



Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 09:43 PM JST

PDB ID : 7CF9
EMDB ID : EMD-30343
Title : Structure of RyR1 (Ca²⁺/CHL)
Authors : Ma, R.; Haji-Ghassemi, O.; Ma, D.; Lin, L.; Samurkas, A.; Van Petegem, F.; Yuchi, Z.
Deposited on : 2020-06-24
Resolution : 4.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

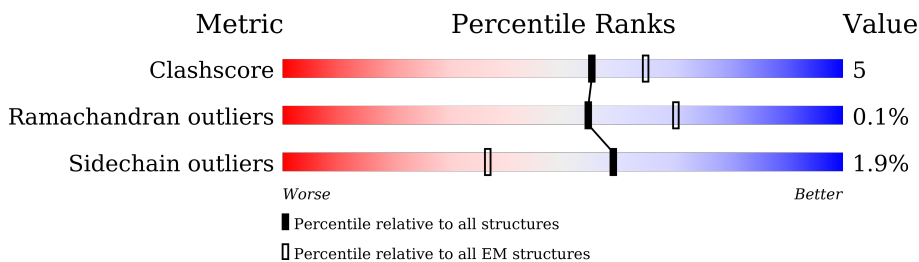
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.70 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	5037	 67% 11% 22%
1	C	5037	 67% 11% 22%
1	E	5037	 67% 11% 22%
1	G	5037	 67% 11% 22%
2	B	107	 77% 21% 2% 2%
2	D	107	 74% 24% 2% 2%
2	F	107	 72% 26% 2% 2%
2	H	107	 77% 21% 2% 2%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 116104 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,RyR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3949	Total	C	N	O	S	0	0
			28192	17975	5027	5013	177		
1	C	3949	Total	C	N	O	S	0	0
			28192	17975	5027	5013	177		
1	E	3949	Total	C	N	O	S	0	0
			28192	17975	5027	5013	177		
1	G	3949	Total	C	N	O	S	0	0
			28192	17975	5027	5013	177		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	107	Total	C	N	O	S	0	0
			804	510	144	146	4		
2	D	107	Total	C	N	O	S	0	0
			804	510	144	146	4		
2	F	107	Total	C	N	O	S	0	0
			804	510	144	146	4		
2	H	107	Total	C	N	O	S	0	0
			804	510	144	146	4		

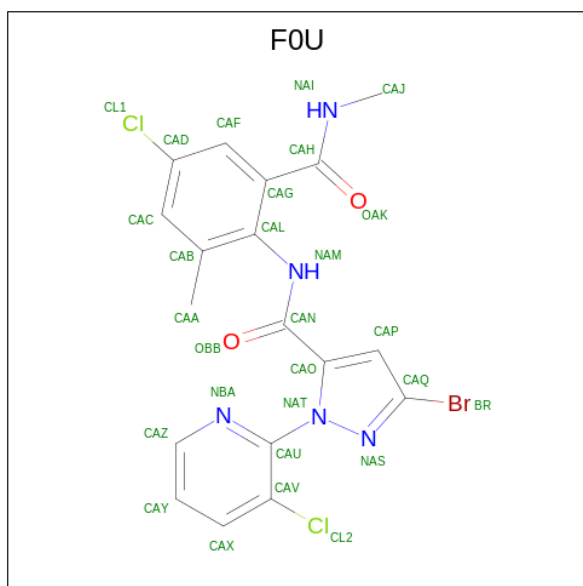
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Zn	0
			1	1	
4	C	1	Total	Zn	0
			1	1	
4	E	1	Total	Zn	0
			1	1	
4	G	1	Total	Zn	0
			1	1	

- Molecule 5 is 5-bromanyl-N-[4-chloranyl-2-methyl-6-(methylcarbamoyl)phenyl]-2-(3-chloranypyridin-2-yl)pyrazole-3-carboxamide (three-letter code: F0U) (formula: $C_{18}H_{14}BrCl_2N_5O_2$) (labeled as "Ligand of Interest" by depositor).

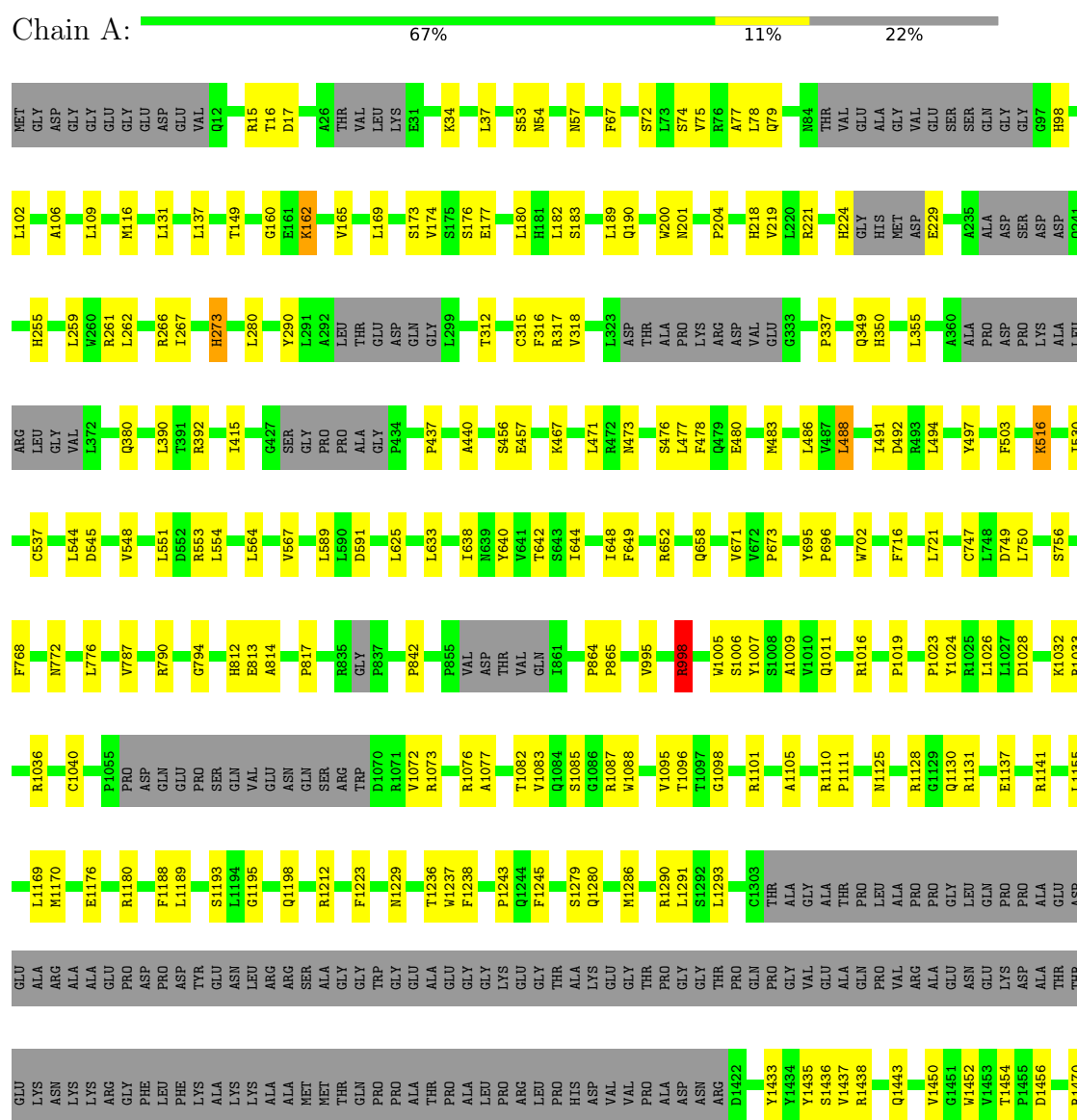


Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total	Br	C	Cl	N	O	0
			28	1	18	2	5	2	
5	C	1	Total	Br	C	Cl	N	O	0
			28	1	18	2	5	2	
5	E	1	Total	Br	C	Cl	N	O	0
			28	1	18	2	5	2	
5	G	1	Total	Br	C	Cl	N	O	0
			28	1	18	2	5	2	

3 Residue-property plots

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

• Molecule 1: Ryanodine receptor 1, RyR1







L2038	L2047	L2058	L2069	L2080	L2091	L2102	L2113	L2124	L2135	L2146	L2157	L2168	L2179	L2190	L2201	L2212	L2223	L2234	L2245	L2256	L2267	L2278	L2289	L2300	L2311	L2322	L2333	L2344	L2355	L2366	L2377	L2388	L2399	L2410	L2421	L2432	L2443	L2454	L2465	L2476	L2487	L2498	L2509	L2520	L2531	L2542	L2553	L2564	L2575	L2586	L2597	L2608	L2619	L2630	L2641	L2652	L2663	L2674	L2685	L2696	L2707	L2718	L2729	L2740	L2751	L2762	L2773	L2784	L2795	L2806	L2817	L2828	L2839	L2850	L2861	L2872	L2883	L2894	L2905	L2916	L2927	L2938	L2949	L2960	L2971	L2982	L2993	L3004	L3015	L3026	L3037	L3048	L3059	L3070	L3081	L3092	L3103	L3114	L3125	L3136	L3147	L3158	L3169	L3180	L3191	L3202	L3213	L3224	L3235	L3246	L3257	L3268	L3279	L3290	L3301	L3312	L3323	L3334	L3345	L3356	L3367	L3378	L3389	L3400	L3411	L3422	L3433	L3444	L3455	L3466	L3477	L3488	L3499	L3510	L3521	L3532	L3543	L3554	L3565	L3576	L3587	L3598	L3609	L3620	L3631	L3642	L3653	L3664	L3675	L3686	L3697	L3708	L3719	L3730	L3741	L3752	L3763	L3774	L3785	L3796	L3807	L3818	L3829	L3840	L3851	L3862	L3873	L3884	L3895	L3906	L3917	L3928	L3939	L3950	L3961	L3972	L3983	L3994	L4005	L4016	L4027	L4038	L4049	L4060	L4071	L4082	L4093	L4104	L4115	L4126	L4137	L4148	L4159	L4170	L4181	L4192	L4203	L4214	L4225	L4236	L4247	L4258	L4269	L4280	L4291	L4302	L4313	L4324	L4335	L4346	L4357	L4368	L4379	L4390	L4401	L4412	L4423	L4434	L4445	L4456	L4467	L4478	L4489	L4500	L4511	L4522	L4533	L4544	L4555	L4566	L4577	L4588	L4599	L4610	L4621	L4632	L4643	L4654	L4665	L4676	L4687	L4698	L4709	L4720	L4731	L4742	L4753	L4764	L4775	L4786	L4797	L4808	L4819	L4830	L4841	L4852	L4863	L4874	L4885	L4896	L4907	L4918	L4929	L4940	L4951	L4962	L4973	L4984	L4995	L5006	L5017	L5028	L5039	L5050	L5061	L5072	L5083	L5094	L5105	L5116	L5127	L5138	L5149	L5160	L5171	L5182	L5193	L5204	L5215	L5226	L5237	L5248	L5259	L5270	L5281	L5292	L5303	L5314	L5325	L5336	L5347	L5358	L5369	L5380	L5391	L5402	L5413	L5424	L5435	L5446	L5457	L5468	L5479	L5490	L5501	L5512	L5523	L5534	L5545	L5556	L5567	L5578	L5589	L5600	L5611	L5622	L5633	L5644	L5655	L5666	L5677	L5688	L5699	L5710	L5721	L5732	L5743	L5754	L5765	L5776	L5787	L5798	L5809	L5820	L5831	L5842	L5853	L5864	L5875	L5886	L5897	L5908	L5919	L5930	L5941	L5952	L5963	L5974	L5985	L5996	L6007	L6018	L6029	L6040	L6051	L6062	L6073	L6084	L6095	L6106	L6117	L6128	L6139	L6150	L6161	L6172	L6183	L6194	L6205	L6216	L6227	L6238	L6249	L6260	L6271	L6282	L6293	L6304	L6315	L6326	L6337	L6348	L6359	L6370	L6381	L6392	L6403	L6414	L6425	L6436	L6447	L6458	L6469	L6480	L6491	L6502	L6513	L6524	L6535	L6546	L6557	L6568	L6579	L6590	L6601	L6612	L6623	L6634	L6645	L6656	L6667	L6678	L6689	L6700	L6711	L6722	L6733	L6744	L6755	L6766	L6777	L6788	L6799	L6810	L6821	L6832	L6843	L6854	L6865	L6876	L6887	L6898	L6909	L6920	L6931	L6942	L6953	L6964	L6975	L6986	L6997	L7008	L7019	L7030	L7041	L7052	L7063	L7074	L7085	L7096	L7107	L7118	L7129	L7140	L7151	L7162	L7173	L7184	L7195	L7206	L7217	L7228	L7239	L7250	L7261	L7272	L7283	L7294	L7305	L7316	L7327	L7338	L7349	L7360	L7371	L7382	L7393	L7404	L7415	L7426	L7437	L7448	L7459	L7470	L7481	L7492	L7503	L7514	L7525	L7536	L7547	L7558	L7569	L7580	L7591	L7602	L7613	L7624	L7635	L7646	L7657	L7668	L7679	L7690	L7701	L7712	L7723	L7734	L7745	L7756	L7767	L7778	L7789	L7800	L7811	L7822	L7833	L7844	L7855	L7866	L7877	L7888	L7899	L7910	L7921	L7932	L7943	L7954	L7965	L7976	L7987	L7998	L8009	L8020	L8031	L8042	L8053	L8064	L8075	L8086	L8097	L8108	L8119	L8130	L8141	L8152	L8163	L8174	L8185	L8196	L8207	L8218	L8229	L8240	L8251	L8262	L8273	L8284	L8295	L8306	L8317	L8328	L8339	L8350	L8361	L8372	L8383	L8394	L8405	L8416	L8427	L8438	L8449	L8460	L8471	L8482	L8493	L8504	L8515	L8526	L8537	L8548	L8559	L8570	L8581	L8592	L8603	L8614	L8625	L8636	L8647	L8658	L8669	L8680	L8691	L8702	L8713	L8724	L8735	L8746	L8757	L8768	L8779	L8790	L8801	L8812	L8823	L8834	L8845	L8856	L8867	L8878	L8889	L8900	L8911	L8922	L8933	L8944	L8955	L8966	L8977	L8988	L8999	L9010	L9021	L9032	L9043	L9054	L9065	L9076	L9087	L9098	L9109	L9120	L9131	L9142	L9153	L9164	L9175	L9186	L9197	L9208	L9219	L9230	L9241	L9252	L9263	L9274	L9285	L9296	L9307	L9318	L9329	L9340	L9351	L9362	L9373	L9384	L9395	L9406	L9417	L9428	L9439	L9450	L9461	L9472	L9483	L9494	L9505	L9516	L9527	L9538	L9549	L9560	L9571	L9582	L9593	L9604	L9615	L9626	L9637	L9648	L9659	L9670	L9681	L9692	L9703	L9714	L9725	L9736	L9747	L9758	L9769	L9780	L9791	L9802	L9813	L9824	L9835	L9846	L9857	L9868	L9879	L9890	L9901	L9912	L9923	L9934	L9945	L9956	L9967	L9978	L9989	L10000	L10011	L10022	L10033	L10044	L10055	L10066	L10077	L10088	L10099	L10100	L10111	L10122	L10133	L10144	L10155	L10166	L10177	L10188	L10199	L10200	L10211	L10222	L10233	L10244	L10255	L10266	L10277	L10288	L10299	L10300	L10311	L10322	L10333	L10344	L10355	L10366	L10377	L10388	L10399	L10400	L10411	L10422	L10433	L10444	L10455	L10466	L10477	L10488	L10499	L10500	L10511	L10522	L10533	L10544	L10555	L10566	L10577	L10588	L10599	L10600	L10611	L10622	L10633	L10644	L10655	L10666	L10677	L10688	L10699	L10700	L10711	L10722	L10733	L10744	L10755	L10766	L10777	L10788	L10799	L10800	L10811	L10822	L10833	L10844	L10855	L10866	L10877	L10888	L10899	L10900	L10911	L10922	L10933	L10944	L10955	L10966	L10977	L10988	L10999	L11000	L11011	L11022	L11033	L11044	L11055	L11066	L11077	L11088	L11099	L11100	L11111	L11122	L11133	L11144	L11155	L11166	L11177	L11188	L11199	L11200	L11211	L11222	L11233	L11244	L11255	L11266	L11277	L11288	L11299	L11300	L11311	L11322	L11333	L11344	L11355	L11366	L11377	L11388	L11399	L11400	L11411	L11422	L11433	L11444	L11455	L11466	L11477	L11488	L11499	L11500	L11511	L11522	L11533	L11544	L11555	L11566	L11577	L11588	L11599	L11600	L11611	L11622	L11633	L11644	L11655	L11666	L11677	L11688	L11699	L11700	L11711	L11722	L11733	L11744	L11755	L11766	L11777	L11788	L11799	L11800	L11811	L11822	L11833	L11844	L11855	L11866	L11877	L11888	L11899	L11900	L11911	L11922	L11933	L11944	L11955	L11966	L11977	L11988	L11999	L12000	L12011	L12022	L12033	L12044	L12055	L12066	L12077	L12088	L12099	L12100	L12111	L12122	L12133	L12144	L12155	L12166	L12177	L12188	L12199	L12200	L12211	L12222	L12233	L12244	L12255	L12266	L12277	L12288	L12299	L12300	L12311	L12322	L12333	L12344	L12355	L12366	L12377	L12388	L12399	L12400	L12411	L12422	L12433	L12444	L12455	L12466	L12477	L12488	L12499	L12500	L12511	L12522	L12533	L12544	L12555	L12566	L12577	L12588	L12599	L12600	L12611	L12622	L12633	L12644	L12655	L12666	L12677	L12688	L12699	L12700	L12711	L12722	L12733	L12744	L12755	L12766	L12777	L12788	L12799	L12800	L12811	L12822	L12833	L12844	L12855	L12866	L12877	L12888	L12899	L12900	L12911	L12922	L12933	L12944	L12955	L12966	L12977	L12988	L12999	L13000	L13011	L13022	L13033	L13044	L13055	L13066	L13077	L13088	L13099	L13100	L13111	L13122	L13133	L13144	L13155	L13166	L13177	L13188	L13199	L13200	L13211	L13222	L13233	L13244	L13255	L13266	L13277	L13288	L13299	L13300	L13311	L13322	L13333	L13344	L13355	L13366	L13377	L13388	L13399	L13400	L13411	L13422	L13433	L13444	L13455	L13466	L13477	L13488	L13499	L13500	L13511	L13522	L13533	L13544	L13555	L13566	L13577	L13588	L13599	L13600	L13611	L13622	L13633	L13644	L13655	L13666	L13677	L13688	L13699	L13700	L13711	L13722	L13733	L13744	L13755	L13766	L13777	L13788	L13799	L13800	L13811	L13822	L13833	L13844	L13855	L13866	L13877	L13888	L13899	L13900	L13911	L13922	L13933	L13944	L13955	L13966	L13977	L13988	L13999	L14000	L14011	L14022	L14033	L14044	L14055	L14066	L14077	L14088	L14099	L14100	L14111	L14122	L14133	L14144	L14155	L14166	L14177	L14188	L14199	L14200	L14211	L14222	L14233	L14244	L14255	L14266	L14277	L14288	L14299	L14300	L14311	L14322	L14333	L14344	L14355	L14366	L14377	L14388	L14399	L14400	L14411	L14422	L14433	L14444	L14455	L14466	L14477	L14488	L14499	L14500	L14511	L14522	L14533	L14544	L14555	L14566	L14577	L14588	L14599	L14600	L14611	L14622	L14633	L14644	L14655	L14666	L14677	L14688	L14699	L14700	L14711	L14722	L14733	L14744	L14755	L14766	L14777	L14788	L14799	L14800	L14811	L14822	L14833	L14844	L14855	L14866	L14877	L14888	L14899	L14900	L14911	L14922	L14933	L14944	L14955	L14966	L14977	L14988	L14999	L15000	L15011	L15022	L15033	L15044	L15055	L15066	L15077	L15088	L15099	L15100	L15111	L15122	L15133	L15144	L15155	L15166	L15177	L15188	L15199	L15200	L15211	L15222	L15233	L15244	L15255	L15266	L15277	L15288	L15299	L15300	L15311	L15322	L15333	L15344	L15355	L15366	L15377	L15388	L15399	L15400	L15411	L15422	L15433	L15444	L15455	L15466	L15477	L15488	L15499	L15500	L15511	L15522	L15533	L15544	L15555	L15566	L15577	L15588	L15599	L15600	L15611	L15622	L15633	L15644	L15655	L15666	L15677	L15688	L15699	L15700	L15711	L157
-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------	------





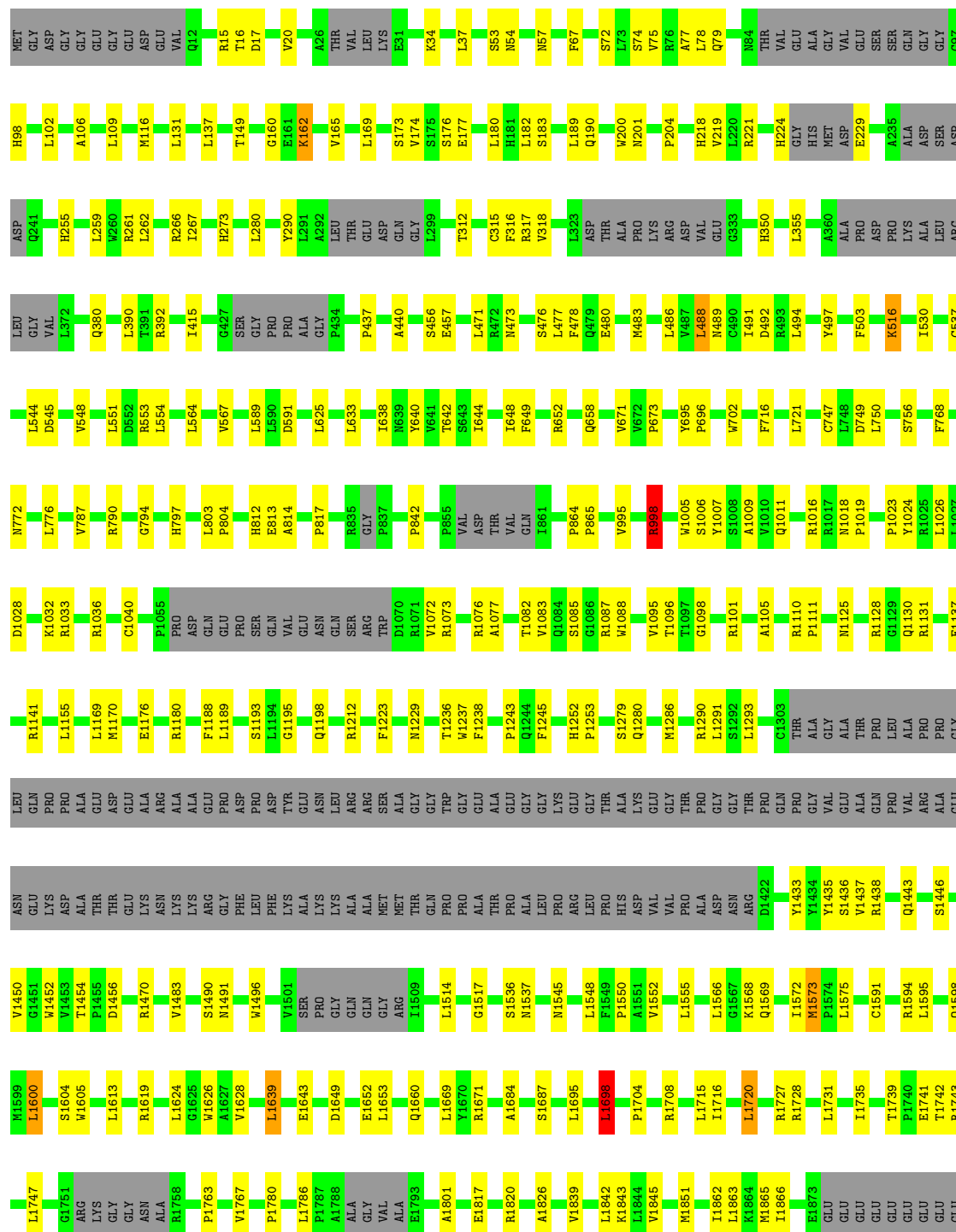






• Molecule 1: Ryanodine receptor 1, RyR1

Chain G: 67% 11% 22%




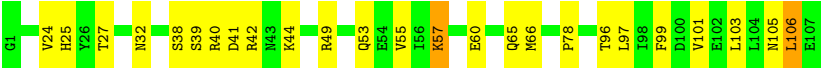


Chain F:  72% 26% .



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

Chain H:  77% 21% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35780	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.001	Depositor
Minimum map value	-0.000	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.0	Depositor
Map size (Å)	483.84003, 483.84003, 483.84003	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.32	0/26486	0.72	40/36018 (0.1%)
1	C	0.32	0/26486	0.72	40/36018 (0.1%)
1	E	0.32	0/26486	0.72	40/36018 (0.1%)
1	G	0.32	0/26486	0.72	40/36018 (0.1%)
2	B	0.33	0/820	0.76	0/1105
2	D	0.34	0/820	0.76	0/1105
2	F	0.34	0/820	0.76	0/1105
2	H	0.34	0/820	0.76	0/1105
All	All	0.32	0/109224	0.72	160/148492 (0.1%)

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	2
1	C	0	2
1	E	0	2
1	G	0	2
All	All	0	8

There are no bond length outliers.

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	998	ARG	CA-CB-CG	8.63	132.39	113.40
1	E	998	ARG	CA-CB-CG	8.61	132.35	113.40
1	A	998	ARG	CA-CB-CG	8.61	132.34	113.40
1	G	998	ARG	CA-CB-CG	8.61	132.34	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4211	LYS	CD-CE-NZ	8.17	130.49	111.70
1	G	4211	LYS	CD-CE-NZ	8.17	130.49	111.70
1	E	4211	LYS	CD-CE-NZ	8.16	130.46	111.70
1	C	4211	LYS	CD-CE-NZ	8.15	130.44	111.70
1	A	78	LEU	CA-CB-CG	7.31	132.11	115.30
1	E	78	LEU	CA-CB-CG	7.30	132.10	115.30
1	G	78	LEU	CA-CB-CG	7.30	132.09	115.30
1	C	78	LEU	CA-CB-CG	7.29	132.06	115.30
1	C	2623	LEU	CA-CB-CG	6.48	130.20	115.30
1	E	2623	LEU	CA-CB-CG	6.48	130.20	115.30
1	A	2623	LEU	CA-CB-CG	6.47	130.18	115.30
1	G	2623	LEU	CA-CB-CG	6.46	130.15	115.30
1	A	516	LYS	CD-CE-NZ	6.45	126.53	111.70
1	G	477	LEU	CA-CB-CG	6.45	130.13	115.30
1	E	477	LEU	CA-CB-CG	6.44	130.12	115.30
1	A	477	LEU	CA-CB-CG	6.44	130.11	115.30
1	C	477	LEU	CA-CB-CG	6.44	130.11	115.30
1	G	516	LYS	CD-CE-NZ	6.43	126.50	111.70
1	C	516	LYS	CD-CE-NZ	6.42	126.47	111.70
1	E	516	LYS	CD-CE-NZ	6.41	126.44	111.70
1	A	4017	LEU	CB-CG-CD2	6.22	121.57	111.00
1	E	4017	LEU	CB-CG-CD2	6.20	121.54	111.00
1	G	4017	LEU	CB-CG-CD2	6.19	121.53	111.00
1	C	4017	LEU	CB-CG-CD2	6.19	121.52	111.00
1	C	1438	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	1438	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	E	1438	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	G	1438	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	C	1720	LEU	CA-CB-CG	6.05	129.21	115.30
1	E	1720	LEU	CA-CB-CG	6.04	129.20	115.30
1	G	1720	LEU	CA-CB-CG	6.04	129.20	115.30
1	A	1720	LEU	CA-CB-CG	6.03	129.17	115.30
1	G	1698	LEU	CA-CB-CG	6.03	129.16	115.30
1	C	1698	LEU	CA-CB-CG	6.02	129.15	115.30
1	E	1698	LEU	CA-CB-CG	6.02	129.15	115.30
1	A	1698	LEU	CA-CB-CG	6.02	129.14	115.30
1	C	488	LEU	CA-CB-CG	6.00	129.09	115.30
1	E	488	LEU	CA-CB-CG	6.00	129.09	115.30
1	A	488	LEU	CA-CB-CG	5.99	129.07	115.30
1	G	488	LEU	CA-CB-CG	5.98	129.06	115.30
1	A	1715	LEU	CA-CB-CG	5.94	128.97	115.30
1	C	1715	LEU	CA-CB-CG	5.94	128.97	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1715	LEU	CA-CB-CG	5.94	128.97	115.30
1	G	1715	LEU	CA-CB-CG	5.94	128.95	115.30
1	G	4677	LEU	CA-CB-CG	5.85	128.76	115.30
1	A	553	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	C	553	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	C	4677	LEU	CA-CB-CG	5.85	128.75	115.30
1	E	4677	LEU	CA-CB-CG	5.85	128.75	115.30
1	A	4677	LEU	CA-CB-CG	5.84	128.73	115.30
1	G	553	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	E	553	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	G	1669	LEU	CA-CB-CG	5.69	128.39	115.30
1	E	1669	LEU	CA-CB-CG	5.68	128.37	115.30
1	A	1669	LEU	CA-CB-CG	5.67	128.34	115.30
1	C	1669	LEU	CA-CB-CG	5.65	128.30	115.30
1	A	544	LEU	CA-CB-CG	5.56	128.08	115.30
1	C	544	LEU	CA-CB-CG	5.55	128.06	115.30
1	E	544	LEU	CA-CB-CG	5.55	128.06	115.30
1	G	544	LEU	CA-CB-CG	5.55	128.06	115.30
1	C	2138	LEU	CA-CB-CG	5.54	128.03	115.30
1	G	2138	LEU	CA-CB-CG	5.54	128.03	115.30
1	A	2138	LEU	CA-CB-CG	5.53	128.01	115.30
1	E	2138	LEU	CA-CB-CG	5.53	128.01	115.30
1	A	1671	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	E	4046	ASP	CB-CG-OD2	5.44	123.20	118.30
1	G	2165	LEU	CA-CB-CG	5.44	127.82	115.30
1	A	2165	LEU	CA-CB-CG	5.42	127.76	115.30
1	A	4046	ASP	CB-CG-OD2	5.42	123.17	118.30
1	C	4046	ASP	CB-CG-OD2	5.42	123.17	118.30
1	G	4046	ASP	CB-CG-OD2	5.42	123.17	118.30
1	C	2165	LEU	CA-CB-CG	5.41	127.75	115.30
1	E	2165	LEU	CA-CB-CG	5.41	127.75	115.30
1	A	998	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	C	998	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	G	998	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	G	1671	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	C	3716	LEU	CA-CB-CG	5.37	127.65	115.30
1	C	37	LEU	CA-CB-CG	5.36	127.62	115.30
1	A	625	LEU	CA-CB-CG	5.35	127.60	115.30
1	A	3716	LEU	CA-CB-CG	5.35	127.60	115.30
1	C	625	LEU	CA-CB-CG	5.35	127.60	115.30
1	E	625	LEU	CA-CB-CG	5.35	127.60	115.30
1	E	3716	LEU	CA-CB-CG	5.35	127.60	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	3716	LEU	CA-CB-CG	5.35	127.60	115.30
1	A	37	LEU	CA-CB-CG	5.34	127.59	115.30
1	G	37	LEU	CA-CB-CG	5.34	127.59	115.30
1	E	1671	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	C	1671	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	E	37	LEU	CA-CB-CG	5.32	127.55	115.30
1	E	4150	LEU	CA-CB-CG	5.32	127.54	115.30
1	G	625	LEU	CA-CB-CG	5.32	127.53	115.30
1	A	4150	LEU	CA-CB-CG	5.32	127.53	115.30
1	E	998	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	C	471	LEU	CA-CB-CG	5.30	127.50	115.30
1	E	471	LEU	CA-CB-CG	5.30	127.50	115.30
1	G	471	LEU	CA-CB-CG	5.30	127.50	115.30
1	C	4150	LEU	CA-CB-CG	5.29	127.48	115.30
1	G	4150	LEU	CA-CB-CG	5.29	127.48	115.30
1	C	2550	LEU	CA-CB-CG	5.28	127.44	115.30
1	E	2550	LEU	CA-CB-CG	5.28	127.44	115.30
1	A	2550	LEU	CA-CB-CG	5.27	127.42	115.30
1	A	471	LEU	CA-CB-CG	5.27	127.41	115.30
1	G	2550	LEU	CA-CB-CG	5.26	127.39	115.30
1	A	1600	LEU	CA-CB-CG	5.25	127.36	115.30
1	C	1600	LEU	CA-CB-CG	5.25	127.36	115.30
1	E	2583	LEU	CA-CB-CG	5.25	127.36	115.30
1	E	1600	LEU	CA-CB-CG	5.24	127.36	115.30
1	G	1600	LEU	CA-CB-CG	5.24	127.36	115.30
1	A	4577	LEU	CA-CB-CG	5.24	127.34	115.30
1	C	2583	LEU	CA-CB-CG	5.24	127.34	115.30
1	G	2583	LEU	CA-CB-CG	5.24	127.34	115.30
1	A	1786	LEU	CA-CB-CG	5.23	127.33	115.30
1	C	1786	LEU	CA-CB-CG	5.23	127.33	115.30
1	E	1786	LEU	CA-CB-CG	5.23	127.34	115.30
1	G	1786	LEU	CA-CB-CG	5.23	127.33	115.30
1	G	2522	LEU	CA-CB-CG	5.23	127.33	115.30
1	A	2583	LEU	CA-CB-CG	5.23	127.32	115.30
1	C	4577	LEU	CA-CB-CG	5.22	127.32	115.30
1	E	4577	LEU	CA-CB-CG	5.22	127.32	115.30
1	G	4577	LEU	CA-CB-CG	5.22	127.32	115.30
1	A	2522	LEU	CA-CB-CG	5.22	127.31	115.30
1	C	2522	LEU	CA-CB-CG	5.22	127.31	115.30
1	E	2522	LEU	CA-CB-CG	5.21	127.30	115.30
1	G	2023	LEU	CA-CB-CG	5.19	127.24	115.30
1	E	4681	LEU	CA-CB-CG	5.19	127.23	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	4681	LEU	CA-CB-CG	5.19	127.23	115.30
1	A	2023	LEU	CA-CB-CG	5.18	127.23	115.30
1	C	2023	LEU	CA-CB-CG	5.18	127.23	115.30
1	C	1514	LEU	CA-CB-CG	5.18	127.21	115.30
1	E	1514	LEU	CA-CB-CG	5.18	127.21	115.30
1	G	1514	LEU	CA-CB-CG	5.18	127.21	115.30
1	C	4555	LEU	CA-CB-CG	5.18	127.21	115.30
1	E	2023	LEU	CA-CB-CG	5.18	127.21	115.30
1	A	4555	LEU	CA-CB-CG	5.17	127.19	115.30
1	A	4681	LEU	CA-CB-CG	5.17	127.19	115.30
1	C	4681	LEU	CA-CB-CG	5.17	127.19	115.30
1	E	4555	LEU	CA-CB-CG	5.17	127.19	115.30
1	G	4555	LEU	CA-CB-CG	5.17	127.19	115.30
1	E	4873	ASP	CB-CG-OD1	5.16	122.95	118.30
1	A	1514	LEU	CA-CB-CG	5.15	127.16	115.30
1	G	1639	LEU	CA-CB-CG	5.13	127.10	115.30
1	A	1639	LEU	CA-CB-CG	5.13	127.09	115.30
1	E	1639	LEU	CA-CB-CG	5.12	127.08	115.30
1	C	1639	LEU	CA-CB-CG	5.12	127.07	115.30
1	G	4873	ASP	CB-CG-OD1	5.11	122.90	118.30
1	A	4873	ASP	CB-CG-OD1	5.10	122.89	118.30
1	C	4873	ASP	CB-CG-OD1	5.10	122.89	118.30
1	E	554	LEU	CA-CB-CG	5.09	127.00	115.30
1	A	554	LEU	CA-CB-CG	5.09	127.00	115.30
1	G	554	LEU	CA-CB-CG	5.08	126.99	115.30
1	C	554	LEU	CA-CB-CG	5.08	126.98	115.30
1	E	2022	PRO	C-N-CA	5.08	134.40	121.70
1	G	2022	PRO	C-N-CA	5.07	134.38	121.70
1	A	2022	PRO	C-N-CA	5.07	134.36	121.70
1	C	2022	PRO	C-N-CA	5.07	134.36	121.70

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4018	ASP	Peptide
1	A	749	ASP	Peptide
1	C	4018	ASP	Peptide
1	C	749	ASP	Peptide
1	E	4018	ASP	Peptide
1	E	749	ASP	Peptide
1	G	4018	ASP	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	G	749	ASP	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	28192	0	24933	290	0
1	C	28192	0	24933	285	0
1	E	28192	0	24933	291	0
1	G	28192	0	24933	291	0
2	B	804	0	812	8	0
2	D	804	0	812	9	0
2	F	804	0	812	11	0
2	H	804	0	812	7	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
5	A	28	0	0	0	0
5	C	28	0	0	0	0
5	E	28	0	0	0	0
5	G	28	0	0	0	0
All	All	116104	0	102980	1155	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 5.

All (1155) 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:C:652:ARG:HD3	1:C:750:LEU:HB3	1.69	0.74
1:E:652:ARG:HD3	1:E:750:LEU:HB3	1.69	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2304:GLY:O	1:E:2308:GLN:HB2	1.88	0.73
1:A:2304:GLY:O	1:A:2308:GLN:HB2	1.88	0.73
1:G:652:ARG:HD3	1:G:750:LEU:HB3	1.69	0.73
1:G:2304:GLY:O	1:G:2308:GLN:HB2	1.88	0.73
1:A:652:ARG:HD3	1:A:750:LEU:HB3	1.69	0.73
1:C:2304:GLY:O	1:C:2308:GLN:HB2	1.88	0.72
1:G:794:GLY:HA3	1:G:812:HIS:HB3	1.72	0.72
1:A:794:GLY:HA3	1:A:812:HIS:HB3	1.72	0.72
1:C:794:GLY:HA3	1:C:812:HIS:HB3	1.72	0.71
1:E:794:GLY:HA3	1:E:812:HIS:HB3	1.72	0.70
1:E:2620:GLN:HA	1:E:2623:LEU:HG	1.76	0.68
1:G:4661:TYR:HH	1:G:4788:SER:HG	1.42	0.68
1:G:2620:GLN:HA	1:G:2623:LEU:HG	1.76	0.68
1:A:2620:GLN:HA	1:A:2623:LEU:HG	1.76	0.67
1:C:2620:GLN:HA	1:C:2623:LEU:HG	1.76	0.66
1:G:74:SER:HB3	1:G:77:ALA:HB2	1.78	0.66
1:C:74:SER:HB3	1:C:77:ALA:HB2	1.78	0.66
1:E:74:SER:HB3	1:E:77:ALA:HB2	1.78	0.66
1:A:74:SER:HB3	1:A:77:ALA:HB2	1.78	0.66
1:A:3767:GLN:NE2	1:A:3803:SER:O	2.29	0.65
1:G:3767:GLN:NE2	1:G:3803:SER:O	2.29	0.65
1:C:3767:GLN:NE2	1:C:3803:SER:O	2.29	0.65
1:E:3767:GLN:NE2	1:E:3803:SER:O	2.29	0.65
1:G:3924:LEU:HA	1:G:3927:GLN:HG3	1.79	0.65
1:A:3924:LEU:HA	1:A:3927:GLN:HG3	1.79	0.65
1:A:176:SER:O	1:G:2452:ARG:NH1	2.30	0.65
1:A:2452:ARG:NH1	1:C:176:SER:O	2.30	0.64
1:C:2452:ARG:NH1	1:E:176:SER:O	2.30	0.64
1:E:2452:ARG:NH1	1:G:176:SER:O	2.30	0.64
1:C:1763:PRO:HG3	1:C:2094:LEU:HD13	1.80	0.64
1:C:3924:LEU:HA	1:C:3927:GLN:HG3	1.79	0.64
1:E:3924:LEU:HA	1:E:3927:GLN:HG3	1.79	0.64
1:A:1763:PRO:HG3	1:A:2094:LEU:HD13	1.80	0.64
1:E:1780:PRO:HD3	1:E:1801:ALA:H	1.63	0.64
1:A:1780:PRO:HD3	1:A:1801:ALA:H	1.63	0.64
1:G:1763:PRO:HG3	1:G:2094:LEU:HD13	1.80	0.63
1:A:4661:TYR:HH	1:A:4788:SER:HG	1.47	0.63
1:G:1780:PRO:HD3	1:G:1801:ALA:H	1.63	0.63
1:C:1780:PRO:HD3	1:C:1801:ALA:H	1.63	0.63
1:G:2143:THR:H	1:G:3651:ASN:HD21	1.45	0.62
1:E:4068:LEU:HD21	1:E:4129:ALA:HA	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2143:THR:H	1:A:3651:ASN:HD21	1.46	0.62
1:G:488:LEU:HA	1:G:491:ILE:HG22	1.82	0.62
1:G:4068:LEU:HD21	1:G:4129:ALA:HA	1.81	0.62
1:A:1704:PRO:O	1:A:1708:ARG:HB2	1.99	0.62
1:A:3889:GLN:NE2	1:A:3967:GLU:OE1	2.33	0.62
1:G:1024:TYR:O	1:G:1032:LYS:NZ	2.32	0.62
1:C:2003:GLN:NE2	1:C:3864:THR:OG1	2.33	0.62
1:C:4680:LYS:HD3	1:C:4686:LEU:HD13	1.82	0.62
1:E:1763:PRO:HG3	1:E:2094:LEU:HD13	1.80	0.62
1:C:1085:SER:HA	1:C:1155:LEU:HD11	1.81	0.62
1:C:1704:PRO:O	1:C:1708:ARG:HB2	1.99	0.62
1:C:4068:LEU:HD21	1:C:4129:ALA:HA	1.82	0.62
1:E:488:LEU:HA	1:E:491:ILE:HG22	1.82	0.62
1:E:1243:PRO:HB2	1:E:1600:LEU:HD21	1.82	0.62
1:G:1243:PRO:HB2	1:G:1600:LEU:HD21	1.82	0.62
1:G:1948:ASP:OD1	1:G:2126:ARG:NH1	2.31	0.62
1:A:488:LEU:HA	1:A:491:ILE:HG22	1.82	0.62
1:A:4068:LEU:HD21	1:A:4129:ALA:HA	1.81	0.62
1:C:1024:TYR:O	1:C:1032:LYS:NZ	2.32	0.62
1:C:3889:GLN:NE2	1:C:3967:GLU:OE1	2.33	0.62
1:E:1085:SER:HA	1:E:1155:LEU:HD11	1.81	0.62
1:E:1704:PRO:O	1:E:1708:ARG:HB2	1.99	0.62
1:E:4680:LYS:HD3	1:E:4686:LEU:HD13	1.82	0.62
1:G:3889:GLN:NE2	1:G:3967:GLU:OE1	2.33	0.62
1:A:1024:TYR:O	1:A:1032:LYS:NZ	2.32	0.62
1:C:1545:ASN:HD21	2:D:32:ASN:HA	1.65	0.62
1:E:2143:THR:H	1:E:3651:ASN:HD21	1.45	0.62
1:A:4680:LYS:HD3	1:A:4686:LEU:HD13	1.82	0.62
1:E:2003:GLN:NE2	1:E:3864:THR:OG1	2.33	0.61
1:G:1085:SER:HA	1:G:1155:LEU:HD11	1.81	0.61
1:C:2143:THR:H	1:C:3651:ASN:HD21	1.45	0.61
1:A:1085:SER:HA	1:A:1155:LEU:HD11	1.81	0.61
1:C:16:THR:HB	1:C:98:HIS:HB3	1.83	0.61
1:A:2003:GLN:NE2	1:A:3864:THR:OG1	2.33	0.61
1:C:488:LEU:HA	1:C:491:ILE:HG22	1.82	0.61
1:E:16:THR:HB	1:E:98:HIS:HB3	1.83	0.61
1:G:1704:PRO:O	1:G:1708:ARG:HB2	1.99	0.61
1:G:4680:LYS:HD3	1:G:4686:LEU:HD13	1.82	0.61
1:A:34:LYS:H	1:A:53:SER:HB3	1.66	0.61
1:G:2003:GLN:NE2	1:G:3864:THR:OG1	2.33	0.61
1:C:1243:PRO:HB2	1:C:1600:LEU:HD21	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1739:THR:HG23	1:C:1741:GLU:H	1.66	0.60
1:E:3889:GLN:NE2	1:E:3967:GLU:OE1	2.33	0.60
1:G:842:PRO:HD3	1:G:1073:ARG:HD2	1.83	0.60
1:E:1739:THR:HG23	1:E:1741:GLU:H	1.66	0.60
1:E:1948:ASP:OD1	1:E:2126:ARG:NH1	2.31	0.60
1:G:16:THR:HB	1:G:98:HIS:HB3	1.83	0.60
1:A:1739:THR:HG23	1:A:1741:GLU:H	1.66	0.60
1:C:34:LYS:H	1:C:53:SER:HB3	1.66	0.60
1:A:842:PRO:HD3	1:A:1073:ARG:HD2	1.83	0.60
1:A:1243:PRO:HB2	1:A:1600:LEU:HD21	1.82	0.60
1:C:1569:GLN:HE21	1:C:1572:ILE:HD13	1.66	0.60
1:E:34:LYS:H	1:E:53:SER:HB3	1.66	0.60
1:G:34:LYS:H	1:G:53:SER:HB3	1.67	0.60
1:G:2477:PRO:HB3	1:G:2487:GLN:HA	1.83	0.60
1:C:633:LEU:HB3	1:C:1639:LEU:HD11	1.83	0.60
1:G:1569:GLN:HE21	1:G:1572:ILE:HD13	1.66	0.60
1:A:644:ILE:HG21	1:A:1628:VAL:HG21	1.83	0.60
2:B:42:ARG:HB3	2:B:44:LYS:HG3	1.83	0.60
1:G:644:ILE:HG21	1:G:1628:VAL:HG21	1.83	0.60
1:A:1569:GLN:HE21	1:A:1572:ILE:HD13	1.66	0.60
1:E:842:PRO:HD3	1:E:1073:ARG:HD2	1.83	0.60
1:E:1545:ASN:HD21	2:F:32:ASN:HA	1.66	0.60
1:A:2094:LEU:HG	1:A:2127:GLN:HE22	1.67	0.60
1:E:644:ILE:HG21	1:E:1628:VAL:HG21	1.83	0.60
1:E:1024:TYR:O	1:E:1032:LYS:NZ	2.32	0.60
1:E:2583:LEU:HB3	1:E:2622:LEU:HG	1.84	0.60
1:G:1739:THR:HG23	1:G:1741:GLU:H	1.66	0.60
1:A:2477:PRO:HB3	1:A:2487:GLN:HA	1.84	0.60
1:C:1948:ASP:OD1	1:C:2126:ARG:NH1	2.31	0.60
1:C:2094:LEU:HG	1:C:2127:GLN:HE22	1.67	0.60
1:C:644:ILE:HG21	1:C:1628:VAL:HG21	1.83	0.59
1:G:2583:LEU:HB3	1:G:2622:LEU:HG	1.84	0.59
2:H:42:ARG:HB3	2:H:44:LYS:HG3	1.83	0.59
1:G:633:LEU:HB3	1:G:1639:LEU:HD11	1.83	0.59
1:G:2094:LEU:HG	1:G:2127:GLN:HE22	1.67	0.59
1:A:16:THR:HB	1:A:98:HIS:HB3	1.83	0.59
1:E:2094:LEU:HG	1:E:2127:GLN:HE22	1.67	0.59
1:E:4661:TYR:HH	1:E:4788:SER:HG	1.50	0.59
1:A:817:PRO:HB2	1:A:1028:ASP:HB2	1.85	0.59
1:E:633:LEU:HB3	1:E:1639:LEU:HD11	1.83	0.59
1:C:2583:LEU:HB3	1:C:2622:LEU:HG	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1569:GLN:HE21	1:E:1572:ILE:HD13	1.66	0.59
1:C:2477:PRO:HB3	1:C:2487:GLN:HA	1.84	0.59
1:C:4661:TYR:HH	1:C:4788:SER:HG	1.49	0.59
1:A:1948:ASP:OD1	1:A:2126:ARG:NH1	2.31	0.59
1:C:842:PRO:HD3	1:C:1073:ARG:HD2	1.83	0.59
1:G:817:PRO:HB2	1:G:1028:ASP:HB2	1.85	0.59
1:A:4025:VAL:HA	1:A:4028:LEU:HB2	1.85	0.59
1:A:1839:VAL:HB	1:A:1935:VAL:HG12	1.85	0.59
1:C:1839:VAL:HB	1:C:1935:VAL:HG12	1.85	0.59
1:E:2196:ASN:HD21	1:E:2245:GLN:HE21	1.51	0.59
1:E:2477:PRO:HB3	1:E:2487:GLN:HA	1.83	0.59
1:A:633:LEU:HB3	1:A:1639:LEU:HD11	1.83	0.59
1:C:2196:ASN:HD21	1:C:2245:GLN:HE21	1.51	0.59
1:C:4025:VAL:HA	1:C:4028:LEU:HB2	1.85	0.59
1:G:1839:VAL:HB	1:G:1935:VAL:HG12	1.85	0.59
2:F:42:ARG:HB3	2:F:44:LYS:HG3	1.83	0.58
1:A:2583:LEU:HB3	1:A:2622:LEU:HG	1.84	0.58
1:C:4818:MET:O	1:C:4824:ARG:NH2	2.36	0.58
2:D:42:ARG:HB3	2:D:44:LYS:HG3	1.83	0.58
1:E:1839:VAL:HB	1:E:1935:VAL:HG12	1.85	0.58
1:G:3645:PRO:HD2	1:G:3648:ARG:HD3	1.86	0.58
1:A:173:SER:OG	1:A:174:VAL:N	2.37	0.58
1:C:4664:LEU:HD23	1:C:4665:LYS:HB3	1.86	0.58
1:G:4025:VAL:HA	1:G:4028:LEU:HB2	1.85	0.58
1:A:437:PRO:HB2	1:A:440:ALA:HB3	1.86	0.58
1:A:1131:ARG:HB2	1:A:1137:GLU:H	1.69	0.58
1:A:3645:PRO:HD2	1:A:3648:ARG:HD3	1.86	0.58
1:C:173:SER:OG	1:C:174:VAL:N	2.37	0.58
1:G:1131:ARG:HB2	1:G:1137:GLU:H	1.69	0.58
1:C:2494:PHE:HE2	1:C:2498:HIS:HB2	1.69	0.58
1:E:1131:ARG:HB2	1:E:1137:GLU:H	1.69	0.58
1:E:4818:MET:O	1:E:4824:ARG:NH2	2.36	0.58
1:C:1727:ARG:NH1	1:C:1851:MET:O	2.37	0.58
1:C:3645:PRO:HD2	1:C:3648:ARG:HD3	1.86	0.58
1:G:4818:MET:O	1:G:4824:ARG:NH2	2.36	0.58
1:A:4818:MET:O	1:A:4824:ARG:NH2	2.36	0.58
1:E:3645:PRO:HD2	1:E:3648:ARG:HD3	1.86	0.58
1:E:4664:LEU:HD23	1:E:4665:LYS:HB3	1.86	0.58
1:A:315:CYS:SG	1:A:316:PHE:N	2.77	0.58
1:A:4182:GLU:HB3	1:A:4190:ILE:HD11	1.86	0.58
1:C:817:PRO:HB2	1:C:1028:ASP:HB2	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:817:PRO:HB2	1:E:1028:ASP:HB2	1.85	0.58
1:E:1727:ARG:NH1	1:E:1851:MET:O	2.37	0.58
1:E:4025:VAL:HA	1:E:4028:LEU:HB2	1.85	0.58
1:G:437:PRO:HB2	1:G:440:ALA:HB3	1.86	0.58
1:A:2196:ASN:HD21	1:A:2245:GLN:HE21	1.51	0.57
1:C:1131:ARG:HB2	1:C:1137:GLU:H	1.69	0.57
1:C:1728:ARG:HA	1:C:1731:LEU:HD23	1.86	0.57
1:E:2494:PHE:HE2	1:E:2498:HIS:HB2	1.69	0.57
1:A:2494:PHE:HE2	1:A:2498:HIS:HB2	1.69	0.57
1:G:2494:PHE:HE2	1:G:2498:HIS:HB2	1.69	0.57
1:G:4215:ARG:HA	1:G:4218:ILE:HB	1.86	0.57
1:G:4664:LEU:HD23	1:G:4665:LYS:HB3	1.86	0.57
1:G:4182:GLU:HB3	1:G:4190:ILE:HD11	1.86	0.57
1:C:4215:ARG:HA	1:C:4218:ILE:HB	1.86	0.57
1:E:173:SER:OG	1:E:174:VAL:N	2.37	0.57
1:E:315:CYS:SG	1:E:316:PHE:N	2.77	0.57
1:G:315:CYS:SG	1:G:316:PHE:N	2.77	0.57
1:G:2196:ASN:HD21	1:G:2245:GLN:HE21	1.51	0.57
1:E:4215:ARG:HA	1:E:4218:ILE:HB	1.86	0.57
1:G:1728:ARG:HA	1:G:1731:LEU:HD23	1.86	0.57
1:C:74:SER:OG	1:C:75:VAL:N	2.38	0.57
1:G:173:SER:OG	1:G:174:VAL:N	2.37	0.57
1:A:1727:ARG:NH1	1:A:1851:MET:O	2.37	0.57
1:A:4664:LEU:HD23	1:A:4665:LYS:HB3	1.86	0.57
1:A:4704:LEU:HB3	1:A:4774:LYS:HD3	1.87	0.57
1:C:315:CYS:SG	1:C:316:PHE:N	2.77	0.57
1:C:4704:LEU:HB3	1:C:4774:LYS:HD3	1.87	0.57
1:A:1728:ARG:HA	1:A:1731:LEU:HD23	1.86	0.56
1:E:437:PRO:HB2	1:E:440:ALA:HB3	1.86	0.56
1:C:437:PRO:HB2	1:C:440:ALA:HB3	1.86	0.56
1:E:4182:GLU:HB3	1:E:4190:ILE:HD11	1.86	0.56
1:G:640:TYR:HB3	1:G:1613:LEU:HD11	1.88	0.56
1:E:3917:ILE:HA	1:E:3920:VAL:HG12	1.88	0.56
1:G:74:SER:OG	1:G:75:VAL:N	2.38	0.56
1:G:1727:ARG:NH1	1:G:1851:MET:O	2.37	0.56
1:C:4125:PHE:HA	1:C:4128:PHE:HB3	1.87	0.56
1:E:3757:GLU:HA	1:E:3760:LYS:HG2	1.88	0.56
1:E:4125:PHE:HA	1:E:4128:PHE:HB3	1.87	0.56
1:G:3757:GLU:HA	1:G:3760:LYS:HG2	1.88	0.56
1:A:4215:ARG:HA	1:A:4218:ILE:HB	1.86	0.56
1:C:4182:GLU:HB3	1:C:4190:ILE:HD11	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2138:LEU:HD11	1:C:3658:LYS:HB2	1.88	0.56
1:C:3917:ILE:HA	1:C:3920:VAL:HG12	1.88	0.56
2:F:105:ASN:OD1	2:F:106:LEU:N	2.39	0.56
1:A:491:ILE:HA	1:A:494:LEU:HB2	1.88	0.56
1:A:3917:ILE:HA	1:A:3920:VAL:HG12	1.88	0.56
1:E:74:SER:OG	1:E:75:VAL:N	2.38	0.56
1:E:491:ILE:HA	1:E:494:LEU:HB2	1.88	0.56
1:G:3958:ALA:HA	1:G:3961:VAL:HG12	1.87	0.56
1:A:1594:ARG:NH2	1:A:1643:GLU:OE2	2.39	0.56
2:B:105:ASN:OD1	2:B:106:LEU:N	2.39	0.56
1:C:1291:LEU:HB3	1:C:1595:LEU:HD22	1.87	0.56
1:C:106:ALA:HA	1:C:149:THR:HA	1.88	0.56
1:E:106:ALA:HA	1:E:149:THR:HA	1.88	0.56
1:G:3917:ILE:HA	1:G:3920:VAL:HG12	1.88	0.56
1:G:4704:LEU:HB3	1:G:4774:LYS:HD3	1.87	0.56
1:A:3624:LEU:HD13	1:A:3629:ARG:HH12	1.71	0.56
1:C:3757:GLU:HA	1:C:3760:LYS:HG2	1.88	0.56
1:E:1452:TRP:HB3	1:E:1548:LEU:HB3	1.88	0.56
1:E:1594:ARG:NH2	1:E:1643:GLU:OE2	2.39	0.55
1:A:3958:ALA:HA	1:A:3961:VAL:HG12	1.87	0.55
1:C:491:ILE:HA	1:C:494:LEU:HB2	1.88	0.55
1:E:1291:LEU:HB3	1:E:1595:LEU:HD22	1.87	0.55
1:E:1728:ARG:HA	1:E:1731:LEU:HD23	1.86	0.55
1:E:4704:LEU:HB3	1:E:4774:LYS:HD3	1.87	0.55
1:G:1594:ARG:NH2	1:G:1643:GLU:OE2	2.39	0.55
1:A:2138:LEU:HD11	1:A:3658:LYS:HB2	1.88	0.55
1:G:491:ILE:HA	1:G:494:LEU:HB2	1.88	0.55
1:G:1545:ASN:HD21	2:H:32:ASN:HA	1.71	0.55
1:A:640:TYR:HB3	1:A:1613:LEU:HD11	1.88	0.55
1:A:1649:ASP:HB3	1:A:1652:GLU:HG3	1.88	0.55
1:C:640:TYR:HB3	1:C:1613:LEU:HD11	1.87	0.55
2:D:78:PRO:HD3	2:D:96:THR:HG22	1.88	0.55
1:C:1452:TRP:HB3	1:C:1548:LEU:HB3	1.88	0.55
1:C:1594:ARG:NH2	1:C:1643:GLU:OE2	2.39	0.55
1:E:1006:SER:OG	1:E:1007:TYR:N	2.40	0.55
1:E:640:TYR:HB3	1:E:1613:LEU:HD11	1.87	0.55
1:E:2138:LEU:HD11	1:E:3658:LYS:HB2	1.88	0.55
2:F:78:PRO:HD3	2:F:96:THR:HG22	1.88	0.55
1:E:224:HIS:O	1:E:229:GLU:N	2.40	0.55
1:G:3624:LEU:HD13	1:G:3629:ARG:HH12	1.71	0.55
1:A:3757:GLU:HA	1:A:3760:LYS:HG2	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:813:GLU:HG2	1:C:1009:ALA:HB3	1.89	0.55
1:C:3958:ALA:HA	1:C:3961:VAL:HG12	1.87	0.55
2:H:105:ASN:OD1	2:H:106:LEU:N	2.39	0.55
1:C:4714:ASN:ND2	1:C:4775:TYR:OH	2.40	0.55
1:E:4247:ILE:HD13	1:E:4667:PRO:HG2	1.89	0.55
1:G:4125:PHE:HA	1:G:4128:PHE:HB3	1.87	0.55
2:H:57:LYS:HA	2:H:60:GLU:HG2	1.89	0.55
1:C:3624:LEU:HD13	1:C:3629:ARG:HH12	1.71	0.55
1:E:3958:ALA:HA	1:E:3961:VAL:HG12	1.87	0.55
1:G:106:ALA:HA	1:G:149:THR:HA	1.88	0.55
1:C:224:HIS:O	1:C:229:GLU:N	2.40	0.54
1:E:4714:ASN:ND2	1:E:4775:TYR:OH	2.40	0.54
2:F:57:LYS:HA	2:F:60:GLU:HG2	1.89	0.54
1:G:102:LEU:HD13	1:G:160:GLY:HA2	1.89	0.54
1:A:1291:LEU:HB3	1:A:1595:LEU:HD22	1.87	0.54
1:C:1279:SER:OG	1:C:1280:GLN:N	2.41	0.54
1:E:1279:SER:OG	1:E:1280:GLN:N	2.41	0.54
1:E:1649:ASP:HB3	1:E:1652:GLU:HG3	1.88	0.54
1:G:813:GLU:HG2	1:G:1009:ALA:HB3	1.89	0.54
1:G:1279:SER:OG	1:G:1280:GLN:N	2.41	0.54
1:G:1286:MET:HG3	1:G:1555:LEU:HB2	1.90	0.54
1:G:1291:LEU:HB3	1:G:1595:LEU:HD22	1.87	0.54
1:A:415:ILE:HD11	1:A:486:LEU:HD11	1.89	0.54
1:A:4125:PHE:HA	1:A:4128:PHE:HB3	1.87	0.54
1:C:1286:MET:HG3	1:C:1555:LEU:HB2	1.90	0.54
1:C:4247:ILE:HD13	1:C:4667:PRO:HG2	1.89	0.54
1:E:165:VAL:HG23	1:E:204:PRO:HD2	1.90	0.54
1:E:3752:SER:OG	1:E:3753:PHE:N	2.41	0.54
1:G:1649:ASP:HB3	1:G:1652:GLU:HG3	1.88	0.54
1:A:54:ASN:HB2	1:A:57:ASN:HD21	1.73	0.54
2:B:78:PRO:HD3	2:B:96:THR:HG22	1.88	0.54
1:C:1006:SER:OG	1:C:1007:TYR:N	2.40	0.54
1:E:3624:LEU:HD13	1:E:3629:ARG:HH12	1.71	0.54
1:E:4851:TYR:HE1	1:E:4919:THR:HG23	1.73	0.54
1:G:224:HIS:O	1:G:229:GLU:N	2.40	0.54
1:G:1452:TRP:HB3	1:G:1548:LEU:HB3	1.88	0.54
1:G:2138:LEU:HD11	1:G:3658:LYS:HB2	1.88	0.54
1:G:4851:TYR:HE1	1:G:4919:THR:HG23	1.73	0.54
1:A:102:LEU:HD13	1:A:160:GLY:HA2	1.89	0.54
1:A:4133:GLN:HA	1:A:4136:ALA:HB3	1.90	0.54
1:C:3771:HIS:HB3	1:C:3804:ILE:HD11	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:165:VAL:HG23	1:G:204:PRO:HD2	1.90	0.54
1:A:106:ALA:HA	1:A:149:THR:HA	1.88	0.54
1:A:317:ARG:NH2	1:A:350:HIS:O	2.41	0.54
1:A:1452:TRP:HB3	1:A:1548:LEU:HB3	1.88	0.54
1:E:1286:MET:HG3	1:E:1555:LEU:HB2	1.90	0.54
1:E:4051:SER:HB2	1:E:4054:ASN:HD21	1.73	0.54
1:E:4823:LEU:HD11	1:G:4839:MET:HG2	1.90	0.54
2:H:78:PRO:HD3	2:H:96:THR:HG22	1.88	0.54
1:A:131:LEU:HD11	1:G:2460:LEU:HB2	1.90	0.54
1:A:224:HIS:O	1:A:229:GLU:N	2.40	0.54
1:A:4823:LEU:HD11	1:C:4839:MET:HG2	1.90	0.54
2:B:57:LYS:HA	2:B:60:GLU:HG2	1.89	0.54
1:C:1170:MET:HA	1:C:1176:GLU:HA	1.89	0.54
1:C:1649:ASP:HB3	1:C:1652:GLU:HG3	1.88	0.54
2:D:105:ASN:OD1	2:D:106:LEU:N	2.39	0.54
1:E:54:ASN:HB2	1:E:57:ASN:HD21	1.73	0.54
1:E:2159:LEU:HA	1:E:2162:ILE:HG22	1.90	0.54
1:G:3771:HIS:HB3	1:G:3804:ILE:HD11	1.90	0.54
1:A:4714:ASN:ND2	1:A:4775:TYR:OH	2.40	0.54
1:C:2460:LEU:HB2	1:E:131:LEU:HD11	1.90	0.54
2:D:57:LYS:HA	2:D:60:GLU:HG2	1.89	0.54
1:E:415:ILE:HD11	1:E:486:LEU:HD11	1.89	0.54
1:E:3771:HIS:HB3	1:E:3804:ILE:HD11	1.90	0.54
1:G:3752:SER:OG	1:G:3753:PHE:N	2.41	0.54
1:A:3752:SER:OG	1:A:3753:PHE:N	2.41	0.54
1:C:317:ARG:NH2	1:C:350:HIS:O	2.41	0.54
1:C:4823:LEU:HD11	1:E:4839:MET:HG2	1.90	0.54
1:E:2460:LEU:HB2	1:G:131:LEU:HD11	1.90	0.54
1:G:2159:LEU:HA	1:G:2162:ILE:HG22	1.89	0.54
1:A:1286:MET:HG3	1:A:1555:LEU:HB2	1.90	0.54
1:A:2460:LEU:HB2	1:C:131:LEU:HD11	1.90	0.54
1:C:2258:LEU:HD12	1:C:2297:LYS:HE2	1.90	0.54
1:C:4051:SER:HB2	1:C:4054:ASN:HD21	1.73	0.54
1:C:54:ASN:HB2	1:C:57:ASN:HD21	1.73	0.53
1:G:2258:LEU:HD12	1:G:2297:LYS:HE2	1.90	0.53
1:G:4247:ILE:HD13	1:G:4667:PRO:HG2	1.89	0.53
1:A:813:GLU:HG2	1:A:1009:ALA:HB3	1.89	0.53
1:C:102:LEU:HD13	1:C:160:GLY:HA2	1.89	0.53
1:G:4133:GLN:HA	1:G:4136:ALA:HB3	1.90	0.53
1:A:3771:HIS:HB3	1:A:3804:ILE:HD11	1.90	0.53
1:C:1695:LEU:HA	1:C:1698:LEU:HD22	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:813:GLU:HG2	1:E:1009:ALA:HB3	1.89	0.53
1:E:2258:LEU:HD12	1:E:2297:LYS:HE2	1.90	0.53
1:G:415:ILE:HD11	1:G:486:LEU:HD11	1.89	0.53
1:G:1011:GLN:HB3	1:G:1019:PRO:HD3	1.91	0.53
1:A:2013:LYS:NZ	1:A:3660:ALA:O	2.41	0.53
1:C:1011:GLN:HB3	1:C:1019:PRO:HD3	1.91	0.53
1:C:3878:ASP:OD1	1:C:3878:ASP:N	2.42	0.53
1:A:1695:LEU:HA	1:A:1698:LEU:HD22	1.91	0.53
1:A:2159:LEU:HA	1:A:2162:ILE:HG22	1.90	0.53
1:C:415:ILE:HD11	1:C:486:LEU:HD11	1.89	0.53
1:E:1170:MET:HA	1:E:1176:GLU:HA	1.89	0.53
1:E:1695:LEU:HA	1:E:1698:LEU:HD22	1.91	0.53
1:G:1695:LEU:HA	1:G:1698:LEU:HD22	1.91	0.53
1:G:4714:ASN:ND2	1:G:4775:TYR:OH	2.40	0.53
1:A:4247:ILE:HD13	1:A:4667:PRO:HG2	1.89	0.53
1:C:2159:LEU:HA	1:C:2162:ILE:HG22	1.90	0.53
1:E:317:ARG:NH2	1:E:350:HIS:O	2.41	0.53
1:E:4133:GLN:HA	1:E:4136:ALA:HB3	1.90	0.53
1:G:1170:MET:HA	1:G:1176:GLU:HA	1.89	0.53
1:A:1011:GLN:HB3	1:A:1019:PRO:HD3	1.91	0.53
1:E:1011:GLN:HB3	1:E:1019:PRO:HD3	1.91	0.53
1:G:54:ASN:HB2	1:G:57:ASN:HD21	1.73	0.53
1:A:165:VAL:HG23	1:A:204:PRO:HD2	1.90	0.53
1:A:1170:MET:HA	1:A:1176:GLU:HA	1.89	0.53
1:C:165:VAL:HG23	1:C:204:PRO:HD2	1.90	0.53
1:E:1089:TYR:HH	1:E:1163:THR:HG1	1.51	0.53
1:G:4051:SER:HB2	1:G:4054:ASN:HD21	1.73	0.53
1:A:1279:SER:OG	1:A:1280:GLN:N	2.41	0.53
1:E:530:ILE:HG21	1:E:567:VAL:HG12	1.91	0.53
1:E:4031:LEU:HA	1:E:4034:ASN:HD22	1.74	0.53
1:G:4031:LEU:HA	1:G:4034:ASN:HD22	1.74	0.53
1:A:1006:SER:OG	1:A:1007:TYR:N	2.40	0.53
1:A:4839:MET:HG2	1:G:4823:LEU:HD11	1.90	0.53
1:E:102:LEU:HD13	1:E:160:GLY:HA2	1.89	0.53
1:G:530:ILE:HG21	1:G:567:VAL:HG12	1.91	0.53
1:G:1006:SER:OG	1:G:1007:TYR:N	2.40	0.53
1:G:1141:ARG:HG3	1:G:1169:LEU:HD11	1.91	0.53
1:A:2258:LEU:HD12	1:A:2297:LYS:HE2	1.90	0.52
1:A:4851:TYR:HE1	1:A:4919:THR:HG23	1.73	0.52
1:A:530:ILE:HG21	1:A:567:VAL:HG12	1.91	0.52
1:A:1454:THR:HG23	1:A:1456:ASP:H	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4133:GLN:HA	1:C:4136:ALA:HB3	1.90	0.52
1:C:4851:TYR:HE1	1:C:4919:THR:HG23	1.73	0.52
1:E:1141:ARG:HG3	1:E:1169:LEU:HD11	1.91	0.52
1:C:545:ASP:HA	1:C:548:VAL:HG22	1.92	0.52
1:C:1023:PRO:HG2	1:C:1026:LEU:HB2	1.92	0.52
1:G:3814:GLN:HE22	1:G:3896:ASN:HD21	1.57	0.52
1:C:3814:GLN:HE22	1:C:3896:ASN:HD21	1.57	0.52
1:A:1072:VAL:HG23	1:A:1195:GLY:HA2	1.92	0.52
1:A:2552:ARG:O	1:A:2556:LEU:HB2	2.10	0.52
1:A:3878:ASP:N	1:A:3878:ASP:OD1	2.42	0.52
1:G:3781:GLN:NE2	1:G:3819:TYR:OH	2.42	0.52
1:A:1023:PRO:HG2	1:A:1026:LEU:HB2	1.92	0.52
1:A:2575:ARG:HH12	1:A:2578:MET:HE3	1.75	0.52
1:E:1291:LEU:HB2	1:E:1550:PRO:HG2	1.91	0.52
1:E:4820:VAL:HG22	1:E:4822:THR:H	1.75	0.52
1:A:591:ASP:O	1:A:1594:ARG:NH1	2.43	0.52
1:A:1291:LEU:HB2	1:A:1550:PRO:HG2	1.91	0.52
1:A:4051:SER:HB2	1:A:4054:ASN:HD21	1.73	0.52
1:C:1072:VAL:HG23	1:C:1195:GLY:HA2	1.92	0.52
1:C:1454:THR:HG23	1:C:1456:ASP:H	1.74	0.52
1:C:4820:VAL:HG22	1:C:4822:THR:H	1.75	0.52
1:G:1291:LEU:HB2	1:G:1550:PRO:HG2	1.92	0.52
1:G:2432:LEU:O	1:G:2436:CYS:HB3	2.10	0.52
1:G:2552:ARG:O	1:G:2556:LEU:HB2	2.10	0.52
1:A:2432:LEU:O	1:A:2436:CYS:HB3	2.10	0.52
1:A:2467:VAL:HA	1:A:2470:ILE:HG22	1.92	0.52
1:C:530:ILE:HG21	1:C:567:VAL:HG12	1.91	0.52
1:E:591:ASP:O	1:E:1594:ARG:NH1	2.43	0.52
1:A:1141:ARG:HG3	1:A:1169:LEU:HD11	1.91	0.51
1:A:4031:LEU:HA	1:A:4034:ASN:HD22	1.74	0.51
1:C:3752:SER:OG	1:C:3753:PHE:N	2.41	0.51
1:A:3814:GLN:HE22	1:A:3896:ASN:HD21	1.57	0.51
1:G:180:LEU:HB2	1:G:200:TRP:HE1	1.76	0.51
1:G:1454:THR:HG23	1:G:1456:ASP:H	1.74	0.51
1:A:74:SER:OG	1:A:75:VAL:N	2.38	0.51
1:C:591:ASP:O	1:C:1594:ARG:NH1	2.43	0.51
1:C:2432:LEU:O	1:C:2436:CYS:HB3	2.10	0.51
1:C:4031:LEU:HA	1:C:4034:ASN:HD22	1.74	0.51
1:E:1023:PRO:HG2	1:E:1026:LEU:HB2	1.92	0.51
1:E:1072:VAL:HG23	1:E:1195:GLY:HA2	1.92	0.51
1:A:2466:LEU:HD11	1:A:2506:LEU:HB2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3904:ARG:NH2	1:A:3976:ASN:OD1	2.43	0.51
1:C:2467:VAL:HA	1:C:2470:ILE:HG22	1.92	0.51
1:E:456:SER:OG	1:E:457:GLU:N	2.44	0.51
1:E:2467:VAL:HA	1:E:2470:ILE:HG22	1.92	0.51
1:E:3814:GLN:HE22	1:E:3896:ASN:HD21	1.57	0.51
1:E:2432:LEU:O	1:E:2436:CYS:HB3	2.10	0.51
1:E:2552:ARG:O	1:E:2556:LEU:HB2	2.10	0.51
1:E:3781:GLN:NE2	1:E:3819:TYR:OH	2.43	0.51
1:E:4187:SER:O	1:E:4187:SER:OG	2.27	0.51
1:G:545:ASP:HA	1:G:548:VAL:HG22	1.92	0.51
1:G:591:ASP:O	1:G:1594:ARG:NH1	2.43	0.51
1:G:1023:PRO:HG2	1:G:1026:LEU:HB2	1.92	0.51
1:C:1141:ARG:HG3	1:C:1169:LEU:HD11	1.91	0.51
1:E:180:LEU:HB2	1:E:200:TRP:HE1	1.76	0.51
1:A:3781:GLN:NE2	1:A:3819:TYR:OH	2.43	0.51
1:C:3904:ARG:NH2	1:C:3976:ASN:OD1	2.43	0.51
1:E:545:ASP:HA	1:E:548:VAL:HG22	1.92	0.51
1:E:2030:ASP:OD2	1:E:2030:ASP:N	2.44	0.51
1:E:3904:ARG:NH2	1:E:3976:ASN:OD1	2.43	0.51
1:G:456:SER:OG	1:G:457:GLU:N	2.44	0.51
1:G:2549:ALA:HA	1:G:2552:ARG:HD3	1.93	0.51
1:A:642:THR:HG23	1:A:1613:LEU:HD13	1.93	0.51
1:C:2021:CYS:HB2	1:C:2028:ARG:HH22	1.76	0.51
1:C:2552:ARG:O	1:C:2556:LEU:HB2	2.10	0.51
1:E:1454:THR:HG23	1:E:1456:ASP:H	1.75	0.51
1:E:2021:CYS:HB2	1:E:2028:ARG:HH22	1.76	0.51
1:G:551:LEU:HB3	1:G:589:LEU:HD13	1.93	0.51
1:G:642:THR:HG23	1:G:1613:LEU:HD13	1.93	0.51
1:G:1653:LEU:HB3	1:G:1660:GLN:HB3	1.93	0.51
1:C:456:SER:OG	1:C:457:GLU:N	2.44	0.51
1:C:2549:ALA:HA	1:C:2552:ARG:HD3	1.93	0.51
1:E:2549:ALA:HA	1:E:2552:ARG:HD3	1.93	0.51
1:G:2021:CYS:HB2	1:G:2028:ARG:HH22	1.76	0.51
1:G:2467:VAL:HA	1:G:2470:ILE:HG22	1.92	0.51
1:A:4820:VAL:HG22	1:A:4822:THR:H	1.75	0.50
1:G:1072:VAL:HG23	1:G:1195:GLY:HA2	1.92	0.50
1:A:545:ASP:HA	1:A:548:VAL:HG22	1.92	0.50
1:A:2021:CYS:HB2	1:A:2028:ARG:HH22	1.76	0.50
1:A:2549:ALA:HA	1:A:2552:ARG:HD3	1.93	0.50
1:A:4022:ASP:HA	1:A:4025:VAL:HG12	1.94	0.50
1:C:1291:LEU:HB2	1:C:1550:PRO:HG2	1.91	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1653:LEU:HB3	1:E:1660:GLN:HB3	1.93	0.50
1:C:1089:TYR:HH	1:C:1163:THR:HG1	1.56	0.50
1:C:2575:ARG:HH12	1:C:2578:MET:HE3	1.76	0.50
1:G:2433:LEU:HB3	1:G:2457:LEU:HD11	1.94	0.50
1:G:2575:ARG:HH12	1:G:2578:MET:HE3	1.76	0.50
1:A:4892:ARG:HE	1:C:4896:GLY:HA3	1.76	0.50
1:C:1076:ARG:O	1:C:1237:TRP:N	2.45	0.50
1:E:1076:ARG:O	1:E:1237:TRP:N	2.45	0.50
1:A:456:SER:OG	1:A:457:GLU:N	2.44	0.50
1:E:671:VAL:HG22	1:E:787:VAL:HG13	1.93	0.50
1:G:3904:ARG:NH2	1:G:3976:ASN:OD1	2.43	0.50
1:A:180:LEU:HB2	1:A:200:TRP:HE1	1.76	0.50
1:A:1653:LEU:HB3	1:A:1660:GLN:HB3	1.93	0.50
1:C:642:THR:HG23	1:C:1613:LEU:HD13	1.93	0.50
1:E:2433:LEU:HB3	1:E:2457:LEU:HD11	1.94	0.50
1:G:317:ARG:NH2	1:G:350:HIS:O	2.41	0.50
1:G:1076:ARG:O	1:G:1237:TRP:N	2.45	0.50
1:G:4022:ASP:HA	1:G:4025:VAL:HG12	1.94	0.50
1:C:3626:LYS:HA	1:C:3629:ARG:HG2	1.93	0.50
1:C:4022:ASP:HA	1:C:4025:VAL:HG12	1.94	0.50
1:G:648:ILE:HG23	1:G:814:ALA:HB3	1.94	0.50
1:A:551:LEU:HB3	1:A:589:LEU:HD13	1.93	0.50
1:A:671:VAL:HG22	1:A:787:VAL:HG13	1.93	0.50
1:C:2013:LYS:NZ	1:C:3660:ALA:O	2.41	0.50
1:C:2466:LEU:HD11	1:C:2506:LEU:HB2	1.93	0.50
1:G:2466:LEU:HD11	1:G:2506:LEU:HB2	1.93	0.50
1:C:3781:GLN:NE2	1:C:3819:TYR:OH	2.43	0.50
1:C:4187:SER:O	1:C:4187:SER:OG	2.27	0.50
1:E:3626:LYS:HA	1:E:3629:ARG:HG2	1.94	0.50
1:G:4820:VAL:HG22	1:G:4822:THR:H	1.75	0.50
1:C:551:LEU:HB3	1:C:589:LEU:HD13	1.93	0.49
1:E:551:LEU:HB3	1:E:589:LEU:HD13	1.93	0.49
1:A:2149:VAL:HA	1:A:2152:THR:HG22	1.95	0.49
1:A:4896:GLY:HA3	1:G:4892:ARG:HE	1.76	0.49
1:C:1653:LEU:HB3	1:C:1660:GLN:HB3	1.93	0.49
1:C:2149:VAL:HA	1:C:2152:THR:HG22	1.95	0.49
1:E:642:THR:HG23	1:E:1613:LEU:HD13	1.93	0.49
1:E:648:ILE:HG23	1:E:814:ALA:HB3	1.94	0.49
1:C:478:PHE:HB3	1:C:483:MET:HG2	1.95	0.49
1:C:1229:ASN:HB3	1:C:1826:ALA:HA	1.94	0.49
1:E:1229:ASN:HB3	1:E:1826:ALA:HA	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4022:ASP:HA	1:E:4025:VAL:HG12	1.94	0.49
1:G:1817:GLU:HA	1:G:1820:ARG:HE	1.77	0.49
1:A:478:PHE:HB3	1:A:483:MET:HG2	1.95	0.49
1:A:1862:ILE:HA	1:A:1865:MET:HB2	1.95	0.49
1:C:1443:GLN:NE2	1:C:1555:LEU:O	2.45	0.49
1:E:2466:LEU:HD11	1:E:2506:LEU:HB2	1.93	0.49
1:G:1862:ILE:HA	1:G:1865:MET:HB2	1.95	0.49
1:A:648:ILE:HG23	1:A:814:ALA:HB3	1.94	0.49
1:A:1229:ASN:HB3	1:A:1826:ALA:HA	1.95	0.49
1:C:671:VAL:HG22	1:C:787:VAL:HG13	1.93	0.49
1:G:1229:ASN:HB3	1:G:1826:ALA:HA	1.94	0.49
1:G:2597:LYS:HA	1:G:2600:ARG:HG2	1.95	0.49
1:C:995:VAL:HA	1:C:998:ARG:HB3	1.95	0.49
1:E:478:PHE:HB3	1:E:483:MET:HG2	1.95	0.49
1:G:3626:LYS:HA	1:G:3629:ARG:HG2	1.94	0.49
1:A:995:VAL:HA	1:A:998:ARG:HB3	1.95	0.49
1:C:2433:LEU:HB3	1:C:2457:LEU:HD11	1.94	0.49
1:G:671:VAL:HG22	1:G:787:VAL:HG13	1.93	0.49
1:G:995:VAL:HA	1:G:998:ARG:HB3	1.95	0.49
1:A:4187:SER:O	1:A:4187:SER:OG	2.27	0.49
1:C:355:LEU:HD11	1:C:380:GLN:HA	1.94	0.49
1:C:2559:LEU:HD12	1:C:2602:VAL:HG23	1.95	0.49
1:E:4892:ARG:HE	1:G:4896:GLY:HA3	1.76	0.49
1:A:1735:ILE:HD11	1:A:2156:LEU:HD21	1.95	0.49
1:A:1817:GLU:HA	1:A:1820:ARG:HE	1.77	0.49
1:A:2433:LEU:HB3	1:A:2457:LEU:HD11	1.94	0.49
1:E:355:LEU:HD11	1:E:380:GLN:HA	1.94	0.49
1:E:995:VAL:HA	1:E:998:ARG:HB3	1.95	0.49
1:G:1443:GLN:NE2	1:G:1555:LEU:O	2.45	0.49
1:G:2467:VAL:O	1:G:2471:SER:HB2	2.13	0.49
1:C:1817:GLU:HA	1:C:1820:ARG:HE	1.77	0.49
1:A:1076:ARG:O	1:A:1237:TRP:N	2.45	0.48
1:A:2467:VAL:O	1:A:2471:SER:HB2	2.13	0.48
1:A:2559:LEU:HD12	1:A:2602:VAL:HG23	1.95	0.48
1:C:180:LEU:HB2	1:C:200:TRP:HE1	1.76	0.48
1:C:1862:ILE:HA	1:C:1865:MET:HB2	1.95	0.48
1:C:4667:PRO:HA	1:C:4670:ILE:HB	1.95	0.48
1:C:4892:ARG:HE	1:E:4896:GLY:HA3	1.76	0.48
1:E:1443:GLN:NE2	1:E:1555:LEU:O	2.45	0.48
1:E:1862:ILE:HA	1:E:1865:MET:HB2	1.95	0.48
1:A:3626:LYS:HA	1:A:3629:ARG:HG2	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:772:ASN:HB2	1:C:1470:ARG:HG2	1.95	0.48
1:C:2467:VAL:O	1:C:2471:SER:HB2	2.13	0.48
1:E:1105:ALA:O	1:E:1189:LEU:N	2.46	0.48
1:E:1863:LEU:HD23	1:E:1866:ILE:HD11	1.95	0.48
1:E:2149:VAL:HA	1:E:2152:THR:HG22	1.94	0.48
1:G:478:PHE:HB3	1:G:483:MET:HG2	1.95	0.48
1:G:2149:VAL:HA	1:G:2152:THR:HG22	1.95	0.48
1:E:772:ASN:HB2	1:E:1470:ARG:HG2	1.95	0.48
1:E:4667:PRO:HA	1:E:4670:ILE:HB	1.95	0.48
1:G:1735:ILE:HD11	1:G:2156:LEU:HD21	1.95	0.48
1:G:3705:PHE:HA	1:G:3708:THR:HG22	1.95	0.48
1:A:772:ASN:HB2	1:A:1470:ARG:HG2	1.95	0.48
1:A:1443:GLN:NE2	1:A:1555:LEU:O	2.45	0.48
1:C:1105:ALA:O	1:C:1189:LEU:N	2.46	0.48
1:A:3628:ARG:HH12	1:A:3858:MET:H	1.62	0.48
1:C:1735:ILE:HD11	1:C:2156:LEU:HD21	1.95	0.48
1:C:2030:ASP:OD2	1:C:2030:ASP:N	2.44	0.48
1:C:3674:ILE:HG23	1:C:3769:ARG:HH12	1.79	0.48
1:C:3705:PHE:HA	1:C:3708:THR:HG22	1.95	0.48
1:G:355:LEU:HD11	1:G:380:GLN:HA	1.94	0.48
1:A:355:LEU:HD11	1:A:380:GLN:HA	1.94	0.48
1:A:1036:ARG:O	1:A:1040:CYS:HB2	2.14	0.48
1:C:3794:VAL:HA	1:C:3797:THR:HG22	1.96	0.48
1:G:772:ASN:HB2	1:G:1470:ARG:HG2	1.95	0.48
1:G:1036:ARG:O	1:G:1040:CYS:HB2	2.14	0.48
1:C:648:ILE:HG23	1:C:814:ALA:HB3	1.94	0.48
1:E:1817:GLU:HA	1:E:1820:ARG:HE	1.78	0.48
1:E:2013:LYS:NZ	1:E:3660:ALA:O	2.41	0.48
1:E:2559:LEU:HD12	1:E:2602:VAL:HG23	1.95	0.48
1:E:2621:HIS:HA	1:E:2624:ARG:HG2	1.96	0.48
1:G:1843:LYS:HB2	1:G:1938:GLN:HE21	1.79	0.48
1:G:3628:ARG:HH12	1:G:3858:MET:H	1.62	0.48
1:A:116:MET:HB2	1:A:137:LEU:HD23	1.95	0.48
1:A:3705:PHE:HA	1:A:3708:THR:HG22	1.95	0.48
1:C:1435:TYR:HB3	1:C:1575:LEU:HD21	1.96	0.48
1:C:3628:ARG:HH12	1:C:3858:MET:H	1.62	0.48
1:E:1435:TYR:HB3	1:E:1575:LEU:HD21	1.96	0.48
1:E:1735:ILE:HD11	1:E:2156:LEU:HD21	1.95	0.48
1:E:1843:LYS:HB2	1:E:1938:GLN:HE21	1.79	0.48
1:E:3705:PHE:HA	1:E:3708:THR:HG22	1.95	0.48
1:G:2013:LYS:NZ	1:G:3660:ALA:O	2.41	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2458:ARG:HE	1:A:2510:TYR:HA	1.79	0.48
1:E:497:TYR:HB3	1:E:503:PHE:HB3	1.96	0.48
1:E:3674:ILE:HG23	1:E:3769:ARG:HH12	1.79	0.48
1:G:1105:ALA:O	1:G:1189:LEU:N	2.46	0.48
1:A:1073:ARG:HH21	1:A:1238:PHE:HE2	1.62	0.47
1:A:1863:LEU:HD23	1:A:1866:ILE:HD11	1.95	0.47
1:C:2597:LYS:HA	1:C:2600:ARG:HG2	1.95	0.47
1:C:3916:ILE:HG21	1:C:3980:LEU:HD21	1.97	0.47
1:E:1073:ARG:HH21	1:E:1238:PHE:HE2	1.62	0.47
1:E:3628:ARG:HH12	1:E:3858:MET:H	1.62	0.47
1:G:1073:ARG:HH21	1:G:1238:PHE:HE2	1.62	0.47
1:G:2621:HIS:HA	1:G:2624:ARG:HG2	1.96	0.47
1:C:497:TYR:HB3	1:C:503:PHE:HB3	1.96	0.47
1:C:1073:ARG:HH21	1:C:1238:PHE:HE2	1.62	0.47
1:C:5004:THR:H	1:C:5007:GLU:HB2	1.80	0.47
1:E:1036:ARG:O	1:E:1040:CYS:HB2	2.14	0.47
1:E:2597:LYS:HA	1:E:2600:ARG:HG2	1.95	0.47
1:E:3794:VAL:HA	1:E:3797:THR:HG22	1.96	0.47
1:G:1863:LEU:HD23	1:G:1866:ILE:HD11	1.95	0.47
1:C:2254:LEU:HA	1:C:2257:LEU:HB2	1.96	0.47
1:C:4870:ASP:OD1	1:C:4870:ASP:N	2.48	0.47
1:G:4667:PRO:HA	1:G:4670:ILE:HB	1.95	0.47
1:A:492:ASP:OD1	1:A:492:ASP:N	2.48	0.47
1:A:1545:ASN:HD21	2:B:32:ASN:HA	1.78	0.47
1:A:1604:SER:OG	1:A:1605:TRP:N	2.48	0.47
1:A:3674:ILE:HG23	1:A:3769:ARG:HH12	1.79	0.47
1:C:1863:LEU:HD23	1:C:1866:ILE:HD11	1.95	0.47
1:E:2467:VAL:O	1:E:2471:SER:HB2	2.13	0.47
1:G:3674:ILE:HG23	1:G:3769:ARG:HH12	1.79	0.47
1:A:2254:LEU:HA	1:A:2257:LEU:HB2	1.96	0.47
1:A:2597:LYS:HA	1:A:2600:ARG:HG2	1.95	0.47
1:A:4667:PRO:HA	1:A:4670:ILE:HB	1.95	0.47
1:G:492:ASP:OD1	1:G:492:ASP:N	2.48	0.47
1:G:1435:TYR:HB3	1:G:1575:LEU:HD21	1.96	0.47
1:A:1105:ALA:O	1:A:1189:LEU:N	2.46	0.47
1:A:3916:ILE:HG21	1:A:3980:LEU:HD21	1.97	0.47
1:C:1036:ARG:O	1:C:1040:CYS:HB2	2.14	0.47
1:C:1604:SER:OG	1:C:1605:TRP:N	2.48	0.47
1:G:497:TYR:HB3	1:G:503:PHE:HB3	1.96	0.47
1:G:2030:ASP:OD2	1:G:2030:ASP:N	2.44	0.47
1:G:2458:ARG:HE	1:G:2510:TYR:HA	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2559:LEU:HD12	1:G:2602:VAL:HG23	1.95	0.47
1:G:3916:ILE:HG21	1:G:3980:LEU:HD21	1.97	0.47
1:G:4048:LEU:HD23	1:G:4055:VAL:HG11	1.97	0.47
1:A:1101:ARG:HB2	1:A:1193:SER:HB3	1.97	0.47
1:A:1436:SER:HA	1:A:1517:GLY:HA2	1.96	0.47
1:A:2621:HIS:HA	1:A:2624:ARG:HG2	1.96	0.47
1:C:1436:SER:HA	1:C:1517:GLY:HA2	1.96	0.47
1:C:2458:ARG:HE	1:C:2510:TYR:HA	1.79	0.47
1:C:2621:HIS:HA	1:C:2624:ARG:HG2	1.96	0.47
1:E:492:ASP:N	1:E:492:ASP:OD1	2.48	0.47
1:E:3916:ILE:HG21	1:E:3980:LEU:HD21	1.97	0.47
1:E:4884:LEU:HD21	1:G:4914:VAL:HG11	1.97	0.47
1:G:72:SER:O	1:G:72:SER:OG	2.32	0.47
1:G:564:LEU:HA	1:G:567:VAL:HG22	1.97	0.47
1:G:2254:LEU:HA	1:G:2257:LEU:HB2	1.97	0.47
1:G:3794:VAL:HA	1:G:3797:THR:HG22	1.96	0.47
1:A:564:LEU:HA	1:A:567:VAL:HG22	1.97	0.47
1:A:3794:VAL:HA	1:A:3797:THR:HG22	1.96	0.47
1:E:3675:ASP:OD1	1:E:3675:ASP:N	2.48	0.47
1:E:4244:GLU:HA	1:E:4247:ILE:HG22	1.97	0.47
1:G:116:MET:HB2	1:G:137:LEU:HD23	1.96	0.47
1:A:4870:ASP:N	1:A:4870:ASP:OD1	2.48	0.47
1:A:4884:LEU:HD21	1:C:4914:VAL:HG11	1.97	0.47
1:C:3772:THR:HG23	1:C:3773:ARG:HG3	1.97	0.47
1:E:5004:THR:H	1:E:5007:GLU:HB2	1.80	0.47
1:A:1435:TYR:HB3	1:A:1575:LEU:HD21	1.96	0.47
1:A:3772:THR:HG23	1:A:3773:ARG:HG3	1.97	0.47
1:A:4048:LEU:HD23	1:A:4055:VAL:HG11	1.97	0.47
1:A:4914:VAL:HG11	1:G:4884:LEU:HD21	1.97	0.47
1:C:116:MET:HB2	1:C:137:LEU:HD23	1.96	0.47
1:E:183:SER:HB3	1:E:190:GLN:H	1.80	0.47
1:E:1536:SER:OG	1:E:1537:ASN:N	2.47	0.47
1:E:4048:LEU:HD23	1:E:4055:VAL:HG11	1.97	0.47
1:G:1101:ARG:HB2	1:G:1193:SER:HB3	1.97	0.47
1:G:5004:THR:H	1:G:5007:GLU:HB2	1.80	0.47
1:A:497:TYR:HB3	1:A:503:PHE:HB3	1.96	0.46
1:A:5004:THR:H	1:A:5007:GLU:HB2	1.80	0.46
1:C:1101:ARG:HB2	1:C:1193:SER:HB3	1.97	0.46
1:C:4048:LEU:HD23	1:C:4055:VAL:HG11	1.96	0.46
1:C:4884:LEU:HD21	1:E:4914:VAL:HG11	1.97	0.46
1:C:183:SER:HB3	1:C:190:GLN:H	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:116:MET:HB2	1:E:137:LEU:HD23	1.96	0.46
1:E:649:PHE:HB3	1:E:776:LEU:HD22	1.97	0.46
1:G:2515:GLN:HG3	1:G:2518:LEU:HB3	1.96	0.46
1:G:4244:GLU:HA	1:G:4247:ILE:HG22	1.97	0.46
1:A:649:PHE:HB3	1:A:776:LEU:HD22	1.97	0.46
1:E:2254:LEU:HA	1:E:2257:LEU:HB2	1.96	0.46
1:E:2332:LEU:HD12	1:E:2432:LEU:HD13	1.98	0.46
1:G:1436:SER:HA	1:G:1517:GLY:HA2	1.96	0.46
1:A:1436:SER:OG	1:A:1437:VAL:N	2.49	0.46
1:A:1536:SER:OG	1:A:1537:ASN:N	2.47	0.46
1:A:2515:GLN:HG3	1:A:2518:LEU:HB3	1.96	0.46
1:C:652:ARG:HG2	1:C:658:GLN:HG2	1.98	0.46
1:C:3960:GLN:O	1:C:3964:SER:OG	2.34	0.46
1:E:1436:SER:HA	1:E:1517:GLY:HA2	1.96	0.46
1:G:183:SER:HB3	1:G:190:GLN:H	1.80	0.46
1:G:1436:SER:OG	1:G:1437:VAL:N	2.49	0.46
1:C:1619:ARG:HB2	1:C:1626:TRP:HA	1.97	0.46
1:C:2515:GLN:HG3	1:C:2518:LEU:HB3	1.96	0.46
1:E:1101:ARG:HB2	1:E:1193:SER:HB3	1.97	0.46
1:E:3960:GLN:O	1:E:3964:SER:OG	2.34	0.46
1:G:1604:SER:OG	1:G:1605:TRP:N	2.48	0.46
1:A:183:SER:HB3	1:A:190:GLN:H	1.80	0.46
1:E:2458:ARG:HE	1:E:2510:TYR:HA	1.79	0.46
1:E:3878:ASP:OD1	1:E:3878:ASP:N	2.42	0.46
1:G:649:PHE:HB3	1:G:776:LEU:HD22	1.97	0.46
1:G:1082:THR:OG1	1:G:1188:PHE:O	2.27	0.46
1:G:1536:SER:OG	1:G:1537:ASN:N	2.48	0.46
1:C:162:LYS:HD2	1:C:162:LYS:HA	1.69	0.46
1:E:1604:SER:OG	1:E:1605:TRP:N	2.48	0.46
1:G:162:LYS:HD2	1:G:162:LYS:HA	1.69	0.46
1:A:1619:ARG:HB2	1:A:1626:TRP:HA	1.97	0.46
1:C:564:LEU:HA	1:C:567:VAL:HG22	1.97	0.46
1:G:1619:ARG:HB2	1:G:1626:TRP:HA	1.97	0.46
1:G:3948:LYS:HD3	1:G:3948:LYS:HA	1.77	0.46
1:A:162:LYS:HD2	1:A:162:LYS:HA	1.69	0.46
1:A:1843:LYS:HB2	1:A:1938:GLN:HE21	1.79	0.46
1:A:1949:GLN:HA	1:A:1952:GLN:HB2	1.98	0.46
1:A:2030:ASP:OD2	1:A:2030:ASP:N	2.44	0.46
1:C:4244:GLU:HA	1:C:4247:ILE:HG22	1.97	0.46
1:G:1949:GLN:HA	1:G:1952:GLN:HB2	1.98	0.46
1:A:4000:MET:HB3	1:A:4013:LEU:HD11	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1843:LYS:HB2	1:C:1938:GLN:HE21	1.79	0.46
1:C:4837:LEU:HA	1:C:4840:THR:HG22	1.98	0.46
1:E:4000:MET:HB3	1:E:4013:LEU:HD11	1.98	0.46
1:G:3878:ASP:OD1	1:G:3878:ASP:N	2.42	0.46
1:A:652:ARG:HG2	1:A:658:GLN:HG2	1.98	0.45
1:A:2623:LEU:HA	1:A:2626:LEU:HB3	1.98	0.45
1:E:564:LEU:HA	1:E:567:VAL:HG22	1.97	0.45
1:E:2515:GLN:HG3	1:E:2518:LEU:HB3	1.96	0.45
1:G:3960:GLN:O	1:G:3964:SER:OG	2.34	0.45
1:A:3844:LEU:HD21	1:A:3933:PHE:HA	1.99	0.45
1:A:3960:GLN:O	1:A:3964:SER:OG	2.34	0.45
1:C:649:PHE:HB3	1:C:776:LEU:HD22	1.97	0.45
1:G:1739:THR:HG22	1:G:1742:THR:HG23	1.99	0.45
1:G:4000:MET:HB3	1:G:4013:LEU:HD11	1.98	0.45
1:E:3772:THR:HG23	1:E:3773:ARG:HG3	1.97	0.45
1:E:4571:PHE:HD1	1:E:4813:LEU:HD21	1.82	0.45
1:G:4187:SER:O	1:G:4187:SER:OG	2.27	0.45
1:C:2623:LEU:HA	1:C:2626:LEU:HB3	1.98	0.45
1:E:1619:ARG:HB2	1:E:1626:TRP:HA	1.97	0.45
1:A:72:SER:O	1:A:72:SER:OG	2.32	0.45
1:C:266:ARG:HD3	1:C:267:ILE:H	1.82	0.45
1:C:492:ASP:N	1:C:492:ASP:OD1	2.48	0.45
1:C:2155:LEU:HB2	1:C:2188:ASN:ND2	2.31	0.45
1:C:2332:LEU:HD12	1:C:2432:LEU:HD13	1.97	0.45
1:C:4571:PHE:HD1	1:C:4813:LEU:HD21	1.82	0.45
1:E:290:TYR:HB3	1:E:312:THR:HG21	1.99	0.45
1:E:1739:THR:HG22	1:E:1742:THR:HG23	1.99	0.45
1:E:4837:LEU:HA	1:E:4840:THR:HG22	1.98	0.45
1:A:2332:LEU:HD12	1:A:2432:LEU:HD13	1.98	0.45
1:A:4244:GLU:HA	1:A:4247:ILE:HG22	1.97	0.45
1:E:2155:LEU:HB2	1:E:2188:ASN:ND2	2.31	0.45
1:G:3772:THR:HG23	1:G:3773:ARG:HG3	1.97	0.45
1:G:4060:LYS:HA	1:G:4060:LYS:HD3	1.74	0.45
1:G:4837:LEU:HA	1:G:4840:THR:HG22	1.98	0.45
1:A:4837:LEU:HA	1:A:4840:THR:HG22	1.98	0.45
1:C:3844:LEU:HD21	1:C:3933:PHE:HA	1.99	0.45
1:E:2623:LEU:HA	1:E:2626:LEU:HB3	1.98	0.45
1:E:4060:LYS:HA	1:E:4060:LYS:HD3	1.74	0.45
1:G:3921:ASP:HA	1:G:3924:LEU:HG	1.99	0.45
1:A:266:ARG:HD3	1:A:267:ILE:H	1.82	0.45
1:A:1128:ARG:HB2	1:A:1130:GLN:HE22	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3675:ASP:OD1	1:C:3675:ASP:N	2.48	0.45
1:E:790:ARG:HE	1:E:1624:LEU:HB3	1.82	0.45
1:G:290:TYR:HB3	1:G:312:THR:HG21	1.99	0.45
1:G:2155:LEU:HB2	1:G:2188:ASN:ND2	2.31	0.45
1:G:2623:LEU:HA	1:G:2626:LEU:HB3	1.99	0.45
1:G:4180:ARG:HD3	1:G:4192:ARG:NH2	2.32	0.45
1:A:4180:ARG:HD3	1:A:4192:ARG:NH2	2.32	0.45
1:C:790:ARG:HE	1:C:1624:LEU:HB3	1.82	0.45
1:C:1128:ARG:HB2	1:C:1130:GLN:HE22	1.82	0.45
1:C:4000:MET:HB3	1:C:4013:LEU:HD11	1.98	0.45
1:G:3754:GLU:O	1:G:3758:MET:HB2	2.17	0.45
1:G:4047:MET:HB3	1:G:4048:LEU:HD12	1.99	0.45
1:A:790:ARG:HE	1:A:1624:LEU:HB3	1.82	0.45
1:A:3921:ASP:HA	1:A:3924:LEU:HG	1.99	0.45
1:A:290:TYR:HB3	1:A:312:THR:HG21	1.99	0.44
1:A:3754:GLU:O	1:A:3758:MET:HB2	2.17	0.44
1:A:3850:GLN:HA	1:A:3853:ALA:HB3	2.00	0.44
1:C:4180:ARG:HD3	1:C:4192:ARG:NH2	2.32	0.44
1:G:652:ARG:HG2	1:G:658:GLN:HG2	1.98	0.44
1:G:2332:LEU:HD12	1:G:2432:LEU:HD13	1.98	0.44
1:A:2155:LEU:HB2	1:A:2188:ASN:ND2	2.31	0.44
1:A:4879:MET:HA	1:A:4882:CYS:HB3	1.99	0.44
1:C:1739:THR:HG22	1:C:1742:THR:HG23	1.99	0.44
1:C:1949:GLN:HA	1:C:1952:GLN:HB2	1.98	0.44
1:C:4936:ILE:HG21	1:E:4927:ILE:HG23	1.99	0.44
1:E:182:LEU:HD22	1:E:189:LEU:HD21	2.00	0.44
1:E:3754:GLU:O	1:E:3758:MET:HB2	2.17	0.44
1:G:790:ARG:HE	1:G:1624:LEU:HB3	1.82	0.44
1:G:1095:VAL:HG13	1:G:1096:THR:HG23	1.99	0.44
1:G:4879:MET:HA	1:G:4882:CYS:HB3	1.99	0.44
1:A:1095:VAL:HG13	1:A:1096:THR:HG23	1.99	0.44
1:A:4217:PHE:HZ	1:A:4233:LEU:HD22	1.83	0.44
1:C:1436:SER:OG	1:C:1437:VAL:N	2.49	0.44
1:C:3850:GLN:HA	1:C:3853:ALA:HB3	2.00	0.44
1:C:4060:LYS:HD3	1:C:4060:LYS:HA	1.74	0.44
1:E:4879:MET:HA	1:E:4882:CYS:HB3	2.00	0.44
1:G:266:ARG:HD3	1:G:267:ILE:H	1.82	0.44
1:G:1128:ARG:HB2	1:G:1130:GLN:HE22	1.82	0.44
1:G:4217:PHE:HZ	1:G:4233:LEU:HD22	1.83	0.44
1:A:1739:THR:HG22	1:A:1742:THR:HG23	1.99	0.44
1:A:4047:MET:HB3	1:A:4048:LEU:HD12	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4707:ASN:HA	1:C:4742:GLY:HA3	1.99	0.44
1:C:4879:MET:HA	1:C:4882:CYS:HB3	2.00	0.44
1:E:266:ARG:HD3	1:E:267:ILE:H	1.82	0.44
1:E:652:ARG:HG2	1:E:658:GLN:HG2	1.98	0.44
1:E:1128:ARG:HB2	1:E:1130:GLN:HE22	1.82	0.44
1:E:4047:MET:HB3	1:E:4048:LEU:HD12	1.99	0.44
1:E:4707:ASN:HA	1:E:4742:GLY:HA3	1.99	0.44
1:G:4571:PHE:HD1	1:G:4813:LEU:HD21	1.82	0.44
1:A:1684:ALA:O	1:A:1687:SER:OG	2.35	0.44
1:A:3675:ASP:N	1:A:3675:ASP:OD1	2.48	0.44
1:A:4571:PHE:HD1	1:A:4813:LEU:HD21	1.82	0.44
1:C:2244:ARG:NH2	1:C:2283:ASN:HB2	2.33	0.44
1:C:4047:MET:HB3	1:C:4048:LEU:HD12	1.99	0.44
1:A:1005:TRP:HA	1:A:1016:ARG:HG3	2.00	0.44
1:A:4707:ASN:HA	1:A:4742:GLY:HA3	1.99	0.44
1:C:1566:LEU:HG	1:C:1591:CYS:HB2	1.99	0.44
1:E:721:LEU:HB3	1:E:768:PHE:HZ	1.83	0.44
1:E:1436:SER:OG	1:E:1437:VAL:N	2.49	0.44
1:E:4069:LYS:HD2	1:E:4069:LYS:HA	1.85	0.44
1:E:4936:ILE:HG21	1:G:4927:ILE:HG23	1.99	0.44
1:A:1077:ALA:HA	1:A:1236:THR:HA	2.00	0.44
1:A:2243:SER:OG	1:A:2244:ARG:N	2.51	0.44
1:C:290:TYR:HB3	1:C:312:THR:HG21	1.99	0.44
1:C:721:LEU:HB3	1:C:768:PHE:HZ	1.83	0.44
1:C:1077:ALA:HA	1:C:1236:THR:HA	2.00	0.44
1:C:2243:SER:OG	1:C:2244:ARG:N	2.51	0.44
1:E:1490:SER:OG	1:E:1491:ASN:N	2.51	0.44
1:G:182:LEU:HD22	1:G:189:LEU:HD21	2.00	0.44
1:C:182:LEU:HD22	1:C:189:LEU:HD21	2.00	0.44
1:C:1245:PHE:HA	1:C:1600:LEU:HA	1.99	0.44
1:E:719:LEU:HD21	2:F:7:ILE:HG12	1.99	0.44
1:E:3844:LEU:HD21	1:E:3933:PHE:HA	1.99	0.44
1:G:3850:GLN:HA	1:G:3853:ALA:HB3	2.00	0.44
1:A:4662:ASN:HA	1:A:4666:VAL:HG13	2.00	0.44
1:C:3754:GLU:O	1:C:3758:MET:HB2	2.17	0.44
1:C:3921:ASP:HA	1:C:3924:LEU:HG	1.99	0.44
1:E:173:SER:HB3	1:E:177:GLU:H	1.83	0.44
1:E:1245:PHE:HA	1:E:1600:LEU:HA	1.99	0.44
1:E:1566:LEU:HG	1:E:1591:CYS:HB2	1.99	0.44
1:E:1716:ILE:HA	1:E:1720:LEU:HD23	2.00	0.44
1:E:1949:GLN:HA	1:E:1952:GLN:HB2	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2155:LEU:HB2	1:E:2188:ASN:HD21	1.83	0.44
1:G:1077:ALA:HA	1:G:1236:THR:HA	2.00	0.44
1:G:4707:ASN:HA	1:G:4742:GLY:HA3	1.99	0.44
1:C:173:SER:HB3	1:C:177:GLU:H	1.83	0.43
1:C:2155:LEU:HB2	1:C:2188:ASN:HD21	1.83	0.43
1:C:3771:HIS:O	1:C:3815:LYS:NZ	2.51	0.43
1:E:3850:GLN:HA	1:E:3853:ALA:HB3	2.00	0.43
1:A:3771:HIS:O	1:A:3815:LYS:NZ	2.51	0.43
1:C:1490:SER:OG	1:C:1491:ASN:N	2.51	0.43
1:C:1864:LYS:NZ	1:C:1871:PHE:O	2.48	0.43
1:E:219:VAL:HG13	1:E:261:ARG:HD3	2.00	0.43
1:E:2244:ARG:NH2	1:E:2283:ASN:HB2	2.33	0.43
1:E:3921:ASP:HA	1:E:3924:LEU:HG	1.99	0.43
1:G:173:SER:HB3	1:G:177:GLU:H	1.83	0.43
1:G:864:PRO:HA	1:G:865:PRO:HD3	1.89	0.43
1:G:1490:SER:OG	1:G:1491:ASN:N	2.51	0.43
1:G:1566:LEU:HG	1:G:1591:CYS:HB2	1.99	0.43
1:G:2155:LEU:HB2	1:G:2188:ASN:HD21	1.83	0.43
1:G:4662:ASN:HA	1:G:4666:VAL:HG13	2.00	0.43
1:C:2113:SER:HA	1:C:2114:PRO:HD3	1.89	0.43
1:E:162:LYS:HA	1:E:162:LYS:HD2	1.69	0.43
1:E:4180:ARG:HD3	1:E:4192:ARG:NH2	2.32	0.43
1:E:4217:PHE:HZ	1:E:4233:LEU:HD22	1.83	0.43
1:G:638:ILE:HD13	1:G:702:TRP:HD1	1.83	0.43
1:G:1716:ILE:HA	1:G:1720:LEU:HD23	2.00	0.43
1:A:1245:PHE:HA	1:A:1600:LEU:HA	1.99	0.43
1:C:1095:VAL:HG13	1:C:1096:THR:HG23	1.99	0.43
1:C:1684:ALA:O	1:C:1687:SER:OG	2.35	0.43
1:C:1716:ILE:HA	1:C:1720:LEU:HD23	2.00	0.43
1:G:1083:VAL:HG21	1:G:1088:TRP:CD1	2.54	0.43
1:G:1245:PHE:HA	1:G:1600:LEU:HA	1.99	0.43
1:G:1842:LEU:HA	1:G:1845:VAL:HG12	2.01	0.43
1:A:182:LEU:HD22	1:A:189:LEU:HD21	2.00	0.43
1:A:1082:THR:OG1	1:A:1188:PHE:O	2.27	0.43
1:A:1566:LEU:HG	1:A:1591:CYS:HB2	1.99	0.43
1:A:1842:LEU:HA	1:A:1845:VAL:HG12	2.01	0.43
1:A:4927:ILE:HG23	1:G:4936:ILE:HG21	1.99	0.43
1:E:1095:VAL:HG13	1:E:1096:THR:HG23	1.99	0.43
1:E:4870:ASP:OD1	1:E:4870:ASP:N	2.48	0.43
1:G:67:PHE:HD2	1:G:109:LEU:HD13	1.84	0.43
1:A:4936:ILE:HG21	1:C:4927:ILE:HG23	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:SER:O	1:C:72:SER:OG	2.32	0.43
1:C:638:ILE:HD13	1:C:702:TRP:HD1	1.83	0.43
1:C:1005:TRP:HA	1:C:1016:ARG:HG3	2.00	0.43
1:C:1842:LEU:HA	1:C:1845:VAL:HG12	2.01	0.43
1:C:4692:PRO:O	1:C:4700:GLN:NE2	2.52	0.43
1:E:20:VAL:N	1:E:67:PHE:O	2.46	0.43
1:E:1005:TRP:HA	1:E:1016:ARG:HG3	2.00	0.43
1:E:1842:LEU:HA	1:E:1845:VAL:HG12	2.01	0.43
1:E:3771:HIS:O	1:E:3815:LYS:NZ	2.51	0.43
1:E:3924:LEU:HB3	1:E:3988:ALA:HB2	2.00	0.43
1:G:2244:ARG:NH2	1:G:2283:ASN:HB2	2.33	0.43
1:A:1083:VAL:HG21	1:A:1088:TRP:CD1	2.54	0.43
1:A:2244:ARG:NH2	1:A:2283:ASN:HB2	2.33	0.43
1:C:1083:VAL:HG21	1:C:1088:TRP:CD1	2.54	0.43
1:C:1125:ASN:HB3	1:C:1130:GLN:H	1.84	0.43
1:C:2615:ARG:HA	1:C:2616:PRO:HD3	1.88	0.43
1:C:3924:LEU:HB3	1:C:3988:ALA:HB2	2.00	0.43
1:C:3952:SER:HA	1:C:3955:MET:HG2	2.01	0.43
1:E:1077:ALA:HA	1:E:1236:THR:HA	2.00	0.43
1:E:1125:ASN:HB3	1:E:1130:GLN:H	1.84	0.43
1:E:4586:PRO:HA	1:E:4587:PRO:HD3	1.92	0.43
1:G:262:LEU:HG	1:G:280:LEU:HD22	2.01	0.43
1:G:3924:LEU:HB3	1:G:3988:ALA:HB2	2.00	0.43
1:A:1125:ASN:HB3	1:A:1130:GLN:H	1.84	0.43
1:A:4570:ALA:HB2	1:A:4650:HIS:CD2	2.54	0.43
1:C:262:LEU:HG	1:C:280:LEU:HD22	2.01	0.43
1:C:4570:ALA:HB2	1:C:4650:HIS:CD2	2.54	0.43
1:E:221:ARG:HG3	1:E:259:LEU:HD23	2.01	0.43
1:E:1110:ARG:HH11	1:E:1111:PRO:HD2	1.84	0.43
1:E:4692:PRO:O	1:E:4700:GLN:NE2	2.52	0.43
2:F:47:LYS:HB3	2:F:47:LYS:HE3	1.85	0.43
1:G:721:LEU:HB3	1:G:768:PHE:HZ	1.83	0.43
1:G:2615:ARG:HA	1:G:2616:PRO:HD3	1.88	0.43
1:G:3675:ASP:OD1	1:G:3675:ASP:N	2.48	0.43
1:G:3844:LEU:HD21	1:G:3933:PHE:HA	1.99	0.43
1:A:173:SER:HB3	1:A:177:GLU:H	1.83	0.43
1:A:221:ARG:HG3	1:A:259:LEU:HD23	2.01	0.43
1:A:1110:ARG:HH11	1:A:1111:PRO:HD2	1.84	0.43
1:A:1747:LEU:HD13	1:A:2038:LEU:HD12	2.01	0.43
1:A:2155:LEU:HB2	1:A:2188:ASN:HD21	1.83	0.43
1:C:221:ARG:HG3	1:C:259:LEU:HD23	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:530:ILE:HG23	1:E:537:CYS:HB3	2.01	0.43
1:E:1743:ARG:O	1:E:1964:ARG:NH2	2.52	0.43
1:E:2243:SER:OG	1:E:2244:ARG:N	2.51	0.43
1:E:4570:ALA:HB2	1:E:4650:HIS:CD2	2.54	0.43
1:G:221:ARG:HG3	1:G:259:LEU:HD23	2.01	0.43
1:G:1747:LEU:HD13	1:G:2038:LEU:HD12	2.01	0.43
1:G:2243:SER:OG	1:G:2244:ARG:N	2.51	0.43
1:G:3952:SER:HA	1:G:3955:MET:HG2	2.01	0.43
1:G:4570:ALA:HB2	1:G:4650:HIS:CD2	2.54	0.43
1:C:169:LEU:HD13	1:C:201:ASN:HA	2.01	0.43
1:C:219:VAL:HG13	1:C:261:ARG:HD3	2.00	0.43
1:C:1110:ARG:HH11	1:C:1111:PRO:HD2	1.84	0.43
2:D:47:LYS:HB3	2:D:47:LYS:HE3	1.85	0.43
1:E:169:LEU:HD13	1:E:201:ASN:HA	2.01	0.43
1:E:262:LEU:HG	1:E:280:LEU:HD22	2.01	0.43
1:E:1684:ALA:O	1:E:1687:SER:OG	2.35	0.43
1:E:2354:VAL:HG11	1:E:2453:ILE:HG23	2.01	0.43
1:E:4813:LEU:HD23	1:E:4813:LEU:HA	1.87	0.43
1:G:219:VAL:HG13	1:G:261:ARG:HD3	2.00	0.43
1:G:1110:ARG:HH11	1:G:1111:PRO:HD2	1.84	0.43
1:G:1743:ARG:O	1:G:1964:ARG:NH2	2.52	0.43
1:G:3771:HIS:O	1:G:3815:LYS:NZ	2.51	0.43
1:A:3952:SER:HA	1:A:3955:MET:HG2	2.01	0.42
1:C:2489:LYS:HZ2	1:C:2492:ALA:HB2	1.84	0.42
1:C:2530:MET:HG3	1:C:2554:LEU:HD11	2.01	0.42
1:E:1082:THR:OG1	1:E:1188:PHE:O	2.27	0.42
1:G:1005:TRP:HA	1:G:1016:ARG:HG3	2.00	0.42
1:G:4692:PRO:O	1:G:4700:GLN:NE2	2.52	0.42
1:A:721:LEU:HB3	1:A:768:PHE:HZ	1.83	0.42
1:A:1490:SER:OG	1:A:1491:ASN:N	2.51	0.42
1:A:1743:ARG:O	1:A:1964:ARG:NH2	2.52	0.42
1:A:2533:ALA:HB2	1:A:2550:LEU:HD11	2.01	0.42
1:A:3806:ASN:HA	1:A:3890:LEU:HD23	2.02	0.42
1:C:530:ILE:HG23	1:C:537:CYS:HB3	2.01	0.42
1:C:1536:SER:OG	1:C:1537:ASN:N	2.48	0.42
1:C:1743:ARG:O	1:C:1964:ARG:NH2	2.52	0.42
1:E:2533:ALA:HB2	1:E:2550:LEU:HD11	2.01	0.42
1:G:1684:ALA:O	1:G:1687:SER:OG	2.35	0.42
1:G:2533:ALA:HB2	1:G:2550:LEU:HD11	2.01	0.42
1:G:3806:ASN:HA	1:G:3890:LEU:HD23	2.01	0.42
1:A:638:ILE:HD13	1:A:702:TRP:HD1	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1716:ILE:HA	1:A:1720:LEU:HD23	2.00	0.42
1:C:4217:PHE:HZ	1:C:4233:LEU:HD22	1.83	0.42
1:E:638:ILE:HD13	1:E:702:TRP:HD1	1.83	0.42
1:E:1747:LEU:HD13	1:E:2038:LEU:HD12	2.01	0.42
1:E:2487:GLN:HA	1:E:2488:PRO:HD3	1.88	0.42
1:E:3952:SER:HA	1:E:3955:MET:HG2	2.01	0.42
1:G:1433:TYR:HD1	1:G:1573:MET:HB3	1.85	0.42
1:A:262:LEU:HG	1:A:280:LEU:HD22	2.01	0.42
1:C:1851:MET:HE2	1:C:1851:MET:HB3	1.90	0.42
1:C:4662:ASN:HA	1:C:4666:VAL:HG13	2.00	0.42
1:E:2530:MET:HG3	1:E:2554:LEU:HD11	2.01	0.42
1:E:3806:ASN:HA	1:E:3890:LEU:HD23	2.02	0.42
1:A:169:LEU:HD13	1:A:201:ASN:HA	2.01	0.42
1:A:4692:PRO:O	1:A:4700:GLN:NE2	2.52	0.42
1:C:2307:LEU:HD12	1:C:2307:LEU:HA	1.94	0.42
1:C:2533:ALA:HB2	1:C:2550:LEU:HD11	2.01	0.42
1:C:3756:LYS:HA	1:C:3759:GLU:HG3	2.01	0.42
1:E:1083:VAL:HG21	1:E:1088:TRP:CD1	2.54	0.42
2:H:25:HIS:HE1	2:H:40:ARG:HD3	1.85	0.42
1:A:3898:ASP:O	1:A:3902:TYR:HB2	2.20	0.42
1:A:4145:VAL:HA	1:A:4148:THR:HG22	2.01	0.42
1:C:1087:ARG:HB2	1:C:1223:PHE:CE2	2.54	0.42
1:C:1290:ARG:O	1:C:1598:GLN:N	2.53	0.42
1:C:1433:TYR:HD1	1:C:1573:MET:HB3	1.85	0.42
1:E:4662:ASN:HA	1:E:4666:VAL:HG13	2.00	0.42
2:F:25:HIS:HE1	2:F:40:ARG:HD3	1.84	0.42
1:G:1087:ARG:HB2	1:G:1223:PHE:CE2	2.54	0.42
1:G:2489:LYS:HB3	1:G:2492:ALA:HB3	2.01	0.42
1:A:1433:TYR:HD1	1:A:1573:MET:HB3	1.84	0.42
1:A:3924:LEU:HB3	1:A:3988:ALA:HB2	2.00	0.42
1:A:4060:LYS:HA	1:A:4060:LYS:HD3	1.74	0.42
1:C:1747:LEU:HD13	1:C:2038:LEU:HD12	2.00	0.42
1:C:3806:ASN:HA	1:C:3890:LEU:HD23	2.01	0.42
1:C:3835:LEU:HD22	1:C:3880:PHE:HZ	1.85	0.42
1:C:3948:LYS:HA	1:C:3948:LYS:HD3	1.77	0.42
2:D:25:HIS:HE1	2:D:40:ARG:HD3	1.84	0.42
1:G:1446:SER:O	1:G:1496:TRP:NE1	2.35	0.42
1:G:2530:MET:HG3	1:G:2554:LEU:HD11	2.01	0.42
1:A:1293:LEU:HD12	1:A:1595:LEU:HG	2.02	0.42
1:C:4145:VAL:HA	1:C:4148:THR:HG22	2.01	0.42
1:E:1290:ARG:O	1:E:1598:GLN:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4145:VAL:HA	1:E:4148:THR:HG22	2.01	0.42
1:G:20:VAL:N	1:G:67:PHE:O	2.46	0.42
1:G:4145:VAL:HA	1:G:4148:THR:HG22	2.01	0.42
1:A:219:VAL:HG13	1:A:261:ARG:HD3	2.00	0.42
1:A:1780:PRO:O	2:B:42:ARG:NH2	2.43	0.42
1:A:2354:VAL:HG11	1:A:2453:ILE:HG23	2.01	0.42
2:B:25:HIS:HE1	2:B:40:ARG:HD3	1.84	0.42
1:A:1087:ARG:HB2	1:A:1223:PHE:CE2	2.54	0.42
1:A:1098:GLY:HA3	1:A:1198:GLN:HG2	2.02	0.42
1:A:1290:ARG:O	1:A:1598:GLN:N	2.53	0.42
1:C:15:ARG:HG3	1:C:16:THR:H	1.85	0.42
1:C:67:PHE:HD2	1:C:109:LEU:HD13	1.84	0.42
1:C:315:CYS:O	1:C:349:GLN:N	2.53	0.42
1:C:4586:PRO:HA	1:C:4587:PRO:HD3	1.92	0.42
1:E:15:ARG:HG3	1:E:16:THR:H	1.85	0.42
1:E:2489:LYS:HB3	1:E:2492:ALA:HB3	2.01	0.42
1:G:169:LEU:HD13	1:G:201:ASN:HA	2.01	0.42
1:G:218:HIS:HB3	1:G:392:ARG:HH12	1.85	0.42
1:G:262:LEU:HD11	1:G:280:LEU:HD13	2.02	0.42
1:G:1098:GLY:HA3	1:G:1198:GLN:HG2	2.02	0.42
1:G:3756:LYS:HA	1:G:3759:GLU:HG3	2.01	0.42
1:A:1450:VAL:HA	1:A:1552:VAL:HG12	2.01	0.41
1:C:1450:VAL:HA	1:C:1552:VAL:HG12	2.01	0.41
1:E:218:HIS:HB3	1:E:392:ARG:HH12	1.85	0.41
1:E:2113:SER:HA	1:E:2114:PRO:HD3	1.89	0.41
1:A:530:ILE:HG23	1:A:537:CYS:HB3	2.01	0.41
1:C:2166:LEU:HD12	1:C:2167:ILE:HG23	2.02	0.41
1:C:2354:VAL:HG11	1:C:2453:ILE:HG23	2.01	0.41
1:E:67:PHE:HD2	1:E:109:LEU:HD13	1.84	0.41
1:E:4157:ASP:HA	1:E:4158:PRO:HD3	1.94	0.41
1:G:803:LEU:HA	1:G:804:PRO:HD3	1.93	0.41
1:G:1125:ASN:HB3	1:G:1130:GLN:H	1.84	0.41
1:A:67:PHE:HD2	1:A:109:LEU:HD13	1.84	0.41
1:A:2489:LYS:HB3	1:A:2492:ALA:HB3	2.01	0.41
1:C:2489:LYS:HB3	1:C:2492:ALA:HB3	2.01	0.41
1:E:262:LEU:HD11	1:E:280:LEU:HD13	2.03	0.41
1:E:1087:ARG:HB2	1:E:1223:PHE:CE2	2.54	0.41
1:E:1595:LEU:HD23	1:E:1595:LEU:HA	1.85	0.41
1:G:15:ARG:HG3	1:G:16:THR:H	1.85	0.41
1:G:3672:ARG:O	1:G:3672:ARG:NH2	2.53	0.41
1:A:315:CYS:O	1:A:349:GLN:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:LYS:HB3	1:A:467:LYS:HE2	1.86	0.41
1:A:864:PRO:HA	1:A:865:PRO:HD3	1.89	0.41
1:C:218:HIS:HB3	1:C:392:ARG:HH12	1.85	0.41
1:C:473:ASN:HA	1:C:476:SER:HB3	2.02	0.41
1:E:2166:LEU:HD12	1:E:2167:ILE:HG23	2.02	0.41
1:E:3897:ASN:HD22	1:E:3973:CYS:HB2	1.86	0.41
1:G:530:ILE:HG23	1:G:537:CYS:HB3	2.01	0.41
1:A:218:HIS:HB3	1:A:392:ARG:HH12	1.85	0.41
1:A:255:HIS:CD2	1:A:480:GLU:HG3	2.55	0.41
2:B:38:SER:OG	2:B:39:SER:N	2.53	0.41
1:C:3898:ASP:O	1:C:3902:TYR:HB2	2.20	0.41
1:C:4894:GLY:HA2	1:C:4925:ILE:HG12	2.03	0.41
1:E:716:PHE:HB2	1:E:721:LEU:HD23	2.03	0.41
1:E:1450:VAL:HA	1:E:1552:VAL:HG12	2.01	0.41
1:E:3835:LEU:HD22	1:E:3880:PHE:HZ	1.85	0.41
1:E:3898:ASP:O	1:E:3902:TYR:HB2	2.20	0.41
1:G:1293:LEU:HD12	1:G:1595:LEU:HG	2.02	0.41
1:G:3898:ASP:O	1:G:3902:TYR:HB2	2.20	0.41
1:G:4870:ASP:N	1:G:4870:ASP:OD1	2.48	0.41
1:A:3756:LYS:HA	1:A:3759:GLU:HG3	2.01	0.41
1:C:262:LEU:HD11	1:C:280:LEU:HD13	2.03	0.41
1:E:1433:TYR:HD1	1:E:1573:MET:HB3	1.85	0.41
1:E:4814:LEU:HD21	1:G:4850:LEU:HD22	2.03	0.41
1:G:255:HIS:CD2	1:G:480:GLU:HG3	2.55	0.41
1:G:4247:ILE:O	1:G:4251:ILE:HG12	2.21	0.41
1:A:3644:LEU:HA	1:A:3645:PRO:HD3	1.92	0.41
1:A:4894:GLY:HA2	1:A:4925:ILE:HG12	2.03	0.41
1:C:1098:GLY:HA3	1:C:1198:GLN:HG2	2.02	0.41
1:C:1293:LEU:HD12	1:C:1595:LEU:HG	2.02	0.41
2:D:38:SER:OG	2:D:39:SER:N	2.53	0.41
1:E:315:CYS:O	1:E:349:GLN:N	2.53	0.41
1:E:671:VAL:HG11	1:E:682:LEU:HD22	2.03	0.41
1:E:2489:LYS:HZ2	1:E:2492:ALA:HB2	1.85	0.41
1:G:797:HIS:O	1:G:1619:ARG:NH1	2.54	0.41
1:G:2166:LEU:HD12	1:G:2167:ILE:HG23	2.02	0.41
1:G:4894:GLY:HA2	1:G:4925:ILE:HG12	2.03	0.41
1:A:716:PHE:HB2	1:A:721:LEU:HD23	2.03	0.41
1:A:2530:MET:HG3	1:A:2554:LEU:HD11	2.01	0.41
1:A:3672:ARG:O	1:A:3672:ARG:NH2	2.53	0.41
1:A:3780:LEU:HD12	1:A:3780:LEU:HA	1.90	0.41
1:A:4247:ILE:O	1:A:4251:ILE:HG12	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:486:LEU:HA	1:E:489:ASN:HB2	2.03	0.41
1:E:3756:LYS:HA	1:E:3759:GLU:HG3	2.02	0.41
1:G:486:LEU:HA	1:G:489:ASN:HB2	2.03	0.41
1:G:1018:ASN:OD1	1:G:1018:ASN:N	2.54	0.41
1:G:1290:ARG:O	1:G:1598:GLN:N	2.53	0.41
1:G:3897:ASN:HD22	1:G:3973:CYS:HB2	1.86	0.41
1:A:262:LEU:HD11	1:A:280:LEU:HD13	2.02	0.41
1:A:1595:LEU:HD23	1:A:1595:LEU:HA	1.85	0.41
1:A:2489:LYS:HZ2	1:A:2492:ALA:HB2	1.86	0.41
1:A:2615:ARG:HA	1:A:2616:PRO:HD3	1.88	0.41
1:C:255:HIS:CD2	1:C:480:GLU:HG3	2.55	0.41
1:C:716:PHE:HB2	1:C:721:LEU:HD23	2.03	0.41
1:C:797:HIS:O	1:C:1619:ARG:NH1	2.54	0.41
1:C:1018:ASN:OD1	1:C:1018:ASN:N	2.54	0.41
1:C:3725:TYR:HA	1:C:3728:ILE:HG12	2.03	0.41
1:C:4247:ILE:O	1:C:4251:ILE:HG12	2.21	0.41
1:C:4708:THR:HG21	1:C:4775:TYR:HB2	2.03	0.41
1:E:255:HIS:CD2	1:E:480:GLU:HG3	2.55	0.41
1:E:1098:GLY:HA3	1:E:1198:GLN:HG2	2.02	0.41
1:E:3725:TYR:HA	1:E:3728:ILE:HG12	2.03	0.41
1:E:3913:ILE:HD12	1:E:3913:ILE:HA	1.95	0.41
1:G:473:ASN:HA	1:G:476:SER:HB3	2.02	0.41
1:G:2354:VAL:HG11	1:G:2453:ILE:HG23	2.01	0.41
1:G:3835:LEU:HD22	1:G:3880:PHE:HZ	1.85	0.41
1:G:4248:ALA:O	1:G:4252:SER:HB3	2.21	0.41
1:A:4239:GLU:HA	1:A:4242:ILE:HG22	2.03	0.41
1:C:4248:ALA:O	1:C:4252:SER:HB3	2.21	0.41
1:E:2559:LEU:HD11	1:E:2603:ILE:HG13	2.03	0.41
1:E:3848:GLU:HA	1:E:3851:ASN:HB2	2.03	0.41
1:E:4248:ALA:O	1:E:4252:SER:HB3	2.21	0.41
1:E:4708:THR:HG21	1:E:4775:TYR:HB2	2.03	0.41
2:F:38:SER:OG	2:F:39:SER:N	2.53	0.41
1:G:1450:VAL:HA	1:G:1552:VAL:HG12	2.01	0.41
1:G:4576:ILE:HD12	1:G:4576:ILE:HA	1.91	0.41
2:H:38:SER:OG	2:H:39:SER:N	2.53	0.41
1:A:4814:LEU:HD21	1:C:4850:LEU:HD22	2.03	0.40
1:A:4850:LEU:HD22	1:G:4814:LEU:HD21	2.03	0.40
1:C:3897:ASN:HD22	1:C:3973:CYS:HB2	1.86	0.40
1:G:1252:HIS:HA	1:G:1253:PRO:HD3	1.92	0.40
1:G:2148:SER:O	1:G:2148:SER:OG	2.39	0.40
1:A:2113:SER:HA	1:A:2114:PRO:HD3	1.89	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4157:ASP:HA	1:A:4158:PRO:HD3	1.94	0.40
1:A:4248:ALA:O	1:A:4252:SER:HB3	2.21	0.40
1:C:20:VAL:N	1:C:67:PHE:O	2.46	0.40
1:C:786:GLY:N	1:C:1630:CYS:SG	2.90	0.40
1:C:2175:GLU:OE2	1:C:2175:GLU:N	2.54	0.40
1:E:1293:LEU:HD12	1:E:1595:LEU:HG	2.02	0.40
1:E:4894:GLY:HA2	1:E:4925:ILE:HG12	2.03	0.40
2:F:11:ASP:O	2:F:13:ARG:NH1	2.54	0.40
1:G:716:PHE:HB2	1:G:721:LEU:HD23	2.03	0.40
1:G:747:CYS:SG	1:G:756:SER:HB2	2.62	0.40
1:G:2175:GLU:OE2	1:G:2175:GLU:N	2.54	0.40
1:G:2307:LEU:HD12	1:G:2307:LEU:HA	1.94	0.40
1:G:3644:LEU:HA	1:G:3645:PRO:HD3	1.92	0.40
1:A:15:ARG:HG3	1:A:16:THR:H	1.85	0.40
1:A:273:HIS:ND1	1:A:337:PRO:HA	2.37	0.40
1:A:695:TYR:HA	1:A:696:PRO:HD3	1.97	0.40
1:A:2166:LEU:HD12	1:A:2167:ILE:HG23	2.02	0.40
1:A:2176:ASN:HB2	1:A:2180:GLN:NE2	2.37	0.40
1:A:3897:ASN:HD22	1:A:3973:CYS:HB2	1.86	0.40
1:A:4673:ARG:HE	1:A:4673:ARG:HB2	1.74	0.40
1:A:4843:LEU:HD11	1:G:4823:LEU:HB3	2.03	0.40
1:C:273:HIS:ND1	1:C:337:PRO:HA	2.37	0.40
1:C:3848:GLU:HA	1:C:3851:ASN:HB2	2.03	0.40
1:E:736:HIS:HB3	2:F:9:PRO:HD3	2.03	0.40
1:E:747:CYS:SG	1:E:756:SER:HB2	2.61	0.40
1:E:797:HIS:O	1:E:1619:ARG:NH1	2.54	0.40
1:E:5019:TRP:HD1	1:E:5021:PHE:HE1	1.70	0.40
1:G:2559:LEU:HD11	1:G:2603:ILE:HG13	2.03	0.40
1:A:473:ASN:HA	1:A:476:SER:HB3	2.02	0.40
1:A:747:CYS:SG	1:A:756:SER:HB2	2.62	0.40
1:A:2179:ILE:HA	1:A:2182:ILE:HG12	2.03	0.40
1:A:3725:TYR:HA	1:A:3728:ILE:HG12	2.03	0.40
1:A:4813:LEU:HD23	1:A:4813:LEU:HA	1.87	0.40
2:D:11:ASP:O	2:D:13:ARG:NH1	2.55	0.40
1:E:786:GLY:N	1:E:1630:CYS:SG	2.90	0.40
1:A:3835:LEU:HD22	1:A:3880:PHE:HZ	1.85	0.40
1:A:4823:LEU:HB3	1:C:4843:LEU:HD11	2.03	0.40
1:E:273:HIS:ND1	1:E:337:PRO:HA	2.37	0.40
1:E:473:ASN:HA	1:E:476:SER:HB3	2.02	0.40
1:E:864:PRO:HA	1:E:865:PRO:HD3	1.89	0.40
1:E:1018:ASN:OD1	1:E:1018:ASN:N	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4823:LEU:HB3	1:G:4843:LEU:HD11	2.03	0.40
1:G:695:TYR:HA	1:G:696:PRO:HD3	1.97	0.40
1:G:1110:ARG:HD2	1:G:1110:ARG:HA	1.83	0.40
1:G:2489:LYS:HZ2	1:G:2492:ALA:HB2	1.85	0.40
1:G:5019:TRP:HD1	1:G:5021:PHE:HE1	1.70	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	3427/5037 (68%)	3211 (94%)	214 (6%)	2 (0%)	51	85
1	C	3427/5037 (68%)	3211 (94%)	214 (6%)	2 (0%)	51	85
1	E	3427/5037 (68%)	3211 (94%)	214 (6%)	2 (0%)	51	85
1	G	3427/5037 (68%)	3211 (94%)	214 (6%)	2 (0%)	51	85
2	B	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
2	D	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
2	F	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
2	H	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
All	All	14128/20576 (69%)	13240 (94%)	880 (6%)	8 (0%)	54	85

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	318	VAL
1	A	673	PRO
1	C	318	VAL
1	C	673	PRO
1	E	318	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	673	PRO
1	G	318	VAL
1	G	673	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	2495/3416 (73%)	2460 (99%)	35 (1%)	67	81
1	C	2495/3416 (73%)	2461 (99%)	34 (1%)	67	81
1	E	2495/3416 (73%)	2460 (99%)	35 (1%)	67	81
1	G	2495/3416 (73%)	2461 (99%)	34 (1%)	67	81
2	B	84/88 (96%)	70 (83%)	14 (17%)	2	14
2	D	84/88 (96%)	70 (83%)	14 (17%)	2	14
2	F	84/88 (96%)	70 (83%)	14 (17%)	2	14
2	H	84/88 (96%)	70 (83%)	14 (17%)	2	14
All	All	10316/14016 (74%)	10122 (98%)	194 (2%)	59	75

All (194) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	A	79	GLN
1	A	162	LYS
1	A	273	HIS
1	A	390	LEU
1	A	516	LYS
1	A	998	ARG
1	A	1033	ARG
1	A	1180	ARG
1	A	1212	ARG
1	A	1483	VAL
1	A	1568	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1573	MET
1	A	1634	LEU
1	A	1698	LEU
1	A	1767	VAL
1	A	2035	HIS
1	A	2498	HIS
1	A	3677	LEU
1	A	3959	LYS
1	A	4014	LYS
1	A	4187	SER
1	A	4211	LYS
1	A	4659	ILE
1	A	4665	LYS
1	A	4715	TYR
1	A	4725	LEU
1	A	4779	LYS
1	A	4853	VAL
1	A	4874	MET
1	A	4932	ILE
1	A	4938	ASP
1	A	4985	LEU
1	A	5002	GLU
1	A	5035	GLN
2	B	24	VAL
2	B	27	THR
2	B	41	ASP
2	B	49	ARG
2	B	53	GLN
2	B	55	VAL
2	B	57	LYS
2	B	65	GLN
2	B	66	MET
2	B	97	LEU
2	B	99	PHE
2	B	101	VAL
2	B	103	LEU
2	B	106	LEU
1	C	17	ASP
1	C	79	GLN
1	C	162	LYS
1	C	273	HIS
1	C	390	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	516	LYS
1	C	998	ARG
1	C	1033	ARG
1	C	1180	ARG
1	C	1212	ARG
1	C	1483	VAL
1	C	1568	LYS
1	C	1573	MET
1	C	1698	LEU
1	C	1767	VAL
1	C	2035	HIS
1	C	2498	HIS
1	C	3677	LEU
1	C	3959	LYS
1	C	4014	LYS
1	C	4187	SER
1	C	4211	LYS
1	C	4659	ILE
1	C	4665	LYS
1	C	4715	TYR
1	C	4725	LEU
1	C	4779	LYS
1	C	4853	VAL
1	C	4874	MET
1	C	4932	ILE
1	C	4938	ASP
1	C	4985	LEU
1	C	5002	GLU
1	C	5035	GLN
2	D	24	VAL
2	D	27	THR
2	D	41	ASP
2	D	49	ARG
2	D	53	GLN
2	D	55	VAL
2	D	57	LYS
2	D	65	GLN
2	D	66	MET
2	D	97	LEU
2	D	99	PHE
2	D	101	VAL
2	D	103	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	106	LEU
1	E	17	ASP
1	E	79	GLN
1	E	162	LYS
1	E	273	HIS
1	E	390	LEU
1	E	516	LYS
1	E	998	ARG
1	E	1033	ARG
1	E	1180	ARG
1	E	1212	ARG
1	E	1483	VAL
1	E	1568	LYS
1	E	1573	MET
1	E	1634	LEU
1	E	1698	LEU
1	E	1767	VAL
1	E	2035	HIS
1	E	2498	HIS
1	E	3677	LEU
1	E	3959	LYS
1	E	4014	LYS
1	E	4187	SER
1	E	4211	LYS
1	E	4659	ILE
1	E	4665	LYS
1	E	4715	TYR
1	E	4725	LEU
1	E	4779	LYS
1	E	4853	VAL
1	E	4874	MET
1	E	4932	ILE
1	E	4938	ASP
1	E	4985	LEU
1	E	5002	GLU
1	E	5035	GLN
2	F	24	VAL
2	F	27	THR
2	F	41	ASP
2	F	49	ARG
2	F	53	GLN
2	F	55	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	57	LYS
2	F	65	GLN
2	F	66	MET
2	F	97	LEU
2	F	99	PHE
2	F	101	VAL
2	F	103	LEU
2	F	106	LEU
1	G	17	ASP
1	G	79	GLN
1	G	162	LYS
1	G	273	HIS
1	G	390	LEU
1	G	516	LYS
1	G	998	ARG
1	G	1033	ARG
1	G	1180	ARG
1	G	1212	ARG
1	G	1483	VAL
1	G	1568	LYS
1	G	1573	MET
1	G	1698	LEU
1	G	1767	VAL
1	G	2035	HIS
1	G	2498	HIS
1	G	3677	LEU
1	G	3959	LYS
1	G	4014	LYS
1	G	4187	SER
1	G	4211	LYS
1	G	4659	ILE
1	G	4665	LYS
1	G	4715	TYR
1	G	4725	LEU
1	G	4779	LYS
1	G	4853	VAL
1	G	4874	MET
1	G	4932	ILE
1	G	4938	ASP
1	G	4985	LEU
1	G	5002	GLU
1	G	5035	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	24	VAL
2	H	27	THR
2	H	41	ASP
2	H	49	ARG
2	H	53	GLN
2	H	55	VAL
2	H	57	LYS
2	H	65	GLN
2	H	66	MET
2	H	97	LEU
2	H	99	PHE
2	H	101	VAL
2	H	103	LEU
2	H	106	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (190) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	57	ASN
1	A	201	ASN
1	A	255	HIS
1	A	520	ASN
1	A	533	ASN
1	A	610	ASN
1	A	1229	ASN
1	A	1252	HIS
1	A	1281	ASN
1	A	1458	HIS
1	A	1569	GLN
1	A	1949	GLN
1	A	1973	GLN
1	A	2003	GLN
1	A	2127	GLN
1	A	2180	GLN
1	A	2188	ASN
1	A	2245	GLN
1	A	2551	ASN
1	A	3647	HIS
1	A	3651	ASN
1	A	3766	GLN
1	A	3767	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	3781	GLN
1	A	3837	GLN
1	A	3851	ASN
1	A	3896	ASN
1	A	3906	GLN
1	A	3950	ASN
1	A	3970	GLN
1	A	4005	GLN
1	A	4034	ASN
1	A	4037	ASN
1	A	4054	ASN
1	A	4124	ASN
1	A	4223	ASN
1	A	4650	HIS
1	A	4832	HIS
1	A	4833	ASN
1	A	4857	ASN
1	A	4946	GLN
1	A	4978	HIS
2	B	25	HIS
2	B	53	GLN
2	B	65	GLN
2	B	94	ASN
1	C	44	ASN
1	C	57	ASN
1	C	201	ASN
1	C	255	HIS
1	C	520	ASN
1	C	533	ASN
1	C	610	ASN
1	C	1229	ASN
1	C	1252	HIS
1	C	1281	ASN
1	C	1458	HIS
1	C	1545	ASN
1	C	1569	GLN
1	C	1949	GLN
1	C	1973	GLN
1	C	2003	GLN
1	C	2127	GLN
1	C	2180	GLN
1	C	2188	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	2245	GLN
1	C	2551	ASN
1	C	3647	HIS
1	C	3651	ASN
1	C	3766	GLN
1	C	3767	GLN
1	C	3781	GLN
1	C	3837	GLN
1	C	3851	ASN
1	C	3896	ASN
1	C	3906	GLN
1	C	3950	ASN
1	C	3970	GLN
1	C	4005	GLN
1	C	4034	ASN
1	C	4054	ASN
1	C	4124	ASN
1	C	4223	ASN
1	C	4650	HIS
1	C	4832	HIS
1	C	4833	ASN
1	C	4857	ASN
1	C	4946	GLN
1	C	4978	HIS
2	D	25	HIS
2	D	53	GLN
2	D	65	GLN
2	D	94	ASN
1	E	44	ASN
1	E	57	ASN
1	E	201	ASN
1	E	255	HIS
1	E	520	ASN
1	E	533	ASN
1	E	610	ASN
1	E	877	ASN
1	E	1229	ASN
1	E	1252	HIS
1	E	1281	ASN
1	E	1458	HIS
1	E	1545	ASN
1	E	1569	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	1949	GLN
1	E	1973	GLN
1	E	2003	GLN
1	E	2127	GLN
1	E	2180	GLN
1	E	2188	ASN
1	E	2245	GLN
1	E	2551	ASN
1	E	3647	HIS
1	E	3651	ASN
1	E	3766	GLN
1	E	3767	GLN
1	E	3781	GLN
1	E	3837	GLN
1	E	3851	ASN
1	E	3896	ASN
1	E	3906	GLN
1	E	3950	ASN
1	E	3970	GLN
1	E	4005	GLN
1	E	4034	ASN
1	E	4054	ASN
1	E	4124	ASN
1	E	4223	ASN
1	E	4650	HIS
1	E	4832	HIS
1	E	4833	ASN
1	E	4857	ASN
1	E	4946	GLN
1	E	4978	HIS
2	F	25	HIS
2	F	31	GLN
2	F	53	GLN
2	F	65	GLN
2	F	94	ASN
1	G	44	ASN
1	G	57	ASN
1	G	201	ASN
1	G	255	HIS
1	G	520	ASN
1	G	533	ASN
1	G	610	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	1229	ASN
1	G	1252	HIS
1	G	1281	ASN
1	G	1458	HIS
1	G	1545	ASN
1	G	1569	GLN
1	G	1949	GLN
1	G	1973	GLN
1	G	2003	GLN
1	G	2127	GLN
1	G	2180	GLN
1	G	2188	ASN
1	G	2245	GLN
1	G	2551	ASN
1	G	3647	HIS
1	G	3651	ASN
1	G	3766	GLN
1	G	3767	GLN
1	G	3781	GLN
1	G	3837	GLN
1	G	3851	ASN
1	G	3896	ASN
1	G	3906	GLN
1	G	3950	ASN
1	G	3970	GLN
1	G	4005	GLN
1	G	4034	ASN
1	G	4054	ASN
1	G	4124	ASN
1	G	4223	ASN
1	G	4650	HIS
1	G	4832	HIS
1	G	4833	ASN
1	G	4857	ASN
1	G	4946	GLN
1	G	4978	HIS
2	H	25	HIS
2	H	53	GLN
2	H	65	GLN
2	H	94	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	F0U	E	5203	-	29,30,30	2.30	8 (27%)	31,43,43	1.43	4 (12%)
5	F0U	C	5203	-	29,30,30	2.30	8 (27%)	31,43,43	1.43	4 (12%)
5	F0U	A	5203	-	29,30,30	2.30	8 (27%)	31,43,43	1.43	4 (12%)
5	F0U	G	5203	-	29,30,30	2.30	8 (27%)	31,43,43	1.44	4 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	F0U	E	5203	-	-	0/11/18/18	0/3/3/3
5	F0U	C	5203	-	-	0/11/18/18	0/3/3/3
5	F0U	A	5203	-	-	0/11/18/18	0/3/3/3
5	F0U	G	5203	-	-	0/11/18/18	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	5203	F0U	CAU-NAT	-6.50	1.33	1.44
5	G	5203	F0U	CAU-NAT	-6.50	1.33	1.44
5	C	5203	F0U	CAU-NAT	-6.46	1.33	1.44
5	E	5203	F0U	CAU-NAT	-6.46	1.33	1.44
5	E	5203	F0U	CAG-CAH	-5.20	1.39	1.50
5	A	5203	F0U	CAG-CAH	-5.20	1.39	1.50
5	C	5203	F0U	CAG-CAH	-5.20	1.39	1.50
5	G	5203	F0U	CAG-CAH	-5.20	1.39	1.50
5	A	5203	F0U	CAL-NAM	-4.54	1.34	1.43
5	C	5203	F0U	CAL-NAM	-4.54	1.34	1.43
5	G	5203	F0U	CAL-NAM	-4.54	1.34	1.43
5	E	5203	F0U	CAL-NAM	-4.49	1.34	1.43
5	E	5203	F0U	CAP-CAQ	-4.42	1.33	1.39
5	A	5203	F0U	CAP-CAQ	-4.36	1.33	1.39
5	C	5203	F0U	CAP-CAQ	-4.36	1.33	1.39
5	G	5203	F0U	CAP-CAQ	-4.36	1.33	1.39
5	C	5203	F0U	CAP-CAO	-4.31	1.33	1.39
5	A	5203	F0U	CAP-CAO	-4.26	1.33	1.39
5	E	5203	F0U	CAP-CAO	-4.26	1.33	1.39
5	G	5203	F0U	CAP-CAO	-4.26	1.33	1.39
5	E	5203	F0U	CAZ-NBA	2.65	1.40	1.34
5	A	5203	F0U	CAZ-NBA	2.65	1.40	1.34
5	C	5203	F0U	CAZ-NBA	2.65	1.40	1.34
5	G	5203	F0U	CAZ-NBA	2.65	1.40	1.34
5	E	5203	F0U	NAS-NAT	-2.53	1.34	1.39
5	A	5203	F0U	NAS-NAT	-2.50	1.34	1.39
5	C	5203	F0U	NAS-NAT	-2.50	1.34	1.39
5	G	5203	F0U	NAS-NAT	-2.50	1.34	1.39
5	A	5203	F0U	CAO-CAN	-2.49	1.35	1.50
5	C	5203	F0U	CAO-CAN	-2.49	1.35	1.50
5	E	5203	F0U	CAO-CAN	-2.49	1.35	1.50
5	G	5203	F0U	CAO-CAN	-2.49	1.35	1.50

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	5203	F0U	CAJ-NAI-CAH	-4.31	117.00	121.89
5	C	5203	F0U	CAJ-NAI-CAH	-4.30	117.02	121.89
5	A	5203	F0U	CAJ-NAI-CAH	-4.30	117.02	121.89
5	E	5203	F0U	CAJ-NAI-CAH	-4.30	117.02	121.89
5	A	5203	F0U	CAZ-NBA-CAU	4.11	120.63	115.98
5	C	5203	F0U	CAZ-NBA-CAU	4.11	120.63	115.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	5203	F0U	CAZ-NBA-CAU	4.11	120.63	115.98
5	E	5203	F0U	CAZ-NBA-CAU	4.10	120.62	115.98
5	C	5203	F0U	CAY-CAZ-NBA	-2.57	119.24	123.43
5	A	5203	F0U	CAY-CAZ-NBA	-2.56	119.24	123.43
5	G	5203	F0U	CAY-CAZ-NBA	-2.56	119.24	123.43
5	E	5203	F0U	CAY-CAZ-NBA	-2.56	119.25	123.43
5	C	5203	F0U	CAP-CAO-CAN	-2.33	121.29	128.55
5	A	5203	F0U	CAP-CAO-CAN	-2.32	121.30	128.55
5	E	5203	F0U	CAP-CAO-CAN	-2.32	121.30	128.55
5	G	5203	F0U	CAP-CAO-CAN	-2.32	121.30	128.55

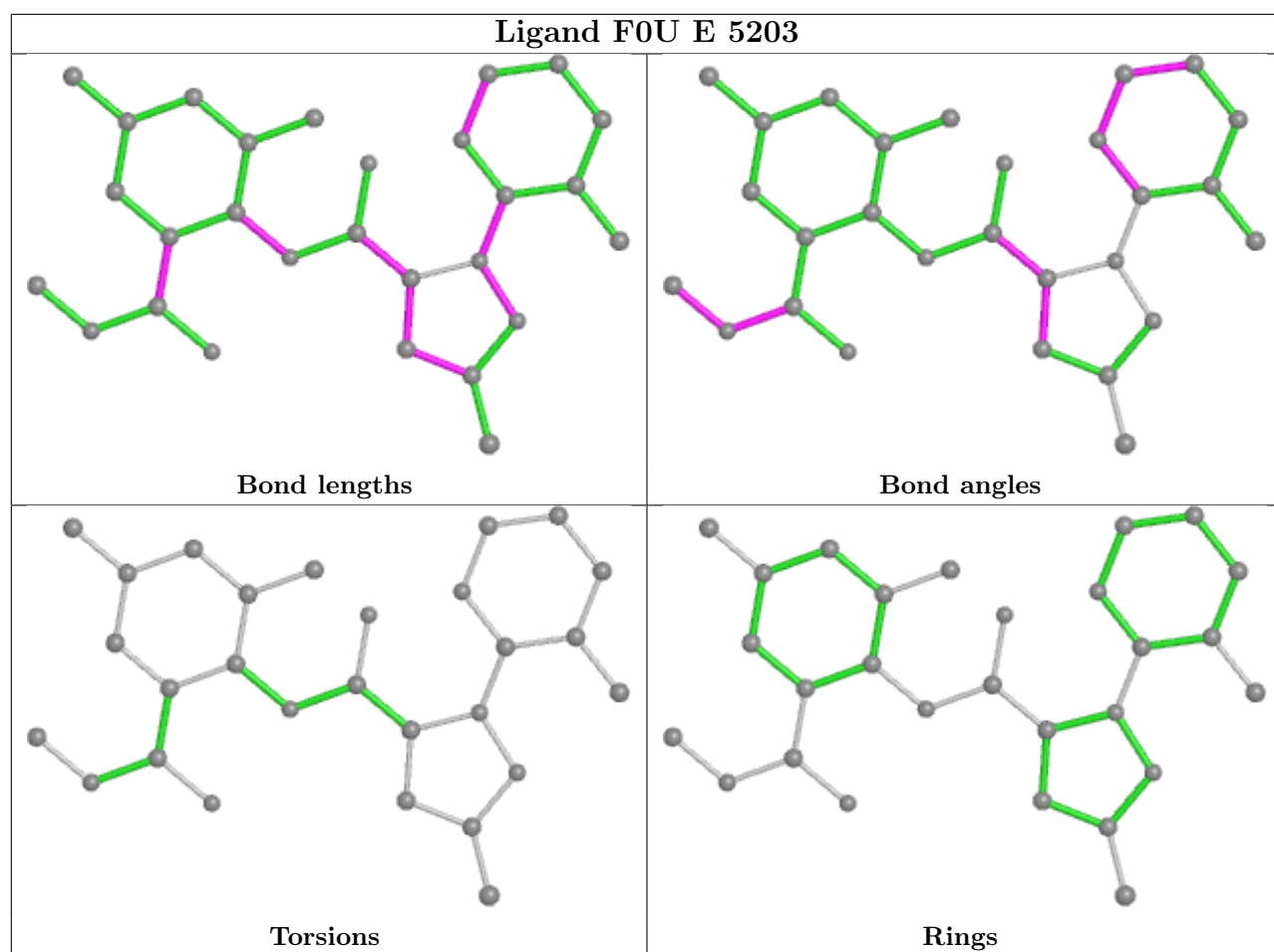
There are no chirality outliers.

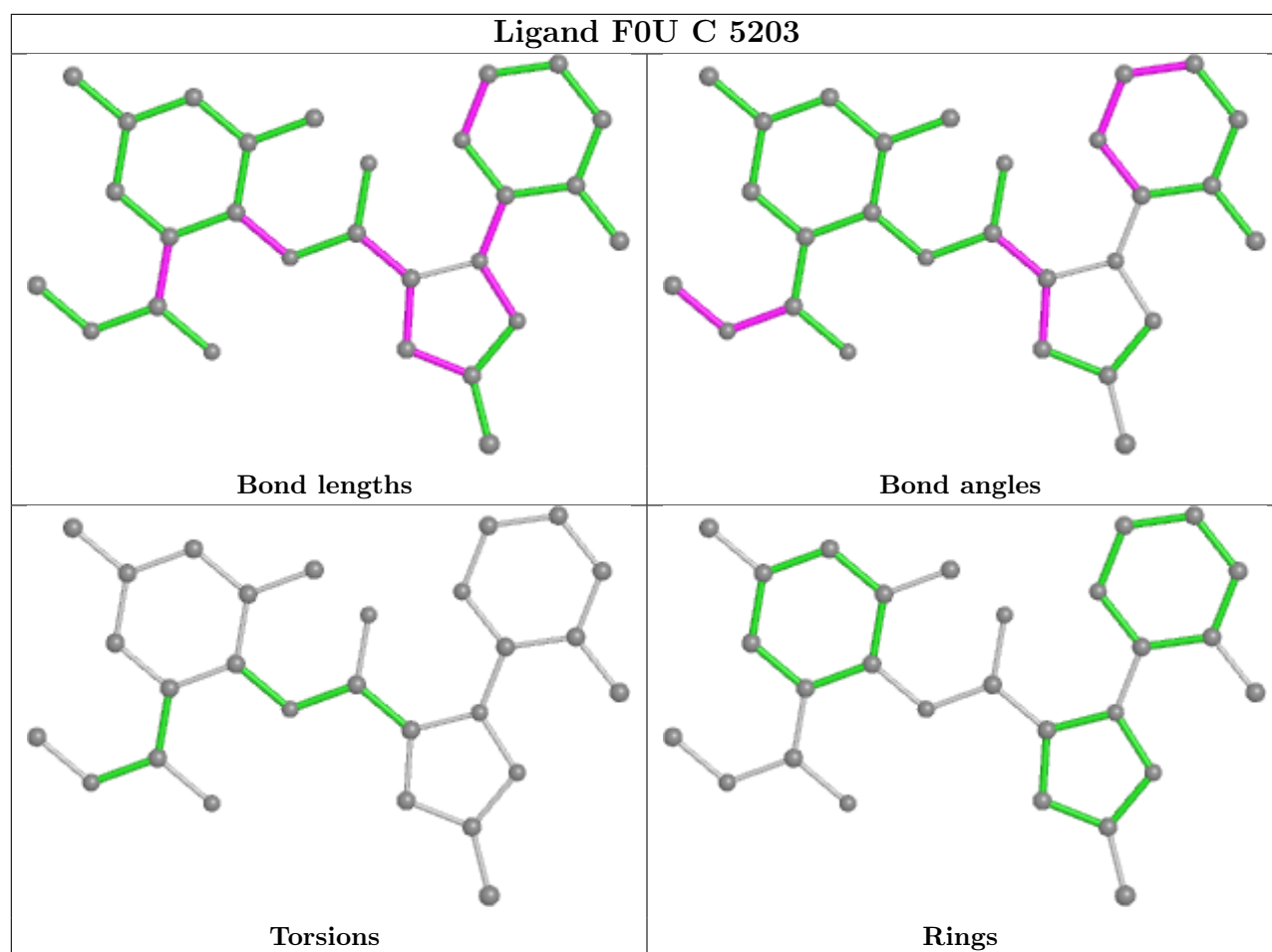
There are no torsion outliers.

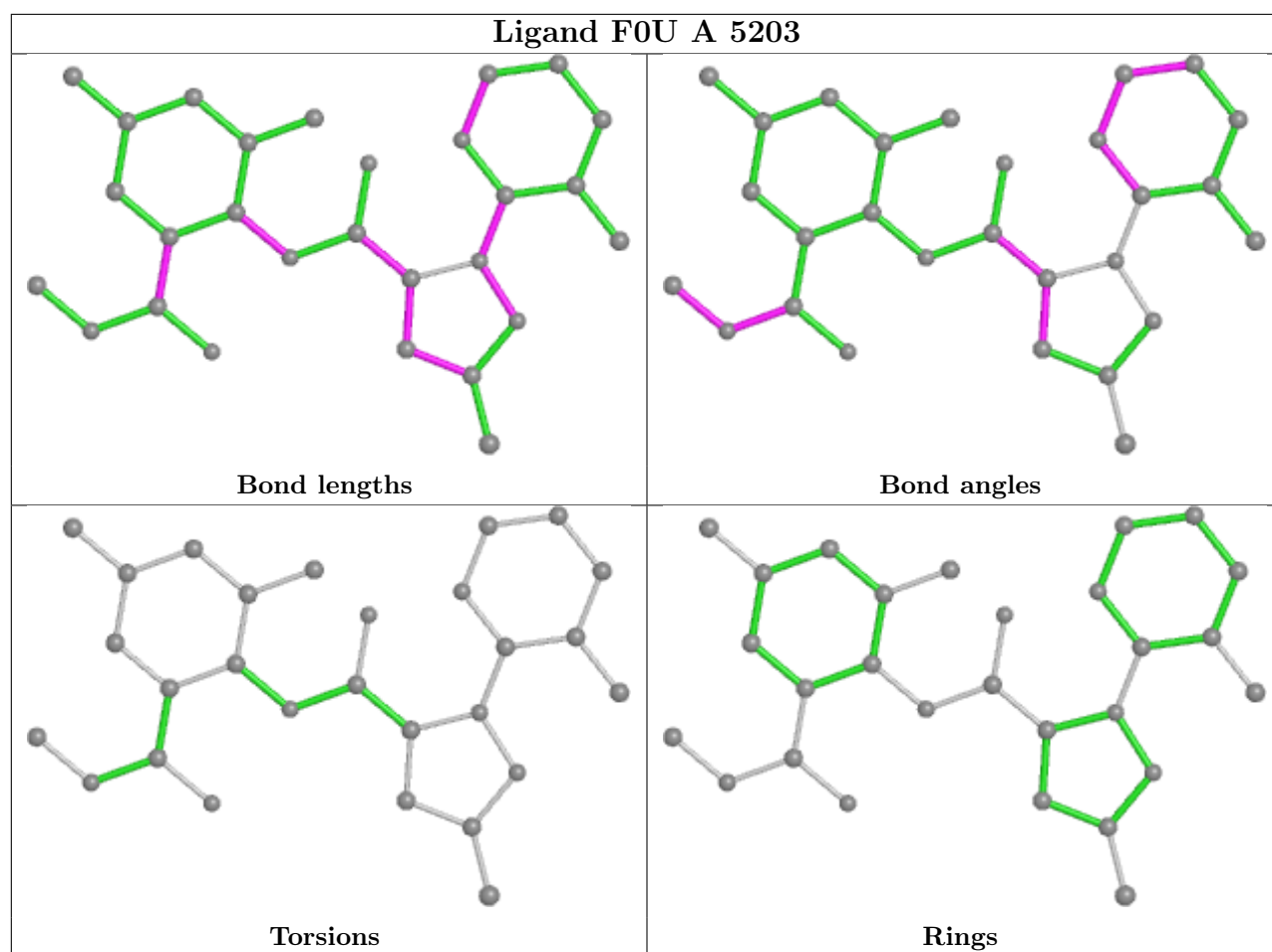
There are no ring outliers.

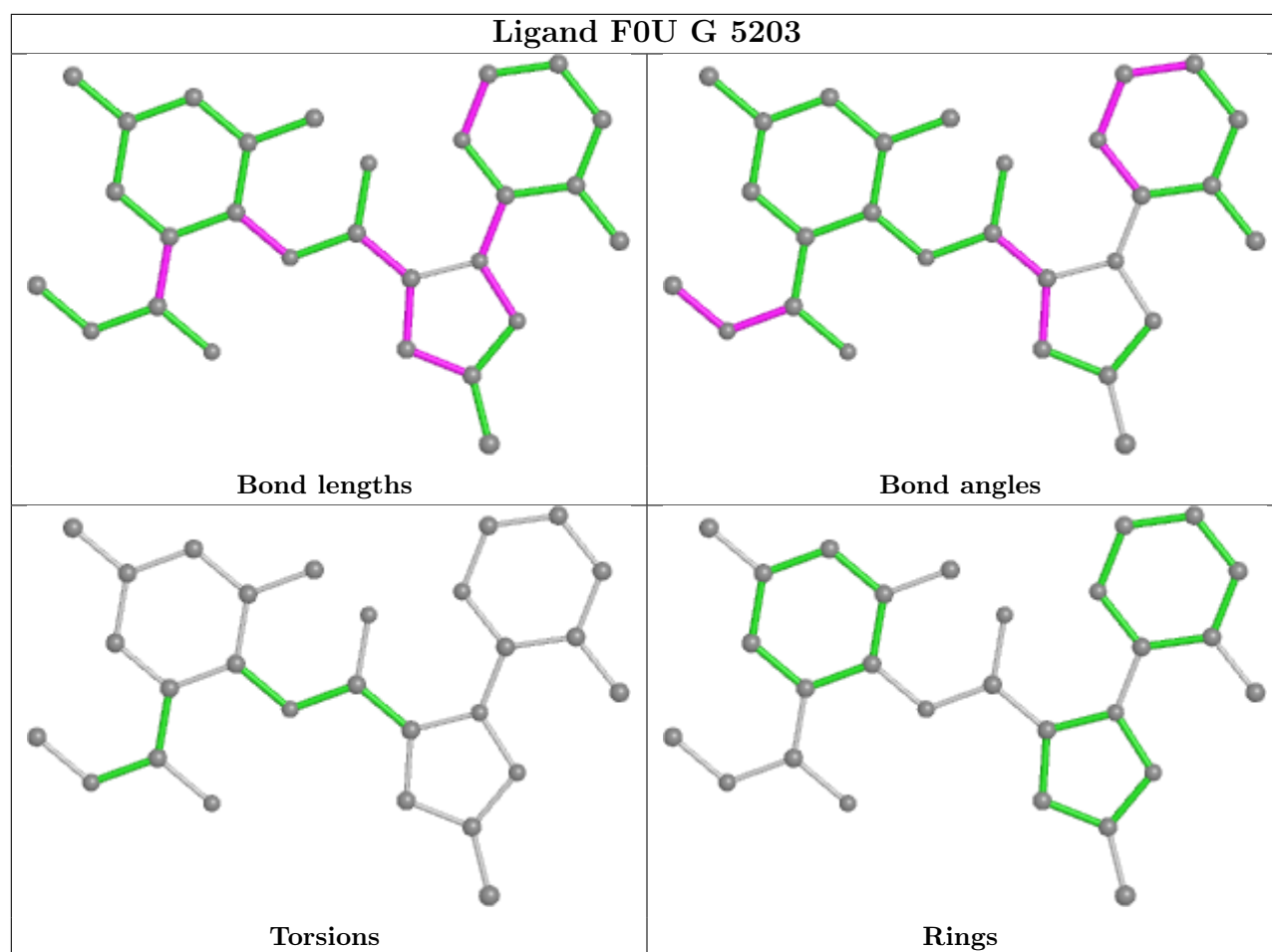
No monomer is involved in short contacts.

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

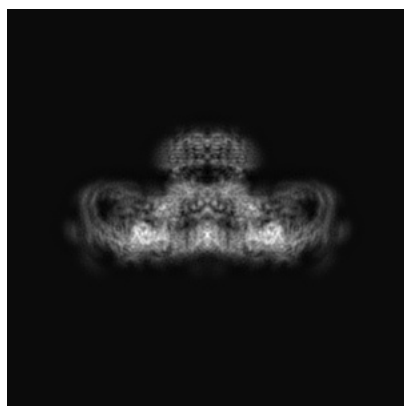
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30343. These allow visual inspection of the internal detail of the map and identification of artifacts.

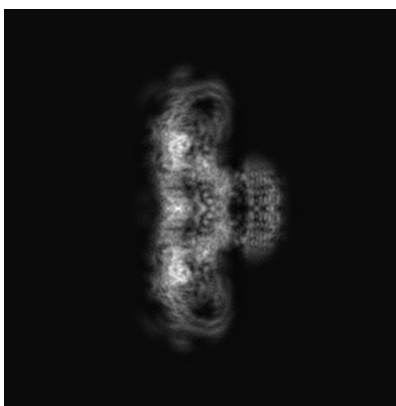
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

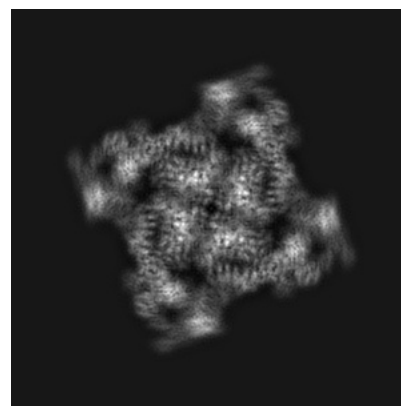
6.1.1 Primary map



X

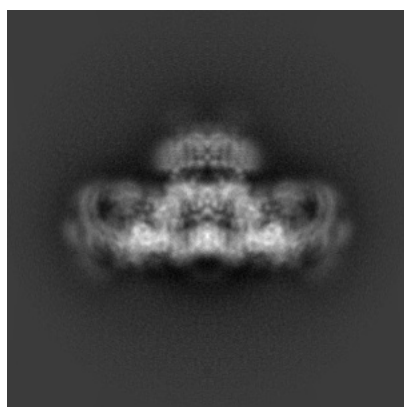


Y

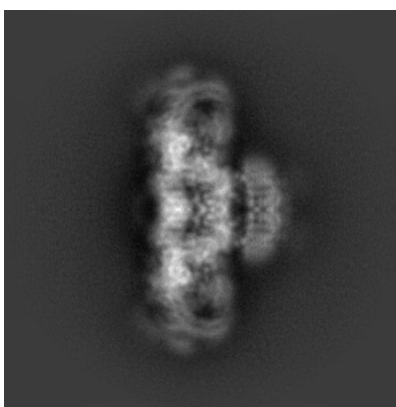


Z

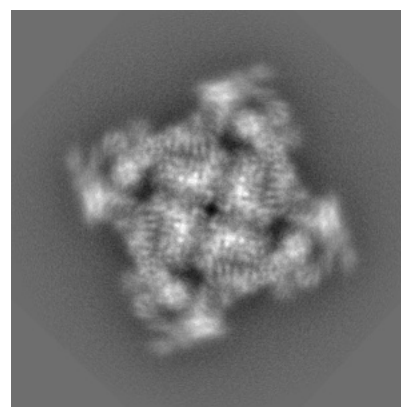
6.1.2 Raw map



X



Y

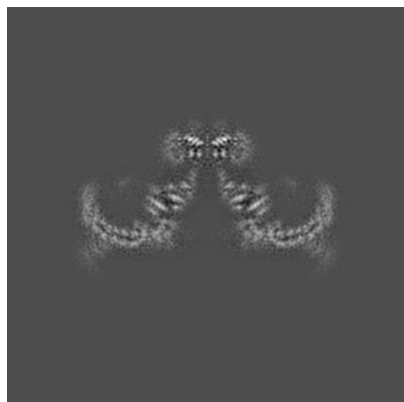


Z

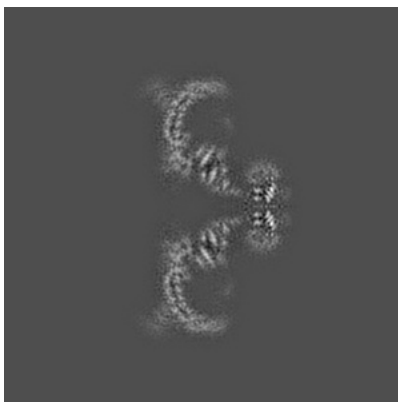
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

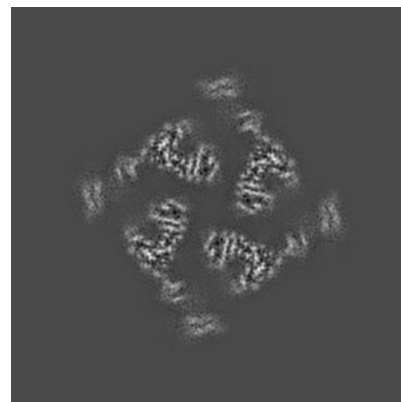
6.2.1 Primary map



X Index: 224

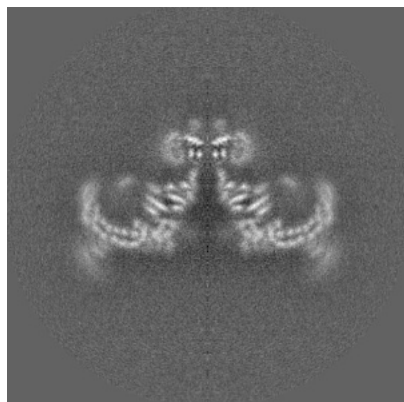


Y Index: 224

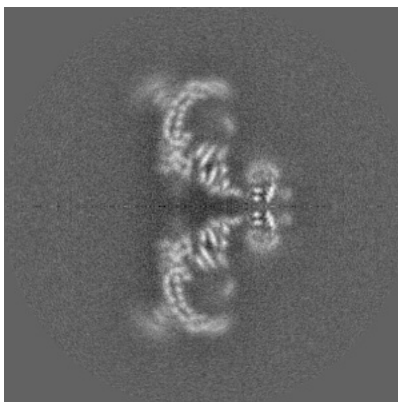


Z Index: 224

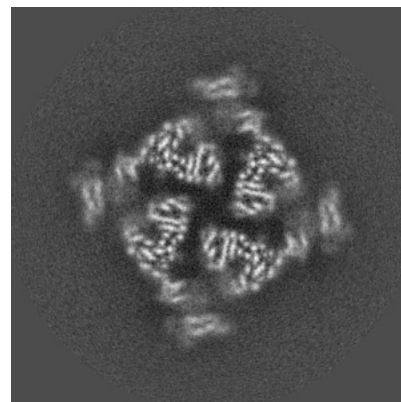
6.2.2 Raw map



X Index: 224



Y Index: 224

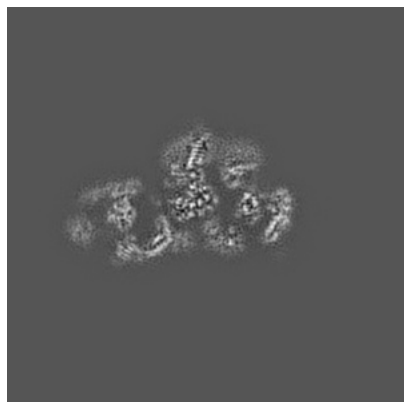


Z Index: 224

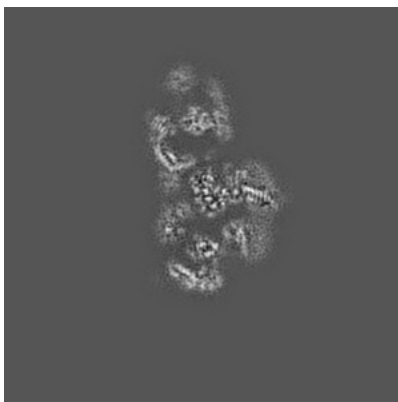
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

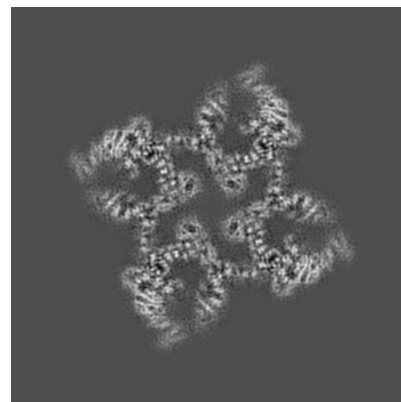
6.3.1 Primary map



X Index: 186

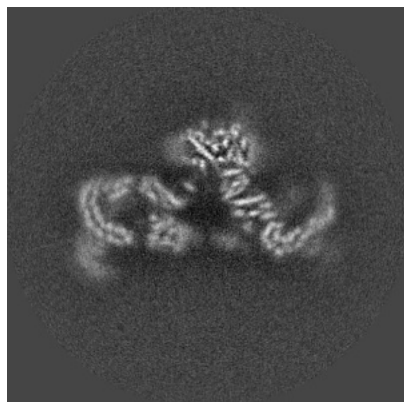


Y Index: 186

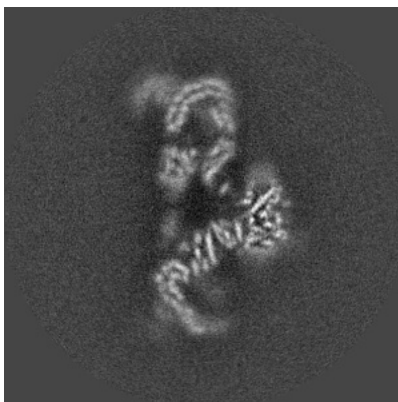


Z Index: 190

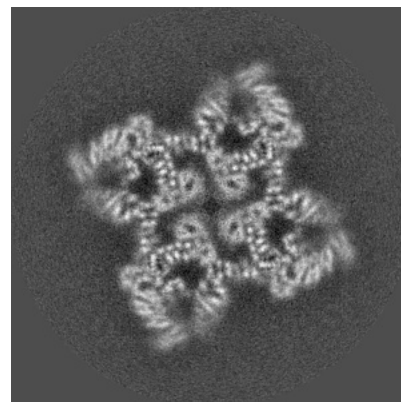
6.3.2 Raw map



X Index: 215



Y Index: 215

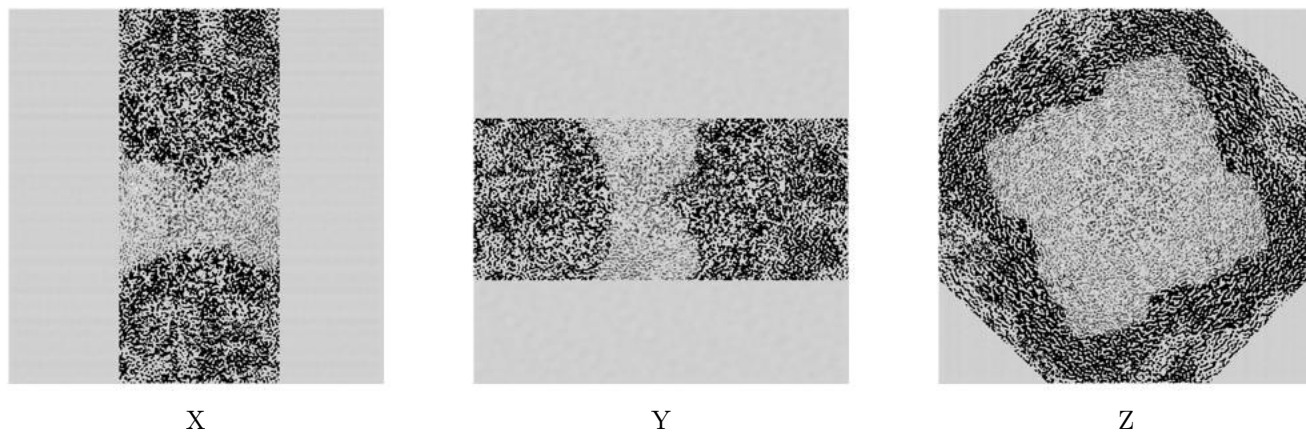


Z Index: 189

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

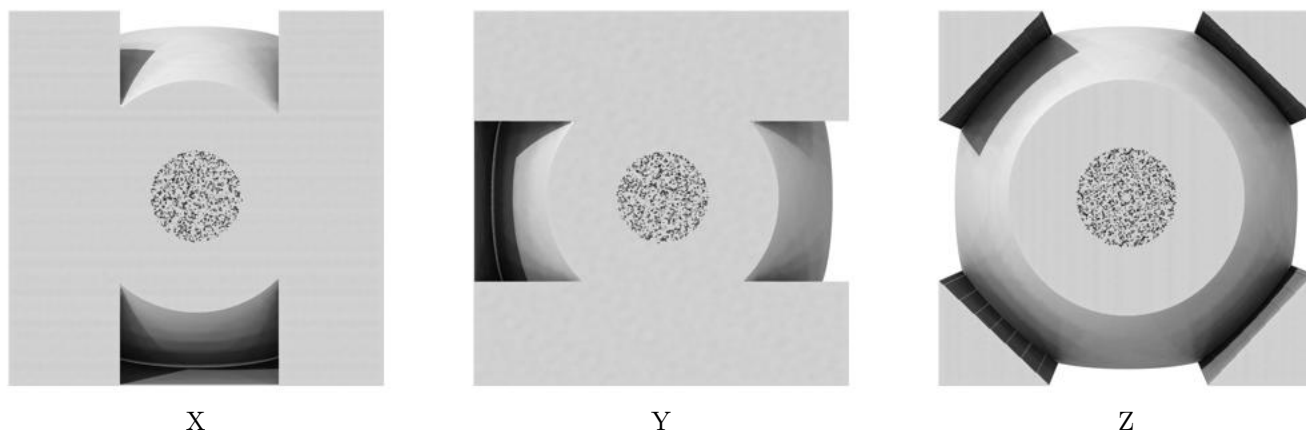
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

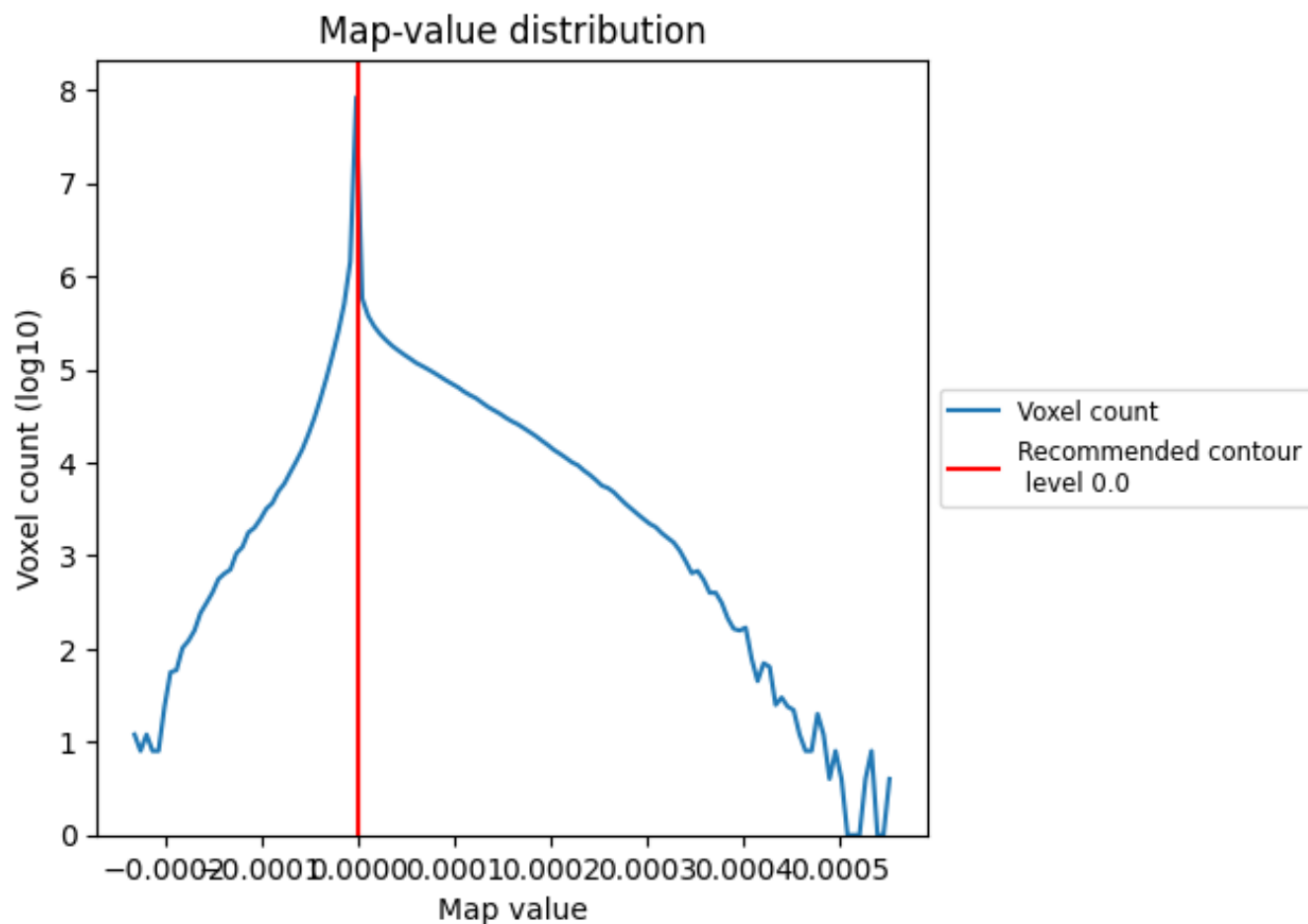
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

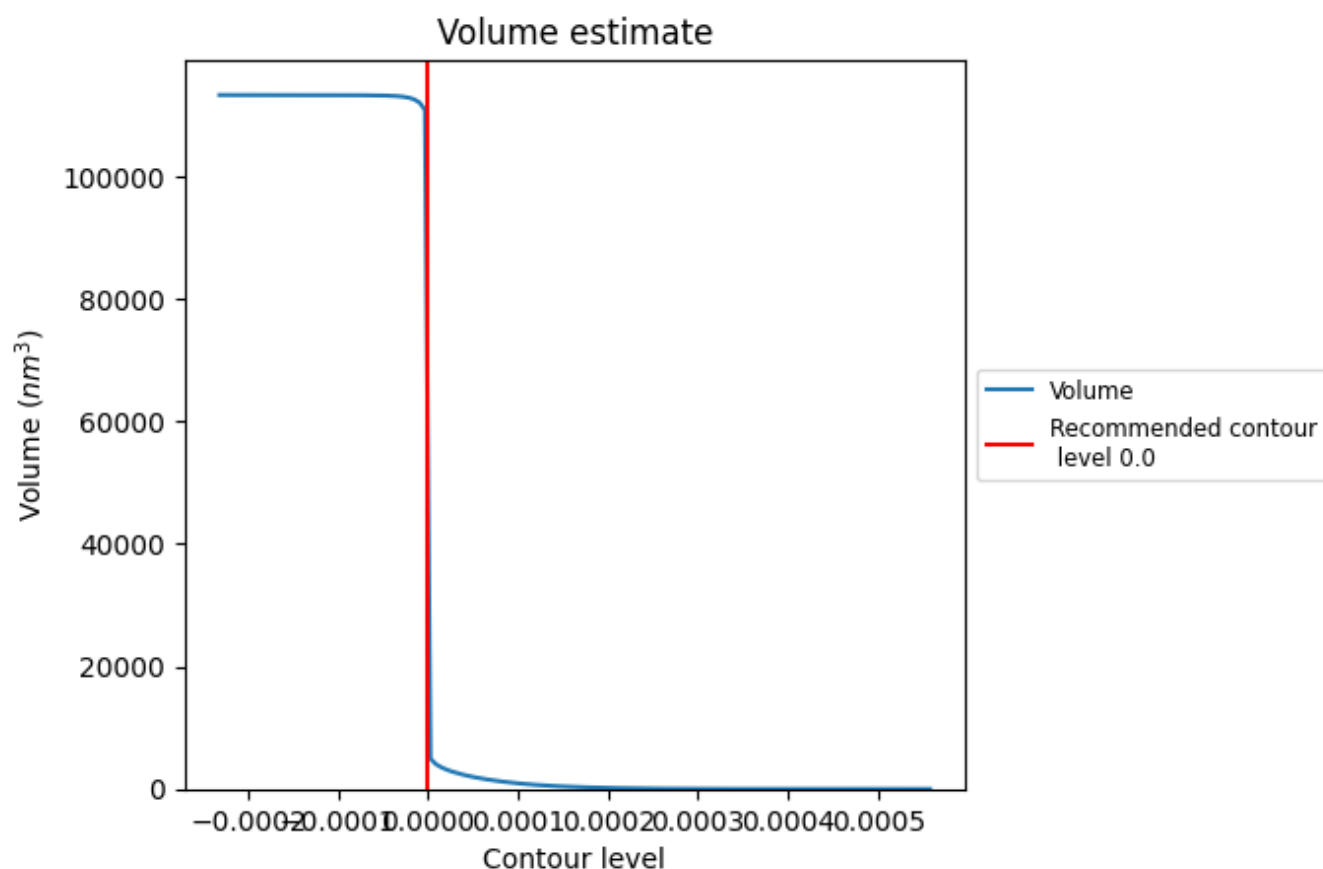
This section contains the results of statistical analysis of the map.

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.

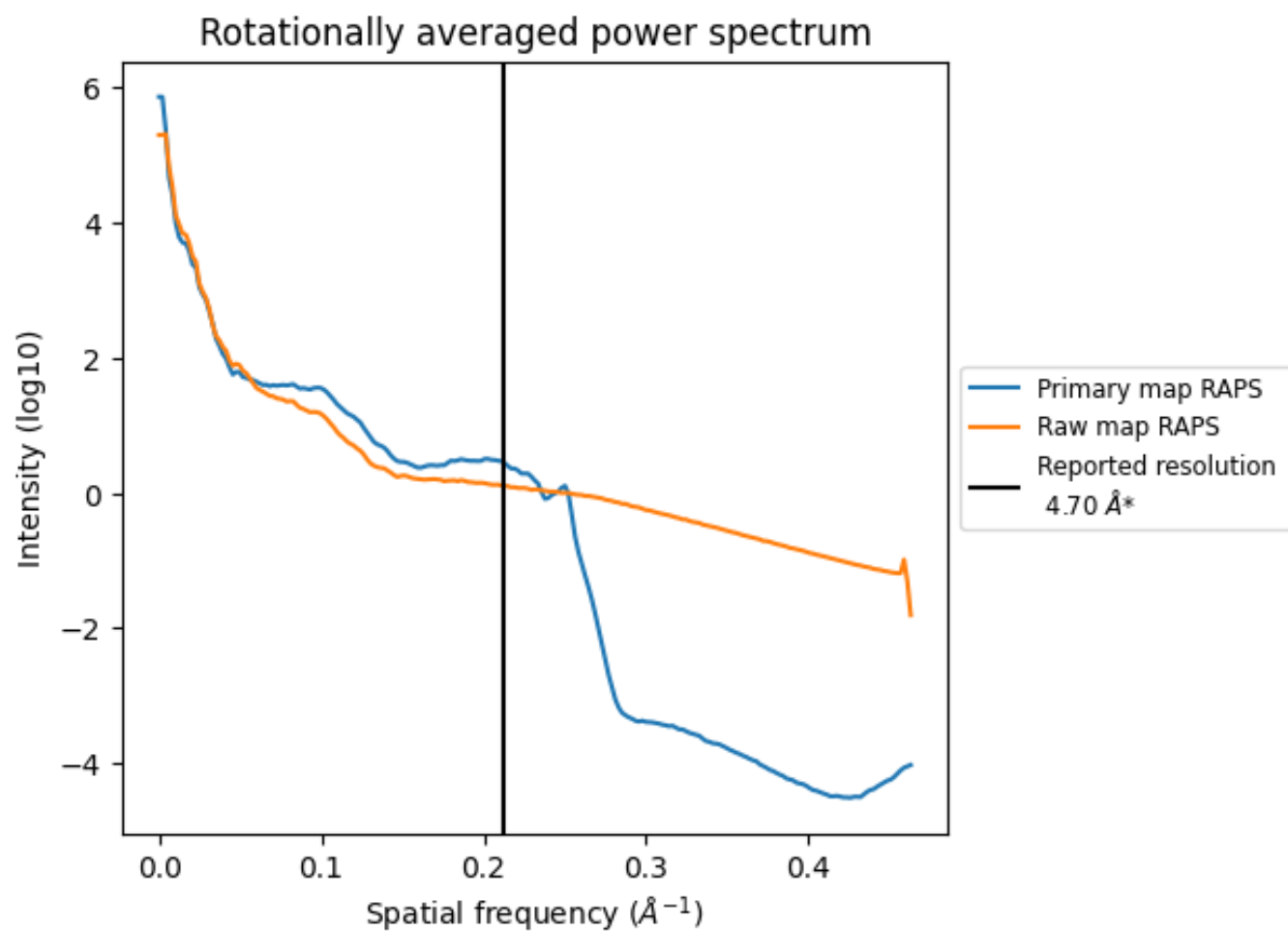
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 51623 nm^3 ; this corresponds to an approximate mass of 46633 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 ⓘ

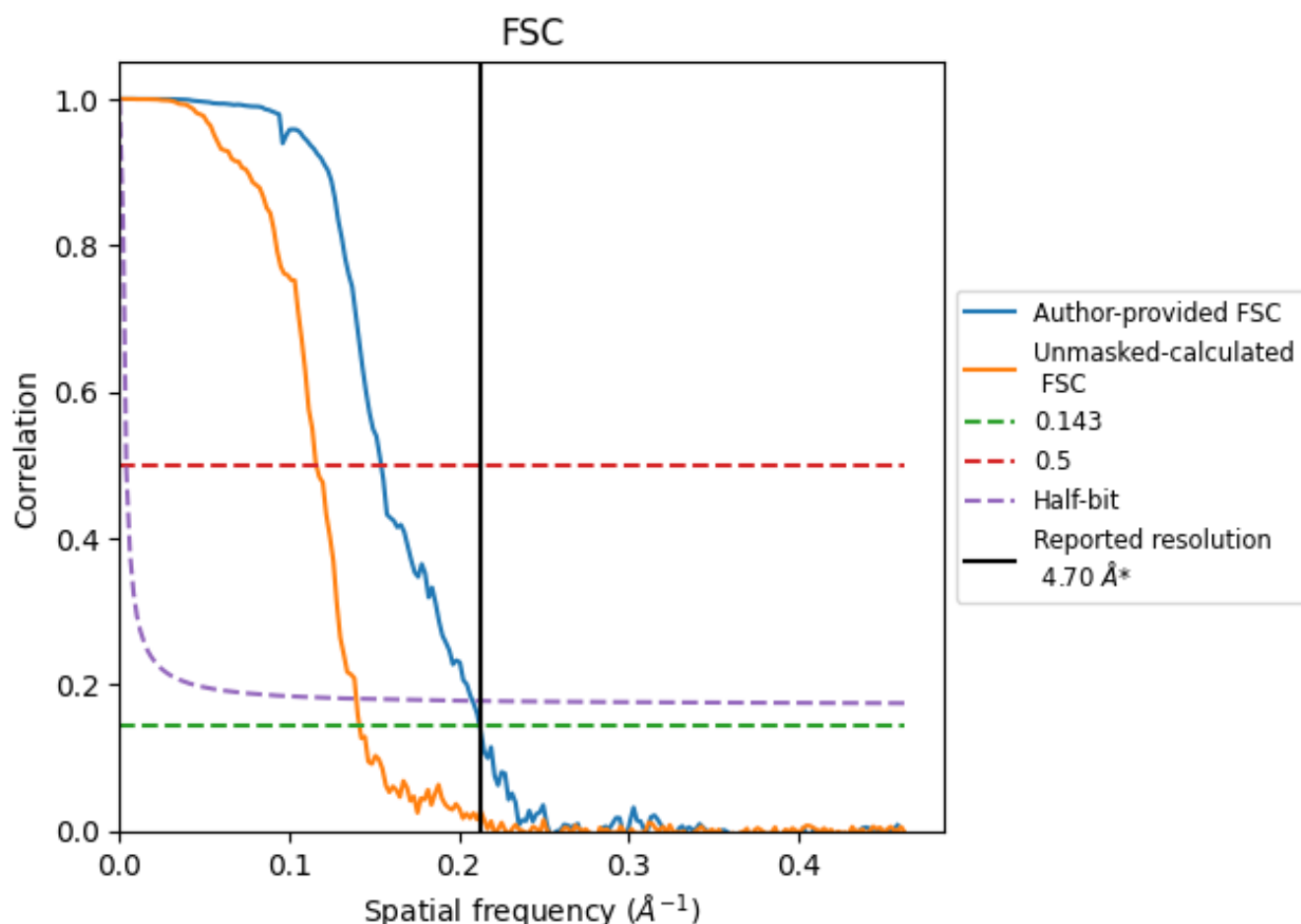


*Reported resolution corresponds to spatial frequency of 0.213 \AA^{-1}

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 0.213 Å⁻¹

8.2 Resolution estimates [i](#)

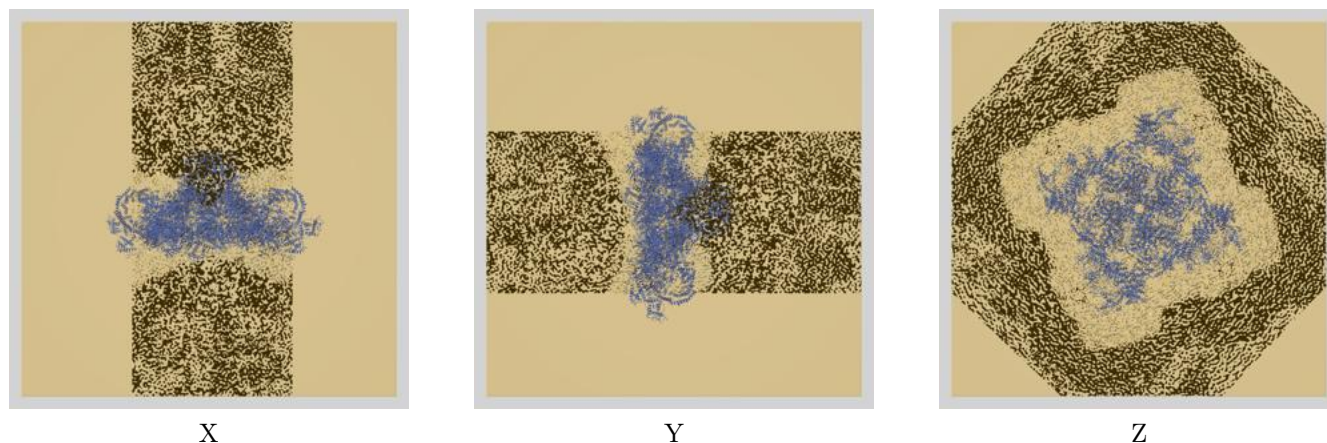
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	4.71	6.48	4.80
Unmasked-calculated*	7.07	8.62	7.16

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.07 differs from the reported value 4.7 by more than 10 %

9 Map-model fit [i](#)

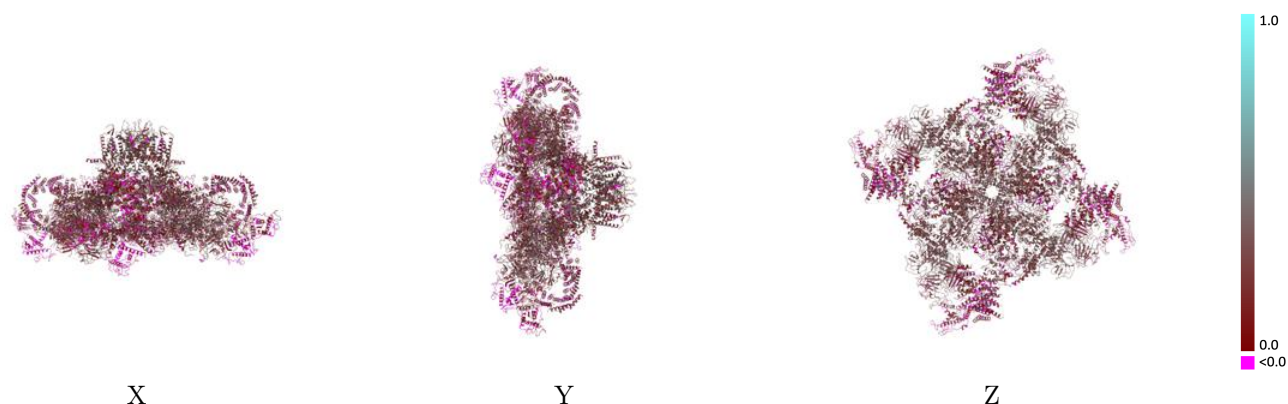
This section contains information regarding the fit between EMDB map EMD-30343 and PDB model 7CF9. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



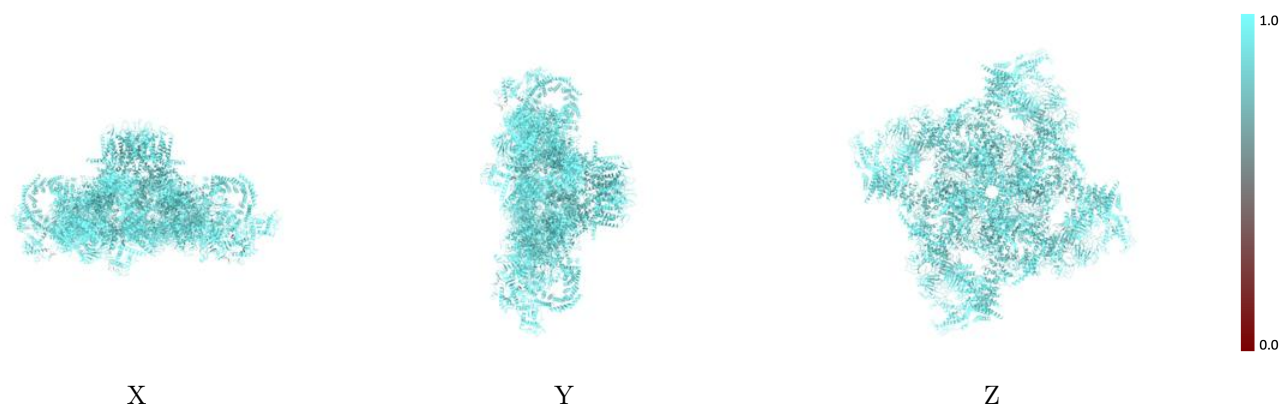
The images above show the 3D surface view of the map at the recommended contour level 0.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



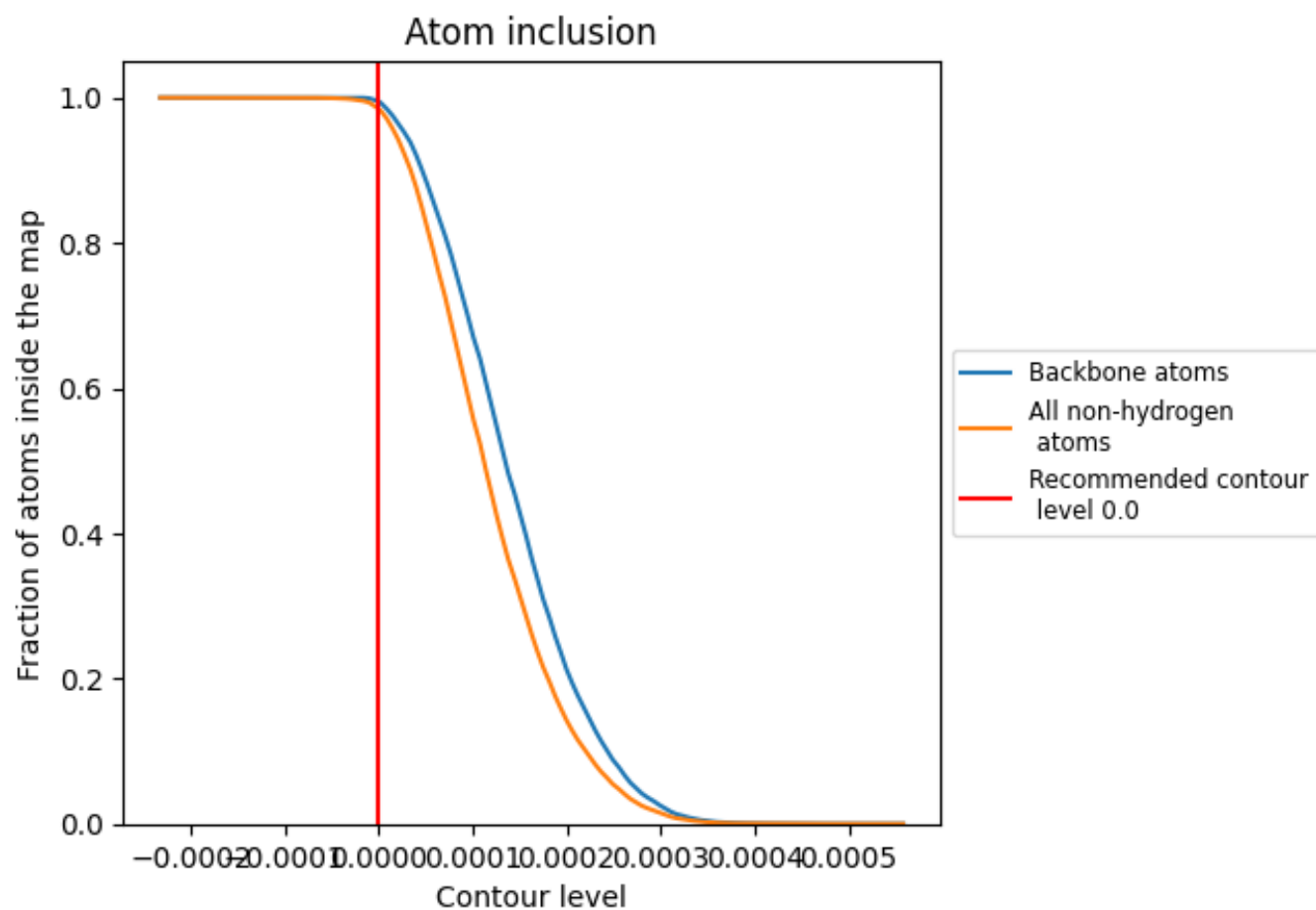
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 98% 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 (0.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.9849</div>	<div><div></div>0.2320</div>
A	<div><div></div>0.9846</div>	<div><div></div>0.2300</div>
B	<div><div></div>0.9975</div>	<div><div></div>0.2860</div>
C	<div><div></div>0.9846</div>	<div><div></div>0.2300</div>
D	<div><div></div>0.9962</div>	<div><div></div>0.2840</div>
E	<div><div></div>0.9845</div>	<div><div></div>0.2300</div>
F	<div><div></div>0.9962</div>	<div><div></div>0.2840</div>
G	<div><div></div>0.9845</div>	<div><div></div>0.2300</div>
H	<div><div></div>0.9975</div>	<div><div></div>0.2860</div>

1.0

0.0

<0.0