:1853:ILE:O	2.34	0.61
1:C:110:ARG:HH21	1:C:115:ARG:HB3	1.65	0.61
1:C:1808:ARG:NH1	1:C:1853:ILE:O	2.34	0.61
1:C:4582:VAL:HG23	1:C:4629:TYR:HA	1.80	0.61
1:C:1764:GLY:HA3	1:C:1859:VAL:HG11	1.83	0.61
1:C:379:HIS:HD2	1:C:382:GLY:H	1.47	0.61
1:D:3751:VAL:O	1:D:3756:LYS:NZ	2.34	0.61
1:B:1764:GLY:HA3	1:B:1859:VAL:HG11	1.83	0.60
1:B:119:SER:H	1:B:137:LEU:HA	1.66	0.60
1:B:4987:ASN:HA	1:B:4990:PHE:HD2	1.67	0.60
1:D:110:ARG:HH21	1:D:115:ARG:HB3	1.65	0.60
1:D:4987:ASN:HA	1:D:4990:PHE:HD2	1.66	0.60
1:B:4960:ILE:HD11	1:B:4985:LEU:HD23	1.83	0.60
1:A:3751:VAL:O	1:A:3756:LYS:NZ	2.34	0.60
1:C:733:PRO:HG2	1:C:763:PRO:HD2	1.82	0.60
1:C:3763:LEU:HD21	1:C:3807:GLY:HA3	1.84	0.60
1:D:853:PRO:HG3	1:D:1024:TYR:H	1.66	0.60
1:A:40:GLU:HB3	1:A:44:ASN:HB3	1.83	0.60
1:A:119:SER:H	1:A:137:LEU:HA	1.66	0.60
1:A:853:PRO:HG3	1:A:1024:TYR:H	1.66	0.60
1:A:1808:ARG:NH1	1:A:1853:ILE:O	2.34	0.60
1:B:494:LEU:HD22	1:B:515:TRP:HE1	1.65	0.60
1:B:3751:VAL:O	1:B:3756:LYS:NZ	2.34	0.60
1:D:119:SER:H	1:D:137:LEU:HA	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2318:TYR:HH	1:D:2414:ASN:N	2.00	0.60
1:A:3763:LEU:HD21	1:A:3807:GLY:HA3	1.83	0.60
1:B:4083:ASP:HA	1:B:4085:ARG:HH11	1.65	0.60
1:B:4864:ASN:ND2	1:B:4871:GLU:OE1	2.35	0.60
1:C:119:SER:H	1:C:137:LEU:HA	1.66	0.60
1:D:1764:GLY:HA3	1:D:1859:VAL:HG11	1.83	0.60
1:D:1808:ARG:NH1	1:D:1853:ILE:O	2.34	0.60
1:A:281:ARG:NH2	1:A:309:THR:OG1	2.35	0.59
1:D:281:ARG:NH2	1:D:309:THR:OG1	2.35	0.59
1:A:1764:GLY:HA3	1:A:1859:VAL:HG11	1.83	0.59
1:A:4960:ILE:HD11	1:A:4985:LEU:HD23	1.83	0.59
1:B:4001:MET:HE3	1:B:4057:MET:HE3	1.84	0.59
1:D:40:GLU:HB3	1:D:44:ASN:HB3	1.83	0.59
1:D:3763:LEU:HD21	1:D:3807:GLY:HA3	1.83	0.59
1:D:286:THR:HA	1:D:405:HIS:HB2	1.85	0.59
1:D:4001:MET:HE3	1:D:4057:MET:HE3	1.84	0.59
1:B:286:THR:HA	1:B:405:HIS:HB2	1.85	0.59
1:B:331:VAL:HG12	1:B:333:GLY:H	1.67	0.59
1:B:853:PRO:HG3	1:B:1024:TYR:H	1.66	0.59
1:C:683:ARG:NH1	1:C:707:VAL:O	2.36	0.59
1:C:853:PRO:HG3	1:C:1024:TYR:H	1.66	0.59
1:C:4987:ASN:HA	1:C:4990:PHE:HD2	1.67	0.59
1:B:1100:MET:HE2	1:B:1198:GLN:HB3	1.85	0.59
1:B:3763:LEU:HD21	1:B:3807:GLY:HA3	1.84	0.59
1:A:331:VAL:HG12	1:A:333:GLY:H	1.67	0.59
1:A:1105:ALA:HB1	1:A:1109:LEU:HD21	1.85	0.59
1:C:331:VAL:HG12	1:C:333:GLY:H	1.67	0.59
1:D:1105:ALA:HB1	1:D:1109:LEU:HD21	1.85	0.59
1:A:4001:MET:HE3	1:A:4057:MET:HE3	1.84	0.59
1:B:683:ARG:NH1	1:B:707:VAL:O	2.36	0.59
1:A:463:GLU:OE2	1:A:467:LYS:NZ	2.36	0.59
1:A:4987:ASN:HA	1:A:4990:PHE:HD2	1.67	0.59
1:B:40:GLU:HB3	1:B:44:ASN:HB3	1.83	0.59
1:C:281:ARG:NH2	1:C:309:THR:OG1	2.35	0.59
1:C:463:GLU:OE2	1:C:467:LYS:NZ	2.36	0.59
1:A:286:THR:HA	1:A:405:HIS:HB2	1.85	0.58
1:A:4864:ASN:ND2	1:A:4871:GLU:OE1	2.35	0.58
1:D:331:VAL:HG12	1:D:333:GLY:H	1.67	0.58
1:C:1105:ALA:HB1	1:C:1109:LEU:HD21	1.85	0.58
1:C:1960:ALA:O	1:C:1964:ARG:NE	2.37	0.58
1:D:683:ARG:NH1	1:D:707:VAL:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:ARG:NH2	1:B:309:THR:OG1	2.35	0.58
1:B:4864:ASN:H	1:B:4874:MET:HG2	1.68	0.58
1:A:1100:MET:HE2	1:A:1198:GLN:HB3	1.84	0.58
1:C:494:LEU:HD22	1:C:515:TRP:HE1	1.65	0.58
1:C:4001:MET:HE3	1:C:4057:MET:HE3	1.84	0.58
1:D:266:ARG:NH1	1:D:331:VAL:O	2.36	0.58
1:A:4104:THR:HG22	1:A:4106:PRO:HD2	1.85	0.58
1:B:4104:THR:HG22	1:B:4106:PRO:HD2	1.85	0.58
1:C:286:THR:HA	1:C:405:HIS:HB2	1.85	0.58
1:C:4864:ASN:H	1:C:4874:MET:HG2	1.68	0.58
1:D:463:GLU:OE2	1:D:467:LYS:NZ	2.36	0.58
1:A:609:CYS:SG	1:A:610:ASN:N	2.77	0.58
1:C:40:GLU:HB3	1:C:44:ASN:HB3	1.83	0.58
1:D:106:ALA:HA	1:D:149:THR:HA	1.85	0.58
1:A:3902:TYR:O	1:A:3906:GLN:NE2	2.37	0.58
1:B:463:GLU:OE2	1:B:467:LYS:NZ	2.36	0.58
1:D:1100:MET:HE2	1:D:1198:GLN:HB3	1.84	0.58
1:A:683:ARG:NH1	1:A:707:VAL:O	2.36	0.58
1:B:1105:ALA:HB1	1:B:1109:LEU:HD21	1.85	0.58
1:B:4180:ARG:HG3	1:B:4194:TYR:HE1	1.69	0.58
1:C:4180:ARG:HG3	1:C:4194:TYR:HE1	1.69	0.58
1:A:1778:SER:N	1:A:1799:SER:O	2.37	0.58
1:A:4864:ASN:H	1:A:4874:MET:HG2	1.68	0.58
1:D:4180:ARG:HG3	1:D:4194:TYR:HE1	1.69	0.58
1:B:106:ALA:HA	1:B:149:THR:HA	1.85	0.57
1:C:609:CYS:SG	1:C:610:ASN:N	2.77	0.57
1:D:717:ASP:OD1	1:D:720:HIS:ND1	2.37	0.57
1:A:57:ASN:HD22	1:A:308:HIS:HB2	1.69	0.57
1:A:1152:MET:HB2	1:A:1161:ILE:HB	1.86	0.57
1:A:2024:PRO:HB2	1:A:2027:ILE:HG12	1.86	0.57
1:B:57:ASN:HD22	1:B:308:HIS:HB2	1.70	0.57
1:B:717:ASP:OD1	1:B:720:HIS:ND1	2.37	0.57
1:C:1100:MET:HE2	1:C:1198:GLN:HB3	1.84	0.57
1:D:1721:GLU:OE2	1:D:1725:ARG:NH2	2.37	0.57
1:D:4104:THR:HG22	1:D:4106:PRO:HD2	1.85	0.57
1:D:4864:ASN:ND2	1:D:4871:GLU:OE1	2.34	0.57
1:C:717:ASP:OD1	1:C:720:HIS:ND1	2.37	0.57
1:C:4104:THR:HG22	1:C:4106:PRO:HD2	1.85	0.57
1:A:1721:GLU:OE2	1:A:1725:ARG:NH2	2.37	0.57
1:C:1152:MET:HB2	1:C:1161:ILE:HB	1.86	0.57
1:B:1152:MET:HB2	1:B:1161:ILE:HB	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:ASN:HD22	1:D:308:HIS:HB2	1.69	0.57
1:D:3902:TYR:O	1:D:3906:GLN:NE2	2.37	0.57
1:A:106:ALA:HA	1:A:149:THR:HA	1.85	0.57
1:A:717:ASP:OD1	1:A:720:HIS:ND1	2.37	0.57
1:A:4180:ARG:HG3	1:A:4194:TYR:HE1	1.69	0.57
1:C:1778:SER:N	1:C:1799:SER:O	2.37	0.57
1:C:106:ALA:HA	1:C:149:THR:HA	1.85	0.57
1:B:3927:GLN:NE2	1:B:3988:ALA:O	2.34	0.57
1:D:1960:ALA:O	1:D:1964:ARG:NE	2.37	0.57
1:A:3927:GLN:NE2	1:A:3988:ALA:O	2.34	0.57
1:C:4864:ASN:ND2	1:C:4871:GLU:OE1	2.35	0.57
1:D:3927:GLN:NE2	1:D:3988:ALA:O	2.34	0.57
1:A:120:CYS:SG	1:A:121:LEU:N	2.78	0.57
1:C:266:ARG:NH1	1:C:331:VAL:O	2.36	0.57
1:C:3902:TYR:O	1:C:3906:GLN:NE2	2.37	0.57
1:D:2024:PRO:HB2	1:D:2027:ILE:HG12	1.86	0.57
1:D:3767:GLN:NE2	1:D:3804:ILE:O	2.38	0.57
1:A:2535:UNK:O	1:A:2540:UNK:N	2.38	0.56
1:B:1721:GLU:OE2	1:B:1725:ARG:NH2	2.37	0.56
1:A:266:ARG:NH1	1:A:331:VAL:O	2.36	0.56
1:A:3767:GLN:NE2	1:A:3804:ILE:O	2.38	0.56
1:B:120:CYS:SG	1:B:121:LEU:N	2.78	0.56
1:D:3772:THR:OG1	1:D:3815:LYS:NZ	2.37	0.56
1:B:4704:LEU:HD21	1:B:4774:LYS:HG2	1.87	0.56
1:C:1721:GLU:OE2	1:C:1725:ARG:NH2	2.37	0.56
1:D:120:CYS:SG	1:D:121:LEU:N	2.78	0.56
1:D:1152:MET:HB2	1:D:1161:ILE:HB	1.86	0.56
1:D:2535:UNK:O	1:D:2540:UNK:N	2.38	0.56
1:D:4864:ASN:H	1:D:4874:MET:HG2	1.68	0.56
1:C:4582:VAL:HG11	1:D:4860:ARG:HD2	1.87	0.56
1:C:4702:ASP:OD1	1:C:4778:TRP:NE1	2.33	0.56
1:B:2042:CYS:SG	1:B:2043:GLY:N	2.79	0.56
1:C:2737:PRO:O	1:C:2888:ARG:NH2	2.39	0.56
1:C:3767:GLN:NE2	1:C:3804:ILE:O	2.38	0.56
1:A:4704:LEU:HD21	1:A:4774:LYS:HG2	1.87	0.56
1:B:3767:GLN:NE2	1:B:3804:ILE:O	2.38	0.56
1:C:57:ASN:HD22	1:C:308:HIS:HB2	1.69	0.56
1:C:2024:PRO:HB2	1:C:2027:ILE:HG12	1.86	0.56
1:A:3830:GLN:HA	1:A:3833:GLN:HG2	1.87	0.56
1:B:1778:SER:N	1:B:1799:SER:O	2.37	0.56
1:C:2535:UNK:O	1:C:2540:UNK:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3927:GLN:NE2	1:C:3988:ALA:O	2.34	0.56
1:A:2420:HIS:ND1	1:A:2523:UNK:O	2.37	0.56
1:A:2830:GLU:HB2	1:A:2932:MET:HE2	1.88	0.56
1:B:2535:UNK:O	1:B:2540:UNK:N	2.38	0.56
1:C:120:CYS:SG	1:C:121:LEU:N	2.78	0.56
1:C:3830:GLN:HA	1:C:3833:GLN:HG2	1.87	0.56
1:B:2830:GLU:HB2	1:B:2932:MET:HE2	1.88	0.56
1:C:2042:CYS:SG	1:C:2043:GLY:N	2.79	0.56
1:D:609:CYS:SG	1:D:610:ASN:N	2.77	0.56
1:D:2830:GLU:HB2	1:D:2932:MET:HE2	1.88	0.56
1:D:4704:LEU:HD21	1:D:4774:LYS:HG2	1.87	0.56
1:A:500:ALA:H	1:A:503:PHE:HB3	1.71	0.56
1:A:2737:PRO:O	1:A:2888:ARG:NH2	2.39	0.56
1:B:3902:TYR:O	1:B:3906:GLN:NE2	2.37	0.56
1:D:315:CYS:SG	1:D:316:PHE:N	2.79	0.56
1:B:500:ALA:H	1:B:503:PHE:HB3	1.72	0.55
1:B:2024:PRO:HB2	1:B:2027:ILE:HG12	1.86	0.55
1:C:1284:UNK:HA	1:C:1471:UNK:HA	1.88	0.55
1:C:4704:LEU:HD21	1:C:4774:LYS:HG2	1.87	0.55
1:A:3981:ALA:HA	1:A:3986:TRP:HE1	1.71	0.55
1:B:1284:UNK:HA	1:B:1471:UNK:HA	1.88	0.55
1:A:4958:CYS:SG	1:A:4978:HIS:NE2	2.65	0.55
1:B:2737:PRO:O	1:B:2888:ARG:NH2	2.39	0.55
1:C:2830:GLU:HB2	1:C:2932:MET:HE2	1.88	0.55
1:D:500:ALA:H	1:D:503:PHE:HB3	1.72	0.55
1:D:3830:GLN:HA	1:D:3833:GLN:HG2	1.87	0.55
1:C:111:HIS:HD2	1:C:114:SER:H	1.53	0.55
1:D:4998:LYS:NZ	1:D:5007:GLU:OE1	2.40	0.55
1:B:609:CYS:SG	1:B:610:ASN:N	2.77	0.55
1:D:313:SER:HB3	1:D:351:VAL:HB	1.88	0.55
1:D:3980:LEU:HD22	1:D:3985:LEU:HD22	1.89	0.55
1:A:111:HIS:HD2	1:A:114:SER:H	1.53	0.55
1:A:3980:LEU:HD22	1:A:3985:LEU:HD22	1.89	0.55
1:D:1778:SER:N	1:D:1799:SER:O	2.37	0.55
1:D:2189:LYS:HA	1:D:2192:TYR:HD2	1.72	0.55
1:A:16:THR:OG1	1:A:98:HIS:ND1	2.40	0.55
1:A:2189:LYS:HA	1:A:2192:TYR:HD2	1.72	0.55
1:A:3696:ASP:O	1:A:3700:GLN:N	2.36	0.55
1:C:500:ALA:H	1:C:503:PHE:HB3	1.71	0.55
1:C:2121:PHE:O	1:C:3725:TYR:OH	2.25	0.55
1:D:1073:ARG:O	1:D:1194:LEU:N	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:ARG:NH1	1:B:331:VAL:O	2.36	0.55
1:B:3980:LEU:HD22	1:B:3985:LEU:HD22	1.89	0.55
1:B:4685:GLY:O	1:B:4689:THR:N	2.39	0.55
1:B:315:CYS:SG	1:B:316:PHE:N	2.79	0.55
1:D:2737:PRO:O	1:D:2888:ARG:NH2	2.39	0.55
1:A:889:GLN:O	1:A:902:ARG:NH1	2.40	0.54
1:B:313:SER:HB3	1:B:351:VAL:HB	1.88	0.54
1:B:889:GLN:O	1:B:902:ARG:NH1	2.40	0.54
1:B:1288:UNK:O	1:B:1598:GLN:N	2.40	0.54
1:C:3980:LEU:HD22	1:C:3985:LEU:HD22	1.89	0.54
1:D:1284:UNK:HA	1:D:1471:UNK:HA	1.88	0.54
1:B:2267:MET:HE3	1:B:2268:GLN:HG2	1.89	0.54
1:B:3830:GLN:HA	1:B:3833:GLN:HG2	1.88	0.54
1:C:2189:LYS:HA	1:C:2192:TYR:HD2	1.72	0.54
1:C:2267:MET:HE3	1:C:2268:GLN:HG2	1.90	0.54
1:C:4904:PRO:HB3	1:C:4913:ARG:HD3	1.89	0.54
1:D:16:THR:OG1	1:D:98:HIS:ND1	2.40	0.54
1:A:1284:UNK:HA	1:A:1471:UNK:HA	1.88	0.54
1:C:16:THR:OG1	1:C:98:HIS:ND1	2.40	0.54
1:C:620:LEU:O	1:C:624:ASN:HB2	2.08	0.54
1:D:110:ARG:HA	1:D:117:TYR:HA	1.90	0.54
1:D:111:HIS:HD2	1:D:114:SER:H	1.53	0.54
1:D:637:LEU:HD23	1:D:1637:MET:HB3	1.89	0.54
1:A:313:SER:HB3	1:A:351:VAL:HB	1.88	0.54
1:A:315:CYS:SG	1:A:316:PHE:N	2.79	0.54
1:D:1743:ARG:O	1:D:1964:ARG:NH2	2.39	0.54
1:A:110:ARG:HA	1:A:117:TYR:HA	1.90	0.54
1:A:1697:ALA:HA	1:A:1708:ARG:HD2	1.89	0.54
1:A:1948:ASP:OD1	1:A:2126:ARG:NH2	2.40	0.54
1:A:2121:PHE:O	1:A:3725:TYR:OH	2.25	0.54
1:A:2894:LEU:HD23	1:A:2897:LYS:HD2	1.89	0.54
1:B:620:LEU:O	1:B:624:ASN:HB2	2.08	0.54
1:B:1743:ARG:O	1:B:1964:ARG:NH2	2.39	0.54
1:B:4998:LYS:NZ	1:B:5007:GLU:OE1	2.40	0.54
1:C:3772:THR:OG1	1:C:3815:LYS:NZ	2.37	0.54
1:A:4177:TYR:HA	1:A:4197:ILE:HB	1.90	0.54
1:B:1948:ASP:OD1	1:B:2126:ARG:NH2	2.40	0.54
1:C:972:LEU:O	1:C:1044:ARG:NH2	2.41	0.54
1:D:3981:ALA:HA	1:D:3986:TRP:HE1	1.72	0.54
1:D:4177:TYR:HA	1:D:4197:ILE:HB	1.90	0.54
1:A:637:LEU:HD23	1:A:1637:MET:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:972:LEU:O	1:B:1044:ARG:NH2	2.41	0.54
1:C:313:SER:HB3	1:C:351:VAL:HB	1.88	0.54
1:C:2894:LEU:HD23	1:C:2897:LYS:HD2	1.89	0.54
1:C:4685:GLY:O	1:C:4689:THR:N	2.39	0.54
1:D:889:GLN:O	1:D:902:ARG:NH1	2.40	0.54
1:D:1948:ASP:OD1	1:D:2126:ARG:NH2	2.40	0.54
1:D:2440:MET:O	1:D:2444:GLN:N	2.41	0.54
1:D:3428:UNK:O	1:D:3432:UNK:N	2.41	0.54
1:A:2384:ILE:HD11	1:A:2472:LEU:HD21	1.90	0.54
1:C:315:CYS:SG	1:C:316:PHE:N	2.79	0.54
1:C:1679:ASN:HA	1:C:1682:ALA:HB3	1.90	0.54
1:C:2440:MET:O	1:C:2444:GLN:N	2.41	0.54
1:C:3981:ALA:HA	1:C:3986:TRP:HE1	1.72	0.54
1:D:4904:PRO:HB3	1:D:4913:ARG:HD3	1.90	0.54
1:B:16:THR:OG1	1:B:98:HIS:ND1	2.40	0.54
1:B:3981:ALA:HA	1:B:3986:TRP:HE1	1.72	0.54
1:C:889:GLN:O	1:C:902:ARG:NH1	2.40	0.54
1:C:2130:GLY:O	1:C:2134:LEU:HB2	2.08	0.54
1:C:2617:UNK:O	1:C:2621:UNK:N	2.41	0.54
1:A:1802:ILE:HG21	1:A:1807:LEU:HD22	1.89	0.54
1:B:111:HIS:HD2	1:B:114:SER:H	1.53	0.54
1:B:1259:ARG:NH1	1:B:1592:PRO:O	2.40	0.54
1:B:4182:GLU:HA	1:B:4192:ARG:HA	1.90	0.54
1:C:395:GLN:NE2	1:C:397:GLU:OE1	2.41	0.54
1:C:637:LEU:HD23	1:C:1637:MET:HB3	1.89	0.54
1:C:1948:ASP:OD1	1:C:2126:ARG:NH2	2.40	0.54
1:D:620:LEU:O	1:D:624:ASN:HB2	2.08	0.54
1:D:2130:GLY:O	1:D:2134:LEU:HB2	2.08	0.54
1:D:2384:ILE:HD11	1:D:2472:LEU:HD21	1.90	0.54
1:A:620:LEU:O	1:A:624:ASN:HB2	2.08	0.53
1:A:972:LEU:O	1:A:1044:ARG:NH2	2.41	0.53
1:A:1960:ALA:O	1:A:1964:ARG:NE	2.37	0.53
1:A:3772:THR:OG1	1:A:3815:LYS:NZ	2.37	0.53
1:A:4724:VAL:O	1:A:4728:HIS:N	2.40	0.53
1:B:1960:ALA:O	1:B:1964:ARG:NE	2.37	0.53
1:B:2121:PHE:O	1:B:3725:TYR:OH	2.25	0.53
1:B:2384:ILE:HD11	1:B:2472:LEU:HD21	1.90	0.53
1:D:1802:ILE:HG21	1:D:1807:LEU:HD22	1.89	0.53
1:A:1073:ARG:O	1:A:1194:LEU:N	2.38	0.53
1:A:2327:GLY:O	1:A:2331:TYR:N	2.40	0.53
1:A:3428:UNK:O	1:A:3432:UNK:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4873:ASP:OD1	1:A:4875:LYS:NZ	2.40	0.53
1:A:4998:LYS:NZ	1:A:5007:GLU:OE1	2.40	0.53
1:B:1802:ILE:HG21	1:B:1807:LEU:HD22	1.90	0.53
1:B:2617:UNK:O	1:B:2621:UNK:N	2.41	0.53
1:B:3428:UNK:O	1:B:3432:UNK:N	2.41	0.53
1:B:3772:THR:OG1	1:B:3815:LYS:NZ	2.37	0.53
1:B:4580:TYR:HB2	1:C:4879:MET:HB2	1.90	0.53
1:C:110:ARG:HA	1:C:117:TYR:HA	1.90	0.53
1:D:4230:LYS:HE3	1:D:4231:MET:HE2	1.91	0.53
1:B:1679:ASN:HA	1:B:1682:ALA:HB3	1.90	0.53
1:C:1697:ALA:HA	1:C:1708:ARG:HD2	1.89	0.53
1:C:1802:ILE:HG21	1:C:1807:LEU:HD22	1.89	0.53
1:C:4133:GLN:HE21	1:C:4137:ARG:HD3	1.74	0.53
1:D:395:GLN:NE2	1:D:397:GLU:OE1	2.42	0.53
1:D:1697:ALA:HA	1:D:1708:ARG:HD2	1.89	0.53
1:D:1727:ARG:HH12	1:D:1773:PRO:HD2	1.73	0.53
1:D:4133:GLN:HE21	1:D:4137:ARG:HD3	1.74	0.53
1:B:4133:GLN:HE21	1:B:4137:ARG:HD3	1.74	0.53
1:C:1667:LEU:HD23	1:C:1671:ARG:HH12	1.74	0.53
1:C:2384:ILE:HD11	1:C:2472:LEU:HD21	1.90	0.53
1:C:3428:UNK:O	1:C:3432:UNK:N	2.41	0.53
1:D:1259:ARG:NH1	1:D:1592:PRO:O	2.40	0.53
1:A:111:HIS:CD2	1:A:114:SER:H	2.27	0.53
1:A:2617:UNK:O	1:A:2621:UNK:N	2.41	0.53
1:A:4904:PRO:HB3	1:A:4913:ARG:HD3	1.89	0.53
1:B:485:SER:HA	1:B:488:LEU:HB2	1.91	0.53
1:B:637:LEU:HD23	1:B:1637:MET:HB3	1.89	0.53
1:B:1667:LEU:HD23	1:B:1671:ARG:HH12	1.74	0.53
1:B:2894:LEU:HD23	1:B:2897:LYS:HD2	1.89	0.53
1:C:2339:VAL:HG11	1:C:2344:GLU:HA	1.91	0.53
1:C:4230:LYS:HE3	1:C:4231:MET:HE2	1.91	0.53
1:C:4998:LYS:NZ	1:C:5007:GLU:OE1	2.40	0.53
1:D:972:LEU:O	1:D:1044:ARG:NH2	2.41	0.53
1:D:2420:HIS:ND1	1:D:2523:UNK:O	2.37	0.53
1:A:744:VAL:HG22	1:A:759:ILE:HG12	1.91	0.53
1:A:2352:VAL:HG12	1:A:2355:ARG:HH11	1.73	0.53
1:A:2440:MET:O	1:A:2444:GLN:N	2.41	0.53
1:A:4685:GLY:O	1:A:4689:THR:N	2.39	0.53
1:B:395:GLN:NE2	1:B:397:GLU:OE1	2.41	0.53
1:B:4177:TYR:HA	1:B:4197:ILE:HB	1.90	0.53
1:B:4977:THR:O	1:B:4981:GLU:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4177:TYR:HA	1:C:4197:ILE:HB	1.90	0.53
1:D:1679:ASN:HA	1:D:1682:ALA:HB3	1.90	0.53
1:D:2617:UNK:O	1:D:2621:UNK:N	2.41	0.53
1:A:2130:GLY:O	1:A:2134:LEU:HB2	2.08	0.53
1:B:4230:LYS:HE3	1:B:4231:MET:HE2	1.91	0.53
1:C:3955:MET:HG3	1:C:4019:LEU:HD22	1.91	0.53
1:D:3955:MET:HG3	1:D:4019:LEU:HD22	1.91	0.53
1:A:395:GLN:NE2	1:A:397:GLU:OE1	2.42	0.53
1:A:1679:ASN:HA	1:A:1682:ALA:HB3	1.90	0.53
1:A:4687:TYR:OH	1:A:4699:GLY:O	2.27	0.53
1:B:2440:MET:O	1:B:2444:GLN:N	2.41	0.53
1:B:4088:ILE:HG23	1:B:4123:ILE:HB	1.90	0.53
1:B:4724:VAL:O	1:B:4728:HIS:N	2.40	0.53
1:C:1727:ARG:HH12	1:C:1773:PRO:HD2	1.73	0.53
1:C:2352:VAL:HG12	1:C:2355:ARG:HH11	1.73	0.53
1:D:4182:GLU:HA	1:D:4192:ARG:HA	1.90	0.53
1:A:838:HIS:HA	1:A:1201:HIS:HB3	1.91	0.53
1:A:4182:GLU:HA	1:A:4192:ARG:HA	1.90	0.53
1:A:4702:ASP:OD1	1:A:4778:TRP:NE1	2.33	0.53
1:B:111:HIS:CD2	1:B:114:SER:H	2.27	0.53
1:B:838:HIS:HA	1:B:1201:HIS:HB3	1.91	0.53
1:B:2189:LYS:HA	1:B:2192:TYR:HD2	1.72	0.53
1:B:2339:VAL:HG11	1:B:2344:GLU:HA	1.90	0.53
1:B:2420:HIS:ND1	1:B:2523:UNK:O	2.37	0.53
1:B:4904:PRO:HB3	1:B:4913:ARG:HD3	1.90	0.53
1:C:168:ASP:HB3	1:C:199:LEU:HD22	1.91	0.53
1:D:2267:MET:HE3	1:D:2268:GLN:HG2	1.90	0.53
1:A:4230:LYS:HE3	1:A:4231:MET:HE2	1.91	0.53
1:B:2352:VAL:HG12	1:B:2355:ARG:HH11	1.73	0.53
1:B:110:ARG:HA	1:B:117:TYR:HA	1.90	0.52
1:D:111:HIS:CD2	1:D:114:SER:H	2.27	0.52
1:D:120:CYS:HA	1:D:136:GLY:H	1.74	0.52
1:D:1667:LEU:HD23	1:D:1671:ARG:HH12	1.74	0.52
1:D:2894:LEU:HD23	1:D:2897:LYS:HD2	1.89	0.52
1:D:3696:ASP:O	1:D:3700:GLN:N	2.36	0.52
1:A:1288:UNK:O	1:A:1598:GLN:N	2.39	0.52
1:A:1667:LEU:HD23	1:A:1671:ARG:HH12	1.74	0.52
1:A:2267:MET:HE3	1:A:2268:GLN:HG2	1.89	0.52
1:A:4860:ARG:HD2	1:D:4582:VAL:HG11	1.92	0.52
1:B:168:ASP:HB3	1:B:199:LEU:HD22	1.91	0.52
1:B:1697:ALA:HA	1:B:1708:ARG:HD2	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1727:ARG:HH12	1:B:1773:PRO:HD2	1.74	0.52
1:B:1739:THR:OG1	1:B:1742:THR:N	2.41	0.52
1:B:2327:GLY:O	1:B:2331:TYR:N	2.40	0.52
1:C:4088:ILE:HG23	1:C:4123:ILE:HB	1.90	0.52
1:D:842:PRO:HD3	1:D:1073:ARG:HG3	1.92	0.52
1:D:2339:VAL:HG11	1:D:2344:GLU:HA	1.91	0.52
1:D:4687:TYR:OH	1:D:4699:GLY:O	2.27	0.52
1:B:842:PRO:HD3	1:B:1073:ARG:HG3	1.92	0.52
1:B:4201:ASN:HA	1:B:4204:GLN:HB2	1.92	0.52
1:C:485:SER:HA	1:C:488:LEU:HB2	1.91	0.52
1:C:838:HIS:HA	1:C:1201:HIS:HB3	1.91	0.52
1:A:120:CYS:HA	1:A:136:GLY:H	1.74	0.52
1:A:842:PRO:HD3	1:A:1073:ARG:HG3	1.92	0.52
1:A:3955:MET:HG3	1:A:4019:LEU:HD22	1.91	0.52
1:B:3937:TYR:O	1:B:4002:LYS:NZ	2.43	0.52
1:C:1148:VAL:HB	1:C:1165:ASN:HA	1.91	0.52
1:C:4182:GLU:HA	1:C:4192:ARG:HA	1.90	0.52
1:C:4678:ALA:O	1:C:4682:GLU:CB	2.58	0.52
1:D:1478:UNK:HA	1:D:1495:UNK:HA	1.92	0.52
1:D:2352:VAL:HG12	1:D:2355:ARG:HH11	1.73	0.52
1:D:4088:ILE:HG23	1:D:4123:ILE:HB	1.90	0.52
1:D:4724:VAL:O	1:D:4728:HIS:N	2.40	0.52
1:A:4133:GLN:HE21	1:A:4137:ARG:HD3	1.74	0.52
1:A:4201:ASN:HA	1:A:4204:GLN:HB2	1.92	0.52
1:A:4678:ALA:O	1:A:4682:GLU:CB	2.58	0.52
1:B:744:VAL:HG22	1:B:759:ILE:HG12	1.91	0.52
1:B:1076:ARG:HB3	1:B:1191:VAL:HG23	1.92	0.52
1:B:4678:ALA:O	1:B:4682:GLU:CB	2.58	0.52
1:C:111:HIS:CD2	1:C:114:SER:H	2.27	0.52
1:D:1076:ARG:HB3	1:D:1191:VAL:HG23	1.92	0.52
1:D:1148:VAL:HB	1:D:1165:ASN:HA	1.91	0.52
1:A:1076:ARG:HB3	1:A:1191:VAL:HG23	1.92	0.52
1:B:120:CYS:HA	1:B:136:GLY:H	1.74	0.52
1:D:744:VAL:HG22	1:D:759:ILE:HG12	1.91	0.52
1:A:1727:ARG:HH12	1:A:1773:PRO:HD2	1.74	0.52
1:A:4088:ILE:HG23	1:A:4123:ILE:HB	1.90	0.52
1:C:842:PRO:HD3	1:C:1073:ARG:HG3	1.92	0.52
1:D:838:HIS:HA	1:D:1201:HIS:HB3	1.91	0.52
1:D:4685:GLY:O	1:D:4689:THR:N	2.39	0.52
1:C:1478:UNK:HA	1:C:1495:UNK:HA	1.92	0.52
1:A:742:ASP:HA	1:A:760:ASN:HD21	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2339:VAL:HG11	1:A:2344:GLU:HA	1.90	0.52
1:B:3121:UNK:O	1:B:3125:UNK:N	2.43	0.52
1:C:3121:UNK:O	1:C:3125:UNK:N	2.43	0.52
1:A:235:ALA:HA	1:A:257:ARG:HD3	1.92	0.52
1:B:235:ALA:HA	1:B:257:ARG:HD3	1.92	0.52
1:B:2130:GLY:O	1:B:2134:LEU:HB2	2.08	0.52
1:C:744:VAL:HG22	1:C:759:ILE:HG12	1.91	0.52
1:C:1229:ASN:HB3	1:C:1827:ARG:H	1.75	0.52
1:C:2420:HIS:ND1	1:C:2523:UNK:O	2.37	0.52
1:D:4201:ASN:HA	1:D:4204:GLN:HB2	1.92	0.52
1:A:485:SER:HA	1:A:488:LEU:HB2	1.91	0.51
1:B:4702:ASP:OD1	1:B:4778:TRP:NE1	2.33	0.51
1:C:1259:ARG:NH1	1:C:1592:PRO:O	2.40	0.51
1:A:709:ASP:HA	1:A:725:HIS:H	1.76	0.51
1:A:1148:VAL:HB	1:A:1165:ASN:HA	1.91	0.51
1:B:742:ASP:HA	1:B:760:ASN:HD21	1.75	0.51
1:B:4873:ASP:OD1	1:B:4875:LYS:NZ	2.40	0.51
1:C:1076:ARG:HB3	1:C:1191:VAL:HG23	1.92	0.51
1:C:1743:ARG:O	1:C:1964:ARG:NH2	2.39	0.51
1:D:485:SER:HA	1:D:488:LEU:HB2	1.91	0.51
1:A:913:LEU:O	1:A:918:ARG:NH2	2.44	0.51
1:B:3955:MET:HG3	1:B:4019:LEU:HD22	1.91	0.51
1:C:1465:UNK:O	1:C:1505:UNK:N	2.44	0.51
1:D:168:ASP:HB3	1:D:199:LEU:HD22	1.91	0.51
1:D:3121:UNK:O	1:D:3125:UNK:N	2.43	0.51
1:A:3937:TYR:O	1:A:4002:LYS:NZ	2.43	0.51
1:A:4232:GLU:OE2	1:A:5017:ARG:NH1	2.43	0.51
1:B:1229:ASN:HB3	1:B:1827:ARG:H	1.75	0.51
1:C:742:ASP:HA	1:C:760:ASN:HD21	1.75	0.51
1:C:3937:TYR:O	1:C:4002:LYS:NZ	2.43	0.51
1:D:742:ASP:HA	1:D:760:ASN:HD21	1.75	0.51
1:D:864:PRO:O	1:D:868:GLU:N	2.42	0.51
1:D:1229:ASN:HB3	1:D:1827:ARG:H	1.75	0.51
1:A:168:ASP:HB3	1:A:199:LEU:HD22	1.91	0.51
1:A:1739:THR:OG1	1:A:1742:THR:N	2.41	0.51
1:A:3121:UNK:O	1:A:3125:UNK:N	2.43	0.51
1:B:709:ASP:HA	1:B:725:HIS:H	1.76	0.51
1:B:788:LYS:HG2	1:B:1630:CYS:H	1.75	0.51
1:B:1152:MET:HE1	1:B:1217:CYS:HB3	1.93	0.51
1:C:120:CYS:HA	1:C:136:GLY:H	1.74	0.51
1:C:1152:MET:HE1	1:C:1217:CYS:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4201:ASN:HA	1:C:4204:GLN:HB2	1.92	0.51
1:D:4873:ASP:OD1	1:D:4875:LYS:NZ	2.40	0.51
1:A:1152:MET:HE1	1:A:1217:CYS:HB3	1.93	0.51
1:B:913:LEU:O	1:B:918:ARG:NH2	2.44	0.51
1:B:1148:VAL:HB	1:B:1165:ASN:HA	1.91	0.51
1:C:3696:ASP:O	1:C:3700:GLN:N	2.36	0.51
1:A:646:PRO:HD2	1:A:779:PRO:HB2	1.92	0.51
1:A:1478:UNK:HA	1:A:1495:UNK:HA	1.92	0.51
1:B:229:GLU:HA	1:B:249:GLY:HA2	1.93	0.51
1:B:646:PRO:HD2	1:B:779:PRO:HB2	1.92	0.51
1:C:235:ALA:HA	1:C:257:ARG:HD3	1.93	0.51
1:C:646:PRO:HD2	1:C:779:PRO:HB2	1.92	0.51
1:C:3734:HIS:O	1:C:3738:GLY:N	2.40	0.51
1:C:3960:GLN:HA	1:C:3963:ASN:HD22	1.76	0.51
1:D:1288:UNK:O	1:D:1598:GLN:N	2.40	0.51
1:A:3960:GLN:HA	1:A:3963:ASN:HD22	1.76	0.51
1:B:4687:TYR:OH	1:B:4699:GLY:O	2.27	0.51
1:C:1468:UNK:HA	1:C:1502:UNK:HA	1.93	0.51
1:C:3992:PHE:HB2	1:C:4023:MET:HE1	1.93	0.51
1:A:229:GLU:HA	1:A:249:GLY:HA2	1.93	0.51
1:A:4701:TRP:HE1	1:A:4782:VAL:HG23	1.75	0.51
1:B:3992:PHE:HB2	1:B:4023:MET:HE1	1.93	0.51
1:C:1527:UNK:HA	1:C:1534:UNK:HA	1.93	0.51
1:D:709:ASP:HA	1:D:725:HIS:H	1.76	0.51
1:D:1739:THR:OG1	1:D:1742:THR:N	2.41	0.51
1:D:3992:PHE:HB2	1:D:4023:MET:HE1	1.93	0.51
1:A:1468:UNK:HA	1:A:1502:UNK:HA	1.93	0.51
1:A:2354:VAL:HA	1:A:2357:LEU:HB3	1.93	0.51
1:B:2354:VAL:HA	1:B:2357:LEU:HB3	1.93	0.51
1:D:235:ALA:HA	1:D:257:ARG:HD3	1.93	0.51
1:D:788:LYS:HG2	1:D:1630:CYS:H	1.75	0.51
1:D:1830:VAL:HB	1:D:1837:GLN:HA	1.94	0.51
1:D:2354:VAL:HA	1:D:2357:LEU:HB3	1.93	0.51
1:D:4178:LEU:HD11	1:D:4194:TYR:HB3	1.93	0.51
1:A:842:PRO:O	1:A:1197:GLY:N	2.45	0.50
1:A:3698:LEU:HD23	1:A:3771:HIS:HD2	1.76	0.50
1:A:3992:PHE:HB2	1:A:4023:MET:HE1	1.93	0.50
1:B:1465:UNK:O	1:B:1505:UNK:N	2.44	0.50
1:C:229:GLU:HA	1:C:249:GLY:HA2	1.93	0.50
1:C:788:LYS:HG2	1:C:1630:CYS:H	1.75	0.50
1:C:913:LEU:O	1:C:918:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4687:TYR:OH	1:C:4699:GLY:O	2.27	0.50
1:D:646:PRO:HD2	1:D:779:PRO:HB2	1.92	0.50
1:D:1739:THR:H	1:D:1742:THR:HB	1.76	0.50
1:D:2327:GLY:O	1:D:2331:TYR:N	2.40	0.50
1:D:4701:TRP:HE1	1:D:4782:VAL:HG23	1.76	0.50
1:A:1739:THR:H	1:A:1742:THR:HB	1.76	0.50
1:A:1830:VAL:HB	1:A:1837:GLN:HA	1.93	0.50
1:B:1478:UNK:HA	1:B:1495:UNK:HA	1.92	0.50
1:B:3923:LEU:O	1:B:3927:GLN:HB2	2.12	0.50
1:B:3960:GLN:HA	1:B:3963:ASN:HD22	1.76	0.50
1:C:658:GLN:O	1:C:662:TRP:NE1	2.36	0.50
1:C:709:ASP:HA	1:C:725:HIS:H	1.76	0.50
1:C:2354:VAL:HA	1:C:2357:LEU:HB3	1.93	0.50
1:C:4178:LEU:HD11	1:C:4194:TYR:HB3	1.93	0.50
1:D:3698:LEU:HD23	1:D:3771:HIS:HD2	1.75	0.50
1:D:4958:CYS:SG	1:D:4978:HIS:NE2	2.65	0.50
1:D:4977:THR:O	1:D:4981:GLU:N	2.40	0.50
1:A:952:LYS:HB3	1:A:968:ALA:HB1	1.93	0.50
1:A:1527:UNK:HA	1:A:1534:UNK:HA	1.93	0.50
1:B:109:LEU:O	1:B:118:LEU:N	2.43	0.50
1:C:1092:PHE:N	1:C:1149:VAL:O	2.42	0.50
1:C:1288:UNK:O	1:C:1598:GLN:N	2.40	0.50
1:C:3698:LEU:HD23	1:C:3771:HIS:HD2	1.76	0.50
1:D:2121:PHE:O	1:D:3725:TYR:OH	2.25	0.50
1:A:1465:UNK:O	1:A:1505:UNK:N	2.44	0.50
1:B:1526:UNK:O	1:B:1535:UNK:N	2.45	0.50
1:B:1739:THR:H	1:B:1742:THR:HB	1.76	0.50
1:B:4178:LEU:HD11	1:B:4194:TYR:HB3	1.93	0.50
1:A:621:ILE:O	1:A:625:LEU:N	2.39	0.50
1:C:4701:TRP:HE1	1:C:4782:VAL:HG23	1.76	0.50
1:D:660:GLY:HA2	1:D:750:LEU:HD12	1.94	0.50
1:D:913:LEU:O	1:D:918:ARG:NH2	2.44	0.50
1:D:1526:UNK:O	1:D:1535:UNK:N	2.45	0.50
1:D:3923:LEU:O	1:D:3927:GLN:HB2	2.12	0.50
1:D:3962:PHE:HA	1:D:3965:LEU:HD12	1.94	0.50
1:A:1229:ASN:HB3	1:A:1827:ARG:H	1.75	0.50
1:A:1506:UNK:N	1:A:1542:UNK:O	2.45	0.50
1:C:952:LYS:HB3	1:C:968:ALA:HB1	1.93	0.50
1:C:2272:PRO:HA	1:C:2275:VAL:HG12	1.94	0.50
1:C:3778:MET:HA	1:C:3781:GLN:HG2	1.94	0.50
1:D:1465:UNK:O	1:D:1505:UNK:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1843:LYS:HB2	1:D:1938:GLN:HE22	1.76	0.50
1:D:4763:GLY:O	1:D:4766:THR:OG1	2.28	0.50
1:A:426:ARG:NH1	1:A:429:GLY:O	2.45	0.50
1:A:1106:ARG:HB2	1:A:1120:LEU:HD12	1.93	0.50
1:A:1843:LYS:HB2	1:A:1938:GLN:HE22	1.76	0.50
1:A:3923:LEU:O	1:A:3927:GLN:HB2	2.11	0.50
1:A:4178:LEU:HD11	1:A:4194:TYR:HB3	1.93	0.50
1:B:658:GLN:O	1:B:662:TRP:NE1	2.36	0.50
1:B:952:LYS:HB3	1:B:968:ALA:HB1	1.93	0.50
1:B:1073:ARG:O	1:B:1194:LEU:N	2.38	0.50
1:B:1830:VAL:HB	1:B:1837:GLN:HA	1.93	0.50
1:B:2212:VAL:HA	1:B:2215:LEU:HB2	1.94	0.50
1:C:1073:ARG:O	1:C:1194:LEU:N	2.38	0.50
1:C:1739:THR:H	1:C:1742:THR:HB	1.76	0.50
1:C:3962:PHE:HA	1:C:3965:LEU:HD12	1.94	0.50
1:D:1152:MET:HE1	1:D:1217:CYS:HB3	1.93	0.50
1:D:3937:TYR:O	1:D:4002:LYS:NZ	2.43	0.50
1:A:660:GLY:HA2	1:A:750:LEU:HD12	1.94	0.50
1:A:1743:ARG:O	1:A:1964:ARG:NH2	2.39	0.50
1:B:426:ARG:HE	1:B:431:PRO:HA	1.77	0.50
1:B:4701:TRP:HE1	1:B:4782:VAL:HG23	1.75	0.50
1:C:3923:LEU:O	1:C:3927:GLN:HB2	2.11	0.50
1:C:4232:GLU:OE2	1:C:5017:ARG:NH1	2.43	0.50
1:D:4192:ARG:NH1	1:D:4982:GLU:OE2	2.45	0.50
1:B:3698:LEU:HD23	1:B:3771:HIS:HD2	1.76	0.50
1:C:426:ARG:NH1	1:C:429:GLY:O	2.45	0.50
1:C:2327:GLY:O	1:C:2331:TYR:N	2.40	0.50
1:C:4192:ARG:NH1	1:C:4982:GLU:OE2	2.45	0.50
1:D:21:VAL:HG22	1:D:203:ASN:HB2	1.93	0.50
1:D:426:ARG:NH1	1:D:429:GLY:O	2.45	0.50
1:C:132:ALA:HA	1:C:194:SER:HB2	1.94	0.49
1:C:1269:CYS:HA	1:C:1481:UNK:HA	1.94	0.49
1:C:1830:VAL:HB	1:C:1837:GLN:HA	1.94	0.49
1:D:1506:UNK:N	1:D:1542:UNK:O	2.45	0.49
1:D:2022:PRO:O	1:D:2028:ARG:NH2	2.42	0.49
1:D:3960:GLN:HA	1:D:3963:ASN:HD22	1.76	0.49
1:A:151:HIS:HB2	1:A:170:ILE:HB	1.95	0.49
1:A:788:LYS:HG2	1:A:1630:CYS:H	1.75	0.49
1:A:2479:LEU:O	1:A:2517:UNK:N	2.45	0.49
1:A:3962:PHE:HA	1:A:3965:LEU:HD12	1.94	0.49
1:B:842:PRO:O	1:B:1197:GLY:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1506:UNK:N	1:B:1542:UNK:O	2.45	0.49
1:B:2479:LEU:O	1:B:2517:UNK:N	2.45	0.49
1:D:952:LYS:HB3	1:D:968:ALA:HB1	1.93	0.49
1:D:1527:UNK:HA	1:D:1534:UNK:HA	1.93	0.49
1:A:132:ALA:HA	1:A:194:SER:HB2	1.94	0.49
1:A:864:PRO:O	1:A:868:GLU:N	2.42	0.49
1:A:1269:CYS:HA	1:A:1481:UNK:HA	1.94	0.49
1:B:793:LEU:HB2	1:B:797:HIS:H	1.77	0.49
1:B:1843:LYS:HB2	1:B:1938:GLN:HE22	1.76	0.49
1:B:4763:GLY:O	1:B:4766:THR:OG1	2.28	0.49
1:C:1106:ARG:HB2	1:C:1120:LEU:HD12	1.93	0.49
1:C:1506:UNK:N	1:C:1542:UNK:O	2.45	0.49
1:D:109:LEU:O	1:D:118:LEU:N	2.43	0.49
1:D:132:ALA:HA	1:D:194:SER:HB2	1.94	0.49
1:D:2479:LEU:O	1:D:2517:UNK:N	2.45	0.49
1:B:3962:PHE:HA	1:B:3965:LEU:HD12	1.94	0.49
1:C:2479:LEU:O	1:C:2517:UNK:N	2.45	0.49
1:C:4873:ASP:OD1	1:C:4875:LYS:NZ	2.40	0.49
1:D:842:PRO:O	1:D:1197:GLY:N	2.45	0.49
1:D:2212:VAL:HA	1:D:2215:LEU:HB2	1.94	0.49
1:A:596:ASN:HB3	1:A:599:VAL:HG22	1.95	0.49
1:A:3734:HIS:O	1:A:3738:GLY:N	2.40	0.49
1:A:4192:ARG:NH1	1:A:4982:GLU:OE2	2.45	0.49
1:C:660:GLY:HA2	1:C:750:LEU:HD12	1.94	0.49
1:C:1843:LYS:HB2	1:C:1938:GLN:HE22	1.76	0.49
1:C:4977:THR:O	1:C:4981:GLU:N	2.40	0.49
1:D:151:HIS:HB2	1:D:170:ILE:HB	1.94	0.49
1:D:426:ARG:HE	1:D:431:PRO:HA	1.77	0.49
1:D:1092:PHE:N	1:D:1149:VAL:O	2.42	0.49
1:D:3778:MET:HA	1:D:3781:GLN:HG2	1.94	0.49
1:A:21:VAL:HG22	1:A:203:ASN:HB2	1.94	0.49
1:A:247:TYR:HE2	1:A:359:TYR:HB3	1.78	0.49
1:A:658:GLN:O	1:A:662:TRP:NE1	2.36	0.49
1:A:1092:PHE:N	1:A:1149:VAL:O	2.42	0.49
1:B:1468:UNK:HA	1:B:1502:UNK:HA	1.93	0.49
1:B:4181:ILE:HD13	1:B:4987:ASN:HB2	1.95	0.49
1:C:4860:ARG:HG3	1:C:4876:CYS:HB3	1.95	0.49
1:D:621:ILE:O	1:D:625:LEU:N	2.39	0.49
1:D:4860:ARG:HG3	1:D:4876:CYS:HB3	1.95	0.49
1:A:1526:UNK:O	1:A:1535:UNK:N	2.45	0.49
1:D:247:TYR:HE2	1:D:359:TYR:HB3	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1106:ARG:HB2	1:D:1120:LEU:HD12	1.93	0.49
1:D:4957:LYS:HA	1:D:4964:GLY:HA2	1.95	0.49
1:A:793:LEU:HB2	1:A:797:HIS:H	1.77	0.49
1:B:151:HIS:HB2	1:B:170:ILE:HB	1.94	0.49
1:B:426:ARG:NH1	1:B:429:GLY:O	2.45	0.49
1:B:660:GLY:HA2	1:B:750:LEU:HD12	1.94	0.49
1:B:1106:ARG:HB2	1:B:1120:LEU:HD12	1.93	0.49
1:B:3696:ASP:O	1:B:3700:GLN:N	2.36	0.49
1:C:21:VAL:HG22	1:C:203:ASN:HB2	1.93	0.49
1:C:627:PRO:O	1:C:629:ARG:NH1	2.46	0.49
1:C:793:LEU:HB2	1:C:797:HIS:H	1.78	0.49
1:C:1526:UNK:O	1:C:1535:UNK:N	2.45	0.49
1:D:229:GLU:HA	1:D:249:GLY:HA2	1.93	0.49
1:D:3781:GLN:HA	1:D:3784:SER:HB3	1.95	0.49
1:A:206:CYS:SG	1:A:207:SER:N	2.86	0.49
1:A:2212:VAL:HA	1:A:2215:LEU:HB2	1.94	0.49
1:A:3781:GLN:HA	1:A:3784:SER:HB3	1.95	0.49
1:A:3897:ASN:O	1:A:3901:ASN:ND2	2.46	0.49
1:B:21:VAL:HG22	1:B:203:ASN:HB2	1.93	0.49
1:C:4957:LYS:HA	1:C:4964:GLY:HA2	1.95	0.49
1:D:475:GLN:NE2	1:D:531:ARG:O	2.36	0.49
1:D:596:ASN:HB3	1:D:599:VAL:HG22	1.95	0.49
1:D:1468:UNK:HA	1:D:1502:UNK:HA	1.93	0.49
1:D:2272:PRO:HA	1:D:2275:VAL:HG12	1.94	0.49
1:D:3897:ASN:O	1:D:3901:ASN:ND2	2.46	0.49
1:A:426:ARG:HE	1:A:431:PRO:HA	1.77	0.49
1:B:132:ALA:HA	1:B:194:SER:HB2	1.94	0.49
1:B:247:TYR:HE2	1:B:359:TYR:HB3	1.78	0.49
1:B:596:ASN:HB3	1:B:599:VAL:HG22	1.95	0.49
1:B:626:LEU:HD23	1:B:630:GLU:H	1.78	0.49
1:B:864:PRO:O	1:B:868:GLU:N	2.42	0.49
1:B:2816:MET:HE1	1:B:2930:LEU:HD11	1.95	0.49
1:B:3778:MET:HA	1:B:3781:GLN:HG2	1.94	0.49
1:B:3897:ASN:O	1:B:3901:ASN:ND2	2.46	0.49
1:C:842:PRO:O	1:C:1197:GLY:N	2.45	0.49
1:C:2212:VAL:HA	1:C:2215:LEU:HB2	1.94	0.49
1:D:2816:MET:HE1	1:D:2930:LEU:HD11	1.95	0.49
1:D:4678:ALA:O	1:D:4682:GLU:CB	2.58	0.49
1:A:2272:PRO:HA	1:A:2275:VAL:HG12	1.94	0.48
1:A:4977:THR:O	1:A:4981:GLU:N	2.40	0.48
1:C:596:ASN:HB3	1:C:599:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4724:VAL:O	1:C:4728:HIS:N	2.40	0.48
1:D:627:PRO:O	1:D:629:ARG:NH1	2.46	0.48
1:A:475:GLN:NE2	1:A:531:ARG:O	2.36	0.48
1:B:1527:UNK:HA	1:B:1534:UNK:HA	1.93	0.48
1:B:4192:ARG:NH1	1:B:4982:GLU:OE2	2.45	0.48
1:B:4957:LYS:HA	1:B:4964:GLY:HA2	1.95	0.48
1:C:151:HIS:HB2	1:C:170:ILE:HB	1.95	0.48
1:C:206:CYS:SG	1:C:207:SER:N	2.86	0.48
1:C:2022:PRO:O	1:C:2028:ARG:NH2	2.42	0.48
1:D:684:VAL:HA	1:D:781:VAL:HA	1.95	0.48
1:D:1777:PHE:HA	1:D:1799:SER:HB2	1.95	0.48
1:D:4702:ASP:OD1	1:D:4778:TRP:NE1	2.33	0.48
1:A:34:LYS:H	1:A:53:SER:HG	1.60	0.48
1:A:2816:MET:HE1	1:A:2930:LEU:HD11	1.95	0.48
1:C:247:TYR:HE2	1:C:359:TYR:HB3	1.78	0.48
1:D:3734:HIS:O	1:D:3738:GLY:N	2.40	0.48
1:A:233:ILE:HD12	1:A:242:ARG:HB3	1.96	0.48
1:A:3150:UNK:O	1:A:3154:UNK:N	2.46	0.48
1:B:621:ILE:O	1:B:625:LEU:N	2.39	0.48
1:B:627:PRO:O	1:B:629:ARG:NH1	2.46	0.48
1:C:426:ARG:HE	1:C:431:PRO:HA	1.77	0.48
1:C:3781:GLN:HA	1:C:3784:SER:HB3	1.95	0.48
1:D:233:ILE:HD12	1:D:242:ARG:HB3	1.96	0.48
1:D:3150:UNK:O	1:D:3154:UNK:N	2.46	0.48
1:D:4181:ILE:HD13	1:D:4987:ASN:HB2	1.95	0.48
1:A:3778:MET:HA	1:A:3781:GLN:HG2	1.94	0.48
1:B:206:CYS:SG	1:B:207:SER:N	2.86	0.48
1:B:1269:CYS:HA	1:B:1481:UNK:HA	1.95	0.48
1:B:2272:PRO:HA	1:B:2275:VAL:HG12	1.94	0.48
1:B:3734:HIS:O	1:B:3738:GLY:N	2.40	0.48
1:C:3897:ASN:O	1:C:3901:ASN:ND2	2.46	0.48
1:A:684:VAL:HA	1:A:781:VAL:HA	1.95	0.48
1:A:3950:ASN:HA	1:A:3953:LYS:HD3	1.96	0.48
1:A:3963:ASN:O	1:A:3966:THR:OG1	2.32	0.48
1:A:4181:ILE:HD13	1:A:4987:ASN:HB2	1.95	0.48
1:A:4957:LYS:HA	1:A:4964:GLY:HA2	1.95	0.48
1:B:3150:UNK:O	1:B:3154:UNK:N	2.46	0.48
1:D:4697:VAL:O	1:D:4701:TRP:HB2	2.14	0.48
1:A:1865:MET:HB3	1:A:1926:LEU:HB2	1.96	0.48
1:C:1865:MET:SD	1:C:1865:MET:N	2.87	0.48
1:D:626:LEU:HD23	1:D:630:GLU:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:793:LEU:HB2	1:D:797:HIS:H	1.77	0.48
1:D:2042:CYS:SG	1:D:2043:GLY:N	2.79	0.48
1:A:626:LEU:HD23	1:A:630:GLU:H	1.78	0.48
1:B:4232:GLU:OE1	1:B:5019:TRP:NE1	2.47	0.48
1:B:4860:ARG:HG3	1:B:4876:CYS:HB3	1.95	0.48
1:C:626:LEU:HD23	1:C:630:GLU:H	1.78	0.48
1:C:4181:ILE:HD13	1:C:4987:ASN:HB2	1.95	0.48
1:D:206:CYS:SG	1:D:207:SER:N	2.86	0.48
1:D:1269:CYS:HA	1:D:1481:UNK:HA	1.94	0.48
1:A:2328:GLY:HA2	1:A:2331:TYR:HB2	1.96	0.48
1:B:3781:GLN:HA	1:B:3784:SER:HB3	1.95	0.48
1:C:446:GLN:HA	1:C:449:ILE:HD12	1.96	0.48
1:C:2816:MET:HE1	1:C:2930:LEU:HD11	1.95	0.48
1:C:3963:ASN:O	1:C:3966:THR:OG1	2.32	0.48
1:C:4697:VAL:O	1:C:4701:TRP:HB2	2.14	0.48
1:D:446:GLN:HA	1:D:449:ILE:HD12	1.96	0.48
1:D:1235:THR:OG1	1:D:1608:MET:O	2.32	0.48
1:D:3963:ASN:O	1:D:3966:THR:OG1	2.32	0.48
1:D:4976:GLU:O	1:D:4979:THR:OG1	2.29	0.48
1:A:56:GLN:O	1:A:309:THR:OG1	2.28	0.48
1:A:627:PRO:O	1:A:629:ARG:NH1	2.46	0.48
1:A:1153:ILE:HD12	1:A:1160:ILE:HG12	1.96	0.48
1:A:4860:ARG:HG3	1:A:4876:CYS:HB3	1.95	0.48
1:B:684:VAL:HA	1:B:781:VAL:HA	1.95	0.48
1:B:2763:HIS:NE2	1:B:2792:ARG:O	2.47	0.48
1:C:1777:PHE:HA	1:C:1799:SER:HB2	1.96	0.48
1:C:1865:MET:HB3	1:C:1926:LEU:HB2	1.96	0.48
1:A:68:THR:HB	1:A:110:ARG:HB3	1.96	0.47
1:A:1640:HIS:HA	1:A:1647:CYS:HA	1.96	0.47
1:A:1865:MET:N	1:A:1865:MET:SD	2.87	0.47
1:B:1092:PHE:N	1:B:1149:VAL:O	2.42	0.47
1:B:1865:MET:HB3	1:B:1926:LEU:HB2	1.96	0.47
1:B:1991:THR:O	1:B:1995:THR:OG1	2.27	0.47
1:C:2763:HIS:NE2	1:C:2792:ARG:O	2.47	0.47
1:D:1865:MET:HB3	1:D:1926:LEU:HB2	1.96	0.47
1:A:1243:PRO:HB2	1:A:1600:LEU:HB2	1.96	0.47
1:B:4190:ILE:HD12	1:B:5031:GLN:HE21	1.79	0.47
1:B:4242:ILE:HD11	1:B:4993:MET:HG2	1.96	0.47
1:C:233:ILE:HD12	1:C:242:ARG:HB3	1.96	0.47
1:D:215:THR:H	1:D:218:HIS:CE1	2.32	0.47
1:D:1153:ILE:HD12	1:D:1160:ILE:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1649:ASP:HB3	1:D:1652:GLU:HG2	1.97	0.47
1:A:1235:THR:OG1	1:A:1608:MET:O	2.32	0.47
1:A:3639:THR:OG1	1:A:3643:ASN:OD1	2.33	0.47
1:B:233:ILE:HD12	1:B:242:ARG:HB3	1.96	0.47
1:B:4232:GLU:OE2	1:B:5017:ARG:NH1	2.43	0.47
1:C:215:THR:H	1:C:218:HIS:CE1	2.32	0.47
1:C:870:ILE:HD12	1:C:873:LYS:HB2	1.97	0.47
1:C:3150:UNK:O	1:C:3154:UNK:N	2.46	0.47
1:D:719:LEU:HD22	1:D:735:GLN:HG2	1.97	0.47
1:D:3950:ASN:HA	1:D:3953:LYS:HD3	1.96	0.47
1:D:4232:GLU:OE2	1:D:5017:ARG:NH1	2.43	0.47
1:D:4232:GLU:OE1	1:D:5019:TRP:NE1	2.47	0.47
1:A:446:GLN:HA	1:A:449:ILE:HD12	1.96	0.47
1:A:870:ILE:HD12	1:A:873:LYS:HB2	1.96	0.47
1:B:870:ILE:HD12	1:B:873:LYS:HB2	1.97	0.47
1:C:23:GLN:HB2	1:C:203:ASN:HD21	1.80	0.47
1:C:668:VAL:O	1:C:741:GLU:N	2.47	0.47
1:C:684:VAL:HA	1:C:781:VAL:HA	1.95	0.47
1:C:3639:THR:OG1	1:C:3643:ASN:OD1	2.33	0.47
1:D:707:VAL:HG23	1:D:713:SER:HB2	1.97	0.47
1:D:1234:VAL:HG12	1:D:1236:THR:H	1.80	0.47
1:D:1865:MET:N	1:D:1865:MET:SD	2.87	0.47
1:A:5019:TRP:HB3	1:A:5022:PHE:HE2	1.80	0.47
1:B:23:GLN:HB2	1:B:203:ASN:HD21	1.80	0.47
1:B:5019:TRP:HB3	1:B:5022:PHE:HE2	1.80	0.47
1:C:1649:ASP:HB3	1:C:1652:GLU:HG2	1.97	0.47
1:C:1718:ILE:HG13	1:C:1719:HIS:CD2	2.50	0.47
1:D:68:THR:HB	1:D:110:ARG:HB3	1.96	0.47
1:D:263:GLU:N	1:D:281:ARG:O	2.39	0.47
1:D:1243:PRO:HB2	1:D:1600:LEU:HB2	1.96	0.47
1:D:4242:ILE:HD11	1:D:4993:MET:HG2	1.96	0.47
1:A:215:THR:H	1:A:218:HIS:CE1	2.32	0.47
1:A:707:VAL:HG23	1:A:713:SER:HB2	1.97	0.47
1:A:879:HIS:NE2	1:A:908:VAL:O	2.38	0.47
1:A:1109:LEU:O	1:A:1605:TRP:NE1	2.43	0.47
1:A:2763:HIS:NE2	1:A:2792:ARG:O	2.47	0.47
1:A:4697:VAL:O	1:A:4701:TRP:HB2	2.14	0.47
1:B:671:VAL:HG22	1:B:740:PRO:HG3	1.97	0.47
1:B:3762:ARG:O	1:B:3766:GLN:NE2	2.48	0.47
1:C:707:VAL:HG23	1:C:713:SER:HB2	1.96	0.47
1:D:668:VAL:O	1:D:741:GLU:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1718:ILE:HG13	1:D:1719:HIS:CD2	2.50	0.47
1:D:2763:HIS:NE2	1:D:2792:ARG:O	2.47	0.47
1:A:284:HIS:HB3	1:A:287:THR:HB	1.97	0.47
1:A:1649:ASP:HB3	1:A:1652:GLU:HG2	1.97	0.47
1:A:1718:ILE:HG13	1:A:1719:HIS:CD2	2.50	0.47
1:A:1777:PHE:HA	1:A:1799:SER:HB2	1.95	0.47
1:A:4232:GLU:OE1	1:A:5019:TRP:NE1	2.47	0.47
1:B:1234:VAL:HG12	1:B:1236:THR:H	1.80	0.47
1:B:1649:ASP:HB3	1:B:1652:GLU:HG2	1.97	0.47
1:B:1865:MET:N	1:B:1865:MET:SD	2.87	0.47
1:B:2803:GLU:OE1	1:B:2807:TRP:NE1	2.48	0.47
1:B:3963:ASN:O	1:B:3966:THR:OG1	2.32	0.47
1:C:864:PRO:O	1:C:868:GLU:N	2.42	0.47
1:C:2803:GLU:OE1	1:C:2807:TRP:NE1	2.48	0.47
1:C:3950:ASN:HA	1:C:3953:LYS:HD3	1.96	0.47
1:C:4160:LEU:HA	1:C:4163:PHE:HD2	1.80	0.47
1:C:4190:ILE:HD12	1:C:5031:GLN:HE21	1.79	0.47
1:C:4232:GLU:OE1	1:C:5019:TRP:NE1	2.47	0.47
1:D:56:GLN:O	1:D:309:THR:OG1	2.28	0.47
1:D:671:VAL:HG22	1:D:740:PRO:HG3	1.97	0.47
1:D:870:ILE:HD12	1:D:873:LYS:HB2	1.97	0.47
1:D:1640:HIS:HA	1:D:1647:CYS:HA	1.96	0.47
1:D:2328:GLY:HA2	1:D:2331:TYR:HB2	1.96	0.47
1:B:4960:ILE:HG22	1:B:5023:PRO:HG2	1.97	0.47
1:C:173:SER:OG	1:C:174:VAL:N	2.48	0.47
1:C:1234:VAL:HG12	1:C:1236:THR:H	1.80	0.47
1:D:2803:GLU:OE1	1:D:2807:TRP:NE1	2.48	0.47
1:D:4160:LEU:HA	1:D:4163:PHE:HD2	1.80	0.47
1:B:1109:LEU:O	1:B:1605:TRP:NE1	2.43	0.47
1:B:1153:ILE:HD12	1:B:1160:ILE:HG12	1.96	0.47
1:B:1479:UNK:N	1:B:1494:UNK:O	2.48	0.47
1:D:23:GLN:HB2	1:D:203:ASN:HD21	1.80	0.47
1:A:829:TYR:HE2	1:A:1608:MET:HE2	1.80	0.47
1:B:215:THR:H	1:B:218:HIS:CE1	2.32	0.47
1:B:399:GLN:HG2	1:B:403:MET:HE3	1.97	0.47
1:B:1777:PHE:HA	1:B:1799:SER:HB2	1.95	0.47
1:B:2328:GLY:HA2	1:B:2331:TYR:HB2	1.96	0.47
1:C:1640:HIS:HA	1:C:1647:CYS:HA	1.96	0.47
1:C:4580:TYR:HB2	1:D:4879:MET:HB2	1.97	0.47
1:D:173:SER:HB3	1:D:178:ARG:H	1.80	0.47
1:D:776:LEU:HG	1:D:848:HIS:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1092:PHE:HB3	1:D:1149:VAL:HB	1.96	0.47
1:A:23:GLN:HB2	1:A:203:ASN:HD21	1.80	0.46
1:A:4190:ILE:HD12	1:A:5031:GLN:HE21	1.79	0.46
1:B:446:GLN:HA	1:B:449:ILE:HD12	1.96	0.46
1:B:707:VAL:HG23	1:B:713:SER:HB2	1.97	0.46
1:B:1243:PRO:HB2	1:B:1600:LEU:HB2	1.96	0.46
1:B:4697:VAL:O	1:B:4701:TRP:HB2	2.14	0.46
1:C:284:HIS:HB3	1:C:287:THR:HB	1.97	0.46
1:C:671:VAL:HG22	1:C:740:PRO:HG3	1.97	0.46
1:C:1243:PRO:HB2	1:C:1600:LEU:HB2	1.96	0.46
1:C:1739:THR:OG1	1:C:1742:THR:N	2.41	0.46
1:C:4721:LYS:HG2	1:C:4741:LEU:HD13	1.96	0.46
1:D:173:SER:OG	1:D:174:VAL:N	2.48	0.46
1:D:224:HIS:N	1:D:229:GLU:O	2.44	0.46
1:D:1479:UNK:N	1:D:1494:UNK:O	2.48	0.46
1:A:1238:PHE:O	1:A:1606:SER:N	2.45	0.46
1:C:776:LEU:HG	1:C:848:HIS:HA	1.97	0.46
1:C:1479:UNK:N	1:C:1494:UNK:O	2.48	0.46
1:C:4242:ILE:HD11	1:C:4993:MET:HG2	1.96	0.46
1:C:4960:ILE:HG22	1:C:5023:PRO:HG2	1.97	0.46
1:C:5019:TRP:HB3	1:C:5022:PHE:HE2	1.80	0.46
1:D:4190:ILE:HD12	1:D:5031:GLN:HE21	1.79	0.46
1:A:671:VAL:HG22	1:A:740:PRO:HG3	1.97	0.46
1:A:1092:PHE:HB3	1:A:1149:VAL:HB	1.96	0.46
1:A:2006:ILE:HD13	1:A:2009:LEU:HD12	1.97	0.46
1:A:4160:LEU:HA	1:A:4163:PHE:HD2	1.80	0.46
1:B:224:HIS:N	1:B:229:GLU:O	2.44	0.46
1:B:1235:THR:OG1	1:B:1608:MET:O	2.32	0.46
1:B:1718:ILE:HG13	1:B:1719:HIS:CD2	2.50	0.46
1:B:4047:MET:HB2	1:B:4047:MET:HE3	1.75	0.46
1:C:309:THR:O	1:C:313:SER:OG	2.34	0.46
1:C:399:GLN:HG2	1:C:403:MET:HE3	1.97	0.46
1:C:1153:ILE:HD12	1:C:1160:ILE:HG12	1.96	0.46
1:D:5019:TRP:HB3	1:D:5022:PHE:HE2	1.80	0.46
1:A:173:SER:HB3	1:A:178:ARG:H	1.80	0.46
1:A:1466:UNK:HA	1:A:1504:UNK:HA	1.97	0.46
1:A:1637:MET:SD	1:A:1696:HIS:ND1	2.89	0.46
1:B:829:TYR:HE2	1:B:1608:MET:HE2	1.80	0.46
1:B:1637:MET:SD	1:B:1696:HIS:ND1	2.89	0.46
1:B:3950:ASN:HA	1:B:3953:LYS:HD3	1.96	0.46
1:C:2328:GLY:HA2	1:C:2331:TYR:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3829:PHE:HA	1:C:3832:ILE:HD12	1.98	0.46
1:D:716:PHE:HE2	1:D:759:ILE:HD11	1.80	0.46
1:D:1637:MET:SD	1:D:1696:HIS:ND1	2.89	0.46
1:D:1684:ALA:O	1:D:1687:SER:OG	2.28	0.46
1:D:1728:ARG:HA	1:D:1731:LEU:HB2	1.97	0.46
1:D:4190:ILE:HD13	1:D:5031:GLN:HB2	1.97	0.46
1:D:4721:LYS:HG2	1:D:4741:LEU:HD13	1.96	0.46
1:A:109:LEU:O	1:A:118:LEU:N	2.43	0.46
1:A:263:GLU:N	1:A:281:ARG:O	2.39	0.46
1:A:2803:GLU:OE1	1:A:2807:TRP:NE1	2.48	0.46
1:B:173:SER:HB3	1:B:178:ARG:H	1.80	0.46
1:B:716:PHE:HE2	1:B:759:ILE:HD11	1.80	0.46
1:B:1092:PHE:HB3	1:B:1149:VAL:HB	1.96	0.46
1:B:4160:LEU:HA	1:B:4163:PHE:HD2	1.80	0.46
1:B:4721:LYS:HG2	1:B:4741:LEU:HD13	1.96	0.46
1:C:68:THR:HB	1:C:110:ARG:HB3	1.96	0.46
1:C:350:HIS:HB3	1:C:355:LEU:H	1.80	0.46
1:D:350:HIS:HB3	1:D:355:LEU:H	1.80	0.46
1:D:829:TYR:HE2	1:D:1608:MET:HE2	1.80	0.46
1:D:1466:UNK:HA	1:D:1504:UNK:HA	1.97	0.46
1:D:1931:LEU:HD13	1:D:1935:VAL:HG11	1.97	0.46
1:A:350:HIS:HB3	1:A:355:LEU:H	1.80	0.46
1:A:1234:VAL:HG12	1:A:1236:THR:H	1.79	0.46
1:A:1479:UNK:N	1:A:1494:UNK:O	2.48	0.46
1:A:4233:LEU:HA	1:A:4236:SER:HB3	1.97	0.46
1:B:173:SER:OG	1:B:174:VAL:N	2.48	0.46
1:B:719:LEU:HD22	1:B:735:GLN:HG2	1.97	0.46
1:B:1728:ARG:HA	1:B:1731:LEU:HB2	1.97	0.46
1:C:719:LEU:HD22	1:C:735:GLN:HG2	1.97	0.46
1:D:2006:ILE:HD13	1:D:2009:LEU:HD12	1.97	0.46
1:D:3829:PHE:HA	1:D:3832:ILE:HD12	1.98	0.46
1:A:1259:ARG:NH1	1:A:1592:PRO:O	2.40	0.46
1:A:3658:LYS:HA	1:A:3661:TRP:CD2	2.51	0.46
1:A:3874:VAL:HG12	1:A:3875:MET:HG2	1.98	0.46
1:B:68:THR:HB	1:B:110:ARG:HB3	1.96	0.46
1:B:309:THR:O	1:B:313:SER:OG	2.34	0.46
1:B:475:GLN:NE2	1:B:531:ARG:O	2.36	0.46
1:B:1640:HIS:HA	1:B:1647:CYS:HA	1.96	0.46
1:C:34:LYS:H	1:C:53:SER:HG	1.60	0.46
1:C:1637:MET:SD	1:C:1696:HIS:ND1	2.89	0.46
1:D:3639:THR:OG1	1:D:3643:ASN:OD1	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:719:LEU:HD22	1:A:735:GLN:HG2	1.97	0.46
1:A:1991:THR:O	1:A:1995:THR:OG1	2.27	0.46
1:B:1931:LEU:HD13	1:B:1935:VAL:HG11	1.98	0.46
1:B:4190:ILE:HD13	1:B:5031:GLN:HB2	1.97	0.46
1:C:829:TYR:HE2	1:C:1608:MET:HE2	1.80	0.46
1:D:284:HIS:HB3	1:D:287:THR:HB	1.97	0.46
1:D:309:THR:O	1:D:313:SER:OG	2.34	0.46
1:D:399:GLN:HG2	1:D:403:MET:HE3	1.97	0.46
1:D:1286:UNK:HA	1:D:1469:UNK:HA	1.98	0.46
1:A:2782:ASP:HB3	1:A:2785:LEU:HB2	1.98	0.46
1:A:4052:SER:O	1:A:4056:GLU:HB2	2.16	0.46
1:A:4242:ILE:HD11	1:A:4993:MET:HG2	1.96	0.46
1:B:4774:LYS:HA	1:B:4777:ILE:HD12	1.98	0.46
1:C:173:SER:HB3	1:C:178:ARG:H	1.80	0.46
1:C:475:GLN:NE2	1:C:531:ARG:O	2.36	0.46
1:C:1671:ARG:HA	1:C:1674:CYS:HB3	1.98	0.46
1:C:2006:ILE:HD13	1:C:2009:LEU:HD12	1.97	0.46
1:C:4052:SER:O	1:C:4056:GLU:HB2	2.16	0.46
1:D:1074:ILE:HA	1:D:1193:SER:HA	1.98	0.46
1:D:1671:ARG:HA	1:D:1674:CYS:HB3	1.98	0.46
1:D:2121:PHE:HA	1:D:2124:LEU:HB3	1.98	0.46
1:D:2782:ASP:HB3	1:D:2785:LEU:HB2	1.98	0.46
1:A:173:SER:OG	1:A:174:VAL:N	2.48	0.46
1:A:399:GLN:HG2	1:A:403:MET:HE3	1.97	0.46
1:A:1728:ARG:HA	1:A:1731:LEU:HB2	1.97	0.46
1:A:3898:ASP:O	1:A:3902:TYR:N	2.49	0.46
1:A:4721:LYS:HG2	1:A:4741:LEU:HD13	1.96	0.46
1:A:4960:ILE:HG22	1:A:5023:PRO:HG2	1.97	0.46
1:B:134:ASP:N	1:B:134:ASP:OD1	2.49	0.46
1:B:1074:ILE:HA	1:B:1193:SER:HA	1.98	0.46
1:B:3639:THR:OG1	1:B:3643:ASN:OD1	2.33	0.46
1:B:4233:LEU:HA	1:B:4236:SER:HB3	1.97	0.46
1:C:586:ILE:HG21	1:C:603:LEU:HD21	1.98	0.46
1:C:2902:HIS:HB3	1:C:2905:LEU:HG	1.98	0.46
1:D:2210:VAL:HA	1:D:2213:ASN:HD22	1.81	0.46
1:D:4052:SER:O	1:D:4056:GLU:HB2	2.16	0.46
1:A:716:PHE:HE2	1:A:759:ILE:HD11	1.80	0.45
1:A:4875:LYS:HB3	1:A:4882:CYS:HA	1.98	0.45
1:B:2747:ILE:HD11	1:B:2814:LYS:HG3	1.98	0.45
1:B:2902:HIS:HB3	1:B:2905:LEU:HG	1.98	0.45
1:C:20:VAL:HG12	1:C:204:PRO:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2210:VAL:HA	1:C:2213:ASN:HD22	1.81	0.45
1:C:2747:ILE:HD11	1:C:2814:LYS:HG3	1.98	0.45
1:C:2782:ASP:HB3	1:C:2785:LEU:HB2	1.98	0.45
1:D:950:LEU:HB3	1:D:970:LEU:HD22	1.99	0.45
1:A:4190:ILE:HD13	1:A:5031:GLN:HB2	1.97	0.45
1:A:4774:LYS:HA	1:A:4777:ILE:HD12	1.98	0.45
1:B:350:HIS:HB3	1:B:355:LEU:H	1.80	0.45
1:B:586:ILE:HG21	1:B:603:LEU:HD21	1.98	0.45
1:B:2022:PRO:O	1:B:2028:ARG:NH2	2.42	0.45
1:B:2829:GLY:HA2	1:B:2933:ASN:H	1.82	0.45
1:C:1466:UNK:HA	1:C:1504:UNK:HA	1.97	0.45
1:C:2121:PHE:HA	1:C:2124:LEU:HB3	1.99	0.45
1:C:2326:CYS:SG	1:C:2327:GLY:N	2.89	0.45
1:C:2829:GLY:HA2	1:C:2933:ASN:H	1.82	0.45
1:B:776:LEU:HG	1:B:848:HIS:HA	1.97	0.45
1:B:929:LEU:HD23	1:B:932:LEU:HD12	1.99	0.45
1:B:950:LEU:HB3	1:B:970:LEU:HD22	1.99	0.45
1:C:929:LEU:HD23	1:C:932:LEU:HD12	1.99	0.45
1:C:950:LEU:HB3	1:C:970:LEU:HD22	1.98	0.45
1:C:1092:PHE:HB3	1:C:1149:VAL:HB	1.96	0.45
1:C:1684:ALA:O	1:C:1687:SER:OG	2.28	0.45
1:D:2902:HIS:HB3	1:D:2905:LEU:HG	1.98	0.45
1:D:3874:VAL:HG12	1:D:3875:MET:HG2	1.98	0.45
1:D:4960:ILE:HG22	1:D:5023:PRO:HG2	1.97	0.45
1:A:950:LEU:HB3	1:A:970:LEU:HD22	1.98	0.45
1:A:3829:PHE:HA	1:A:3832:ILE:HD12	1.98	0.45
1:B:20:VAL:HG12	1:B:204:PRO:HA	1.99	0.45
1:B:1271:ARG:HA	1:B:1479:UNK:HA	1.99	0.45
1:B:2121:PHE:HD1	1:B:2124:LEU:HD22	1.82	0.45
1:B:4875:LYS:HB3	1:B:4882:CYS:HA	1.98	0.45
1:C:879:HIS:NE2	1:C:908:VAL:O	2.38	0.45
1:C:1973:GLN:HE22	1:C:2005:GLN:NE2	2.14	0.45
1:D:586:ILE:HG21	1:D:603:LEU:HD21	1.98	0.45
1:D:4233:LEU:HA	1:D:4236:SER:HB3	1.97	0.45
1:A:776:LEU:HG	1:A:848:HIS:HA	1.97	0.45
1:A:1973:GLN:HE22	1:A:2005:GLN:NE2	2.14	0.45
1:A:2326:CYS:SG	1:A:2327:GLY:N	2.89	0.45
1:B:284:HIS:HB3	1:B:287:THR:HB	1.97	0.45
1:B:945:LYS:O	1:B:949:ASN:ND2	2.49	0.45
1:B:2121:PHE:HA	1:B:2124:LEU:HB3	1.98	0.45
1:B:2196:ASN:OD1	1:B:2199:ARG:NH1	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2782:ASP:HB3	1:B:2785:LEU:HB2	1.98	0.45
1:B:3581:UNK:O	1:B:3585:UNK:N	2.50	0.45
1:B:3874:VAL:HG12	1:B:3875:MET:HG2	1.98	0.45
1:C:1931:LEU:HD13	1:C:1935:VAL:HG11	1.98	0.45
1:C:3658:LYS:HA	1:C:3661:TRP:CD2	2.51	0.45
1:C:4774:LYS:HA	1:C:4777:ILE:HD12	1.98	0.45
1:D:879:HIS:NE2	1:D:908:VAL:O	2.38	0.45
1:D:945:LYS:O	1:D:949:ASN:ND2	2.49	0.45
1:D:1973:GLN:HE22	1:D:2005:GLN:NE2	2.14	0.45
1:D:2747:ILE:HD11	1:D:2814:LYS:HG3	1.98	0.45
1:D:4161:ARG:HD3	1:D:4164:LEU:HD12	1.99	0.45
1:A:309:THR:O	1:A:313:SER:OG	2.34	0.45
1:A:2121:PHE:HA	1:A:2124:LEU:HB3	1.98	0.45
1:A:2121:PHE:HD1	1:A:2124:LEU:HD22	1.82	0.45
1:B:1636:MET:HE2	1:B:1638:ALA:HB2	1.98	0.45
1:B:2827:ARG:H	1:B:2934:GLY:HA3	1.82	0.45
1:C:134:ASP:OD1	1:C:134:ASP:N	2.49	0.45
1:C:1235:THR:OG1	1:C:1608:MET:O	2.32	0.45
1:C:1854:PHE:HD1	1:C:1858:ASP:HB3	1.82	0.45
1:C:4233:LEU:HA	1:C:4236:SER:HB3	1.97	0.45
1:D:1684:ALA:HA	1:D:1782:PHE:HZ	1.82	0.45
1:D:2326:CYS:SG	1:D:2327:GLY:N	2.89	0.45
1:A:945:LYS:O	1:A:949:ASN:ND2	2.49	0.45
1:A:1684:ALA:O	1:A:1687:SER:OG	2.28	0.45
1:A:1931:LEU:HD13	1:A:1935:VAL:HG11	1.97	0.45
1:B:2326:CYS:SG	1:B:2327:GLY:N	2.89	0.45
1:C:1636:MET:HE2	1:C:1638:ALA:HB2	1.98	0.45
1:D:20:VAL:HG12	1:D:204:PRO:HA	1.99	0.45
1:D:3581:UNK:O	1:D:3585:UNK:N	2.50	0.45
1:D:3658:LYS:HA	1:D:3661:TRP:CD2	2.51	0.45
1:D:4875:LYS:HB3	1:D:4882:CYS:HA	1.98	0.45
1:A:1271:ARG:HA	1:A:1479:UNK:HA	1.99	0.45
1:A:1854:PHE:HD1	1:A:1858:ASP:HB3	1.82	0.45
1:A:2902:HIS:HB3	1:A:2905:LEU:HG	1.98	0.45
1:A:4161:ARG:HD3	1:A:4164:LEU:HD12	1.99	0.45
1:A:4976:GLU:O	1:A:4979:THR:OG1	2.29	0.45
1:B:1466:UNK:HA	1:B:1504:UNK:HA	1.97	0.45
1:B:1854:PHE:HD1	1:B:1858:ASP:HB3	1.82	0.45
1:B:2210:VAL:HA	1:B:2213:ASN:HD22	1.81	0.45
1:B:2229:VAL:O	1:B:2233:CYS:HB2	2.17	0.45
1:C:1728:ARG:HA	1:C:1731:LEU:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4190:ILE:HD13	1:C:5031:GLN:HB2	1.97	0.45
1:D:1854:PHE:HD1	1:D:1858:ASP:HB3	1.82	0.45
1:D:2038:LEU:O	1:D:2042:CYS:N	2.47	0.45
1:D:2229:VAL:O	1:D:2233:CYS:HB2	2.17	0.45
1:D:2829:GLY:HA2	1:D:2933:ASN:H	1.82	0.45
1:A:224:HIS:N	1:A:229:GLU:O	2.44	0.45
1:A:1215:ALA:H	1:A:1216:ILE:HD12	1.82	0.45
1:A:2210:VAL:HA	1:A:2213:ASN:HD22	1.81	0.45
1:A:2747:ILE:HD11	1:A:2814:LYS:HG3	1.98	0.45
1:A:2829:GLY:HA2	1:A:2933:ASN:H	1.82	0.45
1:A:3762:ARG:O	1:A:3766:GLN:NE2	2.48	0.45
1:B:668:VAL:O	1:B:741:GLU:N	2.47	0.45
1:B:682:LEU:HA	1:B:783:PHE:HA	1.99	0.45
1:B:2002:PRO:HA	1:B:2005:GLN:HB3	1.99	0.45
1:B:2006:ILE:HD13	1:B:2009:LEU:HD12	1.97	0.45
1:B:4052:SER:O	1:B:4056:GLU:HB2	2.16	0.45
1:C:716:PHE:HE2	1:C:759:ILE:HD11	1.80	0.45
1:C:1293:UNK:N	1:C:1464:UNK:O	2.50	0.45
1:C:3581:UNK:O	1:C:3585:UNK:N	2.50	0.45
1:C:4161:ARG:HD3	1:C:4164:LEU:HD12	1.99	0.45
1:C:4875:LYS:HB3	1:C:4882:CYS:HA	1.98	0.45
1:A:111:HIS:N	1:A:116:MET:O	2.43	0.45
1:A:682:LEU:HA	1:A:783:PHE:HA	1.99	0.45
1:A:2022:PRO:O	1:A:2028:ARG:NH2	2.42	0.45
1:B:1719:HIS:CD2	1:B:1802:ILE:HD11	2.52	0.45
1:B:1973:GLN:HE22	1:B:2005:GLN:NE2	2.14	0.45
1:B:3829:PHE:HA	1:B:3832:ILE:HD12	1.98	0.45
1:C:263:GLU:N	1:C:281:ARG:O	2.40	0.45
1:C:2229:VAL:O	1:C:2233:CYS:HB2	2.17	0.45
1:C:4584:ASP:HA	1:C:4627:MET:HA	1.99	0.45
1:D:116:MET:HB2	1:D:137:LEU:HD12	1.99	0.45
1:D:1215:ALA:H	1:D:1216:ILE:HD12	1.82	0.45
1:D:1725:ARG:HA	1:D:1728:ARG:HG2	1.99	0.45
1:A:586:ILE:HG21	1:A:603:LEU:HD21	1.98	0.44
1:A:1074:ILE:HA	1:A:1193:SER:HA	1.98	0.44
1:A:1671:ARG:HA	1:A:1674:CYS:HB3	1.98	0.44
1:B:263:GLU:N	1:B:281:ARG:O	2.39	0.44
1:B:1671:ARG:HA	1:B:1674:CYS:HB3	1.98	0.44
1:B:3658:LYS:HA	1:B:3661:TRP:CD2	2.51	0.44
1:B:3663:LEU:H	1:B:3663:LEU:HG	1.57	0.44
1:C:109:LEU:O	1:C:118:LEU:N	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:945:LYS:O	1:C:949:ASN:ND2	2.49	0.44
1:C:1271:ARG:HA	1:C:1479:UNK:HA	1.99	0.44
1:D:1238:PHE:O	1:D:1606:SER:N	2.45	0.44
1:D:1719:HIS:CD2	1:D:1802:ILE:HD11	2.52	0.44
1:D:2365:GLY:O	1:D:2369:ARG:N	2.42	0.44
1:A:134:ASP:OD1	1:A:134:ASP:N	2.49	0.44
1:A:668:VAL:O	1:A:741:GLU:N	2.47	0.44
1:A:4879:MET:HB2	1:D:4580:TYR:HB2	2.00	0.44
1:B:989:ALA:O	1:B:1035:ASN:ND2	2.50	0.44
1:B:1286:UNK:HA	1:B:1469:UNK:HA	1.98	0.44
1:B:1684:ALA:HA	1:B:1782:PHE:HZ	1.82	0.44
1:C:2827:ARG:H	1:C:2934:GLY:HA3	1.82	0.44
1:D:41:GLY:O	1:D:45:ARG:NH1	2.48	0.44
1:D:2827:ARG:H	1:D:2934:GLY:HA3	1.82	0.44
1:A:20:VAL:HG12	1:A:204:PRO:HA	1.99	0.44
1:A:1684:ALA:HA	1:A:1782:PHE:HZ	1.82	0.44
1:C:1286:UNK:HA	1:C:1469:UNK:HA	1.98	0.44
1:D:134:ASP:N	1:D:134:ASP:OD1	2.49	0.44
1:D:929:LEU:HD23	1:D:932:LEU:HD12	1.99	0.44
1:D:1170:MET:HE1	1:D:1176:GLU:HG3	1.99	0.44
1:A:1164:LEU:HB3	1:A:1169:LEU:HD21	1.99	0.44
1:A:1636:MET:HE2	1:A:1638:ALA:HB2	1.98	0.44
1:B:4161:ARG:HD3	1:B:4164:LEU:HD12	1.99	0.44
1:C:468:LEU:HB3	1:C:472:ARG:HH12	1.82	0.44
1:C:1719:HIS:CD2	1:C:1802:ILE:HD11	2.52	0.44
1:C:3874:VAL:HG12	1:C:3875:MET:HG2	1.98	0.44
1:D:4774:LYS:HA	1:D:4777:ILE:HD12	1.98	0.44
1:B:1164:LEU:HB3	1:B:1169:LEU:HD21	1.99	0.44
1:B:2285:GLU:HA	1:B:2288:LEU:HD12	2.00	0.44
1:B:4746:ALA:O	1:B:4750:ILE:N	2.51	0.44
1:C:221:ARG:NE	1:C:253:CYS:O	2.51	0.44
1:C:1109:LEU:O	1:C:1605:TRP:NE1	2.43	0.44
1:D:468:LEU:HB3	1:D:472:ARG:HH12	1.82	0.44
1:D:4047:MET:HB2	1:D:4047:MET:HE3	1.75	0.44
1:A:929:LEU:HD23	1:A:932:LEU:HD12	1.99	0.44
1:A:989:ALA:O	1:A:1035:ASN:ND2	2.50	0.44
1:A:2042:CYS:SG	1:A:2043:GLY:N	2.79	0.44
1:A:4584:ASP:HA	1:A:4627:MET:HA	1.99	0.44
1:B:1170:MET:HE1	1:B:1176:GLU:HG3	1.99	0.44
1:B:1215:ALA:H	1:B:1216:ILE:HD12	1.82	0.44
1:B:1238:PHE:O	1:B:1606:SER:N	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3898:ASP:O	1:B:3902:TYR:N	2.49	0.44
1:C:1074:ILE:HA	1:C:1193:SER:HA	1.98	0.44
1:C:2121:PHE:HD1	1:C:2124:LEU:HD22	1.82	0.44
1:D:1636:MET:HE2	1:D:1638:ALA:HB2	1.98	0.44
1:D:2121:PHE:HD1	1:D:2124:LEU:HD22	1.82	0.44
1:D:2285:GLU:HG3	1:D:2286:LEU:HG	2.00	0.44
1:A:1719:HIS:CD2	1:A:1802:ILE:HD11	2.52	0.44
1:A:1848:LEU:HD22	1:A:1853:ILE:HG13	2.00	0.44
1:A:3581:UNK:O	1:A:3585:UNK:N	2.50	0.44
1:B:4745:LEU:O	1:B:4749:GLU:N	2.50	0.44
1:C:621:ILE:HA	1:C:624:ASN:HB3	2.00	0.44
1:C:2002:PRO:HA	1:C:2005:GLN:HB3	1.99	0.44
1:C:2285:GLU:HA	1:C:2288:LEU:HD12	2.00	0.44
1:C:2285:GLU:HG3	1:C:2286:LEU:HG	2.00	0.44
1:C:4746:ALA:O	1:C:4750:ILE:N	2.51	0.44
1:D:658:GLN:O	1:D:662:TRP:NE1	2.36	0.44
1:D:1240:LYS:HG3	1:D:1242:LEU:H	1.83	0.44
1:D:1271:ARG:HA	1:D:1479:UNK:HA	1.99	0.44
1:A:221:ARG:NE	1:A:253:CYS:O	2.51	0.44
1:A:3225:UNK:O	1:A:3229:UNK:N	2.51	0.44
1:A:3817:LEU:HA	1:A:3820:LEU:HD12	2.00	0.44
1:B:116:MET:HB2	1:B:137:LEU:HD12	2.00	0.44
1:C:1130:GLN:HG2	1:C:1138:PRO:HA	2.00	0.44
1:D:266:ARG:NH2	1:D:272:SER:OG	2.51	0.44
1:D:682:LEU:HA	1:D:783:PHE:HA	1.99	0.44
1:D:870:ILE:HD12	1:D:870:ILE:HA	1.85	0.44
1:D:1293:UNK:N	1:D:1464:UNK:O	2.50	0.44
1:A:1286:UNK:HA	1:A:1469:UNK:HA	1.98	0.44
1:B:221:ARG:NE	1:B:253:CYS:O	2.51	0.44
1:C:116:MET:HB2	1:C:137:LEU:HD12	1.99	0.44
1:C:873:LYS:HB3	1:C:1049:TYR:CZ	2.53	0.44
1:C:4147:LEU:HD23	1:C:4150:LEU:HD12	2.00	0.44
1:D:1101:ARG:HE	1:D:1115:LEU:HD23	1.83	0.44
1:D:4584:ASP:HA	1:D:4627:MET:HA	1.99	0.44
1:D:4746:ALA:O	1:D:4750:ILE:N	2.51	0.44
1:A:621:ILE:HA	1:A:624:ASN:HB3	2.00	0.43
1:A:2827:ARG:H	1:A:2934:GLY:HA3	1.82	0.43
1:B:266:ARG:NH2	1:B:272:SER:OG	2.51	0.43
1:B:1293:UNK:N	1:B:1464:UNK:O	2.50	0.43
1:C:1640:HIS:HD2	1:C:1647:CYS:HB2	1.83	0.43
1:C:1684:ALA:HA	1:C:1782:PHE:HZ	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3762:ARG:O	1:C:3766:GLN:NE2	2.48	0.43
1:A:1101:ARG:HE	1:A:1115:LEU:HD23	1.83	0.43
1:A:2271:THR:HG22	1:A:2273:LEU:H	1.83	0.43
1:B:3225:UNK:O	1:B:3229:UNK:N	2.51	0.43
1:B:3528:UNK:O	1:B:3532:UNK:N	2.51	0.43
1:C:621:ILE:O	1:C:625:LEU:N	2.39	0.43
1:C:989:ALA:O	1:C:1035:ASN:ND2	2.50	0.43
1:C:1101:ARG:HE	1:C:1115:LEU:HD23	1.83	0.43
1:C:1725:ARG:HA	1:C:1728:ARG:HG2	1.99	0.43
1:C:1735:ILE:HG23	1:C:1771:LEU:HD23	1.99	0.43
1:C:3767:GLN:HB3	1:C:3772:THR:HG22	2.00	0.43
1:D:221:ARG:NE	1:D:253:CYS:O	2.51	0.43
1:A:266:ARG:NH2	1:A:272:SER:OG	2.51	0.43
1:A:2365:GLY:O	1:A:2369:ARG:N	2.42	0.43
1:A:4651:THR:HG23	1:A:4799:SER:HB3	2.01	0.43
1:B:359:TYR:HA	1:B:376:ALA:HA	2.00	0.43
1:B:1101:ARG:HE	1:B:1115:LEU:HD23	1.83	0.43
1:B:1640:HIS:HD2	1:B:1647:CYS:HB2	1.83	0.43
1:B:2285:GLU:HG3	1:B:2286:LEU:HG	2.00	0.43
1:B:4651:THR:HG23	1:B:4799:SER:HB3	2.01	0.43
1:C:224:HIS:N	1:C:229:GLU:O	2.44	0.43
1:C:1215:ALA:H	1:C:1216:ILE:HD12	1.82	0.43
1:C:1991:THR:O	1:C:1995:THR:OG1	2.27	0.43
1:C:3225:UNK:O	1:C:3229:UNK:N	2.51	0.43
1:D:1991:THR:O	1:D:1995:THR:OG1	2.27	0.43
1:A:262:LEU:HB3	1:A:280:LEU:HD13	2.00	0.43
1:A:1293:UNK:N	1:A:1464:UNK:O	2.50	0.43
1:A:1725:ARG:HA	1:A:1728:ARG:HG2	1.99	0.43
1:A:2095:GLN:O	1:A:2127:GLN:NE2	2.52	0.43
1:B:4147:LEU:HD23	1:B:4150:LEU:HD12	2.00	0.43
1:B:4584:ASP:HA	1:B:4627:MET:HA	1.99	0.43
1:C:359:TYR:HA	1:C:376:ALA:HA	2.00	0.43
1:C:1115:LEU:HG	1:C:1123:VAL:HG11	2.01	0.43
1:D:3898:ASP:HA	1:D:3901:ASN:HD22	1.83	0.43
1:A:1170:MET:HE1	1:A:1176:GLU:HG3	1.99	0.43
1:A:1735:ILE:HG23	1:A:1771:LEU:HD23	1.99	0.43
1:A:2229:VAL:O	1:A:2233:CYS:HB2	2.17	0.43
1:A:3898:ASP:HA	1:A:3901:ASN:HD22	1.83	0.43
1:B:621:ILE:HA	1:B:624:ASN:HB3	2.00	0.43
1:B:873:LYS:HB3	1:B:1049:TYR:CZ	2.53	0.43
1:B:1651:LEU:O	1:B:1654:SER:OG	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1848:LEU:HD22	1:B:1853:ILE:HG13	2.00	0.43
1:B:3653:PHE:HA	1:B:3656:SER:HB3	2.00	0.43
1:B:3817:LEU:HA	1:B:3820:LEU:HD12	2.00	0.43
1:B:4174:PHE:HA	1:B:4177:TYR:HD2	1.84	0.43
1:C:682:LEU:HA	1:C:783:PHE:HA	1.99	0.43
1:C:1170:MET:HE1	1:C:1176:GLU:HG3	1.99	0.43
1:C:4047:MET:HE3	1:C:4047:MET:HB2	1.75	0.43
1:D:873:LYS:HB3	1:D:1049:TYR:CZ	2.53	0.43
1:D:1130:GLN:HG2	1:D:1138:PRO:HA	2.00	0.43
1:D:3225:UNK:O	1:D:3229:UNK:N	2.51	0.43
1:D:3653:PHE:HA	1:D:3656:SER:HB3	2.00	0.43
1:A:1240:LYS:HG3	1:A:1242:LEU:H	1.83	0.43
1:A:3676:ASP:OD1	1:A:3676:ASP:N	2.51	0.43
1:A:4582:VAL:HG11	1:B:4860:ARG:HD2	2.01	0.43
1:B:468:LEU:HB3	1:B:472:ARG:HH12	1.82	0.43
1:B:1735:ILE:HG23	1:B:1771:LEU:HD23	1.99	0.43
1:B:2095:GLN:O	1:B:2127:GLN:NE2	2.52	0.43
1:C:111:HIS:N	1:C:116:MET:O	2.43	0.43
1:C:484:LEU:O	1:C:488:LEU:N	2.44	0.43
1:C:1164:LEU:HB3	1:C:1169:LEU:HD21	1.99	0.43
1:C:1240:LYS:HG3	1:C:1242:LEU:H	1.83	0.43
1:C:4651:THR:HG23	1:C:4799:SER:HB3	2.01	0.43
1:D:37:LEU:HD11	1:D:47:CYS:HB3	2.01	0.43
1:D:621:ILE:HA	1:D:624:ASN:HB3	2.00	0.43
1:D:2285:GLU:HA	1:D:2288:LEU:HD12	2.00	0.43
1:D:3528:UNK:O	1:D:3532:UNK:N	2.52	0.43
1:D:4147:LEU:HD23	1:D:4150:LEU:HD12	2.00	0.43
1:D:4634:GLU:HG3	1:D:4636:THR:HG23	2.01	0.43
1:A:1130:GLN:HG2	1:A:1138:PRO:HA	2.00	0.43
1:A:2285:GLU:HG3	1:A:2286:LEU:HG	2.00	0.43
1:B:1115:LEU:HG	1:B:1123:VAL:HG11	2.01	0.43
1:B:3767:GLN:HB3	1:B:3772:THR:HG22	2.00	0.43
1:C:56:GLN:O	1:C:309:THR:OG1	2.28	0.43
1:C:2271:THR:HG22	1:C:2273:LEU:H	1.83	0.43
1:C:3676:ASP:N	1:C:3676:ASP:OD1	2.51	0.43
1:C:4745:LEU:O	1:C:4749:GLU:N	2.50	0.43
1:D:1270:LEU:N	1:D:1480:UNK:O	2.52	0.43
1:D:1848:LEU:HD22	1:D:1853:ILE:HG13	2.00	0.43
1:D:2271:THR:HG22	1:D:2273:LEU:H	1.83	0.43
1:D:2739:PRO:HB3	1:D:2884:ASN:HB3	2.00	0.43
1:D:3767:GLN:HB3	1:D:3772:THR:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4174:PHE:HA	1:D:4177:TYR:HD2	1.84	0.43
1:A:2002:PRO:HA	1:A:2005:GLN:HB3	1.99	0.43
1:A:2285:GLU:HA	1:A:2288:LEU:HD12	2.00	0.43
1:A:4174:PHE:HA	1:A:4177:TYR:HD2	1.84	0.43
1:A:4667:PRO:HA	1:A:4670:ILE:HB	2.01	0.43
1:B:23:GLN:HB3	1:B:201:ASN:HB2	2.01	0.43
1:B:1240:LYS:HG3	1:B:1242:LEU:H	1.83	0.43
1:B:2739:PRO:HB3	1:B:2884:ASN:HB3	2.00	0.43
1:C:560:ILE:HA	1:C:563:VAL:HG12	2.01	0.43
1:C:3898:ASP:O	1:C:3902:TYR:N	2.49	0.43
1:C:4174:PHE:HA	1:C:4177:TYR:HD2	1.84	0.43
1:D:4651:THR:HG23	1:D:4799:SER:HB3	2.01	0.43
1:D:4667:PRO:HA	1:D:4670:ILE:HB	2.01	0.43
1:A:2823:ILE:HG12	1:A:2937:VAL:HG22	2.01	0.43
1:B:583:ILE:H	1:B:583:ILE:HG13	1.72	0.43
1:B:1130:GLN:HG2	1:B:1138:PRO:HA	2.00	0.43
1:B:4966:ASP:HA	1:B:4969:ASP:HB2	2.01	0.43
1:C:37:LEU:HD11	1:C:47:CYS:HB3	2.01	0.43
1:C:266:ARG:NH2	1:C:272:SER:OG	2.51	0.43
1:C:1270:LEU:N	1:C:1480:UNK:O	2.52	0.43
1:D:1735:ILE:HG23	1:D:1771:LEU:HD23	2.00	0.43
1:D:2002:PRO:HA	1:D:2005:GLN:HB3	1.99	0.43
1:D:3817:LEU:HA	1:D:3820:LEU:HD12	2.00	0.43
1:D:3898:ASP:O	1:D:3902:TYR:N	2.49	0.43
1:A:3658:LYS:HA	1:A:3661:TRP:CE2	2.54	0.43
1:B:56:GLN:O	1:B:309:THR:OG1	2.28	0.43
1:B:560:ILE:HA	1:B:563:VAL:HG12	2.01	0.43
1:B:1095:VAL:HB	1:B:1199:VAL:HG23	2.01	0.43
1:B:3934:TYR:HB2	1:B:3999:MET:HE2	2.01	0.43
1:B:4667:PRO:HA	1:B:4670:ILE:HB	2.01	0.43
1:C:1152:MET:O	1:C:1161:ILE:N	2.37	0.43
1:C:2196:ASN:OD1	1:C:2199:ARG:NH1	2.39	0.43
1:C:3595:UNK:O	1:C:3599:UNK:N	2.52	0.43
1:C:3653:PHE:HA	1:C:3656:SER:HB3	2.00	0.43
1:C:3658:LYS:HA	1:C:3661:TRP:CE2	2.54	0.43
1:C:4634:GLU:HG3	1:C:4636:THR:HG23	2.01	0.43
1:D:4966:ASP:HA	1:D:4969:ASP:HB2	2.01	0.43
1:A:23:GLN:HB3	1:A:201:ASN:HB2	2.01	0.42
1:A:59:PRO:HB3	1:A:281:ARG:HH11	1.84	0.42
1:A:773:LEU:HA	1:A:777:PHE:HZ	1.84	0.42
1:A:1078:GLU:HB3	1:A:1081:TYR:HD2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1115:LEU:HG	1:A:1123:VAL:HG11	2.01	0.42
1:A:2152:THR:O	1:A:2156:LEU:HB2	2.19	0.42
1:A:4746:ALA:O	1:A:4750:ILE:N	2.51	0.42
1:B:2038:LEU:O	1:B:2042:CYS:N	2.47	0.42
1:B:3898:ASP:HA	1:B:3901:ASN:HD22	1.83	0.42
1:C:262:LEU:HB3	1:C:280:LEU:HD13	2.00	0.42
1:D:2823:ILE:HG12	1:D:2937:VAL:HG22	2.01	0.42
1:A:37:LEU:HD11	1:A:47:CYS:HB3	2.01	0.42
1:A:116:MET:HB2	1:A:137:LEU:HD12	2.00	0.42
1:A:1270:LEU:N	1:A:1480:UNK:O	2.52	0.42
1:A:1640:HIS:HD2	1:A:1647:CYS:HB2	1.83	0.42
1:A:2739:PRO:HB3	1:A:2884:ASN:HB3	2.00	0.42
1:B:37:LEU:HD11	1:B:47:CYS:HB3	2.01	0.42
1:B:484:LEU:O	1:B:488:LEU:N	2.44	0.42
1:B:4563:ARG:NH1	1:B:4815:ASP:OD1	2.52	0.42
1:C:379:HIS:CD2	1:C:382:GLY:H	2.33	0.42
1:C:2739:PRO:HB3	1:C:2884:ASN:HB3	2.00	0.42
1:C:3528:UNK:O	1:C:3532:UNK:N	2.52	0.42
1:C:4966:ASP:HA	1:C:4969:ASP:HB2	2.01	0.42
1:D:359:TYR:HA	1:D:376:ALA:HA	2.00	0.42
1:D:773:LEU:HA	1:D:777:PHE:HZ	1.84	0.42
1:D:1640:HIS:HD2	1:D:1647:CYS:HB2	1.83	0.42
1:D:3595:UNK:O	1:D:3599:UNK:N	2.52	0.42
1:D:3953:LYS:O	1:D:3956:SER:OG	2.35	0.42
1:A:468:LEU:HB3	1:A:472:ARG:HH12	1.82	0.42
1:A:708:GLY:HA3	1:A:722:TRP:HB3	2.01	0.42
1:A:4966:ASP:HA	1:A:4969:ASP:HB2	2.01	0.42
1:B:1575:LEU:HD12	1:B:1578:ALA:HB3	2.01	0.42
1:B:3658:LYS:HA	1:B:3661:TRP:CE2	2.54	0.42
1:C:379:HIS:CD2	1:C:381:GLU:H	2.38	0.42
1:C:792:LEU:HD13	1:C:800:PHE:HD1	1.85	0.42
1:C:1095:VAL:HB	1:C:1199:VAL:HG23	2.01	0.42
1:C:3934:TYR:HB2	1:C:3999:MET:HE2	2.01	0.42
1:C:4767:TRP:HE3	1:C:4770:SER:HB2	1.84	0.42
1:D:59:PRO:HB3	1:D:281:ARG:HH11	1.84	0.42
1:D:116:MET:HB3	1:D:139:GLU:HA	2.02	0.42
1:A:649:PHE:HB3	1:A:776:LEU:HD13	2.02	0.42
1:A:3653:PHE:HA	1:A:3656:SER:HB3	2.00	0.42
1:A:4147:LEU:HD23	1:A:4150:LEU:HD12	2.00	0.42
1:A:4745:LEU:O	1:A:4749:GLU:N	2.50	0.42
1:B:379:HIS:CD2	1:B:382:GLY:H	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:792:LEU:HD13	1:B:800:PHE:HD1	1.85	0.42
1:B:1725:ARG:HA	1:B:1728:ARG:HG2	1.99	0.42
1:B:2105:TRP:HE3	1:B:2120:MET:HE3	1.85	0.42
1:C:649:PHE:HB3	1:C:776:LEU:HD13	2.02	0.42
1:C:1848:LEU:HD22	1:C:1853:ILE:HG13	2.00	0.42
1:C:3898:ASP:HA	1:C:3901:ASN:HD22	1.83	0.42
1:C:4563:ARG:NH1	1:C:4815:ASP:OD1	2.52	0.42
1:D:1041:GLN:O	1:D:1045:THR:OG1	2.35	0.42
1:D:1109:LEU:O	1:D:1605:TRP:NE1	2.43	0.42
1:D:1164:LEU:HB3	1:D:1169:LEU:HD21	1.99	0.42
1:D:3762:ARG:O	1:D:3766:GLN:NE2	2.48	0.42
1:D:4865:LYS:HB2	1:D:4873:ASP:HB3	2.01	0.42
1:A:116:MET:HB3	1:A:139:GLU:HA	2.02	0.42
1:A:3528:UNK:O	1:A:3532:UNK:N	2.52	0.42
1:B:379:HIS:CD2	1:B:381:GLU:H	2.38	0.42
1:B:756:SER:HB3	1:B:767:VAL:HG22	2.01	0.42
1:B:838:HIS:CE1	1:B:1201:HIS:HD2	2.38	0.42
1:B:1704:PRO:HG2	1:B:1707:LEU:HB2	2.02	0.42
1:B:2271:THR:HG22	1:B:2273:LEU:H	1.83	0.42
1:B:3595:UNK:O	1:B:3599:UNK:N	2.52	0.42
1:B:3676:ASP:N	1:B:3676:ASP:OD1	2.51	0.42
1:B:3898:ASP:OD1	1:B:3898:ASP:N	2.44	0.42
1:B:4976:GLU:O	1:B:4979:THR:OG1	2.29	0.42
1:C:838:HIS:CE1	1:C:1201:HIS:HD2	2.38	0.42
1:C:1238:PHE:O	1:C:1606:SER:N	2.45	0.42
1:C:1575:LEU:HD12	1:C:1578:ALA:HB3	2.01	0.42
1:C:3817:LEU:HA	1:C:3820:LEU:HD12	2.00	0.42
1:C:4558:ASN:OD1	1:C:4558:ASN:N	2.50	0.42
1:D:23:GLN:HB3	1:D:201:ASN:HB2	2.01	0.42
1:D:262:LEU:HB3	1:D:280:LEU:HD13	2.01	0.42
1:D:1685:LEU:HD22	1:D:1718:ILE:HG21	2.02	0.42
1:D:1867:GLU:HA	1:D:1870:VAL:HB	2.02	0.42
1:D:2095:GLN:O	1:D:2127:GLN:NE2	2.52	0.42
1:D:2152:THR:O	1:D:2156:LEU:HB2	2.20	0.42
1:D:3658:LYS:HA	1:D:3661:TRP:CE2	2.54	0.42
1:D:4563:ARG:NH1	1:D:4815:ASP:OD1	2.52	0.42
1:D:4968:PHE:O	1:D:4975:PHE:N	2.53	0.42
1:A:41:GLY:O	1:A:45:ARG:NH1	2.48	0.42
1:A:2105:TRP:HE3	1:A:2120:MET:HE3	1.85	0.42
1:A:3595:UNK:O	1:A:3599:UNK:N	2.52	0.42
1:B:574:VAL:HA	1:B:577:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:649:PHE:HB3	1:B:776:LEU:HD13	2.02	0.42
1:B:708:GLY:HA3	1:B:722:TRP:HB3	2.01	0.42
1:B:2152:THR:O	1:B:2156:LEU:HB2	2.19	0.42
1:B:3661:TRP:HB3	1:B:3662:ILE:H	1.68	0.42
1:C:1078:GLU:HB3	1:C:1081:TYR:HD2	1.84	0.42
1:C:2038:LEU:O	1:C:2042:CYS:N	2.48	0.42
1:D:2305:CYS:SG	1:D:2328:GLY:N	2.93	0.42
1:A:1685:LEU:HD22	1:A:1718:ILE:HG21	2.02	0.42
1:A:2364:PHE:HD1	1:A:2429:LEU:HD21	1.85	0.42
1:A:4047:MET:HE3	1:A:4047:MET:HB2	1.75	0.42
1:B:1867:GLU:HA	1:B:1870:VAL:HB	2.02	0.42
1:C:116:MET:HB3	1:C:139:GLU:HA	2.02	0.42
1:C:1708:ARG:HG2	1:C:1711:TYR:CD2	2.55	0.42
1:C:4854:VAL:O	1:C:4858:PHE:N	2.45	0.42
1:D:15:ARG:HG2	1:D:100:THR:HA	2.02	0.42
1:D:1115:LEU:HG	1:D:1123:VAL:HG11	2.01	0.42
1:D:4558:ASN:OD1	1:D:4558:ASN:N	2.50	0.42
1:D:4581:LYS:HB3	1:D:4632:LEU:HB2	2.02	0.42
1:A:574:VAL:HA	1:A:577:ILE:HG12	2.01	0.42
1:A:685:GLY:N	1:A:780:VAL:O	2.37	0.42
1:A:873:LYS:HB3	1:A:1049:TYR:CZ	2.53	0.42
1:A:1704:PRO:HG2	1:A:1707:LEU:HB2	2.02	0.42
1:A:4968:PHE:O	1:A:4975:PHE:N	2.53	0.42
1:B:2318:TYR:OH	1:B:2414:ASN:N	2.53	0.42
1:B:2878:LEU:HD12	1:B:2927:LEU:HG	2.02	0.42
1:C:1651:LEU:O	1:C:1654:SER:OG	2.33	0.42
1:C:2095:GLN:O	1:C:2127:GLN:NE2	2.52	0.42
1:C:2823:ILE:HG12	1:C:2937:VAL:HG22	2.01	0.42
1:C:4667:PRO:HA	1:C:4670:ILE:HB	2.01	0.42
1:C:4976:GLU:O	1:C:4979:THR:OG1	2.29	0.42
1:D:649:PHE:HB3	1:D:776:LEU:HD13	2.02	0.42
1:D:3934:TYR:HB2	1:D:3999:MET:HE2	2.01	0.42
1:A:838:HIS:CE1	1:A:1201:HIS:HD2	2.38	0.42
1:A:1867:GLU:HA	1:A:1870:VAL:HB	2.02	0.42
1:A:2130:GLY:O	1:A:2134:LEU:CB	2.68	0.42
1:A:3767:GLN:HB3	1:A:3772:THR:HG22	2.00	0.42
1:A:4763:GLY:O	1:A:4766:THR:OG1	2.28	0.42
1:B:15:ARG:HG2	1:B:100:THR:HA	2.02	0.42
1:B:773:LEU:HA	1:B:777:PHE:HZ	1.84	0.42
1:B:4865:LYS:HB2	1:B:4873:ASP:HB3	2.01	0.42
1:C:756:SER:HB3	1:C:767:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4865:LYS:HB2	1:C:4873:ASP:HB3	2.01	0.42
1:C:4968:PHE:O	1:C:4975:PHE:N	2.53	0.42
1:D:1575:LEU:HD12	1:D:1578:ALA:HB3	2.01	0.42
1:D:2364:PHE:HD1	1:D:2429:LEU:HD21	1.85	0.42
1:A:792:LEU:HD13	1:A:800:PHE:HD1	1.85	0.42
1:A:2456:ILE:HG12	1:B:178:ARG:NH1	2.35	0.42
1:A:2762:THR:O	1:A:2766:TRP:HB2	2.20	0.42
1:A:4563:ARG:NH1	1:A:4815:ASP:OD1	2.52	0.42
1:B:59:PRO:HB3	1:B:281:ARG:HH11	1.84	0.42
1:B:262:LEU:HB3	1:B:280:LEU:HD13	2.00	0.42
1:B:4581:LYS:HB3	1:B:4632:LEU:HB2	2.02	0.42
1:B:4634:GLU:HG3	1:B:4636:THR:HG23	2.01	0.42
1:C:15:ARG:HG2	1:C:100:THR:HA	2.02	0.42
1:C:59:PRO:HB3	1:C:281:ARG:HH11	1.84	0.42
1:C:273:HIS:CE1	1:C:337:PRO:HB3	2.55	0.42
1:C:2305:CYS:SG	1:C:2328:GLY:N	2.93	0.42
1:C:2878:LEU:HD12	1:C:2927:LEU:HG	2.02	0.42
1:C:4581:LYS:HB3	1:C:4632:LEU:HB2	2.02	0.42
1:D:379:HIS:CD2	1:D:381:GLU:H	2.38	0.42
1:D:583:ILE:H	1:D:583:ILE:HG13	1.72	0.42
1:D:756:SER:HB3	1:D:767:VAL:HG22	2.01	0.42
1:D:989:ALA:O	1:D:1035:ASN:ND2	2.50	0.42
1:A:1131:ARG:N	1:A:1137:GLU:O	2.53	0.41
1:A:2305:CYS:SG	1:A:2328:GLY:N	2.93	0.41
1:B:2130:GLY:O	1:B:2134:LEU:CB	2.68	0.41
1:B:2364:PHE:HD1	1:B:2429:LEU:HD21	1.85	0.41
1:B:4767:TRP:HE3	1:B:4770:SER:HB2	1.84	0.41
1:C:2152:THR:O	1:C:2156:LEU:HB2	2.20	0.41
1:C:2203:MET:O	1:C:2206:THR:OG1	2.34	0.41
1:D:792:LEU:HD13	1:D:800:PHE:HD1	1.85	0.41
1:D:838:HIS:CE1	1:D:1201:HIS:HD2	2.38	0.41
1:D:2130:GLY:O	1:D:2134:LEU:CB	2.68	0.41
1:D:2739:PRO:HD2	1:D:2888:ARG:HH21	1.85	0.41
1:D:4181:ILE:HD12	1:D:4181:ILE:HA	1.91	0.41
1:A:113:HIS:CE1	1:A:399:GLN:HA	2.55	0.41
1:A:359:TYR:HA	1:A:376:ALA:HA	2.00	0.41
1:A:880:GLU:OE1	1:A:968:ALA:N	2.53	0.41
1:A:1575:LEU:HD12	1:A:1578:ALA:HB3	2.01	0.41
1:A:3934:TYR:HB2	1:A:3999:MET:HE2	2.01	0.41
1:A:4581:LYS:HB3	1:A:4632:LEU:HB2	2.02	0.41
1:B:468:LEU:HB3	1:B:472:ARG:NH1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1131:ARG:N	1:B:1137:GLU:O	2.53	0.41
1:B:2006:ILE:HD11	1:B:3641:LEU:HD13	2.02	0.41
1:B:4968:PHE:O	1:B:4975:PHE:N	2.53	0.41
1:D:273:HIS:CE1	1:D:337:PRO:HB3	2.55	0.41
1:D:560:ILE:HA	1:D:563:VAL:HG12	2.01	0.41
1:D:1704:PRO:HG2	1:D:1707:LEU:HB2	2.02	0.41
1:D:2105:TRP:HE3	1:D:2120:MET:HE3	1.85	0.41
1:D:2780:ASN:O	1:D:2787:THR:OG1	2.36	0.41
1:A:1708:ARG:HG2	1:A:1711:TYR:CD2	2.55	0.41
1:A:2739:PRO:HD2	1:A:2888:ARG:HH21	1.86	0.41
1:A:4708:THR:HA	1:A:4709:PRO:HD3	1.94	0.41
1:A:4865:LYS:HB2	1:A:4873:ASP:HB3	2.01	0.41
1:B:1270:LEU:N	1:B:1480:UNK:O	2.52	0.41
1:B:1685:LEU:HD22	1:B:1718:ILE:HG21	2.02	0.41
1:B:2823:ILE:HG12	1:B:2937:VAL:HG22	2.01	0.41
1:B:3767:GLN:HA	1:B:3770:LEU:HB3	2.02	0.41
1:C:3999:MET:O	1:C:4003:LEU:N	2.43	0.41
1:C:4738:ALA:HA	1:C:4743:MET:HE3	2.02	0.41
1:D:468:LEU:HB3	1:D:472:ARG:NH1	2.35	0.41
1:D:708:GLY:HA3	1:D:722:TRP:HB3	2.01	0.41
1:D:717:ASP:OD1	1:D:717:ASP:N	2.53	0.41
1:D:4767:TRP:HE3	1:D:4770:SER:HB2	1.85	0.41
1:A:379:HIS:CD2	1:A:381:GLU:H	2.38	0.41
1:A:560:ILE:HA	1:A:563:VAL:HG12	2.01	0.41
1:B:273:HIS:CE1	1:B:337:PRO:HB3	2.55	0.41
1:B:717:ASP:OD1	1:B:717:ASP:N	2.53	0.41
1:B:2095:GLN:NE2	1:B:2127:GLN:O	2.54	0.41
1:B:2739:PRO:HD2	1:B:2888:ARG:HH21	1.86	0.41
1:B:4708:THR:HA	1:B:4709:PRO:HD3	1.94	0.41
1:C:708:GLY:HA3	1:C:722:TRP:HB3	2.01	0.41
1:C:880:GLU:OE1	1:C:968:ALA:N	2.53	0.41
1:D:880:GLU:OE1	1:D:968:ALA:N	2.53	0.41
1:D:3676:ASP:OD1	1:D:3676:ASP:N	2.51	0.41
1:A:213:TYR:CG	1:A:337:PRO:HB2	2.56	0.41
1:A:583:ILE:H	1:A:583:ILE:HG13	1.72	0.41
1:B:21:VAL:HG12	1:B:66:CYS:HA	2.03	0.41
1:B:116:MET:HB3	1:B:139:GLU:HA	2.02	0.41
1:C:34:LYS:N	1:C:53:SER:OG	2.44	0.41
1:C:468:LEU:HB3	1:C:472:ARG:NH1	2.36	0.41
1:C:1524:UNK:N	1:C:1537:UNK:O	2.53	0.41
1:C:1867:GLU:HA	1:C:1870:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2758:PHE:HD2	1:D:2809:ILE:HG12	1.85	0.41
1:D:3767:GLN:HA	1:D:3770:LEU:HB3	2.02	0.41
1:A:15:ARG:HG2	1:A:100:THR:HA	2.02	0.41
1:A:21:VAL:HG12	1:A:66:CYS:HA	2.03	0.41
1:A:756:SER:HB3	1:A:767:VAL:HG22	2.01	0.41
1:A:1095:VAL:HB	1:A:1199:VAL:HG23	2.01	0.41
1:A:1651:LEU:O	1:A:1654:SER:OG	2.33	0.41
1:A:1774:PRO:HG2	1:A:1776:HIS:CE1	2.56	0.41
1:A:2095:GLN:NE2	1:A:2127:GLN:O	2.54	0.41
1:A:4052:SER:O	1:A:4056:GLU:CB	2.69	0.41
1:B:41:GLY:O	1:B:45:ARG:NH1	2.49	0.41
1:B:113:HIS:CE1	1:B:399:GLN:HA	2.55	0.41
1:B:1078:GLU:HB3	1:B:1081:TYR:HD2	1.84	0.41
1:B:2762:THR:O	1:B:2766:TRP:HB2	2.20	0.41
1:C:717:ASP:OD1	1:C:717:ASP:N	2.53	0.41
1:C:745:SER:HB2	1:C:758:ARG:HB3	2.02	0.41
1:C:773:LEU:HA	1:C:777:PHE:HZ	1.84	0.41
1:C:1704:PRO:HG2	1:C:1707:LEU:HB2	2.02	0.41
1:C:2254:LEU:O	1:C:2258:LEU:HB2	2.21	0.41
1:C:2739:PRO:HD2	1:C:2888:ARG:HH21	1.86	0.41
1:C:4056:GLU:HG3	1:C:4166:LEU:HD21	2.03	0.41
1:D:574:VAL:HA	1:D:577:ILE:HG12	2.01	0.41
1:D:1524:UNK:N	1:D:1537:UNK:O	2.53	0.41
1:D:2006:ILE:HD11	1:D:3641:LEU:HD13	2.02	0.41
1:A:3663:LEU:H	1:A:3663:LEU:HG	1.57	0.41
1:A:3729:MET:O	1:A:3732:SER:OG	2.35	0.41
1:A:4767:TRP:HE3	1:A:4770:SER:HB2	1.84	0.41
1:B:386:ASP:HB3	1:B:388:LEU:HG	2.03	0.41
1:B:2305:CYS:SG	1:B:2328:GLY:N	2.93	0.41
1:B:2806:ARG:HG2	1:B:2810:LYS:HG3	2.03	0.41
1:B:4738:ALA:HA	1:B:4743:MET:HE3	2.02	0.41
1:B:4848:VAL:HG23	1:B:4883:TYR:HE1	1.86	0.41
1:C:23:GLN:HB3	1:C:201:ASN:HB2	2.01	0.41
1:C:386:ASP:HB3	1:C:388:LEU:HG	2.03	0.41
1:C:574:VAL:HA	1:C:577:ILE:HG12	2.01	0.41
1:C:1109:LEU:HD23	1:C:1109:LEU:HA	1.89	0.41
1:D:1078:GLU:HB3	1:D:1081:TYR:HD2	1.84	0.41
1:D:4738:ALA:HA	1:D:4743:MET:HE3	2.02	0.41
1:A:2182:ILE:HD13	1:A:2185:ILE:HD11	2.03	0.41
1:A:2758:PHE:HD2	1:A:2809:ILE:HG12	1.85	0.41
1:B:1126:GLY:HA2	1:B:1129:GLY:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1774:PRO:HG2	1:B:1776:HIS:CE1	2.56	0.41
1:C:119:SER:OG	1:C:136:GLY:O	2.34	0.41
1:C:1685:LEU:HD22	1:C:1718:ILE:HG21	2.02	0.41
1:C:2105:TRP:HE3	1:C:2120:MET:HE3	1.84	0.41
1:C:2130:GLY:O	1:C:2134:LEU:CB	2.68	0.41
1:C:2364:PHE:HD1	1:C:2429:LEU:HD21	1.85	0.41
1:C:3695:PRO:HB2	1:C:3700:GLN:HG3	2.03	0.41
1:C:3767:GLN:HA	1:C:3770:LEU:HB3	2.02	0.41
1:D:395:GLN:HG3	1:D:397:GLU:H	1.86	0.41
1:D:893:TYR:HD1	1:D:907:LEU:HB2	1.86	0.41
1:D:1095:VAL:HB	1:D:1199:VAL:HG23	2.01	0.41
1:D:1774:PRO:HG2	1:D:1776:HIS:CE1	2.56	0.41
1:D:3695:PRO:HB2	1:D:3700:GLN:HG3	2.03	0.41
1:D:4034:ASN:HD22	1:D:4035:VAL:H	1.69	0.41
1:A:273:HIS:CE1	1:A:337:PRO:HB3	2.55	0.41
1:A:3695:PRO:HB2	1:A:3700:GLN:HG3	2.03	0.41
1:A:4634:GLU:HG3	1:A:4636:THR:HG23	2.01	0.41
1:A:4821:LYS:HE2	1:A:4821:LYS:HB3	1.88	0.41
1:B:879:HIS:NE2	1:B:908:VAL:O	2.38	0.41
1:B:880:GLU:OE1	1:B:968:ALA:N	2.53	0.41
1:B:1072:VAL:HG22	1:B:1195:GLY:HA2	2.02	0.41
1:B:1524:UNK:N	1:B:1537:UNK:O	2.53	0.41
1:B:3224:UNK:O	1:B:3228:UNK:N	2.54	0.41
1:C:21:VAL:HG12	1:C:66:CYS:HA	2.03	0.41
1:C:57:ASN:HA	1:C:308:HIS:HA	2.03	0.41
1:C:349:GLN:HA	1:C:356:TRP:HA	2.03	0.41
1:C:1126:GLY:HA2	1:C:1129:GLY:H	1.86	0.41
1:C:2095:GLN:NE2	1:C:2127:GLN:O	2.54	0.41
1:C:4763:GLY:O	1:C:4766:THR:OG1	2.28	0.41
1:C:4786:ASP:OD2	1:C:4789:PHE:N	2.43	0.41
1:D:113:HIS:CE1	1:D:399:GLN:HA	2.56	0.41
1:D:213:TYR:CG	1:D:337:PRO:HB2	2.56	0.41
1:D:386:ASP:HB3	1:D:388:LEU:HG	2.03	0.41
1:D:1078:GLU:HB3	1:D:1081:TYR:CD2	2.56	0.41
1:D:1126:GLY:HA2	1:D:1129:GLY:H	1.86	0.41
1:D:2332:LEU:O	1:D:2336:ARG:N	2.48	0.41
1:D:2762:THR:O	1:D:2766:TRP:HB2	2.20	0.41
1:D:3809:ASN:HB3	1:D:3812:VAL:HG22	2.03	0.41
1:A:230:CYS:N	1:A:248:GLU:O	2.48	0.41
1:A:386:ASP:HB3	1:A:388:LEU:HG	2.03	0.41
1:A:1078:GLU:HB3	1:A:1081:TYR:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2038:LEU:O	1:A:2042:CYS:N	2.47	0.41
1:A:3804:ILE:O	1:A:3809:ASN:ND2	2.54	0.41
1:B:213:TYR:CG	1:B:337:PRO:HB2	2.56	0.41
1:B:1708:ARG:HG2	1:B:1711:TYR:CD2	2.55	0.41
1:B:2254:LEU:O	1:B:2258:LEU:HB2	2.21	0.41
1:C:79:GLN:HA	1:C:82:LEU:HD12	2.03	0.41
1:C:113:HIS:CE1	1:C:399:GLN:HA	2.55	0.41
1:C:675:LEU:HG	1:C:677:ALA:H	1.86	0.41
1:C:1640:HIS:CD2	1:C:1647:CYS:HB2	2.56	0.41
1:C:2318:TYR:OH	1:C:2414:ASN:N	2.53	0.41
1:C:4848:VAL:HG23	1:C:4883:TYR:HE1	1.86	0.41
1:D:349:GLN:HA	1:D:356:TRP:HA	2.03	0.41
1:D:675:LEU:HG	1:D:677:ALA:H	1.86	0.41
1:D:4056:GLU:HG3	1:D:4166:LEU:HD21	2.03	0.41
1:A:468:LEU:HB3	1:A:472:ARG:NH1	2.36	0.40
1:A:745:SER:HB2	1:A:758:ARG:HB3	2.02	0.40
1:A:955:LEU:HB2	1:A:966:LYS:HD2	2.02	0.40
1:A:1126:GLY:HA2	1:A:1129:GLY:H	1.86	0.40
1:A:1524:UNK:N	1:A:1537:UNK:O	2.53	0.40
1:A:1973:GLN:HE22	1:A:2005:GLN:HE21	1.69	0.40
1:A:2878:LEU:HD12	1:A:2927:LEU:HG	2.02	0.40
1:A:3809:ASN:HB3	1:A:3812:VAL:HG22	2.03	0.40
1:B:675:LEU:HG	1:B:677:ALA:H	1.86	0.40
1:B:3729:MET:O	1:B:3732:SER:OG	2.35	0.40
1:C:1078:GLU:HB3	1:C:1081:TYR:CD2	2.56	0.40
1:C:1685:LEU:HA	1:C:1688:HIS:HD2	1.86	0.40
1:C:2006:ILE:HD11	1:C:3641:LEU:HD13	2.02	0.40
1:C:2159:LEU:HD13	1:C:2203:MET:HE1	2.03	0.40
1:C:3224:UNK:O	1:C:3228:UNK:N	2.54	0.40
1:D:21:VAL:HG12	1:D:66:CYS:HA	2.03	0.40
1:D:111:HIS:N	1:D:116:MET:O	2.43	0.40
1:D:1109:LEU:HD23	1:D:1109:LEU:HA	1.89	0.40
1:D:1708:ARG:HG2	1:D:1711:TYR:CD2	2.55	0.40
1:D:2095:GLN:NE2	1:D:2127:GLN:O	2.54	0.40
1:A:2006:ILE:HD11	1:A:3641:LEU:HD13	2.02	0.40
1:B:3804:ILE:O	1:B:3809:ASN:ND2	2.54	0.40
1:C:395:GLN:HG3	1:C:397:GLU:H	1.86	0.40
1:C:870:ILE:HD12	1:C:870:ILE:HA	1.85	0.40
1:C:2758:PHE:HD2	1:C:2809:ILE:HG12	1.85	0.40
1:D:955:LEU:HB2	1:D:966:LYS:HD2	2.02	0.40
1:D:1725:ARG:HH21	1:D:1725:ARG:HD2	1.73	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2318:TYR:OH	1:D:2414:ASN:N	2.53	0.40
1:D:4052:SER:O	1:D:4056:GLU:CB	2.69	0.40
1:A:1092:PHE:HD1	1:A:1202:LEU:HD13	1.87	0.40
1:A:2254:LEU:O	1:A:2258:LEU:HB2	2.21	0.40
1:B:548:VAL:HG23	1:B:582:HIS:CE1	2.57	0.40
1:B:1078:GLU:HB3	1:B:1081:TYR:CD2	2.56	0.40
1:B:2365:GLY:O	1:B:2369:ARG:N	2.42	0.40
1:B:3695:PRO:HB2	1:B:3700:GLN:HG3	2.03	0.40
1:B:3923:LEU:O	1:B:3927:GLN:CB	2.69	0.40
1:B:4052:SER:O	1:B:4056:GLU:CB	2.69	0.40
1:D:57:ASN:HA	1:D:308:HIS:HA	2.03	0.40
1:D:2254:LEU:O	1:D:2258:LEU:HB2	2.21	0.40
1:D:2878:LEU:HD12	1:D:2927:LEU:HG	2.02	0.40
1:A:548:VAL:HG23	1:A:582:HIS:CE1	2.57	0.40
1:A:1072:VAL:HG22	1:A:1195:GLY:HA2	2.02	0.40
1:A:1152:MET:O	1:A:1161:ILE:N	2.37	0.40
1:A:2806:ARG:HG2	1:A:2810:LYS:HG3	2.03	0.40
1:B:745:SER:HB2	1:B:758:ARG:HB3	2.02	0.40
1:B:893:TYR:HD1	1:B:907:LEU:HB2	1.86	0.40
1:B:2182:ILE:HD13	1:B:2185:ILE:HD11	2.03	0.40
1:C:213:TYR:CG	1:C:337:PRO:HB2	2.55	0.40
1:C:1774:PRO:HG2	1:C:1776:HIS:CE1	2.56	0.40
1:C:2440:MET:HB2	1:C:2443:ILE:HG12	2.04	0.40
1:C:4034:ASN:HD22	1:C:4035:VAL:H	1.69	0.40
1:C:4822:THR:O	1:C:4825:THR:OG1	2.28	0.40
1:D:79:GLN:HA	1:D:82:LEU:HD12	2.03	0.40
1:D:629:ARG:HB3	1:D:634:GLN:HE21	1.86	0.40
1:D:2440:MET:HB2	1:D:2443:ILE:HG12	2.04	0.40
1:D:3663:LEU:H	1:D:3663:LEU:HG	1.57	0.40
1:A:572:PRO:HB3	1:A:609:CYS:HB2	2.04	0.40
1:A:709:ASP:HB3	1:A:725:HIS:CE1	2.57	0.40
1:A:893:TYR:HD1	1:A:907:LEU:HB2	1.86	0.40
1:A:1640:HIS:CD2	1:A:1647:CYS:HB2	2.56	0.40
1:A:2159:LEU:HD13	1:A:2203:MET:HE1	2.03	0.40
1:A:3575:UNK:O	1:A:3579:UNK:N	2.55	0.40
1:A:4738:ALA:HA	1:A:4743:MET:HE3	2.02	0.40
1:B:252:VAL:HA	1:B:255:HIS:CG	2.56	0.40
1:B:841:GLY:HA2	1:B:1073:ARG:HD2	2.03	0.40
1:C:207:SER:OG	1:C:208:CYS:N	2.54	0.40
1:C:548:VAL:HG23	1:C:582:HIS:CE1	2.57	0.40
1:C:650:VAL:H	1:C:777:PHE:H	1.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1072:VAL:HG22	1:C:1195:GLY:HA2	2.02	0.40
1:C:2182:ILE:HD13	1:C:2185:ILE:HD11	2.03	0.40
1:C:4052:SER:O	1:C:4056:GLU:CB	2.69	0.40
1:D:572:PRO:HB3	1:D:609:CYS:HB2	2.04	0.40
1:D:1131:ARG:N	1:D:1137:GLU:O	2.53	0.40
1:D:1973:GLN:HE22	1:D:2005:GLN:HE21	1.69	0.40
1:D:2467:VAL:HA	1:D:2470:ILE:HB	2.04	0.40
1:D:3224:UNK:O	1:D:3228:UNK:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3235/5037 (64%)	2854 (88%)	376 (12%)	5 (0%)	43	78
1	B	3235/5037 (64%)	2854 (88%)	376 (12%)	5 (0%)	43	78
1	C	3235/5037 (64%)	2853 (88%)	377 (12%)	5 (0%)	43	78
1	D	3235/5037 (64%)	2853 (88%)	377 (12%)	5 (0%)	43	78
All	All	12940/20148 (64%)	11414 (88%)	1506 (12%)	20 (0%)	44	78

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	810	PRO
1	B	810	PRO
1	C	810	PRO
1	D	810	PRO
1	A	553	ARG
1	A	1932	PRO
1	B	1932	PRO

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Mol	Chain	Res	Type
1	C	1932	PRO
1	D	1932	PRO
1	A	1708	ARG
1	B	553	ARG
1	B	1708	ARG
1	C	553	ARG
1	C	1708	ARG
1	D	553	ARG
1	D	1708	ARG
1	A	4641	PRO
1	B	4641	PRO
1	C	4641	PRO
1	D	4641	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	2493/3209 (78%)	2484 (100%)	9 (0%)	84	84
1	B	2493/3209 (78%)	2484 (100%)	9 (0%)	84	84
1	C	2493/3209 (78%)	2484 (100%)	9 (0%)	84	84
1	D	2493/3209 (78%)	2484 (100%)	9 (0%)	84	84
All	All	9972/12836 (78%)	9936 (100%)	36 (0%)	81	84

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	583	ILE
1	A	688	LEU
1	A	719	LEU
1	A	781	VAL
1	A	2010	LEU
1	A	3663	LEU
1	A	3805	LEU
1	A	4034	ASN

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Mol	Chain	Res	Type
1	A	4985	LEU
1	B	583	ILE
1	B	688	LEU
1	B	719	LEU
1	B	781	VAL
1	B	2010	LEU
1	B	3663	LEU
1	B	3805	LEU
1	B	4034	ASN
1	B	4985	LEU
1	C	583	ILE
1	C	688	LEU
1	C	719	LEU
1	C	781	VAL
1	C	2010	LEU
1	C	3663	LEU
1	C	3805	LEU
1	C	4034	ASN
1	C	4985	LEU
1	D	583	ILE
1	D	688	LEU
1	D	719	LEU
1	D	781	VAL
1	D	2010	LEU
1	D	3663	LEU
1	D	3805	LEU
1	D	4034	ASN
1	D	4985	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (255) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	105	HIS
1	A	111	HIS
1	A	156	GLN
1	A	203	ASN
1	A	273	HIS
1	A	379	HIS
1	A	383	HIS
1	A	465	GLN
1	A	536	ASN

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Mol	Chain	Res	Type
1	A	582	HIS
1	A	765	GLN
1	A	838	HIS
1	A	949	ASN
1	A	1158	ASN
1	A	1198	GLN
1	A	1206	GLN
1	A	1220	GLN
1	A	1229	ASN
1	A	1598	GLN
1	A	1679	ASN
1	A	1719	HIS
1	A	1775	HIS
1	A	1861	GLN
1	A	1938	GLN
1	A	1973	GLN
1	A	2011	HIS
1	A	2041	HIS
1	A	2095	GLN
1	A	2127	GLN
1	A	2194	HIS
1	A	2213	ASN
1	A	2260	ASN
1	A	2773	ASN
1	A	2931	GLN
1	A	3761	GLN
1	A	3766	GLN
1	A	3771	HIS
1	A	3809	ASN
1	A	3814	GLN
1	A	3830	GLN
1	A	3850	GLN
1	A	3882	GLN
1	A	3896	ASN
1	A	3909	ASN
1	A	3946	GLN
1	A	3950	ASN
1	A	3963	ASN
1	A	4034	ASN
1	A	4037	ASN
1	A	4054	ASN
1	A	4078	GLN

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Mol	Chain	Res	Type
1	A	4109	GLN
1	A	4133	GLN
1	A	4142	ASN
1	A	4209	GLN
1	A	4246	GLN
1	A	4553	ASN
1	A	4832	HIS
1	A	4833	ASN
1	A	4949	GLN
1	A	4987	ASN
1	A	5031	GLN
1	B	57	ASN
1	B	84	ASN
1	B	105	HIS
1	B	111	HIS
1	B	156	GLN
1	B	273	HIS
1	B	379	HIS
1	B	383	HIS
1	B	465	GLN
1	B	536	ASN
1	B	582	HIS
1	B	765	GLN
1	B	838	HIS
1	B	949	ASN
1	B	1158	ASN
1	B	1206	GLN
1	B	1220	GLN
1	B	1229	ASN
1	B	1598	GLN
1	B	1679	ASN
1	B	1719	HIS
1	B	1775	HIS
1	B	1861	GLN
1	B	1938	GLN
1	B	1941	ASN
1	B	1973	GLN
1	B	2007	ASN
1	B	2011	HIS
1	B	2041	HIS
1	B	2095	GLN
1	B	2127	GLN

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Mol	Chain	Res	Type
1	B	2194	HIS
1	B	2213	ASN
1	B	2931	GLN
1	B	3761	GLN
1	B	3766	GLN
1	B	3771	HIS
1	B	3809	ASN
1	B	3814	GLN
1	B	3830	GLN
1	B	3850	GLN
1	B	3882	GLN
1	B	3896	ASN
1	B	3909	ASN
1	B	3946	GLN
1	B	3950	ASN
1	B	3963	ASN
1	B	3977	GLN
1	B	4034	ASN
1	B	4037	ASN
1	B	4054	ASN
1	B	4078	GLN
1	B	4109	GLN
1	B	4133	GLN
1	B	4142	ASN
1	B	4209	GLN
1	B	4246	GLN
1	B	4553	ASN
1	B	4691	GLN
1	B	4832	HIS
1	B	4833	ASN
1	B	4836	GLN
1	B	4949	GLN
1	B	4987	ASN
1	B	5031	GLN
1	C	57	ASN
1	C	105	HIS
1	C	111	HIS
1	C	113	HIS
1	C	151	HIS
1	C	156	GLN
1	C	201	ASN
1	C	203	ASN

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Mol	Chain	Res	Type
1	C	273	HIS
1	C	379	HIS
1	C	383	HIS
1	C	465	GLN
1	C	495	ASN
1	C	536	ASN
1	C	582	HIS
1	C	765	GLN
1	C	838	HIS
1	C	949	ASN
1	C	1158	ASN
1	C	1206	GLN
1	C	1220	GLN
1	C	1598	GLN
1	C	1679	ASN
1	C	1719	HIS
1	C	1775	HIS
1	C	1861	GLN
1	C	1938	GLN
1	C	1973	GLN
1	C	2007	ASN
1	C	2011	HIS
1	C	2036	GLN
1	C	2041	HIS
1	C	2095	GLN
1	C	2127	GLN
1	C	2194	HIS
1	C	2213	ASN
1	C	2773	ASN
1	C	2931	GLN
1	C	3761	GLN
1	C	3771	HIS
1	C	3809	ASN
1	C	3814	GLN
1	C	3830	GLN
1	C	3850	GLN
1	C	3882	GLN
1	C	3896	ASN
1	C	3909	ASN
1	C	3946	GLN
1	C	3950	ASN
1	C	3963	ASN

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Mol	Chain	Res	Type
1	C	3977	GLN
1	C	4034	ASN
1	C	4037	ASN
1	C	4054	ASN
1	C	4078	GLN
1	C	4109	GLN
1	C	4133	GLN
1	C	4209	GLN
1	C	4246	GLN
1	C	4553	ASN
1	C	4833	ASN
1	C	4949	GLN
1	C	5031	GLN
1	D	57	ASN
1	D	84	ASN
1	D	105	HIS
1	D	111	HIS
1	D	113	HIS
1	D	151	HIS
1	D	156	GLN
1	D	197	GLN
1	D	273	HIS
1	D	379	HIS
1	D	383	HIS
1	D	465	GLN
1	D	536	ASN
1	D	582	HIS
1	D	838	HIS
1	D	949	ASN
1	D	1158	ASN
1	D	1206	GLN
1	D	1220	GLN
1	D	1598	GLN
1	D	1679	ASN
1	D	1719	HIS
1	D	1775	HIS
1	D	1861	GLN
1	D	1938	GLN
1	D	1941	ASN
1	D	1973	GLN
1	D	2007	ASN
1	D	2011	HIS

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Mol	Chain	Res	Type
1	D	2036	GLN
1	D	2041	HIS
1	D	2095	GLN
1	D	2127	GLN
1	D	2194	HIS
1	D	2213	ASN
1	D	2931	GLN
1	D	3761	GLN
1	D	3771	HIS
1	D	3809	ASN
1	D	3814	GLN
1	D	3830	GLN
1	D	3850	GLN
1	D	3882	GLN
1	D	3896	ASN
1	D	3909	ASN
1	D	3946	GLN
1	D	3950	ASN
1	D	3963	ASN
1	D	3977	GLN
1	D	4034	ASN
1	D	4037	ASN
1	D	4054	ASN
1	D	4078	GLN
1	D	4109	GLN
1	D	4133	GLN
1	D	4209	GLN
1	D	4246	GLN
1	D	4553	ASN
1	D	4691	GLN
1	D	4832	HIS
1	D	4833	ASN
1	D	4949	GLN
1	D	4987	ASN
1	D	5031	GLN

5.3.3 RNA ⓘ

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	9
1	B	9
1	C	9
1	D	9

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	3638:UNK	C	3639:THR	N	46.99
1	B	3638:UNK	C	3639:THR	N	46.99
1	C	3638:UNK	C	3639:THR	N	46.99
1	D	3638:UNK	C	3639:THR	N	46.99

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	3246:UNK	C	3247:UNK	N	16.40
1	B	3246:UNK	C	3247:UNK	N	16.40
1	C	3246:UNK	C	3247:UNK	N	16.40
1	D	3246:UNK	C	3247:UNK	N	16.40
1	A	2733:UNK	C	2734:ASN	N	15.78
1	B	2733:UNK	C	2734:ASN	N	15.78
1	C	2733:UNK	C	2734:ASN	N	15.78
1	D	2733:UNK	C	2734:ASN	N	15.78
1	A	3216:UNK	C	3217:UNK	N	15.67
1	B	3216:UNK	C	3217:UNK	N	15.67
1	C	3216:UNK	C	3217:UNK	N	15.67
1	D	3216:UNK	C	3217:UNK	N	15.67
1	A	3535:UNK	C	3536:UNK	N	14.36
1	B	3535:UNK	C	3536:UNK	N	14.36
1	C	3535:UNK	C	3536:UNK	N	14.36
1	D	3535:UNK	C	3536:UNK	N	14.36
1	A	3147:UNK	C	3148:UNK	N	14.16
1	B	3147:UNK	C	3148:UNK	N	14.16
1	C	3147:UNK	C	3148:UNK	N	14.16
1	D	3147:UNK	C	3148:UNK	N	14.16
1	A	3313:UNK	C	3314:UNK	N	12.90
1	B	3313:UNK	C	3314:UNK	N	12.90
1	C	3313:UNK	C	3314:UNK	N	12.90
1	D	3313:UNK	C	3314:UNK	N	12.90
1	A	1572:UNK	C	1573:MET	N	12.63
1	B	1572:UNK	C	1573:MET	N	12.63
1	C	1572:UNK	C	1573:MET	N	12.63
1	D	1572:UNK	C	1573:MET	N	12.63
1	A	3327:UNK	C	3328:UNK	N	7.78
1	B	3327:UNK	C	3328:UNK	N	7.78
1	C	3327:UNK	C	3328:UNK	N	7.78
1	D	3327:UNK	C	3328:UNK	N	7.78

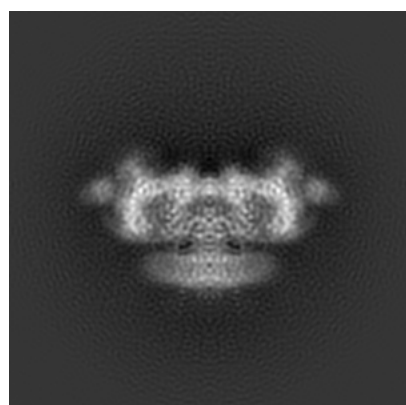
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4258. These allow visual inspection of the internal detail of the map and identification of artifacts.

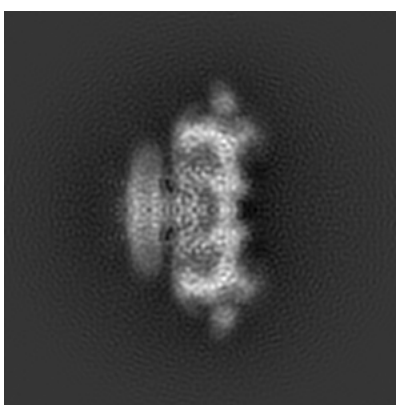
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

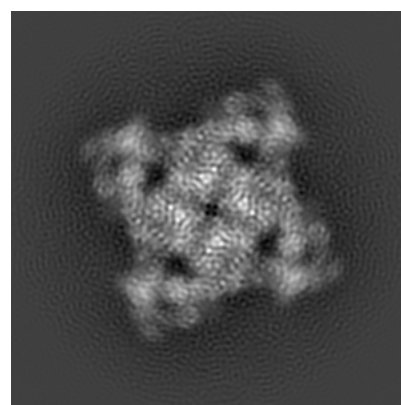
6.1.1 Primary map



X



Y

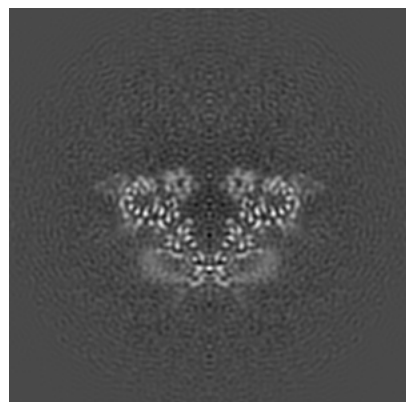


Z

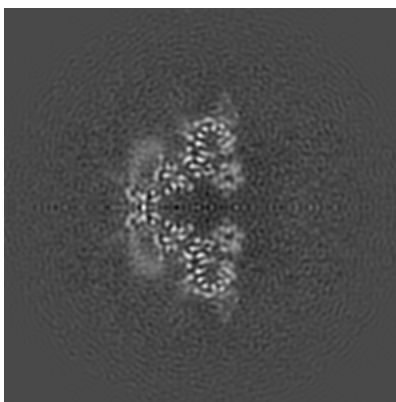
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

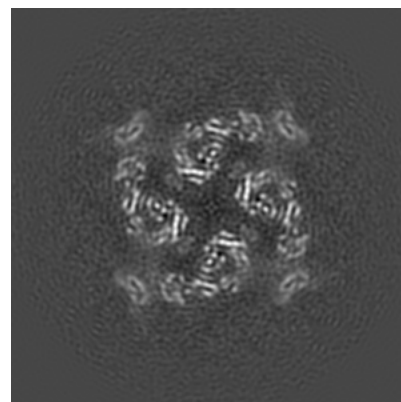
6.2.1 Primary map



X Index: 190



Y Index: 190

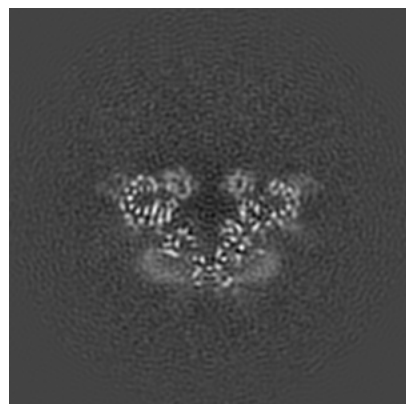


Z Index: 190

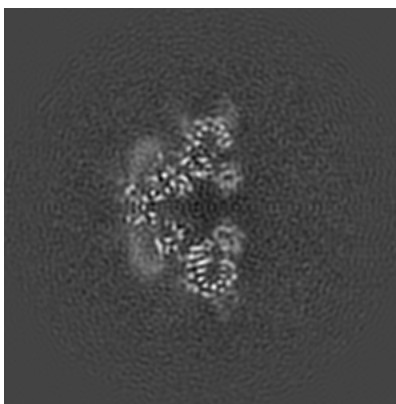
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

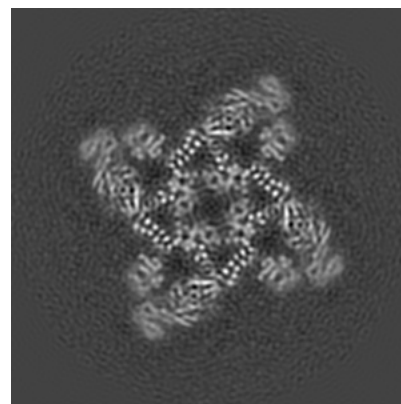
6.3.1 Primary map



X Index: 188



Y Index: 192

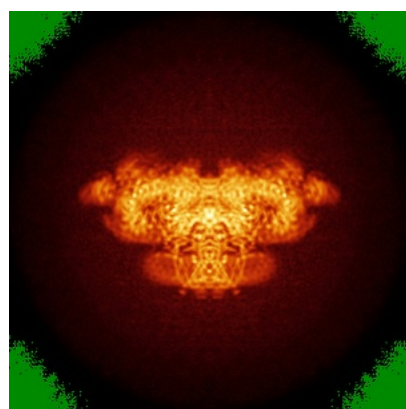


Z Index: 205

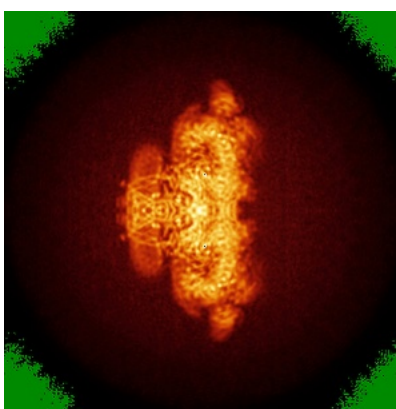
The images above show the largest variance slices of the map in three orthogonal directions.

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

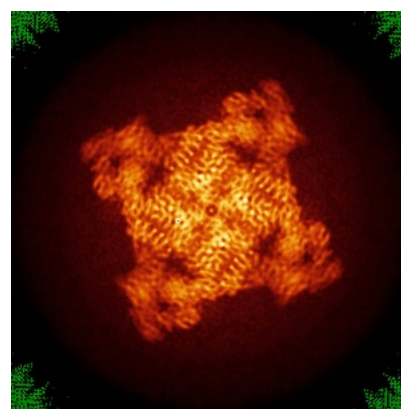
6.4.1 Primary map



X



Y

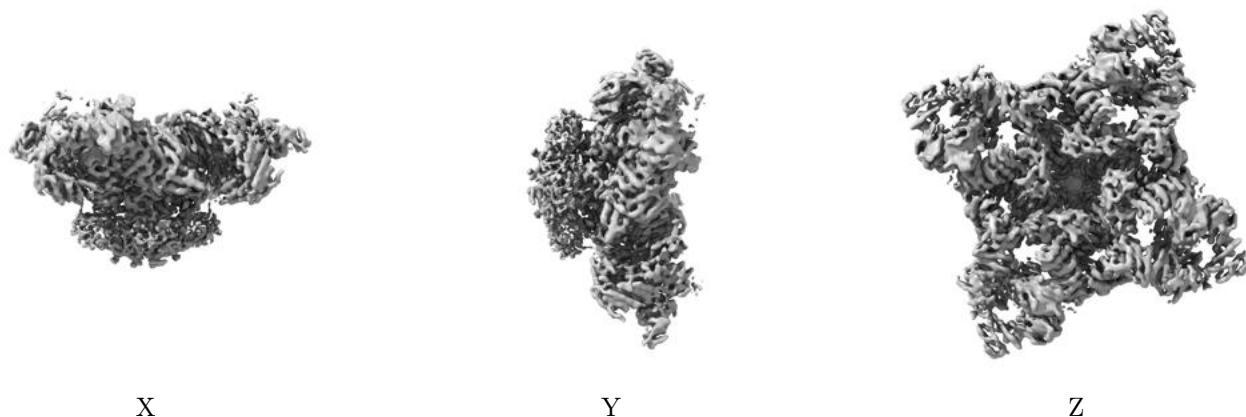


Z

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

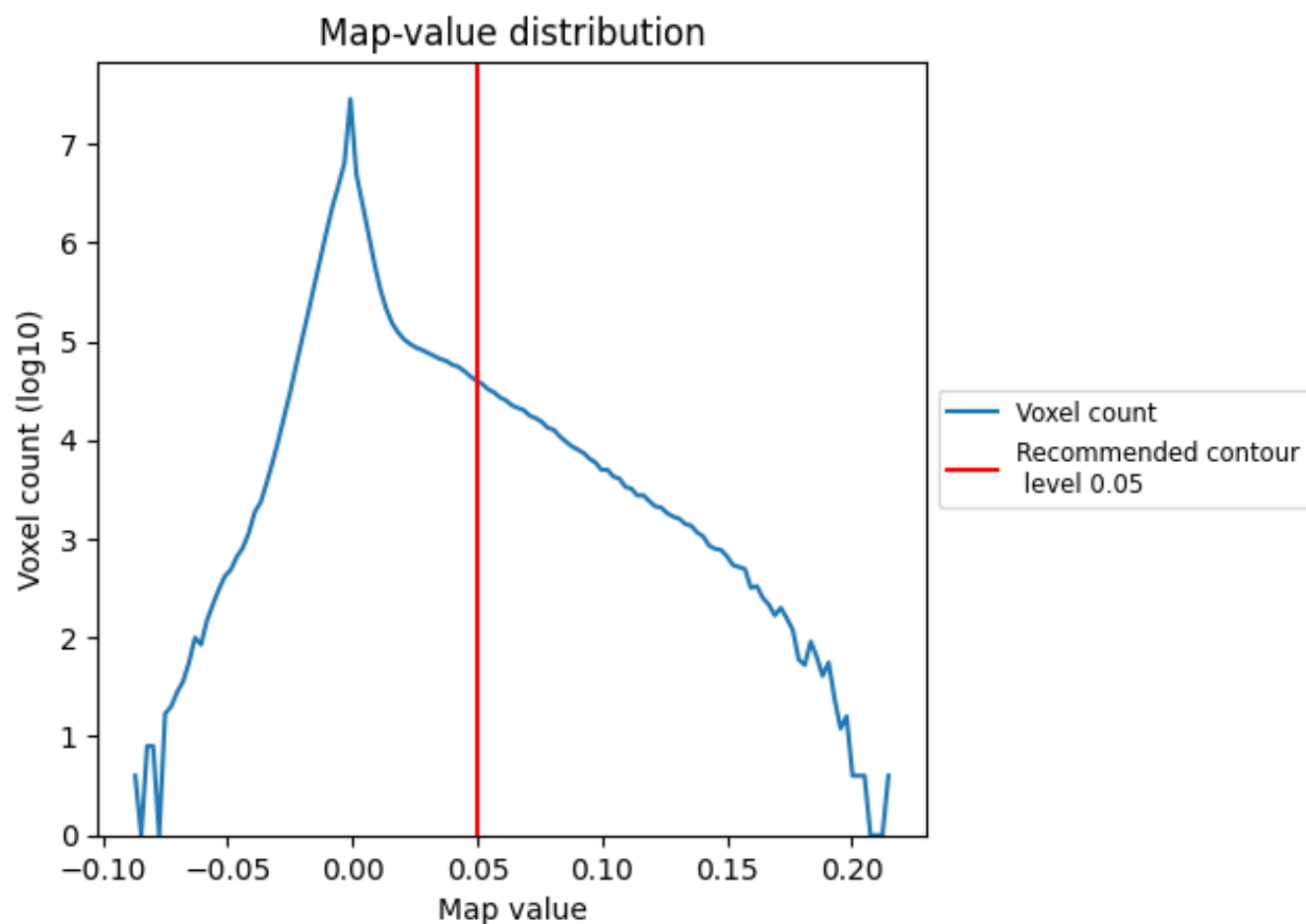
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

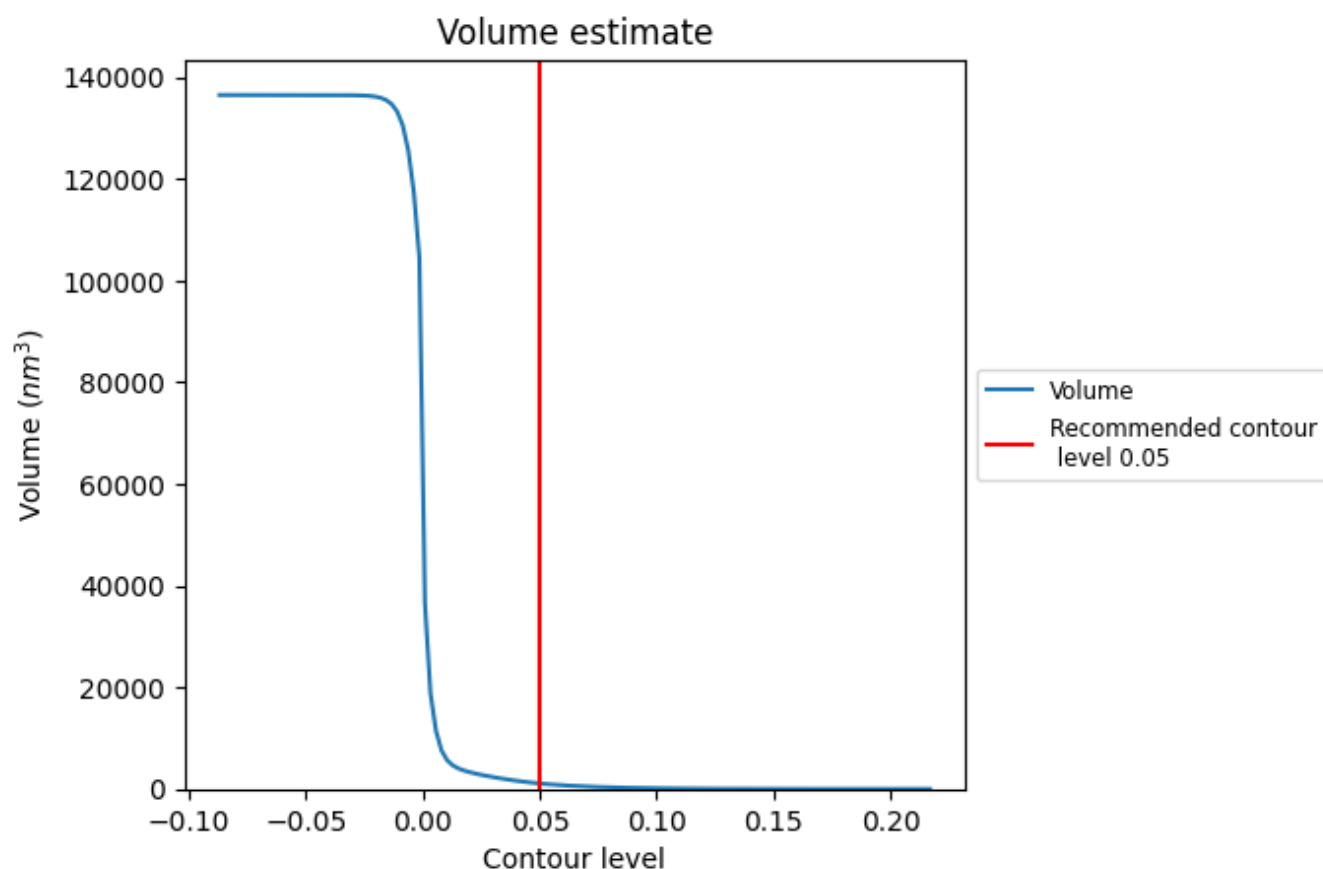
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

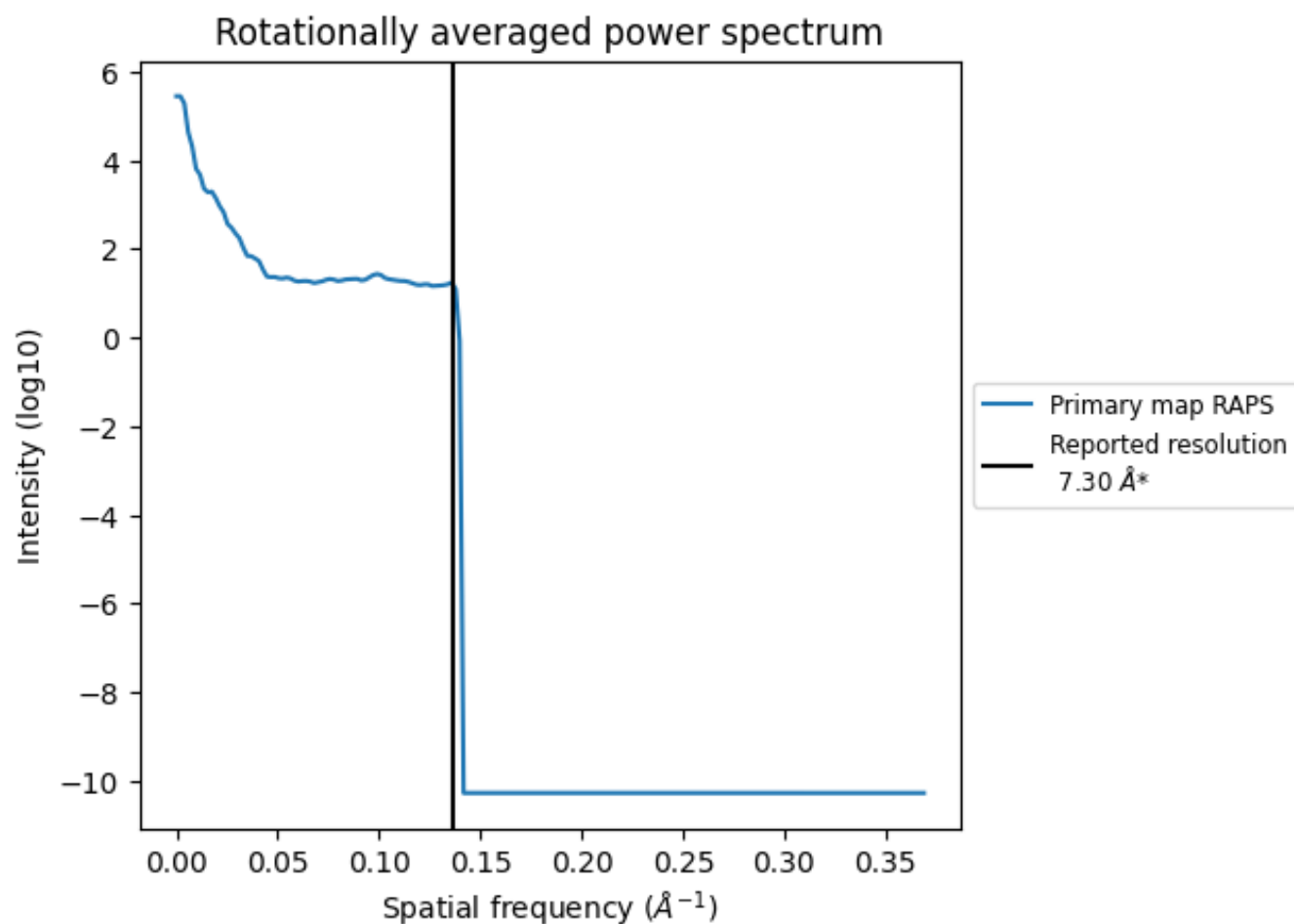
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1080 nm³; this corresponds to an approximate mass of 975 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 ⓘ

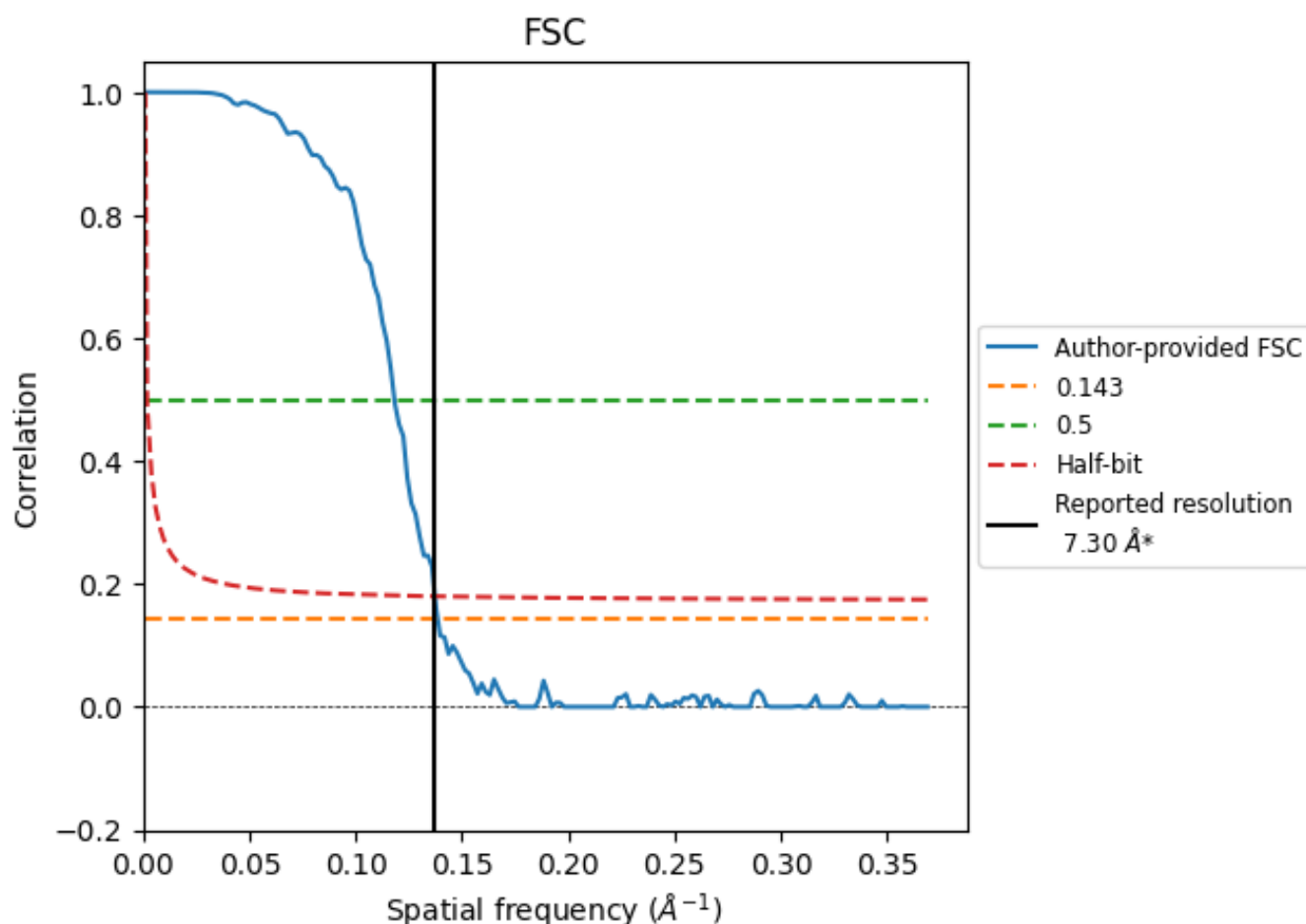


*Reported resolution corresponds to spatial frequency of 0.137 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.137 Å⁻¹

8.2 Resolution estimates [i](#)

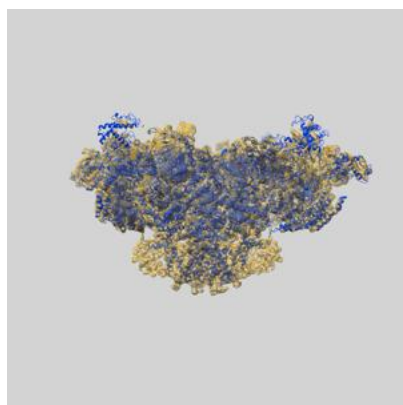
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.30	-	-
Author-provided FSC curve	7.22	8.46	7.28
Unmasked-calculated*	-	-	-

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

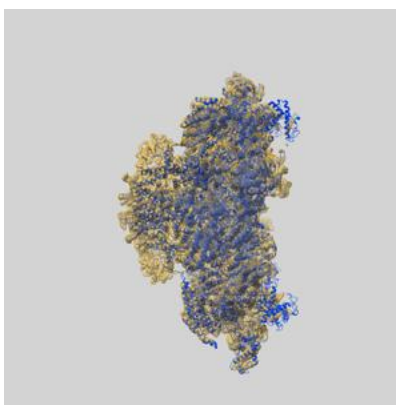
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4258 and PDB model 6FG3. Per-residue inclusion information can be found in section [3](#) on page [4](#).

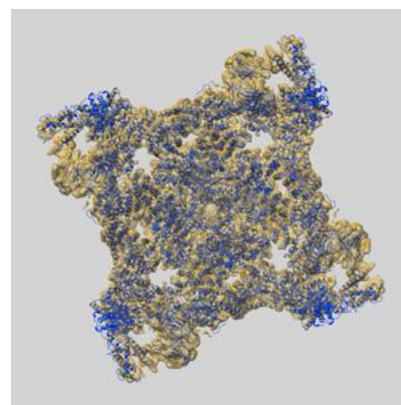
9.1 Map-model overlay [i](#)



X



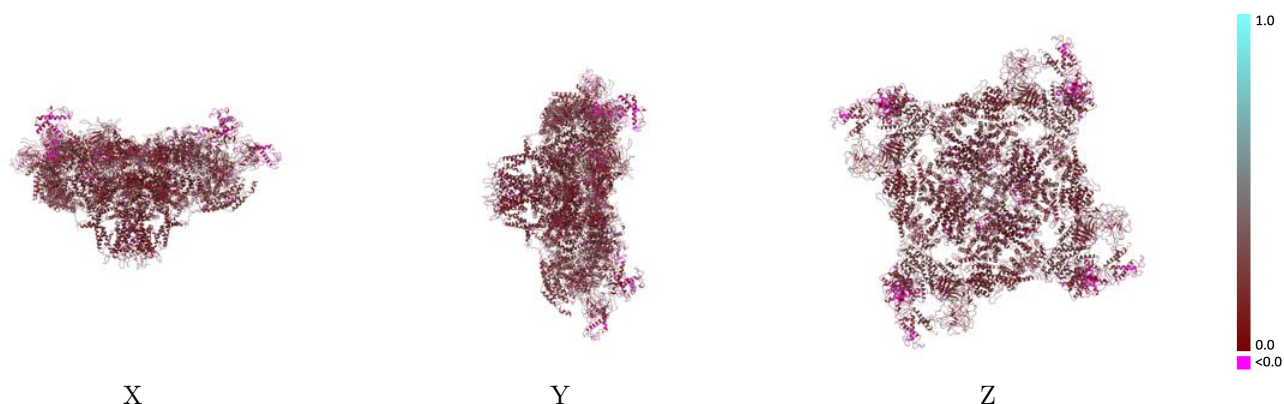
Y



Z

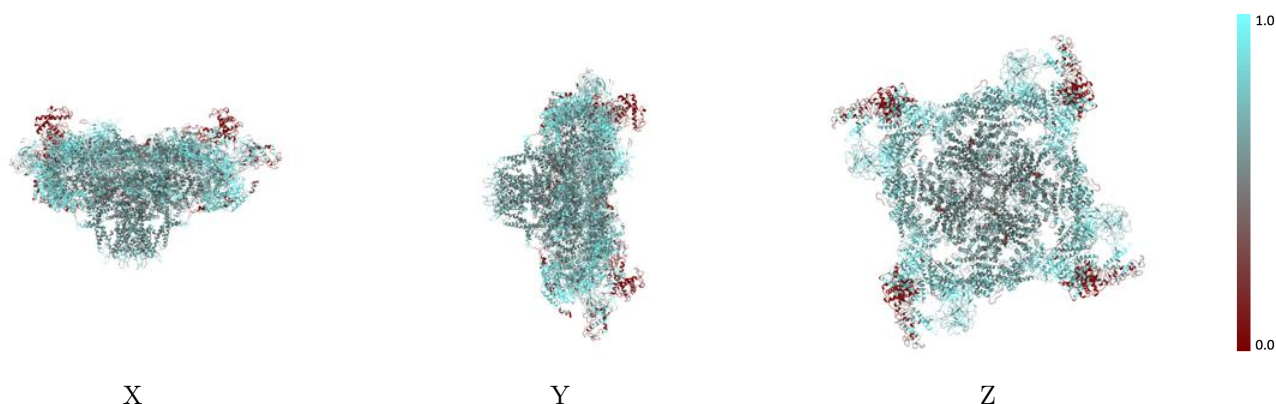
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



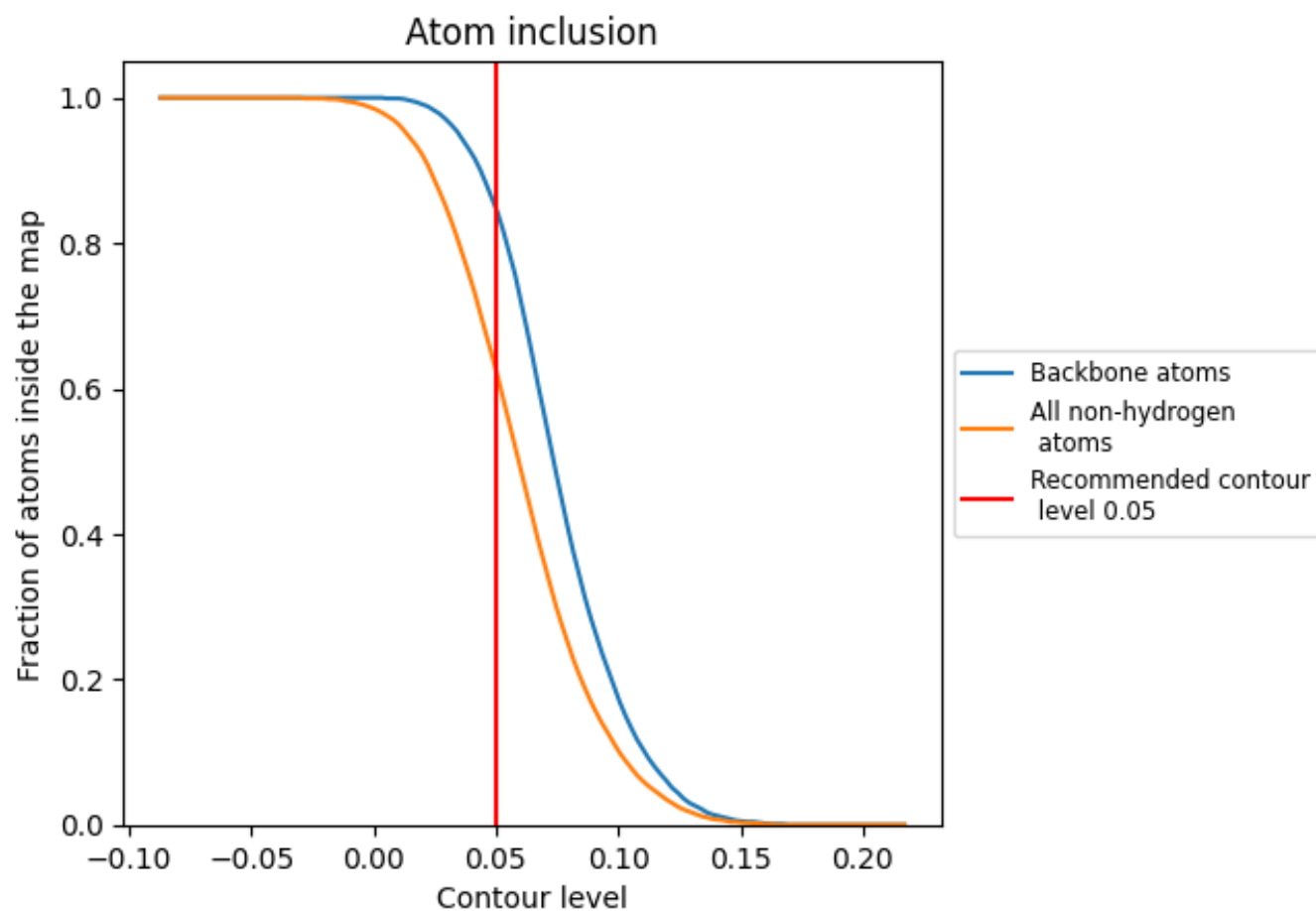
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion ⓘ



At the recommended contour level, 85% of all backbone atoms, 63% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6260	0.1910
A	0.6260	0.1900
B	0.6260	0.1910
C	0.6260	0.1910
D	0.6260	0.1900

