



Full wwPDB EM Validation Report ⓘ

Oct 15, 2024 – 12:05 AM EDT

PDB ID : 8SER
EMDB ID : EMD-40426
Title : Cryo-EM Structure of RyR1 + Adenosine
Authors : Cholak, S.; Saville, J.W.; Zhu, X.; Berezuk, A.M.; Tuttle, K.S.; Haji-Ghassemi, O.; Van Petegem, F.; Subramaniam, S.
Deposited on : 2023-04-10
Resolution : 3.42 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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

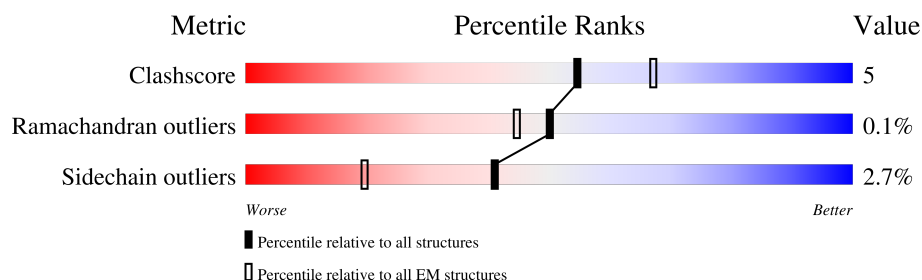
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.42 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	<div> <div>12%</div> <div>74%</div> <div>13%</div> <div>13%</div> </div>
1	B	5037	<div> <div>12%</div> <div>74%</div> <div>13%</div> <div>13%</div> </div>
1	C	5037	<div> <div>13%</div> <div>73%</div> <div>13%</div> <div>13%</div> </div>
1	D	5037	<div> <div>12%</div> <div>74%</div> <div>13%</div> <div>13%</div> </div>
2	E	350	<div> <div>26%</div> <div>5%</div> <div>69%</div> </div>
2	F	350	<div> <div>26%</div> <div>5%</div> <div>69%</div> </div>
2	G	350	<div> <div>26%</div> <div>5%</div> <div>69%</div> </div>
2	H	350	<div> <div>26%</div> <div>5%</div> <div>69%</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 142952 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4376	Total	C	N	O	S	9	0
			34900	22201	6022	6441	236		
1	B	4376	Total	C	N	O	S	9	0
			34900	22201	6022	6441	236		
1	C	4376	Total	C	N	O	S	9	0
			34900	22201	6022	6441	236		
1	D	4376	Total	C	N	O	S	9	0
			34900	22201	6022	6441	236		

- Molecule 2 is a protein called Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	G	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-242	MET	-	expression tag	UNP P08515
E	-241	LYS	-	expression tag	UNP P08515
E	-240	SER	-	expression tag	UNP P08515
E	-239	SER	-	expression tag	UNP P08515
E	-238	HIS	-	expression tag	UNP P08515
E	-237	HIS	-	expression tag	UNP P08515
E	-236	HIS	-	expression tag	UNP P08515
E	-235	HIS	-	expression tag	UNP P08515

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-234	HIS	-	expression tag	UNP P08515
E	-233	HIS	-	expression tag	UNP P08515
E	-232	GLY	-	expression tag	UNP P08515
E	-231	SER	-	expression tag	UNP P08515
E	-230	SER	-	expression tag	UNP P08515
E	-11	GLY	-	linker	UNP P08515
E	-10	ILE	-	linker	UNP P08515
E	-9	GLU	-	linker	UNP P08515
E	-8	GLU	-	linker	UNP P08515
E	-7	ASN	-	linker	UNP P08515
E	-6	LEU	-	linker	UNP P08515
E	-5	TYR	-	linker	UNP P08515
E	-4	PHE	-	linker	UNP P08515
E	-3	GLN	-	linker	UNP P08515
E	-2	SER	-	linker	UNP P08515
E	-1	ASN	-	linker	UNP P08515
E	0	ALA	-	linker	UNP P08515
F	-242	MET	-	expression tag	UNP P08515
F	-241	LYS	-	expression tag	UNP P08515
F	-240	SER	-	expression tag	UNP P08515
F	-239	SER	-	expression tag	UNP P08515
F	-238	HIS	-	expression tag	UNP P08515
F	-237	HIS	-	expression tag	UNP P08515
F	-236	HIS	-	expression tag	UNP P08515
F	-235	HIS	-	expression tag	UNP P08515
F	-234	HIS	-	expression tag	UNP P08515
F	-233	HIS	-	expression tag	UNP P08515
F	-232	GLY	-	expression tag	UNP P08515
F	-231	SER	-	expression tag	UNP P08515
F	-230	SER	-	expression tag	UNP P08515
F	-11	GLY	-	linker	UNP P08515
F	-10	ILE	-	linker	UNP P08515
F	-9	GLU	-	linker	UNP P08515
F	-8	GLU	-	linker	UNP P08515
F	-7	ASN	-	linker	UNP P08515
F	-6	LEU	-	linker	UNP P08515
F	-5	TYR	-	linker	UNP P08515
F	-4	PHE	-	linker	UNP P08515
F	-3	GLN	-	linker	UNP P08515
F	-2	SER	-	linker	UNP P08515
F	-1	ASN	-	linker	UNP P08515
F	0	ALA	-	linker	UNP P08515

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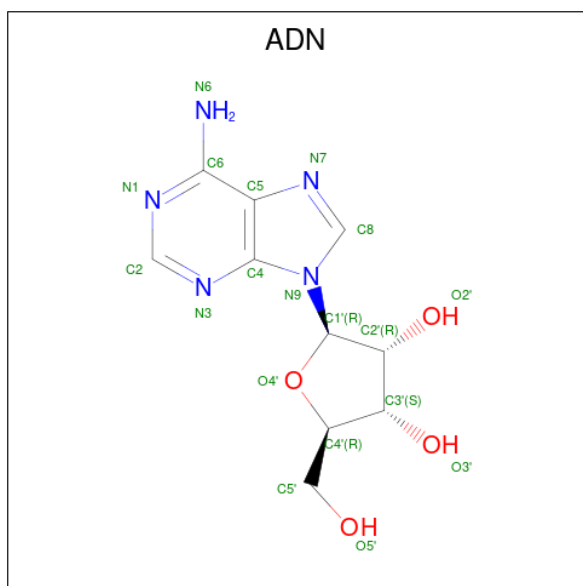
Chain	Residue	Modelled	Actual	Comment	Reference
G	-242	MET	-	expression tag	UNP P08515
G	-241	LYS	-	expression tag	UNP P08515
G	-240	SER	-	expression tag	UNP P08515
G	-239	SER	-	expression tag	UNP P08515
G	-238	HIS	-	expression tag	UNP P08515
G	-237	HIS	-	expression tag	UNP P08515
G	-236	HIS	-	expression tag	UNP P08515
G	-235	HIS	-	expression tag	UNP P08515
G	-234	HIS	-	expression tag	UNP P08515
G	-233	HIS	-	expression tag	UNP P08515
G	-232	GLY	-	expression tag	UNP P08515
G	-231	SER	-	expression tag	UNP P08515
G	-230	SER	-	expression tag	UNP P08515
G	-11	GLY	-	linker	UNP P08515
G	-10	ILE	-	linker	UNP P08515
G	-9	GLU	-	linker	UNP P08515
G	-8	GLU	-	linker	UNP P08515
G	-7	ASN	-	linker	UNP P08515
G	-6	LEU	-	linker	UNP P08515
G	-5	TYR	-	linker	UNP P08515
G	-4	PHE	-	linker	UNP P08515
G	-3	GLN	-	linker	UNP P08515
G	-2	SER	-	linker	UNP P08515
G	-1	ASN	-	linker	UNP P08515
G	0	ALA	-	linker	UNP P08515
H	-242	MET	-	expression tag	UNP P08515
H	-241	LYS	-	expression tag	UNP P08515
H	-240	SER	-	expression tag	UNP P08515
H	-239	SER	-	expression tag	UNP P08515
H	-238	HIS	-	expression tag	UNP P08515
H	-237	HIS	-	expression tag	UNP P08515
H	-236	HIS	-	expression tag	UNP P08515
H	-235	HIS	-	expression tag	UNP P08515
H	-234	HIS	-	expression tag	UNP P08515
H	-233	HIS	-	expression tag	UNP P08515
H	-232	GLY	-	expression tag	UNP P08515
H	-231	SER	-	expression tag	UNP P08515
H	-230	SER	-	expression tag	UNP P08515
H	-11	GLY	-	linker	UNP P08515
H	-10	ILE	-	linker	UNP P08515
H	-9	GLU	-	linker	UNP P08515
H	-8	GLU	-	linker	UNP P08515

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-7	ASN	-	linker	UNP P08515
H	-6	LEU	-	linker	UNP P08515
H	-5	TYR	-	linker	UNP P08515
H	-4	PHE	-	linker	UNP P08515
H	-3	GLN	-	linker	UNP P08515
H	-2	SER	-	linker	UNP P08515
H	-1	ASN	-	linker	UNP P08515
H	0	ALA	-	linker	UNP P08515

- Molecule 3 is ADENOSINE (three-letter code: ADN) (formula: $C_{10}H_{13}N_5O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			19	10	5	4	
3	B	1	Total	C	N	O	0
			19	10	5	4	
3	C	1	Total	C	N	O	0
			19	10	5	4	
3	D	1	Total	C	N	O	0
			19	10	5	4	

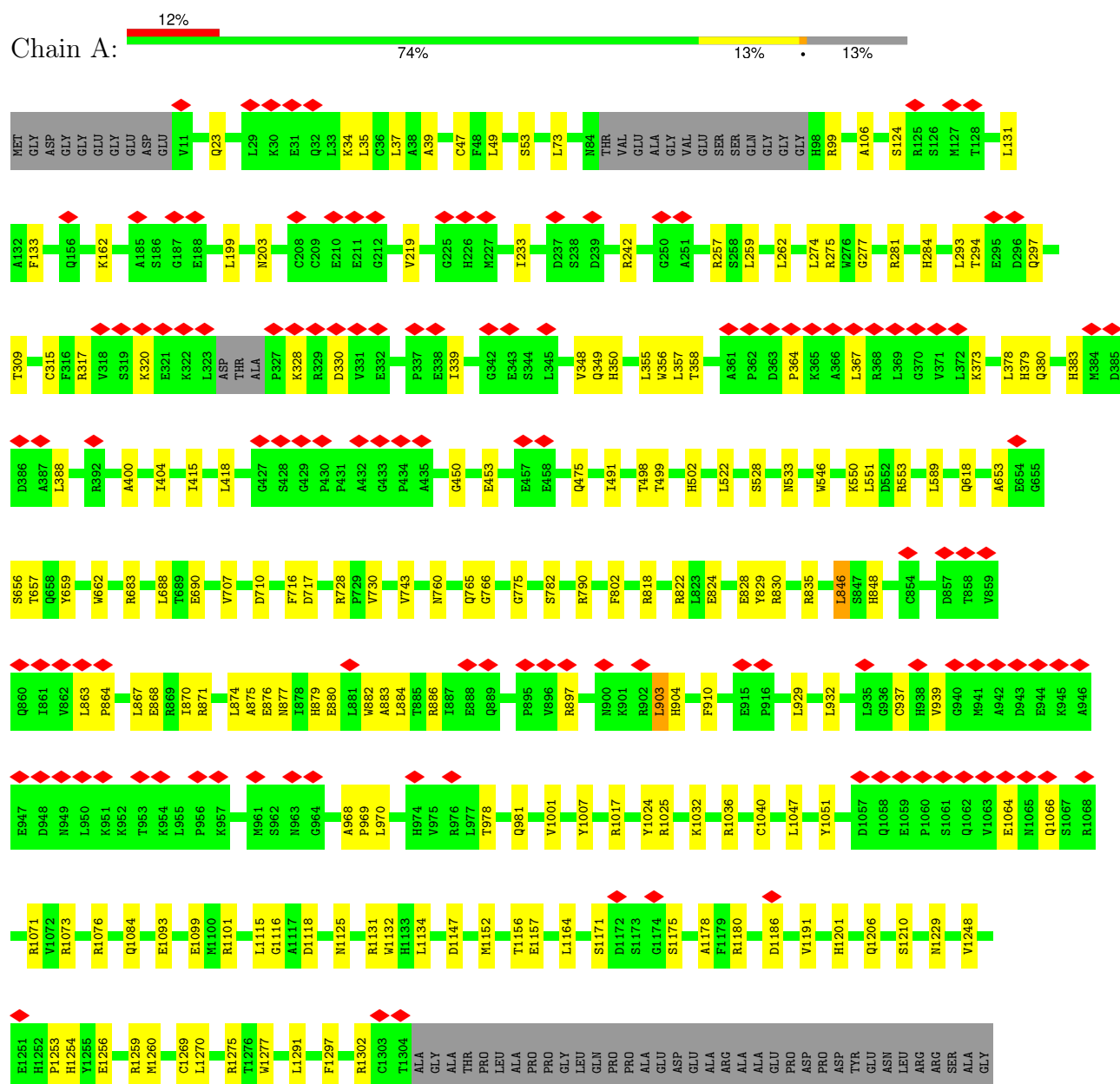
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

3 Residue-property plots

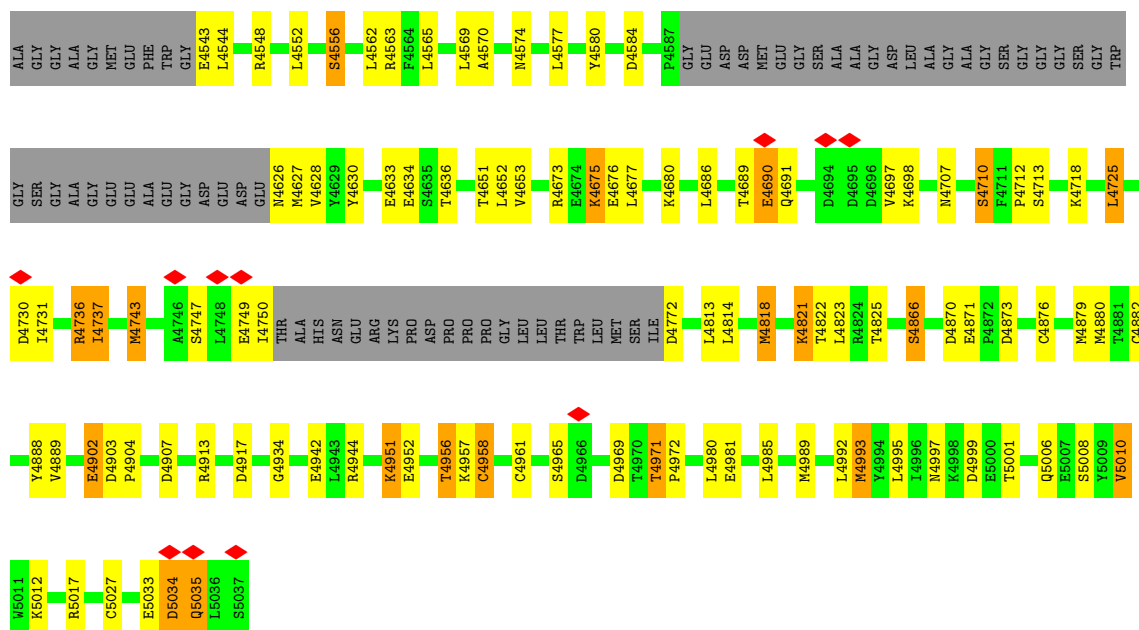
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Ryanodine receptor 1

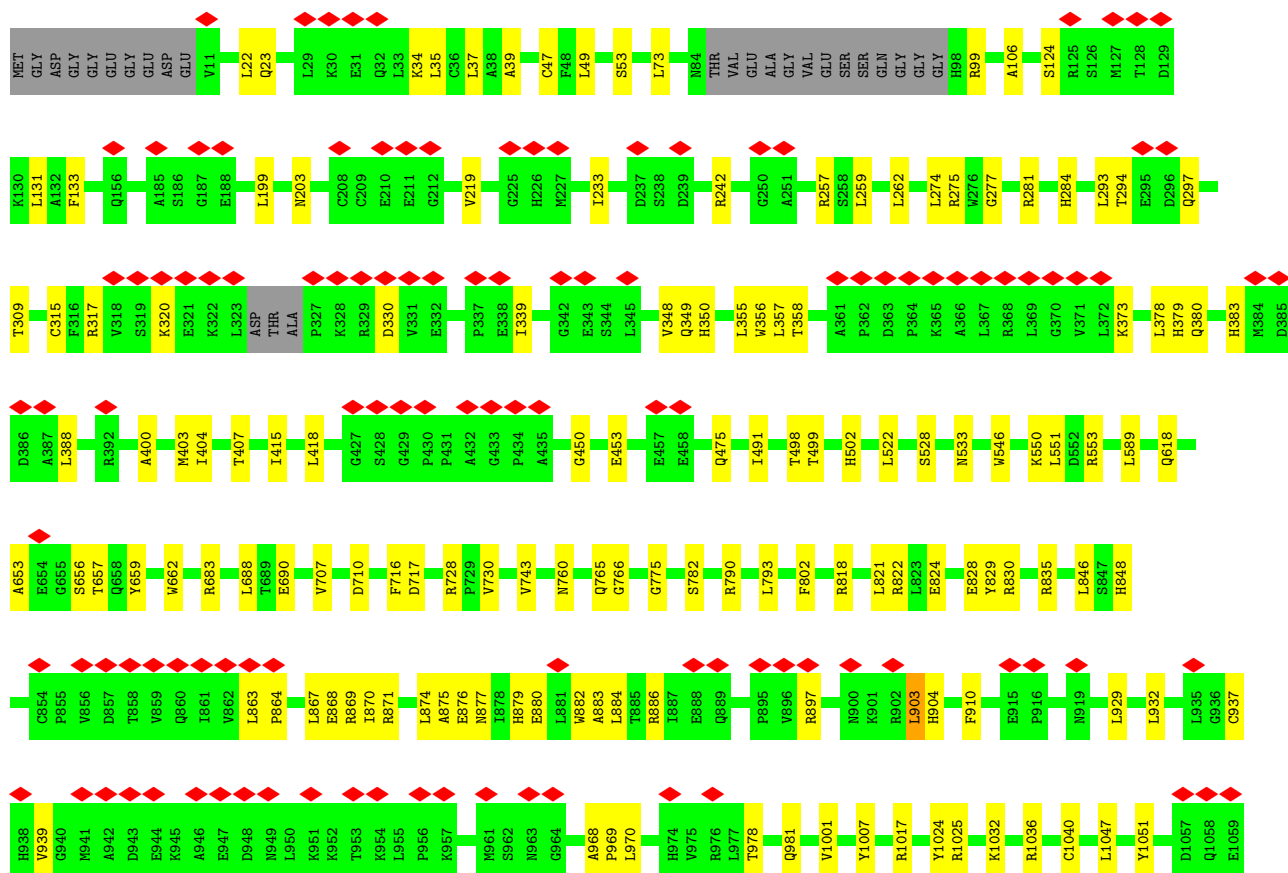






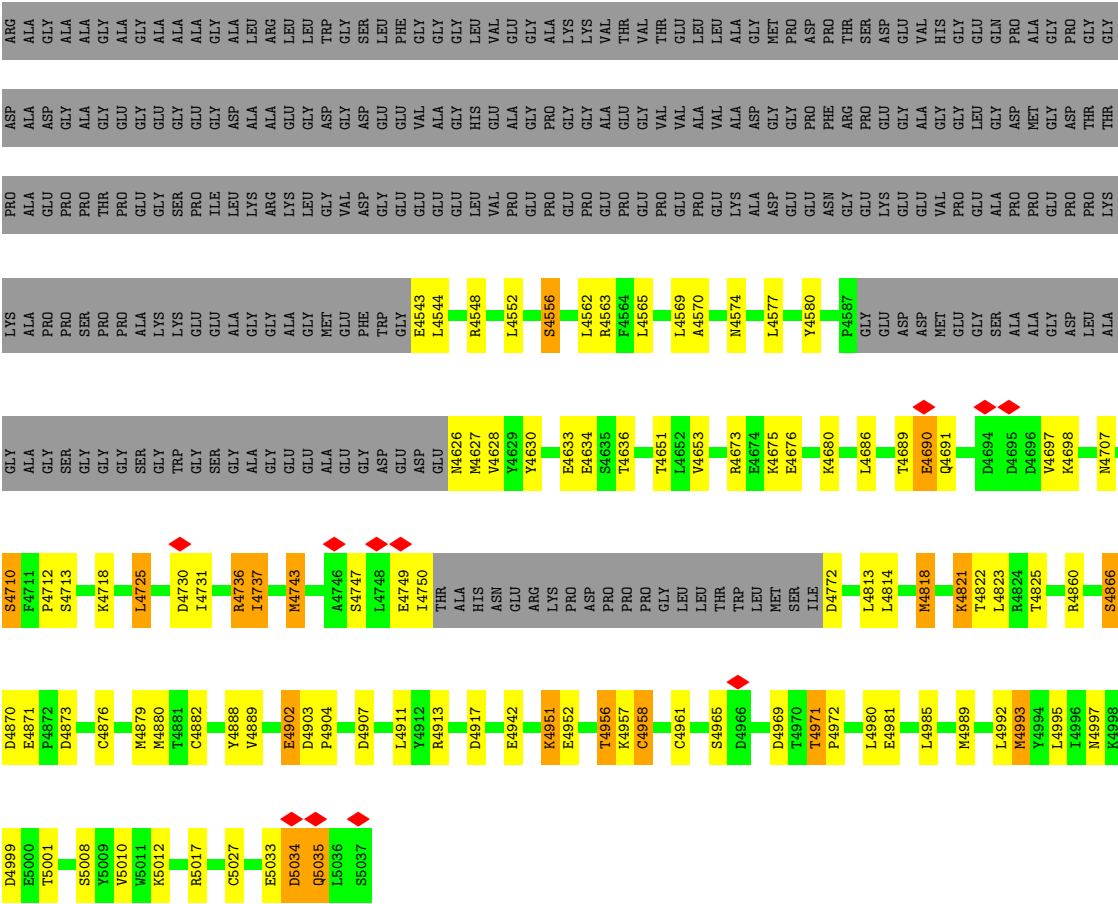


• Molecule 1: Ryanodine receptor 1

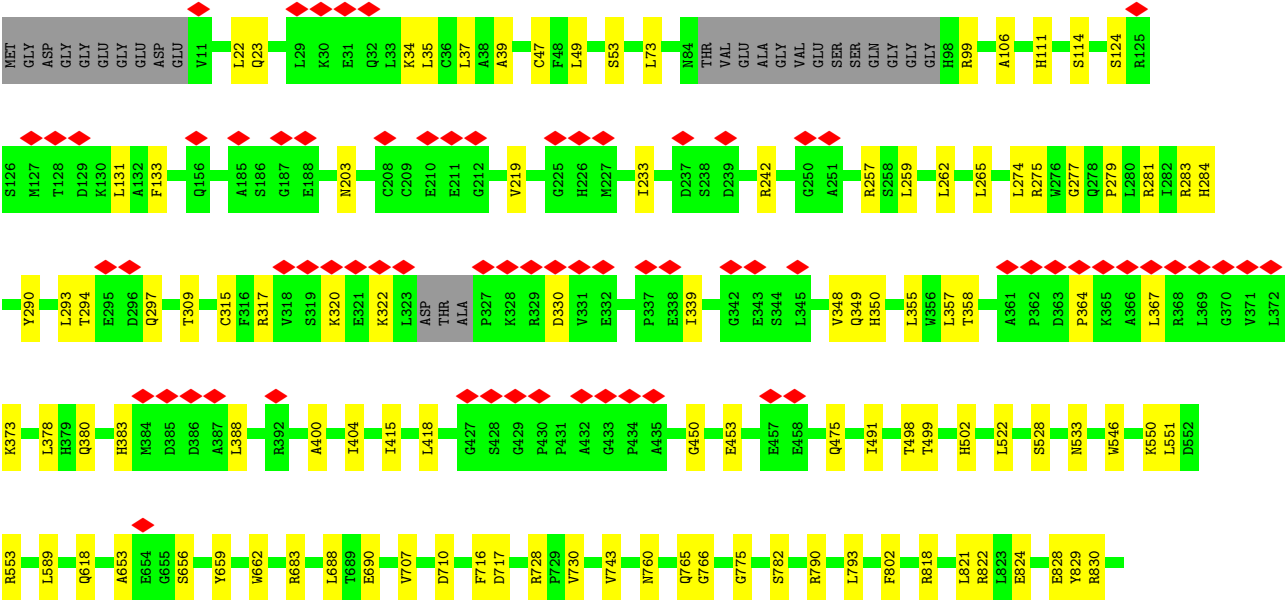


K2795	T2796	F2797	S2798	E2799	K2800	D2801	K2802	E2803	L2804	Y2805	R2806	W2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	W2816	L2817	A2818	W2819	E2820	W2821	T2822	L2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	GLU	ARG	THR	GLU	GLU	LYS	LYS	LYS	THR	ARG	LYS	ILE	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLU	GLY																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
F2735	D2736	P2737	R2738	P2739	V2740	E2741	T2742	L2743	W2744	V2745	L2746	L2747	P2748	E2749	K2750	L2751	S2753	P2754	L2755	W2756	K2757	P2758	E2759	E2760	Y2761	T2762	H2763	E2764	K2765	W2766	A2767	F2768	D2769	K2770	L2771	Q2772	N2773	M2774	S2775	K2776	Y2777	E2778	E2779	M2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	P2788																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
S2590	R2593	S2594	L2595	R2600	M2618	V2627	V2630	P2640	L2643	S2668	E2669	E2670	L2674	T2675	K2676	L2677	F2679	T2682	F2683	S2685	L2686	A2687	H2688	L2706	A2707	P2712	A2717	S2718	Y2719	S2720	S2721	K2722	A2723	E2724	K2725	LYS	ALA	THR	VAL	ASP	ALA	GLU	GLY	N2734																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
ARG	ASP	ARG	ARG	ARG	GLU	HIS	PHE	GLY	GLU	P2410	P2411	E2412	E2413	W2414	L2474	T2478	L2479	G2480	K2481	D2482	G2483	A2484	L2485	F2494	K2499	E2513	D2516	L2527	M2530	T2538	A2539	T2540	F2541	S2542	L2550	G2571	H2574	R2575	A2576	M2582	L2583	V2586	Y2587																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
I2167	N2176	N2196	R2199	E2205	M2208	G2217	G2218	E2219	T2220	K2221	L2236	W2250	L2265	Q2268	A2277	I2281	L2307	C2310	L2313	D2320	R2330	R2336	L2368	R2369	G2370	E2371	G2372	G2373	L2376	R2385	A2391	R2392	G2396	V2397	ARG																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
Q2045	L2046	GLU	GLY	GLU	GLU	GLU	GLU	PRO	GLU	GLU	GLU	THR	SER	SER	ARG	SER	LEU	THR	VAL	ARG	VAL	LYS	LYS	GLU	GLU	PRO	GLU	GLU	LEU	PRO	ALA	ALA	E2088	V2089	Q2095	V2098	S2099	H2100	D2109	R2126	Q2127	L2159	R2163																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
GLU	ALA	PRO	GLY	GLU	GLU	LYS	ASP	L1922	E1923	L1943	D1948	K1968	L1969	R1982	A1983	F1984	T1985	M1986	S1987	A1988	A1989	E1990	R1993	R1994	S2000	P2001	Q2005	L2006	M2008	L2009	L2010	H2011	D2014	E2015	A2016	D2017	E2018	E2019	D2020	C2021	R2028	Q2029	D2030	L2039	L2044																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
G1754	G1755	M1756	A1768	A1789	G1790	V1791	A1792	E1793	R1808	R1827	D1828	I1853	Q1861	M1865	E1874	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU</



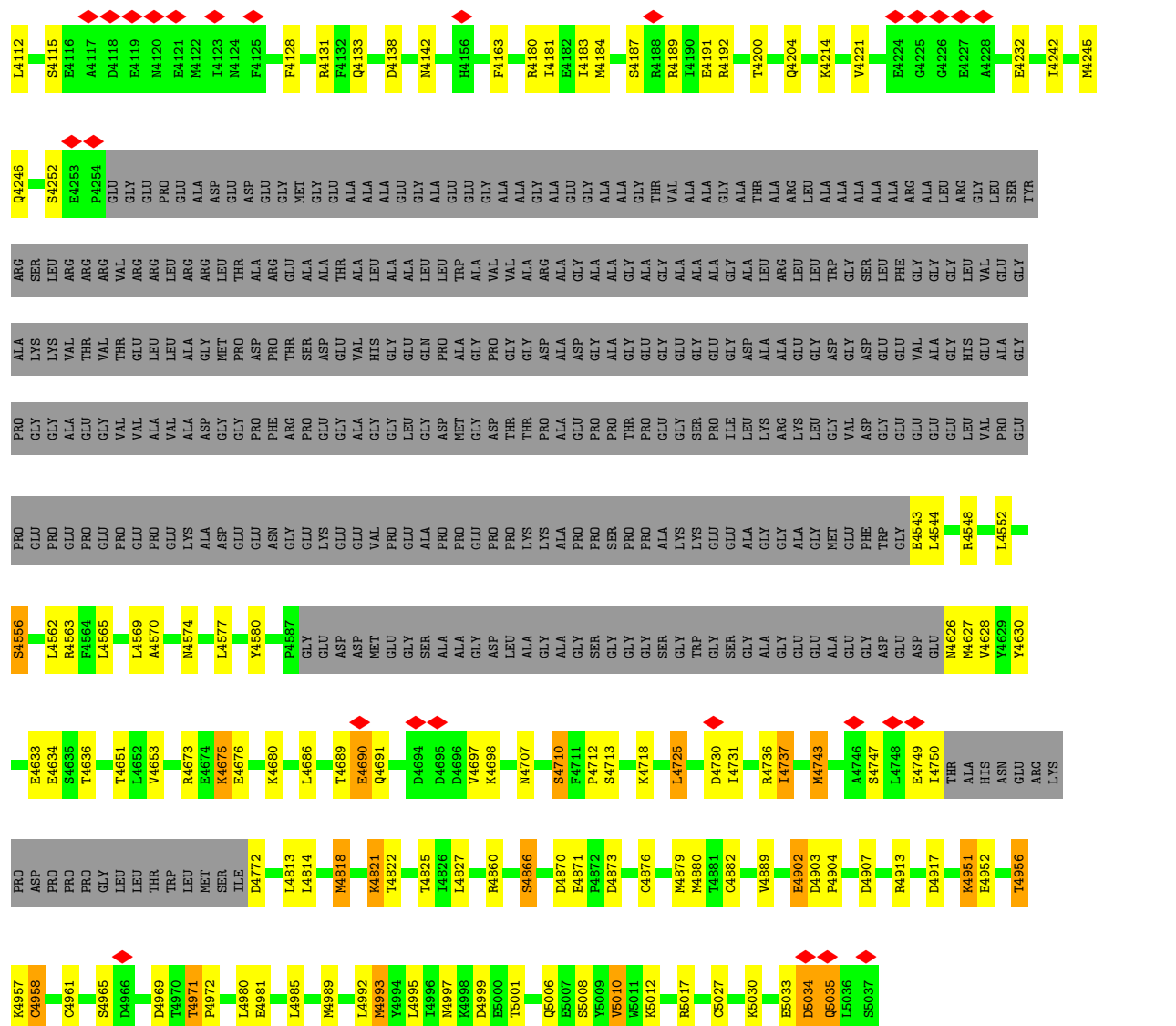


• Molecule 1: Ryanodine receptor 1

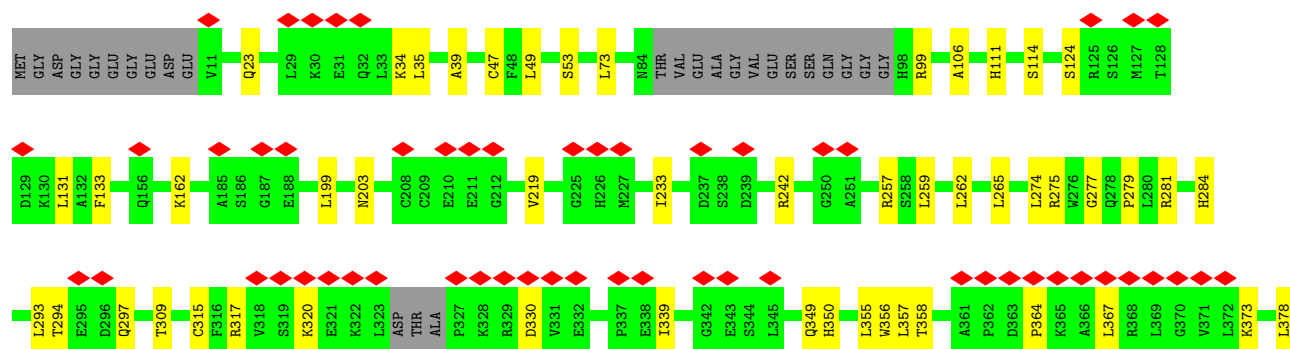
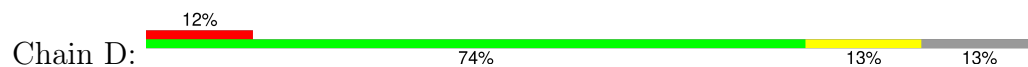




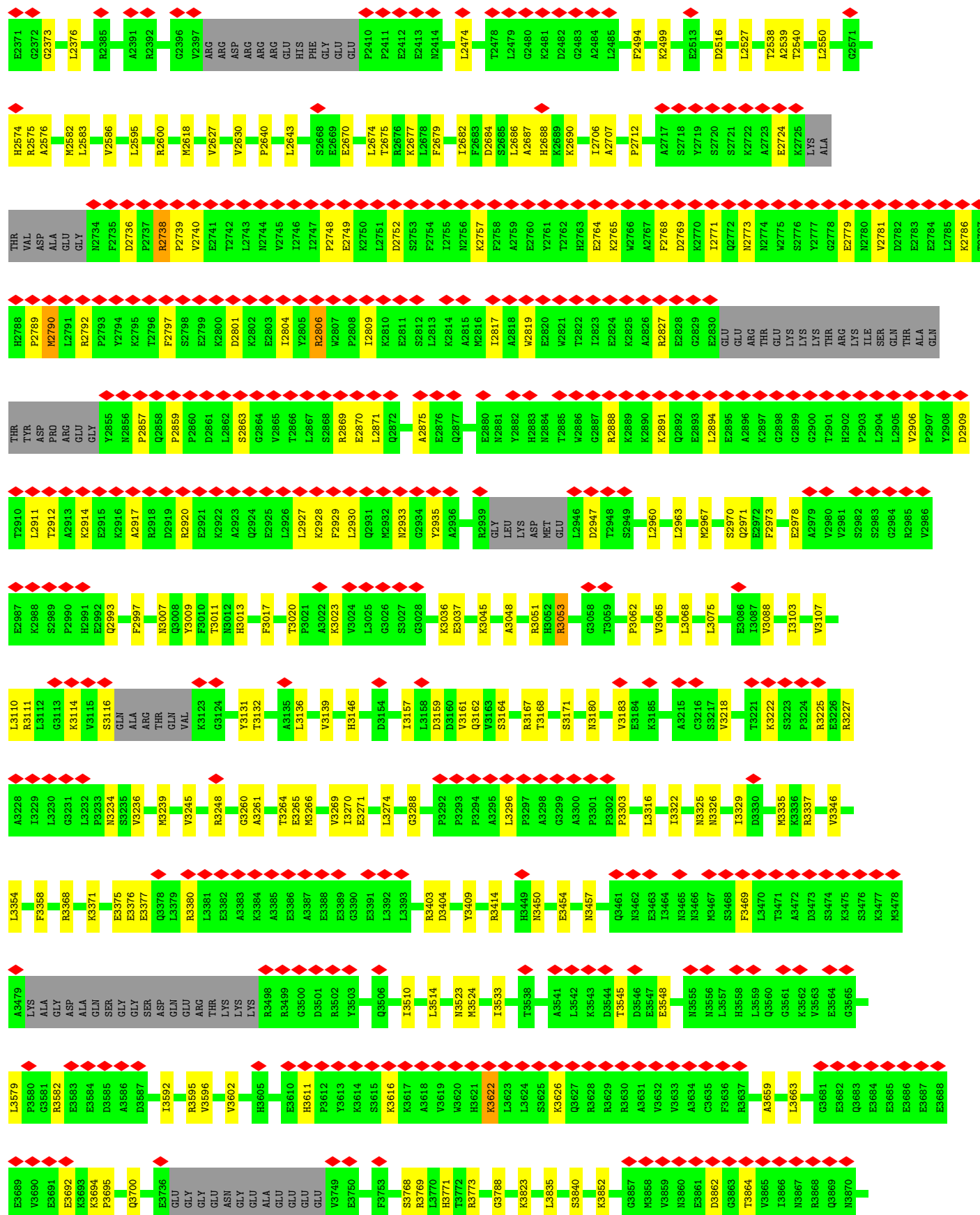


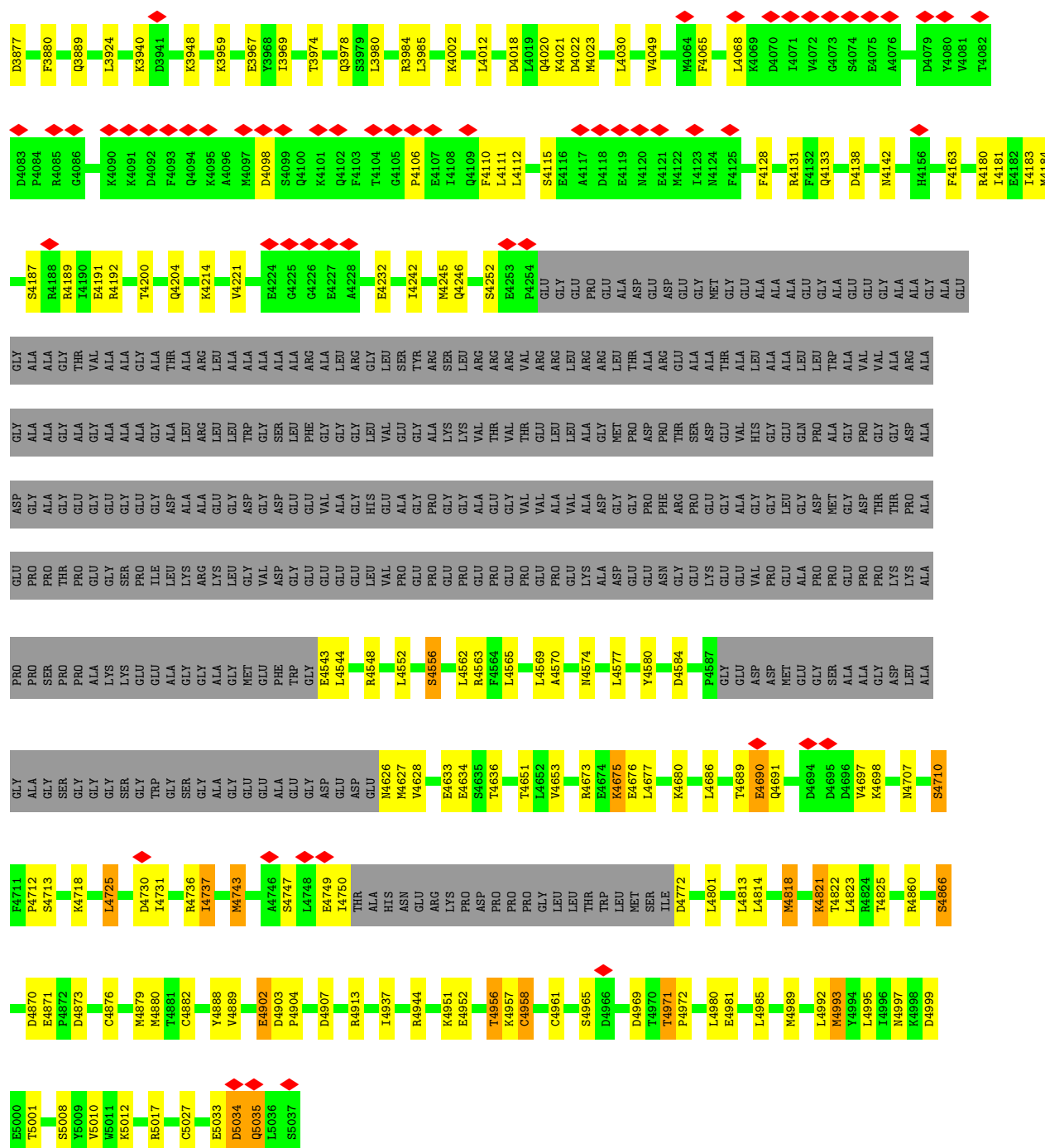


• Molecule 1: Ryanodine receptor 1









Chain E:

26%

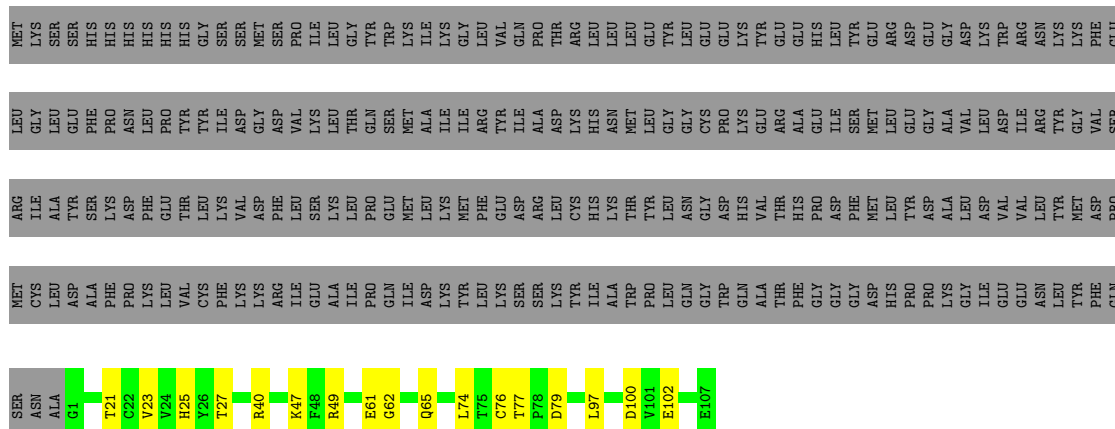
5%

69%

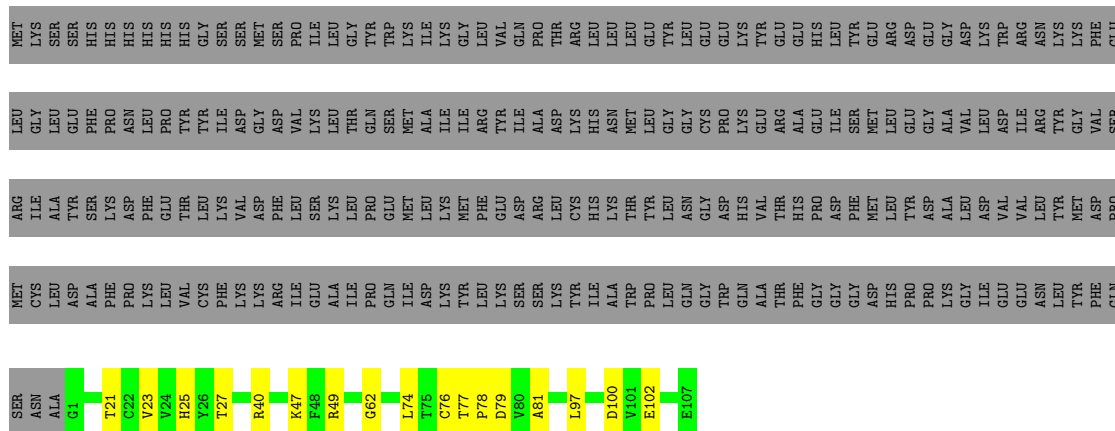
LEU	GLY	SER	THR	ASP	GLY	ASP	VAL	LYS	LEU	THR	GLN	SER	TRP	LYS	ILE	LYS	ILE	ARG	TYR	ILE	ARG	TYR	ILE	ASN	GLY	CYS	PRO	LYS	GLU	ARG	ALA	ILE	SER	MET	LEU	GLU	GLY	ALA	VAL	ASP	LYS	TRP	ARG	ILE	ARG	TYR	GLY	VAL	SER
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Chain F: 26% 5% 69%



Chain G:  26% 5% 69%



Chain H:  26% 5% 69%

SER	ASN	ALA	G1	T21	C22	V23	V24	H25	Y26	T27	R40	K47	F48	R49	G62	L74	T75	C76	T77	P78	D79	V80	A81	L97	D100	V101	E102	E107																												
MET	CYS	LEU	ASP	ALA	PHE	PRO	LYS	LEU	VAL	CYS	PHE	LYS	ARG	ILE	GLU	ALA	ILE	PRO	GLN	ILE	ASP	LYS	TYR	TYR	ILE	ALA	TRP	PRO	LEU	GLN	GLY	GLY	TRP	GLN	ALA	ALA	THR	PHE	GLY	GLY	HIS	ASP	PRO	PRO	LYS	GLY	ILE	GLU	GLU	ASN	LEU	TYR	MET	ASP	VAL	SER
LEU	GLY	LEU	GLU	PHE	PRO	ASN	LEU	PRO	TYR	ILE	ASP	GLY	VAL	LYS	THR	GLN	SER	MET	ALA	ILE	ARG	TYR	ILE	ASP	ALA	LYS	CYS	PRO	HIS	LYS	THR	TYR	LEU	ASN	GLY	CYS	PRO	HIS	VAL	GLU	ARG	ALA	GLU	ILE	ASP	VAL	GLU	GLU	ASP	VAL	ARG	TYR	GLY	VAL	SER	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	51504	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.346	Depositor
Minimum map value	-0.409	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.073	Depositor
Recommended contour level	0.387	Depositor
Map size (Å)	515.2, 515.2, 515.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.288, 1.288, 1.288	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.32	0/35714	0.62	6/48365 (0.0%)
1	B	0.32	0/35714	0.62	6/48365 (0.0%)
1	C	0.32	0/35714	0.62	6/48365 (0.0%)
1	D	0.32	0/35714	0.62	6/48365 (0.0%)
2	E	0.34	0/834	0.62	0/1123
2	F	0.34	0/834	0.62	0/1123
2	G	0.34	0/834	0.62	0/1123
2	H	0.34	0/834	0.62	0/1123
All	All	0.32	0/146192	0.62	24/197952 (0.0%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	903	LEU	CA-CB-CG	6.63	130.54	115.30
1	B	903	LEU	CA-CB-CG	6.63	130.54	115.30
1	C	903	LEU	CA-CB-CG	6.63	130.54	115.30
1	D	903	LEU	CA-CB-CG	6.63	130.54	115.30
1	C	2790	MET	CA-CB-CG	5.77	123.11	113.30
1	D	2790	MET	CA-CB-CG	5.77	123.11	113.30
1	B	2790	MET	CA-CB-CG	5.75	123.08	113.30
1	A	2790	MET	CA-CB-CG	5.72	123.03	113.30
1	D	1478	ASP	CB-CG-OD1	5.67	123.40	118.30
1	B	131	LEU	CA-CB-CG	5.63	128.24	115.30
1	C	131	LEU	CA-CB-CG	5.63	128.24	115.30
1	C	1478	ASP	CB-CG-OD1	5.62	123.35	118.30
1	A	131	LEU	CA-CB-CG	5.61	128.21	115.30
1	D	131	LEU	CA-CB-CG	5.61	128.20	115.30
1	B	1478	ASP	CB-CG-OD1	5.59	123.33	118.30
1	A	1478	ASP	CB-CG-OD1	5.56	123.30	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1152	MET	CA-CB-CG	5.49	122.63	113.30
1	B	1152	MET	CA-CB-CG	5.49	122.63	113.30
1	C	1152	MET	CA-CB-CG	5.47	122.59	113.30
1	D	1152	MET	CA-CB-CG	5.46	122.58	113.30
1	A	3296	LEU	CA-CB-CG	5.42	127.77	115.30
1	D	3296	LEU	CA-CB-CG	5.42	127.76	115.30
1	B	3296	LEU	CA-CB-CG	5.40	127.72	115.30
1	C	3296	LEU	CA-CB-CG	5.40	127.72	115.30

There are no chirality outliers.

There are no planarity outliers.

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	34900	0	34530	340	0
1	B	34900	0	34530	336	0
1	C	34900	0	34530	349	0
1	D	34900	0	34530	336	0
2	E	818	0	824	8	0
2	F	818	0	824	8	0
2	G	818	0	824	8	0
2	H	818	0	824	8	0
3	A	19	0	13	0	0
3	B	19	0	13	0	0
3	C	19	0	13	0	0
3	D	19	0	13	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	142952	0	141468	1384	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 (1384) 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:A:3335:MET:SD	1:A:3403:ARG:NH1	2.64	0.70
1:B:3335:MET:SD	1:B:3403:ARG:NH1	2.64	0.69
1:D:3335:MET:SD	1:D:3403:ARG:NH1	2.65	0.68
1:C:3335:MET:SD	1:C:3403:ARG:NH1	2.65	0.68
1:B:3889:GLN:HG3	1:B:3967:GLU:HG3	1.78	0.65
1:C:2978:GLU:OE2	1:C:3053:ARG:NH1	2.29	0.65
1:D:3889:GLN:HG3	1:D:3967:GLU:HG3	1.78	0.65
1:C:3889:GLN:HG3	1:C:3967:GLU:HG3	1.78	0.65
1:A:1476:MET:HB2	1:A:1485:SER:HB3	1.79	0.64
1:A:3889:GLN:HG3	1:A:3967:GLU:HG3	1.78	0.64
1:B:1943:LEU:HD13	1:B:2098:VAL:HG22	1.79	0.64
1:D:1943:LEU:HD13	1:D:2098:VAL:HG22	1.80	0.64
1:B:2978:GLU:OE2	1:B:3053:ARG:NH1	2.29	0.64
1:D:2978:GLU:OE2	1:D:3053:ARG:NH1	2.29	0.64
1:B:3454:GLU:HA	1:B:3457:ASN:HB2	1.80	0.64
1:C:1476:MET:HB2	1:C:1485:SER:HB3	1.79	0.63
1:C:1943:LEU:HD13	1:C:2098:VAL:HG22	1.79	0.63
1:C:3454:GLU:HA	1:C:3457:ASN:HB2	1.80	0.63
1:C:981:GLN:HG2	1:C:1047:LEU:HD11	1.79	0.63
1:D:981:GLN:HG2	1:D:1047:LEU:HD11	1.79	0.63
1:C:3969:ILE:HD11	1:C:3980:LEU:HD13	1.80	0.63
1:A:981:GLN:HG2	1:A:1047:LEU:HD11	1.79	0.63
1:D:3969:ILE:HD11	1:D:3980:LEU:HD13	1.81	0.63
1:D:1476:MET:HB2	1:D:1485:SER:HB3	1.79	0.63
1:A:1943:LEU:HD13	1:A:2098:VAL:HG22	1.80	0.63
1:B:1476:MET:HB2	1:B:1485:SER:HB3	1.79	0.63
1:B:2630:VAL:HG12	1:B:2682:ILE:HD11	1.81	0.62
1:A:3048:ALA:O	1:A:3053:ARG:NH2	2.33	0.62
1:B:2929:PHE:O	1:B:2933:ASN:ND2	2.33	0.62
1:D:2630:VAL:HG12	1:D:2682:ILE:HD11	1.81	0.62
1:A:4138:ASP:O	1:A:4142:ASN:ND2	2.30	0.62
1:B:3048:ALA:O	1:B:3053:ARG:NH2	2.33	0.62
1:B:4138:ASP:O	1:B:4142:ASN:ND2	2.30	0.62
1:C:1024:TYR:O	1:C:1032:LYS:NZ	2.33	0.62
1:A:978:THR:OG1	1:A:981:GLN:OE1	2.18	0.62
1:B:981:GLN:HG2	1:B:1047:LEU:HD11	1.79	0.62
1:D:3048:ALA:O	1:D:3053:ARG:NH2	2.32	0.62
1:C:2929:PHE:O	1:C:2933:ASN:ND2	2.33	0.62
1:D:3454:GLU:HA	1:D:3457:ASN:HB2	1.80	0.62
1:C:2630:VAL:HG12	1:C:2682:ILE:HD11	1.81	0.61
1:A:3969:ILE:HD11	1:A:3980:LEU:HD13	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3969:ILE:HD11	1:B:3980:LEU:HD13	1.81	0.61
1:C:1653:LEU:O	1:C:1660:GLN:NE2	2.32	0.61
1:C:3048:ALA:O	1:C:3053:ARG:NH2	2.33	0.61
1:A:3454:GLU:HA	1:A:3457:ASN:HB2	1.80	0.61
1:A:1024:TYR:O	1:A:1032:LYS:NZ	2.33	0.61
1:B:1024:TYR:O	1:B:1032:LYS:NZ	2.33	0.61
1:A:2630:VAL:HG12	1:A:2682:ILE:HD11	1.81	0.61
1:B:978:THR:OG1	1:B:981:GLN:OE1	2.18	0.61
1:C:978:THR:OG1	1:C:981:GLN:OE1	2.18	0.61
1:A:2929:PHE:O	1:A:2933:ASN:ND2	2.33	0.61
1:D:2929:PHE:O	1:D:2933:ASN:ND2	2.33	0.61
2:H:40:ARG:NH2	2:H:102:GLU:OE1	2.34	0.61
1:D:1561:VAL:HG12	1:D:1562:ILE:HG23	1.83	0.61
1:A:2875:ALA:HB2	1:A:2927:LEU:HD22	1.83	0.61
1:A:2978:GLU:OE2	1:A:3053:ARG:NH1	2.29	0.61
1:C:2875:ALA:HB2	1:C:2927:LEU:HD22	1.83	0.61
1:D:2875:ALA:HB2	1:D:2927:LEU:HD22	1.83	0.61
1:B:3659:ALA:HA	1:B:3663:LEU:HD12	1.82	0.61
1:D:1024:TYR:O	1:D:1032:LYS:NZ	2.33	0.61
1:D:978:THR:OG1	1:D:981:GLN:OE1	2.18	0.60
1:B:2875:ALA:HB2	1:B:2927:LEU:HD22	1.83	0.60
1:D:1653:LEU:O	1:D:1660:GLN:NE2	2.32	0.60
2:F:40:ARG:NH2	2:F:102:GLU:OE1	2.34	0.60
1:C:1116:GLY:HA3	1:C:1132:TRP:HB3	1.83	0.60
1:D:3659:ALA:HA	1:D:3663:LEU:HD12	1.82	0.60
1:C:1561:VAL:HG12	1:C:1562:ILE:HG23	1.83	0.60
1:A:897:ARG:HB2	1:A:903:LEU:HD11	1.84	0.60
1:A:1561:VAL:HG12	1:A:1562:ILE:HG23	1.83	0.60
1:D:1116:GLY:HA3	1:D:1132:TRP:HB3	1.84	0.60
2:E:40:ARG:NH2	2:E:102:GLU:OE1	2.34	0.60
2:G:40:ARG:NH2	2:G:102:GLU:OE1	2.34	0.60
1:D:897:ARG:HB2	1:D:903:LEU:HD11	1.84	0.60
1:C:317:ARG:NH1	1:C:349:GLN:OE1	2.35	0.60
1:C:4138:ASP:O	1:C:4142:ASN:ND2	2.30	0.60
1:D:317:ARG:NH1	1:D:349:GLN:OE1	2.35	0.60
1:A:275:ARG:HH12	1:A:330:ASP:HA	1.67	0.59
1:A:3659:ALA:HA	1:A:3663:LEU:HD12	1.82	0.59
1:B:2749:GLU:HG3	1:B:2752:ASP:HB3	1.85	0.59
1:A:3020:THR:HG23	1:A:3023:LYS:H	1.68	0.59
1:B:1653:LEU:O	1:B:1660:GLN:NE2	2.32	0.59
1:B:3020:THR:HG23	1:B:3023:LYS:H	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2749:GLU:HG3	1:D:2752:ASP:HB3	1.85	0.59
1:C:3659:ALA:HA	1:C:3663:LEU:HD12	1.82	0.59
1:B:1064:GLU:O	1:B:1071:ARG:NH2	2.32	0.59
1:D:1064:GLU:O	1:D:1071:ARG:NH2	2.32	0.59
1:B:3288:GLY:HA2	1:B:3303:PRO:HB3	1.85	0.59
1:A:2007:ASN:O	1:A:2011:HIS:HB2	2.03	0.59
1:D:275:ARG:HH12	1:D:330:ASP:HA	1.67	0.59
1:B:1561:VAL:HG12	1:B:1562:ILE:HG23	1.83	0.59
1:A:1116:GLY:HA3	1:A:1132:TRP:HB3	1.84	0.59
1:D:3020:THR:HG23	1:D:3023:LYS:H	1.68	0.59
1:A:2749:GLU:HG3	1:A:2752:ASP:HB3	1.85	0.59
1:A:4689:THR:OG1	1:A:4690:GLU:N	2.36	0.59
1:B:275:ARG:HH12	1:B:330:ASP:HA	1.67	0.59
1:B:3051:ARG:O	1:B:3053:ARG:NE	2.36	0.59
1:C:2007:ASN:O	1:C:2011:HIS:HB2	2.03	0.58
1:D:4138:ASP:O	1:D:4142:ASN:ND2	2.30	0.58
1:A:3579:LEU:HB2	1:A:3582:ARG:HG2	1.85	0.58
1:B:1116:GLY:HA3	1:B:1132:TRP:HB3	1.84	0.58
1:C:897:ARG:HB2	1:C:903:LEU:HD11	1.84	0.58
1:C:2749:GLU:HG3	1:C:2752:ASP:HB3	1.85	0.58
1:C:3020:THR:HG23	1:C:3023:LYS:H	1.68	0.58
1:C:3051:ARG:O	1:C:3053:ARG:NE	2.36	0.58
1:D:2007:ASN:O	1:D:2011:HIS:HB2	2.03	0.58
1:A:3051:ARG:O	1:A:3053:ARG:NE	2.36	0.58
1:B:317:ARG:NH1	1:B:349:GLN:OE1	2.35	0.58
1:B:2007:ASN:O	1:B:2011:HIS:HB2	2.03	0.58
1:B:4689:THR:OG1	1:B:4690:GLU:N	2.36	0.58
1:C:4068:LEU:HD22	1:C:4111:LEU:HD11	1.86	0.58
1:C:4689:THR:OG1	1:C:4690:GLU:N	2.36	0.58
1:D:4068:LEU:HD22	1:D:4111:LEU:HD11	1.86	0.58
1:D:1259:ARG:NH2	1:D:1591:CYS:SG	2.77	0.58
1:D:3288:GLY:HA2	1:D:3303:PRO:HB3	1.85	0.58
1:A:1066:GLN:NE2	1:A:1461:ASP:OD1	2.37	0.58
1:A:1131:ARG:NH1	1:A:1178:ALA:O	2.37	0.58
1:A:3288:GLY:HA2	1:A:3303:PRO:HB3	1.85	0.58
1:B:897:ARG:HB2	1:B:903:LEU:HD11	1.84	0.58
1:B:1131:ARG:NH1	1:B:1178:ALA:O	2.37	0.58
1:C:275:ARG:HH12	1:C:330:ASP:HA	1.67	0.58
1:D:3051:ARG:O	1:D:3053:ARG:NE	2.36	0.58
1:A:317:ARG:NH1	1:A:349:GLN:OE1	2.35	0.58
1:B:3579:LEU:HB2	1:B:3582:ARG:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1259:ARG:NH2	1:C:1591:CYS:SG	2.77	0.58
1:A:882:TRP:O	1:A:886:ARG:NH1	2.37	0.58
1:A:1259:ARG:NH2	1:A:1591:CYS:SG	2.77	0.58
1:A:4068:LEU:HD22	1:A:4111:LEU:HD11	1.86	0.58
1:B:1259:ARG:NH2	1:B:1591:CYS:SG	2.77	0.58
1:C:3288:GLY:HA2	1:C:3303:PRO:HB3	1.85	0.58
1:A:1653:LEU:O	1:A:1660:GLN:NE2	2.32	0.58
1:B:4068:LEU:HD22	1:B:4111:LEU:HD11	1.86	0.58
1:C:882:TRP:O	1:C:886:ARG:NH1	2.37	0.58
1:D:4689:THR:OG1	1:D:4690:GLU:N	2.36	0.58
1:B:1066:GLN:NE2	1:B:1461:ASP:OD1	2.37	0.58
1:B:320:LYS:NZ	1:B:383:HIS:O	2.37	0.57
1:B:3132:THR:HG23	1:B:3136:LEU:HB3	1.86	0.57
1:D:882:TRP:O	1:D:886:ARG:NH1	2.37	0.57
1:D:320:LYS:NZ	1:D:383:HIS:O	2.37	0.57
1:D:3132:THR:HG23	1:D:3136:LEU:HB3	1.86	0.57
1:B:882:TRP:O	1:B:886:ARG:NH1	2.37	0.57
1:A:2095:GLN:HA	1:A:2127:GLN:HE21	1.70	0.57
1:C:320:LYS:NZ	1:C:383:HIS:O	2.37	0.57
1:C:1131:ARG:NH1	1:C:1178:ALA:O	2.37	0.57
1:D:1066:GLN:NE2	1:D:1461:ASP:OD1	2.37	0.57
1:D:2595:LEU:O	1:D:2600:ARG:NH2	2.38	0.57
1:A:320:LYS:NZ	1:A:383:HIS:O	2.37	0.57
1:B:765:GLN:NE2	1:B:1479:GLU:OE1	2.38	0.57
1:D:765:GLN:NE2	1:D:1479:GLU:OE1	2.37	0.57
1:D:2196:ASN:OD1	1:D:2199:ARG:NH2	2.38	0.57
1:C:1066:GLN:NE2	1:C:1461:ASP:OD1	2.37	0.57
1:D:1131:ARG:NH1	1:D:1178:ALA:O	2.37	0.57
1:A:1064:GLU:O	1:A:1071:ARG:NH2	2.32	0.57
1:B:2196:ASN:OD1	1:B:2199:ARG:NH2	2.38	0.57
1:D:867:LEU:HD13	1:D:929:LEU:HB3	1.87	0.57
1:A:867:LEU:HD13	1:A:929:LEU:HB3	1.87	0.57
1:B:39:ALA:HB2	1:B:47:CYS:HA	1.86	0.57
1:C:3132:THR:HG23	1:C:3136:LEU:HB3	1.86	0.57
1:D:2095:GLN:HA	1:D:2127:GLN:HE21	1.70	0.57
1:D:3579:LEU:HB2	1:D:3582:ARG:HG2	1.85	0.57
1:A:3132:THR:HG23	1:A:3136:LEU:HB3	1.86	0.56
1:B:4902:GLU:O	1:B:4913:ARG:NH1	2.38	0.56
1:C:765:GLN:NE2	1:C:1479:GLU:OE1	2.38	0.56
1:C:828:GLU:O	1:C:1073:ARG:NH1	2.38	0.56
1:C:2595:LEU:O	1:C:2600:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:ALA:HB2	1:D:47:CYS:HA	1.86	0.56
1:B:828:GLU:O	1:B:1073:ARG:NH1	2.38	0.56
1:D:828:GLU:O	1:D:1073:ARG:NH1	2.38	0.56
1:A:2196:ASN:OD1	1:A:2199:ARG:NH2	2.38	0.56
1:C:867:LEU:HD13	1:C:929:LEU:HB3	1.87	0.56
1:C:3075:LEU:O	1:C:3146:HIS:NE2	2.38	0.56
1:C:3579:LEU:HB2	1:C:3582:ARG:HG2	1.85	0.56
1:B:2095:GLN:HA	1:B:2127:GLN:HE21	1.70	0.56
1:C:4818:MET:SD	1:C:4818:MET:N	2.78	0.56
1:A:39:ALA:HB2	1:A:47:CYS:HA	1.86	0.56
1:C:39:ALA:HB2	1:C:47:CYS:HA	1.86	0.56
1:C:2196:ASN:OD1	1:C:2199:ARG:NH2	2.38	0.56
1:A:4818:MET:SD	1:A:4818:MET:N	2.78	0.56
1:B:2595:LEU:O	1:B:2600:ARG:NH2	2.38	0.56
1:D:4902:GLU:O	1:D:4913:ARG:NH1	2.38	0.56
2:E:21:THR:HG22	2:E:49:ARG:HD2	1.87	0.56
2:G:21:THR:HG22	2:G:49:ARG:HD2	1.87	0.56
1:A:765:GLN:NE2	1:A:1479:GLU:OE1	2.37	0.56
1:C:688:LEU:HD23	1:C:690:GLU:H	1.71	0.56
1:D:4818:MET:SD	1:D:4818:MET:N	2.78	0.56
1:A:828:GLU:O	1:A:1073:ARG:NH1	2.38	0.56
1:B:3075:LEU:O	1:B:3146:HIS:NE2	2.38	0.56
1:B:3157:ILE:HG22	1:B:3162:GLN:HG2	1.87	0.56
1:D:3157:ILE:HG22	1:D:3162:GLN:HG2	1.87	0.56
1:C:1064:GLU:O	1:C:1071:ARG:NH2	2.32	0.56
1:C:2095:GLN:HA	1:C:2127:GLN:HE21	1.70	0.56
1:C:4902:GLU:O	1:C:4913:ARG:NH1	2.38	0.56
1:B:4818:MET:N	1:B:4818:MET:SD	2.78	0.56
1:A:3157:ILE:HG22	1:A:3162:GLN:HG2	1.87	0.55
1:B:867:LEU:HD13	1:B:929:LEU:HB3	1.87	0.55
1:D:2792:ARG:HB2	1:D:2797:PHE:HD1	1.71	0.55
1:D:3075:LEU:O	1:D:3146:HIS:NE2	2.38	0.55
1:A:3075:LEU:O	1:A:3146:HIS:NE2	2.38	0.55
1:A:3377:GLU:HA	1:A:3380:ARG:HG2	1.88	0.55
1:C:35:LEU:HD13	1:C:49:LEU:HD13	1.88	0.55
1:C:3377:GLU:HA	1:C:3380:ARG:HG2	1.88	0.55
1:D:3377:GLU:HA	1:D:3380:ARG:HG2	1.89	0.55
1:A:688:LEU:HD23	1:A:690:GLU:H	1.71	0.55
1:A:2595:LEU:O	1:A:2600:ARG:NH2	2.38	0.55
1:D:2871:LEU:HG	1:D:2927:LEU:HD21	1.89	0.55
2:H:21:THR:HG22	2:H:49:ARG:HD2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2792:ARG:HB2	1:A:2797:PHE:HD1	1.71	0.55
1:B:3948:LYS:HG2	1:B:4012:LEU:HD22	1.89	0.55
1:B:281:ARG:NH2	1:B:309:THR:OG1	2.40	0.55
1:C:2538:THR:HG23	1:C:2540:THR:H	1.71	0.55
1:B:3377:GLU:HA	1:B:3380:ARG:HG2	1.89	0.55
1:C:2677:LYS:NZ	1:C:2909:ASP:OD2	2.37	0.55
1:A:2871:LEU:HG	1:A:2927:LEU:HD21	1.89	0.55
1:C:3157:ILE:HG22	1:C:3162:GLN:HG2	1.87	0.55
1:D:281:ARG:NH2	1:D:309:THR:OG1	2.40	0.55
1:D:475:GLN:NE2	1:D:528:SER:O	2.40	0.55
1:D:688:LEU:HD23	1:D:690:GLU:H	1.71	0.55
1:C:475:GLN:NE2	1:C:528:SER:O	2.40	0.55
1:C:3948:LYS:HG2	1:C:4012:LEU:HD22	1.89	0.55
1:D:350:HIS:HB2	1:D:378:LEU:HD21	1.89	0.55
2:F:21:THR:HG22	2:F:49:ARG:HD2	1.87	0.55
1:A:475:GLN:NE2	1:A:528:SER:O	2.40	0.54
1:A:2538:THR:HG23	1:A:2540:THR:H	1.71	0.54
1:B:2679:PHE:HB2	1:B:2706:ILE:HG21	1.90	0.54
1:A:35:LEU:HD13	1:A:49:LEU:HD13	1.88	0.54
1:B:688:LEU:HD23	1:B:690:GLU:H	1.70	0.54
1:B:3414:ARG:NH1	1:B:3469:PHE:O	2.38	0.54
1:C:277:GLY:HA2	1:C:315:CYS:HB3	1.90	0.54
1:C:2792:ARG:HB2	1:C:2797:PHE:HD1	1.71	0.54
1:D:2765:LYS:NZ	1:D:2859:PRO:O	2.39	0.54
1:A:281:ARG:NH2	1:A:309:THR:OG1	2.40	0.54
1:A:1175:SER:OG	1:A:1180:ARG:NH2	2.38	0.54
1:A:2679:PHE:HB2	1:A:2706:ILE:HG21	1.89	0.54
1:B:475:GLN:NE2	1:B:528:SER:O	2.40	0.54
1:B:2538:THR:HG23	1:B:2540:THR:H	1.71	0.54
1:C:4904:PRO:HB3	1:C:4913:ARG:HG2	1.89	0.54
1:D:35:LEU:HD13	1:D:49:LEU:HD13	1.88	0.54
1:A:2001:PRO:HG2	1:A:3864:THR:HB	1.90	0.54
1:B:35:LEU:HD13	1:B:49:LEU:HD13	1.88	0.54
1:B:277:GLY:HA2	1:B:315:CYS:HB3	1.90	0.54
1:B:886:ARG:HE	1:B:904:HIS:HB2	1.73	0.54
1:A:350:HIS:HB2	1:A:378:LEU:HD21	1.89	0.54
1:A:3940:LYS:O	1:A:4002:LYS:NZ	2.38	0.54
1:A:4904:PRO:HB3	1:A:4913:ARG:HG2	1.89	0.54
1:B:822:ARG:NH1	1:B:824:GLU:OE1	2.40	0.54
1:C:886:ARG:HE	1:C:904:HIS:HB2	1.73	0.54
1:C:2679:PHE:HB2	1:C:2706:ILE:HG21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:822:ARG:NH1	1:D:824:GLU:OE1	2.40	0.54
1:A:886:ARG:HE	1:A:904:HIS:HB2	1.73	0.54
1:B:2792:ARG:HB2	1:B:2797:PHE:HD1	1.72	0.54
1:C:2001:PRO:HG2	1:C:3864:THR:HB	1.90	0.54
1:D:1792:ALA:O	1:D:2176:ASN:ND2	2.40	0.54
1:D:3533:ILE:HD13	1:D:3596:VAL:HG13	1.90	0.54
1:D:3948:LYS:HG2	1:D:4012:LEU:HD22	1.89	0.54
1:B:1792:ALA:O	1:B:2176:ASN:ND2	2.41	0.54
1:D:886:ARG:HE	1:D:904:HIS:HB2	1.73	0.54
1:D:2679:PHE:HB2	1:D:2706:ILE:HG21	1.90	0.54
1:A:4902:GLU:O	1:A:4913:ARG:NH1	2.38	0.54
1:C:1175:SER:OG	1:C:1180:ARG:NH2	2.38	0.54
1:C:2871:LEU:HG	1:C:2927:LEU:HD21	1.89	0.54
1:C:281:ARG:NH2	1:C:309:THR:OG1	2.40	0.54
1:D:277:GLY:HA2	1:D:315:CYS:HB3	1.89	0.54
1:A:277:GLY:HA2	1:A:315:CYS:HB3	1.89	0.54
1:A:683:ARG:HG2	1:A:717:ASP:HB3	1.90	0.54
1:C:3533:ILE:HD13	1:C:3596:VAL:HG13	1.90	0.54
1:D:3524:MET:O	1:D:3595:ARG:NH1	2.41	0.53
1:A:3376:GLU:OE2	1:A:3450:ASN:ND2	2.40	0.53
1:A:3948:LYS:HG2	1:A:4012:LEU:HD22	1.89	0.53
1:B:350:HIS:HB2	1:B:378:LEU:HD21	1.89	0.53
1:B:683:ARG:HG2	1:B:717:ASP:HB3	1.90	0.53
1:B:2871:LEU:HG	1:B:2927:LEU:HD21	1.89	0.53
1:C:822:ARG:NH1	1:C:824:GLU:OE1	2.40	0.53
1:D:3322:ILE:O	1:D:3326:ASN:ND2	2.39	0.53
1:D:3376:GLU:OE2	1:D:3450:ASN:ND2	2.40	0.53
1:B:2682:ILE:O	1:B:2686:LEU:HB2	2.09	0.53
1:B:3533:ILE:HD13	1:B:3596:VAL:HG13	1.90	0.53
1:B:4952:GLU:O	1:B:4956:THR:HB	2.09	0.53
1:C:3524:MET:O	1:C:3595:ARG:NH1	2.41	0.53
1:D:2677:LYS:NZ	1:D:2909:ASP:OD2	2.37	0.53
1:D:4904:PRO:HB3	1:D:4913:ARG:HG2	1.89	0.53
1:A:3980:LEU:HD23	1:A:3985:LEU:HD22	1.90	0.53
1:B:1175:SER:OG	1:B:1180:ARG:NH2	2.38	0.53
1:C:829:TYR:HB3	1:C:1073:ARG:HH11	1.73	0.53
1:C:1302:ARG:HG3	1:C:1523:ALA:HB1	1.91	0.53
1:C:2682:ILE:O	1:C:2686:LEU:HB2	2.09	0.53
1:B:2971:GLN:HE22	1:B:3045:LYS:HD3	1.74	0.53
1:B:3769:ARG:O	1:B:3773:ARG:NH1	2.42	0.53
1:B:3980:LEU:HD23	1:B:3985:LEU:HD22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4232:GLU:OE2	1:B:5017:ARG:NH2	2.41	0.53
1:C:3376:GLU:OE2	1:C:3450:ASN:ND2	2.40	0.53
1:D:683:ARG:HG2	1:D:717:ASP:HB3	1.90	0.53
1:D:829:TYR:HB3	1:D:1073:ARG:HH11	1.73	0.53
1:D:2001:PRO:HG2	1:D:3864:THR:HB	1.90	0.53
1:D:3980:LEU:HD23	1:D:3985:LEU:HD22	1.90	0.53
1:A:499:THR:HG23	1:A:502:HIS:H	1.74	0.53
1:A:2801:ASP:HA	1:A:2804:ILE:HG12	1.91	0.53
1:B:3322:ILE:O	1:B:3326:ASN:ND2	2.39	0.53
1:B:3524:MET:O	1:B:3595:ARG:NH1	2.41	0.53
1:C:350:HIS:HB2	1:C:378:LEU:HD21	1.89	0.53
1:C:683:ARG:HG2	1:C:717:ASP:HB3	1.91	0.53
1:C:1066:GLN:OE1	1:C:1463:ASN:ND2	2.42	0.53
1:C:3227:ARG:NH1	1:C:3234:ASN:OD1	2.42	0.53
1:D:2971:GLN:HE22	1:D:3045:LYS:HD3	1.74	0.53
1:D:3316:LEU:HD11	1:D:3346:VAL:HA	1.91	0.53
1:A:1302:ARG:HG3	1:A:1523:ALA:HB1	1.91	0.53
1:A:1792:ALA:O	1:A:2176:ASN:ND2	2.40	0.53
1:B:1066:GLN:OE1	1:B:1463:ASN:ND2	2.41	0.53
1:B:1302:ARG:HG3	1:B:1523:ALA:HB1	1.91	0.53
1:B:4904:PRO:HB3	1:B:4913:ARG:HG2	1.89	0.53
1:D:2538:THR:HG23	1:D:2540:THR:H	1.71	0.53
1:D:2682:ILE:O	1:D:2686:LEU:HB2	2.09	0.53
1:D:3017:PHE:O	1:D:3036:LYS:NZ	2.42	0.53
1:D:4952:GLU:O	1:D:4956:THR:HB	2.09	0.53
1:A:822:ARG:NH1	1:A:824:GLU:OE1	2.40	0.53
1:A:3227:ARG:NH1	1:A:3234:ASN:OD1	2.42	0.53
1:A:3524:MET:O	1:A:3595:ARG:NH1	2.41	0.53
1:C:2971:GLN:HE22	1:C:3045:LYS:HD3	1.74	0.53
1:D:3227:ARG:NH1	1:D:3234:ASN:OD1	2.42	0.53
1:A:1066:GLN:OE1	1:A:1463:ASN:ND2	2.41	0.53
1:A:2682:ILE:O	1:A:2686:LEU:HB2	2.09	0.53
1:B:499:THR:HG23	1:B:502:HIS:H	1.74	0.53
1:C:2801:ASP:HA	1:C:2804:ILE:HG12	1.91	0.53
1:C:3316:LEU:HD11	1:C:3346:VAL:HA	1.91	0.53
1:A:2971:GLN:HE22	1:A:3045:LYS:HD3	1.74	0.53
1:A:3533:ILE:HD13	1:A:3596:VAL:HG13	1.90	0.53
1:A:743:VAL:HB	1:A:760:ASN:HA	1.90	0.52
1:A:3316:LEU:HD11	1:A:3346:VAL:HA	1.91	0.52
1:C:3414:ARG:NH1	1:C:3469:PHE:O	2.38	0.52
1:D:1066:GLN:OE1	1:D:1463:ASN:ND2	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2687:ALA:O	1:D:2993:GLN:NE2	2.43	0.52
1:D:4232:GLU:OE2	1:D:5017:ARG:NH2	2.41	0.52
1:A:829:TYR:HB3	1:A:1073:ARG:HH11	1.73	0.52
1:B:3376:GLU:OE2	1:B:3450:ASN:ND2	2.40	0.52
1:D:743:VAL:HB	1:D:760:ASN:HA	1.91	0.52
1:D:2801:ASP:HA	1:D:2804:ILE:HG12	1.91	0.52
1:A:3157:ILE:HA	1:A:3161:VAL:HB	1.92	0.52
1:B:3017:PHE:O	1:B:3036:LYS:NZ	2.42	0.52
1:C:707:VAL:HG23	1:C:782:SER:HB3	1.91	0.52
1:C:3322:ILE:O	1:C:3326:ASN:ND2	2.39	0.52
1:C:3769:ARG:O	1:C:3773:ARG:NH1	2.42	0.52
1:C:3980:LEU:HD23	1:C:3985:LEU:HD22	1.90	0.52
1:D:499:THR:HG23	1:D:502:HIS:H	1.74	0.52
1:D:1302:ARG:HG3	1:D:1523:ALA:HB1	1.91	0.52
1:A:3769:ARG:O	1:A:3773:ARG:NH1	2.42	0.52
1:C:2687:ALA:O	1:C:2993:GLN:NE2	2.43	0.52
1:C:4952:GLU:O	1:C:4956:THR:HB	2.09	0.52
1:D:3769:ARG:O	1:D:3773:ARG:NH1	2.42	0.52
1:A:3017:PHE:O	1:A:3036:LYS:NZ	2.42	0.52
1:B:829:TYR:HB3	1:B:1073:ARG:HH11	1.73	0.52
1:B:2001:PRO:HG2	1:B:3864:THR:HB	1.90	0.52
1:B:2677:LYS:NZ	1:B:2909:ASP:OD2	2.37	0.52
1:C:257:ARG:O	1:C:284:HIS:NE2	2.42	0.52
1:A:939:VAL:HB	1:A:1051:TYR:HB3	1.92	0.52
1:B:2687:ALA:O	1:B:2993:GLN:NE2	2.43	0.52
1:C:4020:GLN:HA	1:C:4023:MET:HB3	1.92	0.52
1:D:450:GLY:HA2	1:D:453:GLU:HG3	1.92	0.52
1:A:450:GLY:HA2	1:A:453:GLU:HG3	1.92	0.52
1:A:2765:LYS:NZ	1:A:2859:PRO:O	2.39	0.52
1:A:3322:ILE:O	1:A:3326:ASN:ND2	2.39	0.52
1:A:3414:ARG:NH1	1:A:3469:PHE:O	2.39	0.52
1:B:4020:GLN:HA	1:B:4023:MET:HB3	1.92	0.52
1:C:1792:ALA:O	1:C:2176:ASN:ND2	2.40	0.52
1:D:939:VAL:HB	1:D:1051:TYR:HB3	1.92	0.52
1:D:3835:LEU:HD22	1:D:3880:PHE:HZ	1.75	0.52
1:A:4020:GLN:HA	1:A:4023:MET:HB3	1.92	0.52
1:B:3227:ARG:NH1	1:B:3234:ASN:OD1	2.42	0.52
1:C:499:THR:HG23	1:C:502:HIS:H	1.74	0.52
1:C:3017:PHE:O	1:C:3036:LYS:NZ	2.42	0.52
1:D:3940:LYS:O	1:D:4002:LYS:NZ	2.38	0.52
2:F:27:THR:HB	2:F:100:ASP:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:27:THR:HB	2:H:100:ASP:HB3	1.91	0.52
1:A:4917:ASP:OD2	1:D:4888:TYR:OH	2.18	0.52
1:C:743:VAL:HB	1:C:760:ASN:HA	1.91	0.52
1:C:4112:LEU:O	1:C:4115:SER:OG	2.28	0.52
1:D:1175:SER:OG	1:D:1180:ARG:NH2	2.38	0.52
1:D:3157:ILE:HA	1:D:3161:VAL:HB	1.92	0.52
1:A:4952:GLU:O	1:A:4956:THR:HB	2.09	0.51
1:B:743:VAL:HB	1:B:760:ASN:HA	1.91	0.51
1:B:2801:ASP:HA	1:B:2804:ILE:HG12	1.91	0.51
1:B:3316:LEU:HD11	1:B:3346:VAL:HA	1.91	0.51
1:D:2640:PRO:HA	1:D:2643:LEU:HB3	1.92	0.51
1:D:3368:ARG:NH2	1:D:3404:ASP:OD2	2.43	0.51
1:A:2687:ALA:O	1:A:2993:GLN:NE2	2.43	0.51
1:A:3368:ARG:NH2	1:A:3404:ASP:OD2	2.43	0.51
1:C:450:GLY:HA2	1:C:453:GLU:HG3	1.92	0.51
1:C:1248:VAL:HG22	1:C:1599:MET:HG3	1.93	0.51
2:G:27:THR:HB	2:G:100:ASP:HB3	1.91	0.51
1:A:707:VAL:HG23	1:A:782:SER:HB3	1.91	0.51
1:A:3835:LEU:HD22	1:A:3880:PHE:HZ	1.75	0.51
1:B:3114:LYS:HD3	1:B:3116:SER:H	1.76	0.51
1:B:3368:ARG:NH2	1:B:3404:ASP:OD2	2.43	0.51
1:D:4020:GLN:HA	1:D:4023:MET:HB3	1.92	0.51
1:A:2640:PRO:HA	1:A:2643:LEU:HB3	1.93	0.51
1:B:2640:PRO:HA	1:B:2643:LEU:HB3	1.93	0.51
1:B:3157:ILE:HA	1:B:3161:VAL:HB	1.92	0.51
1:C:2640:PRO:HA	1:C:2643:LEU:HB3	1.92	0.51
1:D:707:VAL:HG23	1:D:782:SER:HB3	1.92	0.51
1:A:3114:LYS:HD3	1:A:3116:SER:H	1.76	0.51
1:B:939:VAL:HB	1:B:1051:TYR:HB3	1.92	0.51
1:C:3157:ILE:HA	1:C:3161:VAL:HB	1.92	0.51
1:C:3368:ARG:NH2	1:C:3404:ASP:OD2	2.43	0.51
1:C:3835:LEU:HD22	1:C:3880:PHE:HZ	1.75	0.51
1:D:4242:ILE:HG12	1:D:4993:MET:HB3	1.93	0.51
1:D:4866:SER:HB2	1:D:4873:ASP:H	1.75	0.51
1:B:3835:LEU:HD22	1:B:3880:PHE:HZ	1.75	0.51
1:A:2369[A]:ARG:HH21	1:A:2373:GLY:HA2	1.75	0.51
1:A:4680:LYS:HE3	1:A:4686:LEU:HD22	1.93	0.51
1:B:274:LEU:HB3	1:B:339:ILE:HD12	1.93	0.51
1:B:4680:LYS:HE3	1:B:4686:LEU:HD22	1.93	0.51
1:A:546:TRP:CE2	1:A:550:LYS:HE2	2.46	0.51
1:A:4866:SER:HB2	1:A:4873:ASP:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:GLY:HA2	1:B:453:GLU:HG3	1.92	0.51
1:B:707:VAL:HG23	1:B:782:SER:HB3	1.92	0.51
1:B:1248:VAL:HG22	1:B:1599:MET:HG3	1.93	0.51
1:B:4866:SER:HB2	1:B:4873:ASP:H	1.76	0.51
1:D:2369[A]:ARG:HH21	1:D:2373:GLY:HA2	1.75	0.51
1:D:2917:ALA:HA	1:D:2920:ARG:HB3	1.92	0.51
1:B:546:TRP:CE2	1:B:550:LYS:HE2	2.46	0.51
1:C:546:TRP:CE2	1:C:550:LYS:HE2	2.46	0.51
1:C:2369[A]:ARG:HH21	1:C:2373:GLY:HA2	1.75	0.51
1:D:3114:LYS:HD3	1:D:3116:SER:H	1.75	0.51
1:D:3959:LYS:NZ	1:D:4022:ASP:OD2	2.43	0.51
1:A:4242:ILE:HG12	1:A:4993:MET:HB3	1.93	0.51
1:B:4112:LEU:O	1:B:4115:SER:OG	2.28	0.51
1:D:1248:VAL:HG22	1:D:1599:MET:HG3	1.93	0.51
1:A:1990:GLU:HG2	1:A:1994:ARG:HH12	1.76	0.50
1:A:2917:ALA:HA	1:A:2920:ARG:HB3	1.92	0.50
1:C:939:VAL:HB	1:C:1051:TYR:HB3	1.92	0.50
2:E:27:THR:HB	2:E:100:ASP:HB3	1.91	0.50
1:A:274:LEU:HB3	1:A:339:ILE:HD12	1.93	0.50
1:B:1578:ALA:O	1:B:1584:ARG:NH2	2.37	0.50
1:B:2369[A]:ARG:HH21	1:B:2373:GLY:HA2	1.75	0.50
1:C:3114:LYS:HD3	1:C:3116:SER:H	1.75	0.50
1:C:4106:PRO:O	1:C:4110:PHE:HB3	2.11	0.50
1:C:4866:SER:HB2	1:C:4873:ASP:H	1.75	0.50
1:D:546:TRP:CE2	1:D:550:LYS:HE2	2.46	0.50
1:D:1270:LEU:HB2	1:D:1564:PHE:HB2	1.93	0.50
1:A:3159:ASP:OD1	1:A:3159:ASP:N	2.44	0.50
1:A:3523:ASN:OD1	1:A:3582:ARG:NH2	2.44	0.50
1:A:3545:THR:HG22	1:A:3548:GLU:HG3	1.93	0.50
1:A:3695:PRO:HB2	1:A:3700:GLN:HG3	1.94	0.50
1:A:4106:PRO:O	1:A:4110:PHE:HB3	2.11	0.50
1:B:1270:LEU:HB2	1:B:1564:PHE:HB2	1.94	0.50
1:B:403:MET:O	1:B:407:THR:OG1	2.26	0.50
1:C:1270:LEU:HB2	1:C:1564:PHE:HB2	1.94	0.50
1:C:4242:ILE:HG12	1:C:4993:MET:HB3	1.93	0.50
1:D:2930:LEU:HB3	1:D:2935:TYR:HB2	1.93	0.50
1:A:3959:LYS:NZ	1:A:4022:ASP:OD2	2.43	0.50
1:C:4232:GLU:OE2	1:C:5017:ARG:NH2	2.41	0.50
1:D:1969:LEU:HD21	1:D:2009:LEU:HD13	1.94	0.50
1:A:4562:LEU:HD22	1:A:4653:VAL:HG13	1.94	0.50
1:B:2869:ARG:NH2	1:B:2870[B]:GLU:OE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2917:ALA:HA	1:B:2920:ARG:HB3	1.92	0.50
1:B:3545:THR:HG22	1:B:3548:GLU:HG3	1.93	0.50
1:C:1260:MET:HB2	1:C:1269:CYS:HB2	1.94	0.50
1:C:3523:ASN:OD1	1:C:3582:ARG:NH2	2.44	0.50
1:A:1270:LEU:HB2	1:A:1564:PHE:HB2	1.93	0.50
1:B:1260:MET:HB2	1:B:1269:CYS:HB2	1.94	0.50
1:B:3695:PRO:HB2	1:B:3700:GLN:HG3	1.94	0.50
1:B:3959:LYS:NZ	1:B:4022:ASP:OD2	2.43	0.50
1:C:3695:PRO:HB2	1:C:3700:GLN:HG3	1.94	0.50
1:C:4562:LEU:HD22	1:C:4653:VAL:HG13	1.94	0.50
1:D:2869:ARG:NH2	1:D:2870[B]:GLU:OE2	2.45	0.50
1:D:3523:ASN:OD1	1:D:3582:ARG:NH2	2.44	0.50
1:D:3695:PRO:HB2	1:D:3700:GLN:HG3	1.94	0.50
1:D:4106:PRO:O	1:D:4110:PHE:HB3	2.11	0.50
1:A:1578:ALA:O	1:A:1584:ARG:NH2	2.37	0.50
1:A:2930:LEU:HB3	1:A:2935:TYR:HB2	1.93	0.50
1:B:4562:LEU:HD22	1:B:4653:VAL:HG13	1.94	0.50
1:C:1969:LEU:HD21	1:C:2009:LEU:HD13	1.94	0.50
1:C:3371:LYS:NZ	1:C:3375:GLU:OE2	2.42	0.50
1:D:4680:LYS:HE3	1:D:4686:LEU:HD22	1.93	0.50
1:A:1248:VAL:HG22	1:A:1599:MET:HG3	1.93	0.50
1:A:2677:LYS:NZ	1:A:2909:ASP:OD2	2.37	0.50
1:A:4232:GLU:OE2	1:A:5017:ARG:NH2	2.41	0.50
1:B:257:ARG:O	1:B:284:HIS:NE2	2.42	0.50
1:B:1969:LEU:HD21	1:B:2009:LEU:HD13	1.94	0.50
1:C:2869:ARG:NH2	1:C:2870[B]:GLU:OE2	2.45	0.50
1:C:2917:ALA:HA	1:C:2920:ARG:HB3	1.92	0.50
1:D:1990:GLU:HG2	1:D:1994:ARG:HH12	1.76	0.50
1:D:3545:THR:HG22	1:D:3548:GLU:HG3	1.93	0.50
1:D:4562:LEU:HD22	1:D:4653:VAL:HG13	1.94	0.50
1:A:551:LEU:HB3	1:A:589:LEU:HD11	1.94	0.49
1:A:618:GLN:OE1	1:A:1678:ASN:ND2	2.40	0.49
1:A:3236:VAL:HA	1:A:3239:MET:HG2	1.94	0.49
1:B:870:ILE:HG13	1:B:874:LEU:HD23	1.94	0.49
1:B:3236:VAL:HA	1:B:3239:MET:HG2	1.94	0.49
1:B:3523:ASN:OD1	1:B:3582:ARG:NH2	2.44	0.49
1:A:2310:CYS:HB3	1:A:2313:LEU:HB2	1.94	0.49
1:B:4106:PRO:O	1:B:4110:PHE:HB3	2.11	0.49
1:C:1093:GLU:HB3	1:C:1201:HIS:HB3	1.94	0.49
1:C:3545:THR:HG22	1:C:3548:GLU:HG3	1.93	0.49
1:D:1260:MET:HB2	1:D:1269:CYS:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1969:LEU:HD21	1:A:2009:LEU:HD13	1.94	0.49
1:A:2869:ARG:NH2	1:A:2870[B]:GLU:OE2	2.45	0.49
1:A:2960:LEU:HD23	1:A:2963:LEU:HD12	1.95	0.49
1:B:1093:GLU:HB3	1:B:1201:HIS:HB3	1.94	0.49
1:B:3159:ASP:OD1	1:B:3159:ASP:N	2.44	0.49
1:B:4242:ILE:HG12	1:B:4993:MET:HB3	1.93	0.49
1:C:2724:GLU:OE1	1:C:2738:ARG:NH2	2.46	0.49
1:C:2930:LEU:HB3	1:C:2935:TYR:HB2	1.93	0.49
1:D:2310:CYS:HB3	1:D:2313:LEU:HB2	1.94	0.49
1:A:2527:LEU:HD13	1:A:2582:MET:HG2	1.95	0.49
1:A:3371:LYS:NZ	1:A:3375:GLU:OE2	2.42	0.49
1:A:4630:TYR:OH	1:B:4860:ARG:NH2	2.42	0.49
1:B:475:GLN:OE1	1:B:533:ASN:ND2	2.46	0.49
1:B:2930:LEU:HB3	1:B:2935:TYR:HB2	1.93	0.49
1:C:274:LEU:HB3	1:C:339:ILE:HD12	1.93	0.49
1:C:3959:LYS:NZ	1:C:4022:ASP:OD2	2.43	0.49
1:D:274:LEU:HB3	1:D:339:ILE:HD12	1.93	0.49
1:D:3236:VAL:HA	1:D:3239:MET:HG2	1.94	0.49
1:A:870:ILE:HG13	1:A:874:LEU:HD23	1.94	0.49
1:A:1260:MET:HB2	1:A:1269:CYS:HB2	1.94	0.49
1:B:2527:LEU:HD13	1:B:2582:MET:HG2	1.95	0.49
1:D:2724:GLU:OE1	1:D:2738:ARG:NH2	2.46	0.49
1:B:1990:GLU:HG2	1:B:1994:ARG:HH12	1.76	0.49
1:B:2724:GLU:OE1	1:B:2738:ARG:NH2	2.46	0.49
1:B:2769:ASP:O	1:B:2773:ASN:HB2	2.13	0.49
1:C:475:GLN:OE1	1:C:533:ASN:ND2	2.46	0.49
1:C:2960:LEU:HD23	1:C:2963:LEU:HD12	1.95	0.49
1:A:932:LEU:HB3	1:A:937:CYS:HB3	1.95	0.49
1:B:2960:LEU:HD23	1:B:2963:LEU:HD12	1.95	0.49
1:A:1093:GLU:HB3	1:A:1201:HIS:HB3	1.94	0.49
1:A:2927:LEU:HD12	1:A:2930:LEU:HD12	1.95	0.49
1:B:551:LEU:HB3	1:B:589:LEU:HD11	1.94	0.49
1:C:3940:LYS:O	1:C:4002:LYS:NZ	2.38	0.49
1:C:4725:LEU:HA	1:C:4737:ILE:HG21	1.95	0.49
1:D:551:LEU:HB3	1:D:589:LEU:HD11	1.95	0.49
1:B:932:LEU:HB3	1:B:937:CYS:HB3	1.95	0.49
1:C:4680:LYS:HE3	1:C:4686:LEU:HD22	1.93	0.49
1:D:2891:LYS:HA	1:D:2894:LEU:HB3	1.95	0.49
1:D:3371:LYS:NZ	1:D:3375:GLU:OE2	2.42	0.49
1:A:475:GLN:OE1	1:A:533:ASN:ND2	2.46	0.49
1:B:3103:ILE:HG21	1:B:3168:THR:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2960:LEU:HD23	1:D:2963:LEU:HD12	1.95	0.49
1:A:1171:SER:OG	1:A:1175:SER:O	2.24	0.48
1:B:3164:SER:HA	1:B:3167:ARG:HE	1.78	0.48
1:C:1171:SER:OG	1:C:1175:SER:O	2.24	0.48
1:C:1990:GLU:HG2	1:C:1994:ARG:HH12	1.77	0.48
1:C:3103:ILE:HG21	1:C:3168:THR:HG23	1.95	0.48
1:C:3236:VAL:HA	1:C:3239:MET:HG2	1.94	0.48
1:D:358:THR:HG21	1:D:383:HIS:H	1.78	0.48
1:D:932:LEU:HB3	1:D:937:CYS:HB3	1.95	0.48
1:D:3414:ARG:NH1	1:D:3469:PHE:O	2.38	0.48
1:A:358:THR:HG21	1:A:383:HIS:H	1.78	0.48
1:A:818:ARG:NH2	1:A:1025:ARG:O	2.47	0.48
1:A:3218:VAL:O	1:A:3222:LYS:HB2	2.13	0.48
1:B:1698:LEU:HD21	1:B:1715:LEU:HD13	1.95	0.48
1:B:2310:CYS:HB3	1:B:2313:LEU:HB2	1.94	0.48
1:C:870:ILE:HG13	1:C:874:LEU:HD23	1.94	0.48
1:C:2527:LEU:HD13	1:C:2582:MET:HG2	1.95	0.48
1:D:1698:LEU:HD21	1:D:1715:LEU:HD13	1.96	0.48
1:D:2527:LEU:HD13	1:D:2582:MET:HG2	1.95	0.48
1:D:2707:ALA:HB1	1:D:3009:TYR:HD1	1.78	0.48
1:D:3218:VAL:O	1:D:3222:LYS:HB2	2.12	0.48
2:E:77:THR:HG22	2:E:79:ASP:H	1.79	0.48
1:A:2891:LYS:HA	1:A:2894:LEU:HB3	1.95	0.48
1:A:3037:GLU:HB3	1:A:3088:VAL:HG21	1.95	0.48
1:A:4112:LEU:O	1:A:4115:SER:OG	2.28	0.48
1:B:358:THR:HG21	1:B:383:HIS:H	1.78	0.48
1:B:818:ARG:NH2	1:B:1025:ARG:O	2.47	0.48
1:B:1076:ARG:HB3	1:B:1191:VAL:HG23	1.96	0.48
1:B:1448:VAL:HG22	1:B:1554:VAL:HG23	1.95	0.48
1:C:358:THR:HG21	1:C:383:HIS:H	1.78	0.48
1:D:475:GLN:OE1	1:D:533:ASN:ND2	2.46	0.48
1:D:1093:GLU:HB3	1:D:1201:HIS:HB3	1.94	0.48
1:A:1076:ARG:HB3	1:A:1191:VAL:HG23	1.96	0.48
1:A:2769:ASP:O	1:A:2773:ASN:HB2	2.13	0.48
1:C:932:LEU:HB3	1:C:937:CYS:HB3	1.95	0.48
1:C:1698:LEU:HD21	1:C:1715:LEU:HD13	1.95	0.48
1:C:1743[A]:ARG:HE	1:C:1743[A]:ARG:HB2	1.49	0.48
1:C:2891:LYS:HA	1:C:2894:LEU:HB3	1.95	0.48
1:C:3164:SER:HA	1:C:3167:ARG:HE	1.79	0.48
1:C:3218:VAL:O	1:C:3222:LYS:HB2	2.13	0.48
1:D:257:ARG:O	1:D:284:HIS:NE2	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1099:GLU:OE2	1:A:1125:ASN:ND2	2.43	0.48
1:A:2724:GLU:OE1	1:A:2738:ARG:NH2	2.46	0.48
1:B:23:GLN:OE1	1:B:203:ASN:ND2	2.47	0.48
1:C:3840:SER:OG	1:C:3877:ASP:OD1	2.26	0.48
1:D:2927:LEU:HD12	1:D:2930:LEU:HD12	1.95	0.48
1:D:3159:ASP:OD1	1:D:3159:ASP:N	2.44	0.48
2:F:77:THR:HG22	2:F:79:ASP:H	1.78	0.48
2:H:77:THR:HG22	2:H:79:ASP:H	1.79	0.48
1:A:2516:ASP:OD1	1:A:2516:ASP:N	2.46	0.48
1:A:3164:SER:HA	1:A:3167:ARG:HE	1.79	0.48
1:B:1171:SER:OG	1:B:1175:SER:O	2.24	0.48
1:B:2765:LYS:NZ	1:B:2859:PRO:O	2.39	0.48
1:B:3218:VAL:O	1:B:3222:LYS:HB2	2.13	0.48
1:B:4018:ASP:HA	1:B:4021:LYS:HB3	1.96	0.48
1:C:551:LEU:HB3	1:C:589:LEU:HD11	1.95	0.48
1:C:2310:CYS:HB3	1:C:2313:LEU:HB2	1.94	0.48
1:C:2707:ALA:HB1	1:C:3009:TYR:HD1	1.78	0.48
1:D:23:GLN:OE1	1:D:203:ASN:ND2	2.47	0.48
1:D:1076:ARG:HB3	1:D:1191:VAL:HG23	1.95	0.48
1:A:1698:LEU:HD21	1:A:1715:LEU:HD13	1.95	0.48
1:B:2927:LEU:HD12	1:B:2930:LEU:HD12	1.95	0.48
1:C:1076:ARG:HB3	1:C:1191:VAL:HG23	1.96	0.48
1:C:3596:VAL:O	1:C:3600:SER:OG	2.21	0.48
1:D:2769:ASP:O	1:D:2773:ASN:HB2	2.13	0.48
1:D:4725:LEU:HA	1:D:4737:ILE:HG21	1.95	0.48
2:F:62:GLY:HA3	2:F:74:LEU:HD21	1.96	0.48
1:A:2739:PRO:HG3	1:A:2888:ARG:HG2	1.96	0.48
1:B:3371:LYS:NZ	1:B:3375:GLU:OE2	2.42	0.48
1:C:2769:ASP:O	1:C:2773:ASN:HB2	2.13	0.48
1:D:1448:VAL:HG22	1:D:1554:VAL:HG23	1.95	0.48
1:D:2516:ASP:OD1	1:D:2516:ASP:N	2.46	0.48
2:G:62:GLY:HA3	2:G:74:LEU:HD21	1.96	0.48
1:A:1653:LEU:HD23	1:A:1660:GLN:HA	1.96	0.48
1:B:2739:PRO:HG3	1:B:2888:ARG:HG2	1.96	0.48
1:C:2739:PRO:HG3	1:C:2888:ARG:HG2	1.96	0.48
1:C:4018:ASP:HA	1:C:4021:LYS:HB3	1.96	0.48
1:D:233:ILE:HD12	1:D:242:ARG:HB3	1.96	0.48
1:D:1171:SER:OG	1:D:1175:SER:O	2.24	0.48
1:D:3037:GLU:HB3	1:D:3088:VAL:HG21	1.95	0.48
1:D:3164:SER:HA	1:D:3167:ARG:HE	1.79	0.48
1:A:3596:VAL:O	1:A:3600:SER:OG	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:GLN:OE1	1:C:203:ASN:ND2	2.47	0.48
1:C:818:ARG:NH2	1:C:1025:ARG:O	2.47	0.48
1:C:1448:VAL:HG22	1:C:1554:VAL:HG23	1.95	0.48
1:D:818:ARG:NH2	1:D:1025:ARG:O	2.47	0.48
1:D:875:ALA:O	1:D:879:HIS:ND1	2.47	0.48
1:D:1653:LEU:HD23	1:D:1660:GLN:HA	1.96	0.48
1:D:3103:ILE:HG21	1:D:3168:THR:HG23	1.95	0.48
1:A:2576:ALA:HB1	1:A:2618:MET:HG2	1.96	0.47
1:A:2707:ALA:HB1	1:A:3009:TYR:HD1	1.78	0.47
1:A:3110:LEU:O	1:A:3180:ASN:ND2	2.47	0.47
1:A:4725:LEU:HA	1:A:4737:ILE:HG21	1.95	0.47
1:B:618:GLN:OE1	1:B:1678:ASN:ND2	2.40	0.47
1:C:1653:LEU:HD23	1:C:1660:GLN:HA	1.95	0.47
1:D:2576:ALA:HB1	1:D:2618:MET:HG2	1.96	0.47
2:G:77:THR:HG22	2:G:79:ASP:H	1.78	0.47
1:A:23:GLN:OE1	1:A:203:ASN:ND2	2.47	0.47
1:A:1448:VAL:HG22	1:A:1554:VAL:HG23	1.95	0.47
1:A:3354:LEU:HA	1:A:3358:PHE:HB2	1.96	0.47
1:B:4725:LEU:HA	1:B:4737:ILE:HG21	1.95	0.47
1:C:3622:LYS:HB2	1:C:3626:LYS:HG2	1.96	0.47
1:D:870:ILE:HG13	1:D:874:LEU:HD23	1.94	0.47
1:D:3354:LEU:HA	1:D:3358:PHE:HB2	1.96	0.47
2:E:62:GLY:HA3	2:E:74:LEU:HD21	1.96	0.47
1:A:233:ILE:HD12	1:A:242:ARG:HB3	1.96	0.47
1:A:257:ARG:O	1:A:284:HIS:NE2	2.42	0.47
1:A:3103:ILE:HG21	1:A:3168:THR:HG23	1.95	0.47
1:B:3007:ASN:O	1:B:3011:THR:OG1	2.22	0.47
1:C:875:ALA:O	1:C:879:HIS:ND1	2.47	0.47
1:D:4112:LEU:O	1:D:4115:SER:OG	2.28	0.47
1:A:4018:ASP:HA	1:A:4021:LYS:HB3	1.96	0.47
1:B:875:ALA:O	1:B:879:HIS:ND1	2.47	0.47
1:B:2891:LYS:HA	1:B:2894:LEU:HB3	1.95	0.47
1:B:3110:LEU:O	1:B:3180:ASN:ND2	2.47	0.47
1:C:2677:LYS:HE2	1:C:2677:LYS:HB3	1.67	0.47
1:C:3110:LEU:O	1:C:3180:ASN:ND2	2.47	0.47
1:D:1099:GLU:OE2	1:D:1125:ASN:ND2	2.43	0.47
1:A:3622:LYS:HB2	1:A:3626:LYS:HG2	1.96	0.47
1:B:884:LEU:HB2	1:B:969:PRO:HD3	1.97	0.47
1:C:355:LEU:HD22	1:C:380:GLN:HA	1.97	0.47
1:B:355:LEU:HD22	1:B:380:GLN:HA	1.97	0.47
1:B:2576:ALA:HB1	1:B:2618:MET:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2707:ALA:HB1	1:B:3009:TYR:HD1	1.78	0.47
1:B:3037:GLU:HB3	1:B:3088:VAL:HG21	1.95	0.47
1:B:3271:GLU:OE2	1:B:3337:ARG:NH2	2.44	0.47
1:B:3354:LEU:HA	1:B:3358:PHE:HB2	1.96	0.47
1:C:2927:LEU:HD12	1:C:2930:LEU:HD12	1.95	0.47
1:C:3354:LEU:HA	1:C:3358:PHE:HB2	1.96	0.47
1:D:1147:ASP:HB3	1:D:1164:LEU:HD11	1.96	0.47
1:D:1698:LEU:HA	1:D:1712:TYR:HE1	1.80	0.47
1:D:4018:ASP:HA	1:D:4021:LYS:HB3	1.96	0.47
1:A:355:LEU:HD22	1:A:380:GLN:HA	1.97	0.47
1:A:710:ASP:OD1	1:A:710:ASP:N	2.48	0.47
1:A:728:ARG:NH2	1:A:1489:CYS:SG	2.88	0.47
1:A:2018:GLU:OE1	1:A:2028:ARG:NH1	2.48	0.47
1:B:1256:GLU:HB3	1:B:1275:ARG:HD2	1.97	0.47
1:B:4965:SER:O	1:B:4969:ASP:HB2	2.15	0.47
1:C:2021:CYS:O	1:C:2028:ARG:NH2	2.48	0.47
1:C:2474:LEU:HD13	1:C:2550:LEU:HD21	1.96	0.47
1:C:3592:ILE:HG22	1:C:3595:ARG:HH21	1.80	0.47
1:D:2018:GLU:OE1	1:D:2028:ARG:NH1	2.48	0.47
1:D:2739:PRO:HG3	1:D:2888:ARG:HG2	1.96	0.47
1:D:3622:LYS:HB2	1:D:3626:LYS:HG2	1.96	0.47
1:A:1147:ASP:HB3	1:A:1164:LEU:HD11	1.96	0.47
1:A:2159:LEU:HG	1:A:2163:ARG:HE	1.80	0.47
1:B:1147:ASP:HB3	1:B:1164:LEU:HD11	1.96	0.47
1:B:1653:LEU:HD23	1:B:1660:GLN:HA	1.96	0.47
1:B:2474:LEU:HD13	1:B:2550:LEU:HD21	1.96	0.47
1:C:728:ARG:NH2	1:C:1489:CYS:SG	2.88	0.47
1:D:728:ARG:NH2	1:D:1489:CYS:SG	2.88	0.47
1:D:2474:LEU:HD13	1:D:2550:LEU:HD21	1.96	0.47
1:D:2677:LYS:HE2	1:D:2677:LYS:HB3	1.67	0.47
1:A:875:ALA:O	1:A:879:HIS:ND1	2.47	0.47
1:B:233:ILE:O	1:B:257:ARG:NH2	2.48	0.47
1:B:2764:GLU:HG3	1:B:2857:PRO:HB3	1.97	0.47
1:B:3622:LYS:HB2	1:B:3626:LYS:HG2	1.96	0.47
1:C:355:LEU:HB2	1:C:378:LEU:HG	1.97	0.47
1:C:2018:GLU:OE1	1:C:2028:ARG:NH1	2.48	0.47
1:C:3037:GLU:HB3	1:C:3088:VAL:HG21	1.95	0.47
1:C:3159:ASP:OD1	1:C:3159:ASP:N	2.44	0.47
1:D:355:LEU:HD22	1:D:380:GLN:HA	1.97	0.47
2:H:62:GLY:HA3	2:H:74:LEU:HD21	1.96	0.47
1:A:1698:LEU:HA	1:A:1712:TYR:HE1	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1743[A]:ARG:HE	1:A:1743[A]:ARG:HB2	1.49	0.47
1:A:2021:CYS:O	1:A:2028:ARG:NH2	2.48	0.47
1:B:1698:LEU:HA	1:B:1712:TYR:HE1	1.80	0.47
1:B:3592:ILE:HG22	1:B:3595:ARG:HH21	1.80	0.47
1:C:1099:GLU:OE2	1:C:1125:ASN:ND2	2.43	0.47
1:D:2021:CYS:O	1:D:2028:ARG:NH2	2.48	0.47
1:D:2768:PHE:HA	1:D:2771:ILE:HG22	1.97	0.47
1:A:1084:GLN:NE2	1:A:1186:ASP:O	2.42	0.46
1:B:1099:GLU:OE2	1:B:1125:ASN:ND2	2.43	0.46
1:B:3329:ILE:O	1:B:3403:ARG:NH2	2.48	0.46
1:B:3840:SER:OG	1:B:3877:ASP:OD1	2.26	0.46
1:C:2764:GLU:HG3	1:C:2857:PRO:HB3	1.97	0.46
1:D:710:ASP:OD1	1:D:710:ASP:N	2.48	0.46
1:D:1297:PHE:HD1	1:D:1522:LEU:HA	1.80	0.46
1:D:2159:LEU:HG	1:D:2163:ARG:HE	1.80	0.46
1:A:1256:GLU:HB3	1:A:1275:ARG:HD2	1.97	0.46
1:B:233:ILE:HD12	1:B:242:ARG:HB3	1.96	0.46
1:B:3264:THR:OG1	1:B:3265:GLU:OE1	2.33	0.46
1:B:3940:LYS:O	1:B:4002:LYS:NZ	2.38	0.46
1:C:233:ILE:HD12	1:C:242:ARG:HB3	1.96	0.46
1:C:1698:LEU:HA	1:C:1712:TYR:HE1	1.80	0.46
1:C:2159:LEU:HG	1:C:2163:ARG:HE	1.80	0.46
1:C:2576:ALA:HB1	1:C:2618:MET:HG2	1.96	0.46
1:D:3110:LEU:O	1:D:3180:ASN:ND2	2.47	0.46
1:A:4965:SER:O	1:A:4969:ASP:HB2	2.15	0.46
1:A:4971:THR:HG22	1:A:4972:PRO:HD2	1.98	0.46
1:B:355:LEU:HB2	1:B:378:LEU:HG	1.97	0.46
1:B:4823:LEU:HD23	1:B:4823:LEU:HA	1.83	0.46
1:C:1968:LYS:NZ	1:C:2030:ASP:OD2	2.49	0.46
1:C:4065:PHE:O	1:C:4133:GLN:NE2	2.49	0.46
1:D:2765:LYS:HA	1:D:2765:LYS:HD3	1.76	0.46
1:A:884:LEU:HB2	1:A:969:PRO:HD3	1.97	0.46
1:A:1968:LYS:NZ	1:A:2030:ASP:OD2	2.49	0.46
1:A:2768:PHE:HA	1:A:2771:ILE:HG22	1.97	0.46
1:B:2021:CYS:O	1:B:2028:ARG:NH2	2.48	0.46
1:C:618:GLN:OE1	1:C:1678:ASN:ND2	2.40	0.46
1:C:1297:PHE:HD1	1:C:1522:LEU:HA	1.80	0.46
1:C:2684:ASP:O	1:C:2688:HIS:ND1	2.46	0.46
1:C:2765:LYS:NZ	1:C:2859:PRO:O	2.39	0.46
1:D:659:TYR:O	1:D:662:TRP:NE1	2.49	0.46
1:D:4065:PHE:O	1:D:4133:GLN:NE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:GLU:HA	1:A:871:ARG:HB2	1.98	0.46
1:A:2863:SER:HA	1:A:2928:LYS:HG3	1.98	0.46
1:A:4736:ARG:HE	1:A:4736:ARG:HB3	1.58	0.46
1:B:2863:SER:HA	1:B:2928:LYS:HG3	1.98	0.46
1:C:659:TYR:O	1:C:662:TRP:NE1	2.49	0.46
1:C:884:LEU:HB2	1:C:969:PRO:HD3	1.97	0.46
1:C:3180:ASN:HB2	1:C:3183:VAL:HG23	1.97	0.46
1:D:355:LEU:HB2	1:D:378:LEU:HG	1.97	0.46
1:D:868:GLU:HA	1:D:871:ARG:HB2	1.98	0.46
1:D:3840:SER:OG	1:D:3877:ASP:OD1	2.26	0.46
1:B:728:ARG:NH2	1:B:1489:CYS:SG	2.88	0.46
1:B:2018:GLU:OE1	1:B:2028:ARG:NH1	2.48	0.46
1:B:4065:PHE:O	1:B:4133:GLN:NE2	2.49	0.46
1:B:4971:THR:HG22	1:B:4972:PRO:HD2	1.98	0.46
1:C:1147:ASP:HB3	1:C:1164:LEU:HD11	1.96	0.46
1:D:2740:VAL:HG21	1:D:2819:TRP:HE1	1.81	0.46
1:A:355:LEU:HB2	1:A:378:LEU:HG	1.97	0.46
1:A:2684:ASP:O	1:A:2688:HIS:ND1	2.46	0.46
1:A:3592:ILE:HG22	1:A:3595:ARG:HH21	1.80	0.46
1:B:2684:ASP:O	1:B:2688:HIS:ND1	2.46	0.46
1:C:357:LEU:HD11	1:C:388:LEU:HD11	1.98	0.46
1:D:1968:LYS:NZ	1:D:2030:ASP:OD2	2.49	0.46
1:D:2764:GLU:HG3	1:D:2857:PRO:HB3	1.97	0.46
1:D:3592:ILE:HG22	1:D:3595:ARG:HH21	1.80	0.46
1:A:3180:ASN:HB2	1:A:3183:VAL:HG23	1.97	0.46
1:D:1232:ARG:NH2	1:D:1828:ASP:O	2.37	0.46
1:D:2863:SER:HA	1:D:2928:LYS:HG3	1.98	0.46
1:A:3840:SER:OG	1:A:3877:ASP:OD1	2.26	0.46
1:A:4049:VAL:HA	1:A:4163:PHE:HZ	1.81	0.46
1:B:2159:LEU:HG	1:B:2163:ARG:HE	1.80	0.46
1:B:3107:VAL:O	1:B:3111:ARG:HB2	2.16	0.46
1:B:4049:VAL:HA	1:B:4163:PHE:HZ	1.81	0.46
1:C:2205:GLU:O	1:C:2208:MET:N	2.49	0.46
1:C:2863:SER:HA	1:C:2928:LYS:HG3	1.98	0.46
1:C:4049:VAL:HA	1:C:4163:PHE:HZ	1.81	0.46
1:D:884:LEU:HB2	1:D:969:PRO:HD3	1.97	0.46
1:D:3107:VAL:O	1:D:3111:ARG:HB2	2.16	0.46
1:D:4965:SER:O	1:D:4969:ASP:HB2	2.15	0.46
1:A:491:ILE:HD11	1:A:522:LEU:HB3	1.98	0.46
1:A:2764:GLU:HG3	1:A:2857:PRO:HB3	1.97	0.46
1:B:1968:LYS:NZ	1:B:2030:ASP:OD2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3180:ASN:HB2	1:B:3183:VAL:HG23	1.97	0.46
1:C:491:ILE:HD11	1:C:522:LEU:HB3	1.98	0.46
1:C:2740:VAL:HG21	1:C:2819:TRP:HE1	1.81	0.46
1:C:3107:VAL:O	1:C:3111:ARG:HB2	2.16	0.46
1:D:3266:MET:HB3	1:D:3269:VAL:HB	1.99	0.46
1:D:4971:THR:HG22	1:D:4972:PRO:HD2	1.98	0.46
1:A:3107:VAL:O	1:A:3111:ARG:HB2	2.16	0.45
1:C:2516:ASP:N	1:C:2516:ASP:OD1	2.46	0.45
1:C:2768:PHE:HA	1:C:2771:ILE:HG22	1.97	0.45
1:C:4965:SER:O	1:C:4969:ASP:HB2	2.15	0.45
1:D:3329:ILE:O	1:D:3403:ARG:NH2	2.48	0.45
1:A:1297:PHE:HD1	1:A:1522:LEU:HA	1.80	0.45
1:A:2205:GLU:O	1:A:2208:MET:N	2.49	0.45
1:A:2474:LEU:HD13	1:A:2550:LEU:HD21	1.96	0.45
1:A:2740:VAL:HG21	1:A:2819:TRP:HE1	1.81	0.45
1:A:3788:GLY:HA2	1:A:3835:LEU:HG	1.98	0.45
1:B:1297:PHE:HD1	1:B:1522:LEU:HA	1.80	0.45
1:D:1118:ASP:OD1	1:D:1118:ASP:N	2.48	0.45
1:D:3409:TYR:HE2	1:D:3510:ILE:HG12	1.82	0.45
1:A:3329:ILE:O	1:A:3403:ARG:NH2	2.48	0.45
1:B:357:LEU:HD11	1:B:388:LEU:HD11	1.98	0.45
1:B:2768:PHE:HA	1:B:2771:ILE:HG22	1.97	0.45
1:C:3980:LEU:HD22	1:C:4030:LEU:HD21	1.98	0.45
1:A:1432:THR:HA	1:A:1520:VAL:O	2.17	0.45
1:A:4823:LEU:HD23	1:A:4823:LEU:HA	1.83	0.45
1:B:3788:GLY:HA2	1:B:3835:LEU:HG	1.98	0.45
1:C:3409:TYR:HE2	1:C:3510:ILE:HG12	1.82	0.45
1:D:1948:ASP:OD1	1:D:2126:ARG:NH2	2.42	0.45
2:E:23:VAL:HG13	2:E:47:LYS:HG2	1.98	0.45
1:A:1465:ASP:OD1	1:A:1465:ASP:N	2.50	0.45
1:B:491:ILE:HD11	1:B:522:LEU:HB3	1.99	0.45
1:C:233:ILE:O	1:C:257:ARG:NH2	2.48	0.45
1:C:868:GLU:HA	1:C:871:ARG:HB2	1.98	0.45
1:C:1578:ALA:O	1:C:1584:ARG:NH2	2.37	0.45
1:C:2670:GLU:HG2	1:C:2912:THR:HB	1.98	0.45
1:C:2765:LYS:HA	1:C:2765:LYS:HD3	1.76	0.45
1:D:2205:GLU:O	1:D:2208:MET:N	2.49	0.45
2:F:23:VAL:HG13	2:F:47:LYS:HG2	1.98	0.45
2:G:23:VAL:HG13	2:G:47:LYS:HG2	1.98	0.45
1:A:4214:LYS:HE2	1:A:4985:LEU:HD11	1.99	0.45
1:B:4214:LYS:HE2	1:B:4985:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1432:THR:HA	1:C:1520:VAL:O	2.17	0.45
1:C:4725:LEU:HD13	1:C:4743:MET:HE1	1.99	0.45
1:D:357:LEU:HD11	1:D:388:LEU:HD11	1.98	0.45
1:D:1256:GLU:HB3	1:D:1275:ARG:HD2	1.97	0.45
1:A:1007:TYR:O	1:A:1017:ARG:NH2	2.49	0.45
1:A:3980:LEU:HD22	1:A:4030:LEU:HD21	1.98	0.45
1:B:710:ASP:N	1:B:710:ASP:OD1	2.48	0.45
1:B:1036:ARG:O	1:B:1040:CYS:HB2	2.17	0.45
1:B:2265:LEU:O	1:B:2330:ARG:NH1	2.50	0.45
1:B:2670:GLU:HG2	1:B:2912:THR:HB	1.98	0.45
1:C:710:ASP:OD1	1:C:710:ASP:N	2.48	0.45
1:C:2368:LEU:HD11	1:C:2376:LEU:HD12	1.99	0.45
1:C:3219:TYR:OH	1:C:3239:MET:SD	2.65	0.45
1:C:3266:MET:HB3	1:C:3269:VAL:HB	1.99	0.45
1:D:233:ILE:O	1:D:257:ARG:NH2	2.48	0.45
1:D:1698:LEU:HA	1:D:1712:TYR:CE1	2.52	0.45
1:A:653:ALA:HB3	1:A:656:SER:HB2	1.99	0.45
1:A:4065:PHE:O	1:A:4133:GLN:NE2	2.49	0.45
1:B:863:LEU:HA	1:B:864:PRO:HD3	1.85	0.45
1:B:2368:LEU:HD11	1:B:2376:LEU:HD12	1.99	0.45
1:C:775:GLY:H	1:C:848:HIS:CE1	2.35	0.45
1:C:2265:LEU:O	1:C:2330:ARG:NH1	2.50	0.45
1:D:2670:GLU:HG2	1:D:2912:THR:HB	1.98	0.45
1:A:294:THR:HG23	1:A:297:GLN:H	1.82	0.45
1:A:2368:LEU:HD11	1:A:2376:LEU:HD12	1.99	0.45
1:C:293:LEU:HD12	1:C:378:LEU:HD23	1.99	0.45
1:C:743:VAL:HG21	1:C:802:PHE:HE2	1.82	0.45
1:C:790:ARG:HA	1:C:1626:TRP:O	2.17	0.45
1:C:1036:ARG:O	1:C:1040:CYS:HB2	2.17	0.45
1:C:4552:LEU:O	1:C:4556:SER:OG	2.34	0.45
1:D:491:ILE:HD11	1:D:522:LEU:HB3	1.98	0.45
1:D:653:ALA:HB3	1:D:656:SER:HB2	1.99	0.45
1:D:743:VAL:HG21	1:D:802:PHE:HE2	1.82	0.45
1:D:1432:THR:HA	1:D:1520:VAL:O	2.17	0.45
1:D:3980:LEU:HD22	1:D:4030:LEU:HD21	1.98	0.45
2:H:23:VAL:HG13	2:H:47:LYS:HG2	1.98	0.45
1:A:1118:ASP:OD1	1:A:1118:ASP:N	2.48	0.45
1:A:2265:LEU:O	1:A:2330:ARG:NH1	2.50	0.45
1:A:3768:SER:HA	1:A:3771:HIS:CD2	2.52	0.45
1:A:4888:TYR:OH	1:B:4917:ASP:OD2	2.27	0.45
1:B:659:TYR:O	1:B:662:TRP:NE1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:743:VAL:HG21	1:B:802:PHE:HE2	1.82	0.45
1:B:868:GLU:HA	1:B:871:ARG:HB2	1.98	0.45
1:B:1465:ASP:N	1:B:1465:ASP:OD1	2.50	0.45
1:C:1256:GLU:HB3	1:C:1275:ARG:HD2	1.97	0.45
1:C:1698:LEU:HA	1:C:1712:TYR:CE1	2.52	0.45
1:C:2686:LEU:HB3	1:C:2997:PHE:HE1	1.82	0.45
1:C:3924:LEU:HD22	1:C:3984:ARG:HG2	1.99	0.45
1:C:4971:THR:HG22	1:C:4972:PRO:HD2	1.98	0.45
1:D:618:GLN:OE1	1:D:1678:ASN:ND2	2.40	0.45
1:D:2265:LEU:O	1:D:2330:ARG:NH1	2.50	0.45
1:A:1698:LEU:HA	1:A:1712:TYR:CE1	2.52	0.44
1:A:2670:GLU:HG2	1:A:2912:THR:HB	1.98	0.44
1:B:2686:LEU:HB3	1:B:2997:PHE:HE1	1.82	0.44
1:C:3271:GLU:OE2	1:C:3337:ARG:NH2	2.44	0.44
1:D:294:THR:HG23	1:D:297:GLN:H	1.82	0.44
1:D:1036:ARG:O	1:D:1040:CYS:HB2	2.17	0.44
1:D:2368:LEU:HD11	1:D:2376:LEU:HD12	1.99	0.44
1:D:3788:GLY:HA2	1:D:3835:LEU:HG	1.98	0.44
1:A:262:LEU:HD13	1:A:274:LEU:HD11	2.00	0.44
1:A:659:TYR:O	1:A:662:TRP:NE1	2.49	0.44
1:B:790:ARG:HA	1:B:1626:TRP:O	2.17	0.44
1:B:3924:LEU:HD22	1:B:3984:ARG:HG2	1.99	0.44
1:B:3980:LEU:HD22	1:B:4030:LEU:HD21	1.98	0.44
1:C:3270:ILE:HA	1:C:3274:LEU:HD12	2.00	0.44
1:D:34:LYS:H	1:D:53:SER:HB3	1.82	0.44
1:D:3180:ASN:HB2	1:D:3183:VAL:HG23	1.98	0.44
1:D:3924:LEU:HD22	1:D:3984:ARG:HG2	1.99	0.44
1:D:4725:LEU:HD13	1:D:4743:MET:HE1	1.99	0.44
1:A:293:LEU:HD12	1:A:378:LEU:HD23	1.99	0.44
1:A:3051:ARG:NH2	1:A:3102:ASP:OD1	2.50	0.44
1:A:3409:TYR:HE2	1:A:3510:ILE:HG12	1.82	0.44
1:B:1007:TYR:O	1:B:1017:ARG:NH2	2.49	0.44
1:B:3266:MET:HB3	1:B:3269:VAL:HB	1.99	0.44
1:C:34:LYS:H	1:C:53:SER:HB3	1.82	0.44
1:C:1101:ARG:NH1	1:C:1115:LEU:O	2.51	0.44
1:C:2309:SER:OG	1:C:2321:ILE:O	2.26	0.44
1:D:2686:LEU:HB3	1:D:2997:PHE:HE1	1.82	0.44
1:A:1036:ARG:O	1:A:1040:CYS:HB2	2.17	0.44
1:A:1277:TRP:HD1	1:A:1559:GLN:HG3	1.82	0.44
1:A:2000:SER:O	1:A:2005:GLN:NE2	2.50	0.44
1:A:3924:LEU:HD22	1:A:3984:ARG:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:LEU:HD12	1:B:378:LEU:HD23	1.99	0.44
1:B:3107:VAL:HG11	1:B:3171:SER:HB2	2.00	0.44
1:C:1007:TYR:O	1:C:1017:ARG:NH2	2.49	0.44
1:C:1864:LYS:NZ	1:C:1871:PHE:O	2.47	0.44
1:D:2018:GLU:HB3	1:D:2028:ARG:HH12	1.82	0.44
1:A:743:VAL:HG21	1:A:802:PHE:HE2	1.82	0.44
1:A:835:ARG:NH2	1:A:1210:SER:O	2.51	0.44
1:A:3301:PRO:HA	1:A:3302:PRO:HD3	1.91	0.44
1:B:1101:ARG:NH1	1:B:1115:LEU:O	2.51	0.44
1:B:1698:LEU:HA	1:B:1712:TYR:CE1	2.52	0.44
1:B:2205:GLU:O	1:B:2208:MET:N	2.49	0.44
1:C:3768:SER:HA	1:C:3771:HIS:CD2	2.52	0.44
1:C:3788:GLY:HA2	1:C:3835:LEU:HG	1.98	0.44
1:D:262:LEU:HD13	1:D:274:LEU:HD11	2.00	0.44
1:D:790:ARG:HA	1:D:1626:TRP:O	2.17	0.44
1:A:34:LYS:H	1:A:53:SER:HB3	1.82	0.44
1:B:1432:THR:HA	1:B:1520:VAL:O	2.17	0.44
1:B:2740:VAL:HG21	1:B:2819:TRP:HE1	1.81	0.44
1:B:3768:SER:HA	1:B:3771:HIS:CD2	2.52	0.44
1:C:73:LEU:O	1:C:106:ALA:N	2.40	0.44
1:D:835:ARG:NH2	1:D:1210:SER:O	2.51	0.44
1:D:3768:SER:HA	1:D:3771:HIS:CD2	2.52	0.44
1:D:3823:LYS:HA	1:D:3823:LYS:HD3	1.82	0.44
1:A:233:ILE:O	1:A:257:ARG:NH2	2.48	0.44
1:B:775:GLY:H	1:B:848:HIS:CE1	2.35	0.44
1:B:2039:LEU:HD22	1:B:2044:ILE:HG13	2.00	0.44
1:B:2869:ARG:NH2	1:B:2947:ASP:OD1	2.51	0.44
1:B:4725:LEU:HD13	1:B:4743:MET:HE1	1.99	0.44
1:B:4736:ARG:HE	1:B:4736:ARG:HB3	1.58	0.44
1:C:835:ARG:NH2	1:C:1210:SER:O	2.51	0.44
1:C:1454:THR:OG1	1:C:1456:ASP:OD1	2.26	0.44
1:C:4958:CYS:HB3	1:C:4961:CYS:SG	2.58	0.44
1:D:775:GLY:H	1:D:848:HIS:CE1	2.35	0.44
1:D:1465:ASP:OD1	1:D:1465:ASP:N	2.50	0.44
1:D:4049:VAL:HA	1:D:4163:PHE:HZ	1.81	0.44
1:D:4214:LYS:HE2	1:D:4985:LEU:HD11	1.99	0.44
1:A:790:ARG:HA	1:A:1626:TRP:O	2.17	0.44
1:A:1454:THR:OG1	1:A:1456:ASP:OD1	2.26	0.44
1:B:3270:ILE:HA	1:B:3274:LEU:HD12	2.00	0.44
1:C:294:THR:HG23	1:C:297:GLN:H	1.82	0.44
1:C:653:ALA:HB3	1:C:656:SER:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2967:MET:HE2	1:C:3045:LYS:HB3	2.00	0.44
1:D:1101:ARG:NH1	1:D:1115:LEU:O	2.51	0.44
1:A:357:LEU:HD11	1:A:388:LEU:HD11	1.98	0.44
1:A:2494:PHE:HE2	1:A:2499:LYS:HE3	1.83	0.44
1:B:653:ALA:HB3	1:B:656:SER:HB2	1.99	0.44
1:B:1277:TRP:HD1	1:B:1559:GLN:HG3	1.83	0.44
1:B:2494:PHE:HE2	1:B:2499:LYS:HE3	1.83	0.44
1:C:1232:ARG:NH2	1:C:1828:ASP:O	2.37	0.44
1:C:1948:ASP:OD1	1:C:2126:ARG:NH2	2.42	0.44
1:C:2159:LEU:HD21	1:C:2163:ARG:HH21	1.83	0.44
1:C:2869:ARG:NH2	1:C:2947:ASP:OD1	2.51	0.44
1:C:4214:LYS:HE2	1:C:4985:LEU:HD11	1.99	0.44
1:D:2869:ARG:NH2	1:D:2947:ASP:OD1	2.51	0.44
1:D:3270:ILE:HA	1:D:3274:LEU:HD12	1.99	0.44
1:D:5034:ASP:OD2	1:D:5035:GLN:NE2	2.51	0.44
1:A:775:GLY:H	1:A:848:HIS:CE1	2.35	0.43
1:A:3264:THR:OG1	1:A:3265:GLU:OE1	2.33	0.43
1:B:1232:ARG:NH2	1:B:1828:ASP:O	2.37	0.43
1:B:1743[A]:ARG:HE	1:B:1743[A]:ARG:HB2	1.49	0.43
1:B:2516:ASP:OD1	1:B:2516:ASP:N	2.46	0.43
1:B:3409:TYR:HE2	1:B:3510:ILE:HG12	1.82	0.43
1:C:2627:VAL:HG21	1:C:2674:LEU:HG	2.00	0.43
1:D:293:LEU:HD12	1:D:378:LEU:HD23	1.99	0.43
1:D:1007:TYR:O	1:D:1017:ARG:NH2	2.49	0.43
1:D:2970:SER:HA	1:D:2973:PHE:CE2	2.53	0.43
1:A:877:ASN:HA	1:A:970:LEU:H	1.84	0.43
1:B:294:THR:HG23	1:B:297:GLN:H	1.82	0.43
1:D:1277:TRP:HD1	1:D:1559:GLN:HG3	1.83	0.43
1:D:3264:THR:OG1	1:D:3265:GLU:OE1	2.33	0.43
1:B:884:LEU:HD13	1:B:968:ALA:H	1.83	0.43
1:C:2018:GLU:HB3	1:C:2028:ARG:HH12	1.82	0.43
1:C:5034:ASP:OD2	1:C:5035:GLN:NE2	2.51	0.43
1:D:2039:LEU:HD22	1:D:2044:ILE:HG13	2.00	0.43
1:D:3107:VAL:HG11	1:D:3171:SER:HB2	1.99	0.43
1:A:2039:LEU:HD22	1:A:2044:ILE:HG13	2.00	0.43
1:A:4725:LEU:HD13	1:A:4743:MET:HE1	1.99	0.43
1:A:4958:CYS:HB3	1:A:4961:CYS:SG	2.58	0.43
1:B:2236:LEU:HD22	1:B:2250:MET:HE1	2.01	0.43
1:C:2675:THR:HG22	1:C:2706:ILE:HG23	2.00	0.43
1:C:4951:LYS:HE3	1:C:4951:LYS:HB3	1.82	0.43
1:D:73:LEU:O	1:D:106:ALA:N	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3271:GLU:OE2	1:D:3337:ARG:NH2	2.44	0.43
1:A:2018:GLU:HB3	1:A:2028:ARG:HH12	1.82	0.43
1:A:2869:ARG:NH2	1:A:2947:ASP:OD1	2.51	0.43
1:A:3266:MET:HB3	1:A:3269:VAL:HB	1.99	0.43
1:A:5034:ASP:OD2	1:A:5035:GLN:NE2	2.51	0.43
1:B:835:ARG:NH2	1:B:1210:SER:O	2.51	0.43
1:C:111:HIS:ND1	1:C:114:SER:OG	2.39	0.43
1:C:877:ASN:HA	1:C:970:LEU:H	1.84	0.43
1:C:4630:TYR:OH	1:D:4860:ARG:NH2	2.47	0.43
1:D:4570:ALA:O	1:D:4574:ASN:ND2	2.52	0.43
1:A:2686:LEU:HB3	1:A:2997:PHE:HE1	1.82	0.43
1:A:3245:VAL:HG23	1:A:3248:ARG:H	1.84	0.43
1:B:34:LYS:H	1:B:53:SER:HB3	1.82	0.43
1:B:2018:GLU:HB3	1:B:2028:ARG:HH12	1.82	0.43
1:B:2277:ALA:O	1:B:2281:ILE:HG13	2.18	0.43
1:B:2712:PRO:HG3	1:B:3013:HIS:CD2	2.54	0.43
1:C:2277:ALA:O	1:C:2281:ILE:HG13	2.18	0.43
1:C:2970:SER:HA	1:C:2973:PHE:CE2	2.53	0.43
1:C:3007:ASN:O	1:C:3011:THR:OG1	2.22	0.43
1:D:403:MET:O	1:D:407:THR:OG1	2.26	0.43
1:A:1101:ARG:NH1	1:A:1115:LEU:O	2.51	0.43
1:A:2159:LEU:HD21	1:A:2163:ARG:HH21	1.83	0.43
1:A:2277:ALA:O	1:A:2281:ILE:HG13	2.18	0.43
1:A:2677:LYS:HE2	1:A:2677:LYS:HB3	1.67	0.43
1:B:1118:ASP:OD1	1:B:1118:ASP:N	2.48	0.43
1:C:863:LEU:HA	1:C:864:PRO:HD3	1.85	0.43
1:C:1465:ASP:OD1	1:C:1465:ASP:N	2.50	0.43
1:C:2494:PHE:HE2	1:C:2499:LYS:HE3	1.83	0.43
1:D:2494:PHE:HE2	1:D:2499:LYS:HE3	1.83	0.43
1:D:2712:PRO:HG3	1:D:3013:HIS:CD2	2.54	0.43
1:A:884:LEU:HD13	1:A:968:ALA:H	1.83	0.43
1:A:3270:ILE:HA	1:A:3274:LEU:HD12	2.00	0.43
1:A:4570:ALA:O	1:A:4574:ASN:ND2	2.52	0.43
1:B:262:LEU:HD13	1:B:274:LEU:HD11	1.99	0.43
1:B:2675:THR:HG22	1:B:2706:ILE:HG23	2.00	0.43
1:C:262:LEU:HD13	1:C:274:LEU:HD11	2.00	0.43
1:C:884:LEU:HD13	1:C:968:ALA:H	1.83	0.43
1:C:2712:PRO:HG3	1:C:3013:HIS:CD2	2.54	0.43
1:D:274:LEU:HD23	1:D:274:LEU:HA	1.84	0.43
1:D:877:ASN:HA	1:D:970:LEU:H	1.84	0.43
1:D:2159:LEU:HD21	1:D:2163:ARG:HH21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2574:HIS:CD2	1:D:2575:ARG:HG2	2.54	0.43
1:D:2779:GLU:HG3	1:D:2792:ARG:HG2	2.01	0.43
1:A:37:LEU:HD23	1:A:37:LEU:HA	1.90	0.43
1:C:1291:LEU:HD12	1:C:1550:PRO:HG2	2.01	0.43
1:C:1812:LEU:HD23	1:C:1812:LEU:HA	1.90	0.43
1:C:2779:GLU:HG3	1:C:2792:ARG:HG2	2.01	0.43
1:C:3107:VAL:HG11	1:C:3171:SER:HB2	1.99	0.43
1:C:3888:LEU:HD23	1:C:3888:LEU:HA	1.91	0.43
1:D:2277:ALA:O	1:D:2281:ILE:HG13	2.18	0.43
1:D:2627:VAL:HG21	1:D:2674:LEU:HG	2.00	0.43
1:D:4958:CYS:HB3	1:D:4961:CYS:SG	2.58	0.43
1:A:2779:GLU:HG3	1:A:2792:ARG:HG2	2.01	0.43
1:A:3051:ARG:HA	1:A:3131:TYR:CE1	2.54	0.43
1:A:4652:LEU:HD12	1:A:4652:LEU:HA	1.92	0.43
1:B:1116:GLY:O	1:B:1134:LEU:N	2.52	0.43
1:B:2627:VAL:HG21	1:B:2674:LEU:HG	2.00	0.43
1:B:4958:CYS:HB3	1:B:4961:CYS:SG	2.58	0.43
1:C:716:PHE:HE1	1:C:730:VAL:HG21	1.84	0.43
1:C:1118:ASP:OD1	1:C:1118:ASP:N	2.48	0.43
1:C:1229:ASN:HB2	1:C:1827:ARG:HG3	2.01	0.43
1:C:1277:TRP:HD1	1:C:1559:GLN:HG3	1.83	0.43
1:C:2583:LEU:HA	1:C:2586:VAL:HG12	2.01	0.43
1:C:3245:VAL:HG23	1:C:3248:ARG:H	1.84	0.43
1:D:2000:SER:O	1:D:2005:GLN:NE2	2.50	0.43
1:D:2583:LEU:HA	1:D:2586:VAL:HG12	2.01	0.43
1:A:1116:GLY:O	1:A:1134:LEU:N	2.52	0.42
1:A:4552:LEU:O	1:A:4556:SER:OG	2.34	0.42
1:B:877:ASN:HA	1:B:970:LEU:H	1.83	0.42
1:B:1229:ASN:HB2	1:B:1827:ARG:HG3	2.01	0.42
1:B:1291:LEU:HD12	1:B:1550:PRO:HG2	2.01	0.42
1:B:2159:LEU:HD21	1:B:2163:ARG:HH21	1.83	0.42
1:B:2970:SER:HA	1:B:2973:PHE:CE2	2.53	0.42
1:B:5034:ASP:OD2	1:B:5035:GLN:NE2	2.51	0.42
1:C:1000:ARG:HA	1:C:1000:ARG:HD3	1.83	0.42
1:C:1256:GLU:HB3	1:C:1275:ARG:HH11	1.84	0.42
1:C:3051:ARG:HA	1:C:3131:TYR:CE1	2.54	0.42
1:D:3051:ARG:HA	1:D:3131:TYR:CE1	2.54	0.42
1:A:162:LYS:H	1:A:162:LYS:HG2	1.67	0.42
1:A:2574:HIS:CD2	1:A:2575:ARG:HG2	2.54	0.42
1:A:2712:PRO:HG3	1:A:3013:HIS:CD2	2.54	0.42
1:A:2970:SER:HA	1:A:2973:PHE:CE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3107:VAL:HG11	1:A:3171:SER:HB2	2.00	0.42
1:A:4675:LYS:HE3	1:A:4675:LYS:HB3	1.83	0.42
1:C:2000:SER:O	1:C:2005:GLN:NE2	2.50	0.42
1:C:4570:ALA:O	1:C:4574:ASN:ND2	2.52	0.42
1:D:716:PHE:HE1	1:D:730:VAL:HG21	1.84	0.42
1:A:2309:SER:OG	1:A:2321:ILE:O	2.26	0.42
1:A:2583:LEU:HA	1:A:2586:VAL:HG12	2.01	0.42
1:B:1269:CYS:HA	1:B:1564:PHE:O	2.20	0.42
1:B:2583:LEU:HA	1:B:2586:VAL:HG12	2.01	0.42
1:B:2779:GLU:HG3	1:B:2792:ARG:HG2	2.01	0.42
1:C:2039:LEU:HD22	1:C:2044:ILE:HG13	2.00	0.42
1:D:2675:THR:HG22	1:D:2706:ILE:HG23	2.00	0.42
1:D:4181:ILE:HD12	1:D:4183:ILE:HG23	2.01	0.42
1:A:124:SER:HB2	1:A:133:PHE:HA	2.01	0.42
1:A:274:LEU:HD23	1:A:274:LEU:HA	1.84	0.42
1:B:4128:PHE:HA	1:B:4131:ARG:HH21	1.85	0.42
1:B:4710:SER:OG	1:B:4772:ASP:OD2	2.38	0.42
1:C:1116:GLY:O	1:C:1134:LEU:N	2.52	0.42
1:C:2574:HIS:CD2	1:C:2575:ARG:HG2	2.54	0.42
1:C:3264:THR:OG1	1:C:3265:GLU:OE1	2.33	0.42
1:C:4181:ILE:HD12	1:C:4183:ILE:HG23	2.01	0.42
1:D:124:SER:HB2	1:D:133:PHE:HA	2.01	0.42
1:D:1269:CYS:HA	1:D:1564:PHE:O	2.20	0.42
1:D:3007:ASN:O	1:D:3011:THR:OG1	2.22	0.42
1:D:3245:VAL:HG23	1:D:3248:ARG:H	1.84	0.42
1:D:4552:LEU:O	1:D:4556:SER:OG	2.34	0.42
1:A:846:LEU:HD22	1:A:846:LEU:HA	1.91	0.42
1:A:2675:THR:HG22	1:A:2706:ILE:HG23	2.00	0.42
1:A:4677:LEU:HD12	1:A:4677:LEU:HA	1.85	0.42
1:B:716:PHE:HE1	1:B:730:VAL:HG21	1.84	0.42
1:B:1156:THR:OG1	1:B:1157:GLU:OE1	2.29	0.42
1:B:2574:HIS:CD2	1:B:2575:ARG:HG2	2.54	0.42
1:B:2677:LYS:HB3	1:B:2677:LYS:HE2	1.67	0.42
1:B:2967:MET:HE2	1:B:3045:LYS:HB3	2.00	0.42
1:B:4630:TYR:OH	1:C:4860:ARG:NH2	2.47	0.42
1:B:4911:LEU:HD13	1:B:4911:LEU:HA	1.90	0.42
1:C:2825:LYS:HE2	1:C:2825:LYS:HB2	1.91	0.42
1:C:3329:ILE:O	1:C:3403:ARG:NH2	2.49	0.42
1:C:3514:LEU:HD11	1:C:3602:VAL:HG13	2.02	0.42
1:D:111:HIS:ND1	1:D:114:SER:OG	2.39	0.42
1:D:400:ALA:O	1:D:404:ILE:HD12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:498:THR:HA	1:D:553:ARG:HH12	1.85	0.42
1:D:884:LEU:HD13	1:D:968:ALA:H	1.83	0.42
1:D:1256:GLU:HB3	1:D:1275:ARG:HH11	1.84	0.42
1:D:1422:ASP:OD2	1:D:1568:LYS:NZ	2.38	0.42
1:D:3862:ASP:OD1	1:D:3862:ASP:N	2.52	0.42
1:A:73:LEU:O	1:A:106:ALA:N	2.40	0.42
1:B:2000:SER:O	1:B:2005:GLN:NE2	2.50	0.42
1:B:3062:PRO:HA	1:B:3065:VAL:HG22	2.02	0.42
1:B:3245:VAL:HG23	1:B:3248:ARG:H	1.84	0.42
1:B:3514:LEU:HD11	1:B:3602:VAL:HG13	2.02	0.42
1:C:400:ALA:O	1:C:404:ILE:HD12	2.19	0.42
1:C:3582:ARG:HA	1:C:3582:ARG:HD3	1.87	0.42
1:D:199:LEU:HD12	1:D:199:LEU:HA	1.87	0.42
1:D:1578:ALA:O	1:D:1584:ARG:NH2	2.37	0.42
1:A:1256:GLU:HB3	1:A:1275:ARG:HH11	1.84	0.42
1:A:2627:VAL:HG21	1:A:2674:LEU:HG	2.00	0.42
1:A:3062:PRO:HA	1:A:3065:VAL:HG22	2.02	0.42
1:B:400:ALA:O	1:B:404:ILE:HD12	2.19	0.42
1:B:2587:TYR:O	1:B:2590:SER:OG	2.26	0.42
1:B:3862:ASP:OD1	1:B:3862:ASP:N	2.52	0.42
1:B:4570:ALA:O	1:B:4574:ASN:ND2	2.52	0.42
1:C:1156:THR:OG1	1:C:1157:GLU:OE1	2.29	0.42
1:C:5030:LYS:HB2	1:C:5030:LYS:HE2	1.90	0.42
1:D:162:LYS:H	1:D:162:LYS:HG2	1.67	0.42
1:D:876:GLU:HG2	1:D:910:PHE:CE2	2.55	0.42
1:D:2967:MET:HE2	1:D:3045:LYS:HB3	2.02	0.42
2:H:76:CYS:HB2	2:H:97:LEU:HB2	2.02	0.42
1:A:876:GLU:HG2	1:A:910:PHE:CE2	2.55	0.42
1:A:2236:LEU:HD22	1:A:2250:MET:HE1	2.02	0.42
1:A:2538:THR:OG1	1:A:2539:ALA:N	2.53	0.42
1:A:4181:ILE:HD12	1:A:4183:ILE:HG23	2.01	0.42
1:A:4944:ARG:NE	1:B:4942:GLU:OE1	2.53	0.42
1:B:876:GLU:HG2	1:B:910:PHE:CE2	2.55	0.42
1:B:3823:LYS:HA	1:B:3823:LYS:HD3	1.82	0.42
1:C:876:GLU:HG2	1:C:910:PHE:CE2	2.55	0.42
1:D:1084:GLN:NE2	1:D:1186:ASP:O	2.42	0.42
1:D:4823:LEU:HD23	1:D:4823:LEU:HA	1.83	0.42
2:E:76:CYS:HB2	2:E:97:LEU:HB2	2.02	0.42
1:A:328:LYS:HE2	1:A:328:LYS:HB2	1.92	0.42
1:B:199:LEU:HD12	1:B:199:LEU:HA	1.87	0.42
1:B:1861:GLN:O	1:B:1865:MET:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4675:LYS:HB3	1:C:4675:LYS:HE3	1.83	0.42
1:D:3068:LEU:HG	1:D:3139:VAL:HG11	2.02	0.42
1:A:657:THR:HG22	1:A:1001:VAL:HG21	2.02	0.42
1:A:2781:VAL:HG22	1:A:2790:MET:HB2	2.02	0.42
1:B:498:THR:HA	1:B:553:ARG:HH12	1.85	0.42
1:B:3051:ARG:HA	1:B:3131:TYR:CE1	2.54	0.42
1:C:1422:ASP:OD2	1:C:1568:LYS:NZ	2.38	0.42
1:C:1861:GLN:O	1:C:1865:MET:HG3	2.20	0.42
1:C:2610:LEU:HD23	1:C:2610:LEU:HA	1.94	0.42
1:C:4128:PHE:HA	1:C:4131:ARG:HH21	1.85	0.42
1:D:1291:LEU:HD12	1:D:1550:PRO:HG2	2.01	0.42
1:D:1676:LEU:HD22	1:D:2167:ILE:HD12	2.02	0.42
1:D:1861:GLN:O	1:D:1865:MET:HG3	2.20	0.42
1:D:3062:PRO:HA	1:D:3065:VAL:HG22	2.02	0.42
1:A:1269:CYS:HA	1:A:1564:PHE:O	2.20	0.41
1:B:37:LEU:HD23	1:B:37:LEU:HA	1.90	0.41
1:B:880:GLU:HB3	1:B:883:ALA:HB3	2.02	0.41
1:B:1256:GLU:HB3	1:B:1275:ARG:HH11	1.84	0.41
1:B:2806:ARG:HA	1:B:2809:ILE:HD13	2.02	0.41
1:B:4181:ILE:HD12	1:B:4183:ILE:HG23	2.01	0.41
1:C:1717:SER:HA	1:C:1721:GLU:HG2	2.02	0.41
1:C:2748:PRO:HG2	1:C:2817:ILE:HD13	2.02	0.41
1:C:3062:PRO:HA	1:C:3065:VAL:HG22	2.02	0.41
1:D:1739:THR:O	1:D:1743[B]:ARG:HG3	2.20	0.41
1:D:1808:ARG:HD3	1:D:1853:ILE:HG22	2.01	0.41
1:D:4584:ASP:OD1	1:D:4584:ASP:N	2.51	0.41
1:A:2527:LEU:HA	1:A:2530:MET:HG3	2.02	0.41
1:A:3514:LEU:HD11	1:A:3602:VAL:HG13	2.01	0.41
1:B:1454:THR:OG1	1:B:1456:ASP:OD1	2.26	0.41
1:B:2781:VAL:HG22	1:B:2790:MET:HB2	2.02	0.41
1:B:3068:LEU:HD23	1:B:3139:VAL:HG21	2.02	0.41
1:B:3068:LEU:HG	1:B:3139:VAL:HG11	2.02	0.41
1:C:1676:LEU:HD22	1:C:2167:ILE:HD12	2.02	0.41
1:D:1229:ASN:HB2	1:D:1827:ARG:HG3	2.01	0.41
1:D:1717:SER:HA	1:D:1721:GLU:HG2	2.02	0.41
1:A:219:VAL:HG12	1:A:259:LEU:HD12	2.03	0.41
1:A:348:VAL:HB	1:A:357:LEU:HD22	2.03	0.41
1:A:400:ALA:O	1:A:404:ILE:HD12	2.19	0.41
1:A:1717:SER:HA	1:A:1721:GLU:HG2	2.02	0.41
1:A:1861:GLN:O	1:A:1865:MET:HG3	2.20	0.41
1:A:3261:ALA:HB1	1:A:3265:GLU:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:SER:HB2	1:B:133:PHE:HA	2.01	0.41
1:B:1717:SER:HA	1:B:1721:GLU:HG2	2.02	0.41
1:B:3110:LEU:HD23	1:B:3183:VAL:HG22	2.02	0.41
1:B:3582:ARG:HD3	1:B:3582:ARG:HA	1.87	0.41
1:C:219:VAL:HG12	1:C:259:LEU:HD12	2.03	0.41
1:C:322:LYS:HD3	1:C:322:LYS:HA	1.95	0.41
1:C:1269:CYS:HA	1:C:1564:PHE:O	2.20	0.41
1:C:1808:ARG:HD3	1:C:1853:ILE:HG22	2.01	0.41
1:C:2781:VAL:HG22	1:C:2790:MET:HB2	2.02	0.41
1:D:2748:PRO:HG2	1:D:2817:ILE:HD13	2.02	0.41
1:A:199:LEU:HD12	1:A:199:LEU:HA	1.87	0.41
1:A:1291:LEU:HD12	1:A:1550:PRO:HG2	2.01	0.41
1:A:3007:ASN:O	1:A:3011:THR:OG1	2.22	0.41
1:A:3110:LEU:HD23	1:A:3183:VAL:HG22	2.02	0.41
1:C:2538:THR:OG1	1:C:2539:ALA:N	2.53	0.41
1:C:2806:ARG:HA	1:C:2809:ILE:HD13	2.02	0.41
1:C:2878:LEU:HD12	1:C:2878:LEU:HA	1.90	0.41
1:C:3051:ARG:NH2	1:C:3102:ASP:OD1	2.50	0.41
1:D:1253:PRO:HG2	1:D:1254:HIS:CD2	2.56	0.41
1:D:4821:LYS:O	1:D:4825:THR:HG23	2.21	0.41
1:A:2748:PRO:HG2	1:A:2817:ILE:HD13	2.02	0.41
1:A:4710:SER:OG	1:A:4772:ASP:OD2	2.38	0.41
1:A:4821:LYS:O	1:A:4825:THR:HG23	2.21	0.41
1:B:348:VAL:HB	1:B:357:LEU:HD22	2.03	0.41
1:B:2748:PRO:HG2	1:B:2817:ILE:HD13	2.02	0.41
1:B:3078:ARG:NE	1:B:3155:ASP:OD2	2.40	0.41
1:B:3260:GLY:HA2	1:B:3325:ASN:ND2	2.36	0.41
1:B:4888:TYR:OH	1:C:4917:ASP:OD2	2.31	0.41
1:C:498:THR:HA	1:C:553:ARG:HH12	1.85	0.41
1:C:3068:LEU:HG	1:C:3139:VAL:HG11	2.02	0.41
1:D:3694:LYS:HA	1:D:3695:PRO:HD3	1.90	0.41
1:A:498:THR:HA	1:A:553:ARG:HH12	1.85	0.41
1:A:1229:ASN:HB2	1:A:1827:ARG:HG3	2.01	0.41
1:A:1739:THR:O	1:A:1743[B]:ARG:HG3	2.20	0.41
1:A:3068:LEU:HG	1:A:3139:VAL:HG11	2.02	0.41
1:B:219:VAL:HG12	1:B:259:LEU:HD12	2.03	0.41
1:B:657:THR:HG22	1:B:1001:VAL:HG21	2.02	0.41
1:B:2538:THR:OG1	1:B:2539:ALA:N	2.53	0.41
1:C:1739:THR:O	1:C:1743[B]:ARG:HG3	2.21	0.41
1:C:2927:LEU:HD12	1:C:2927:LEU:HA	1.92	0.41
1:C:3260:GLY:HA2	1:C:3325:ASN:ND2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4710:SER:OG	1:C:4772:ASP:OD2	2.37	0.41
1:C:4827:LEU:HD23	1:C:4827:LEU:HA	1.94	0.41
1:D:265:LEU:HD22	1:D:279:PRO:HB2	2.03	0.41
1:D:1249:PRO:HA	1:D:1250:PRO:HD3	1.97	0.41
1:D:2684:ASP:O	1:D:2688:HIS:ND1	2.46	0.41
1:D:3110:LEU:HD23	1:D:3183:VAL:HG22	2.02	0.41
1:D:4098:ASP:OD1	1:D:4098:ASP:N	2.54	0.41
2:F:76:CYS:HB2	2:F:97:LEU:HB2	2.02	0.41
2:G:76:CYS:HB2	2:G:97:LEU:HB2	2.02	0.41
1:A:2806:ARG:HA	1:A:2809:ILE:HD13	2.03	0.41
1:A:2967:MET:HE2	1:A:3045:LYS:HB3	2.02	0.41
1:A:4584:ASP:OD1	1:A:4584:ASP:N	2.51	0.41
1:A:4942:GLU:OE1	1:D:4944:ARG:NE	2.53	0.41
1:B:1808:ARG:HD3	1:B:1853:ILE:HG22	2.02	0.41
1:B:2527:LEU:HA	1:B:2530:MET:HG3	2.03	0.41
1:C:124:SER:HB2	1:C:133:PHE:HA	2.01	0.41
1:C:415:ILE:HA	1:C:418:LEU:HD12	2.03	0.41
1:C:3068:LEU:HD23	1:C:3139:VAL:HG21	2.02	0.41
1:C:3696:ASP:OD1	1:C:3696:ASP:N	2.53	0.41
1:D:219:VAL:HG12	1:D:259:LEU:HD12	2.03	0.41
1:D:2757:LYS:HG2	1:D:2929:PHE:HZ	1.86	0.41
1:A:716:PHE:HE1	1:A:730:VAL:HG21	1.84	0.41
1:A:880:GLU:HB3	1:A:883:ALA:HB3	2.02	0.41
1:A:3068:LEU:HD23	1:A:3139:VAL:HG21	2.02	0.41
1:A:4128:PHE:HA	1:A:4131:ARG:HH21	1.85	0.41
1:B:415:ILE:HA	1:B:418:LEU:HD12	2.03	0.41
1:B:1253:PRO:HG2	1:B:1254:HIS:CD2	2.56	0.41
1:B:1948:ASP:OD1	1:B:2126:ARG:NH2	2.42	0.41
1:B:2736:ASP:N	1:B:2736:ASP:OD1	2.54	0.41
1:B:3261:ALA:HB1	1:B:3265:GLU:HG3	2.03	0.41
1:C:2906:VAL:HG23	1:C:2911:LEU:HD23	2.03	0.41
1:C:3852:LYS:HE3	1:C:3852:LYS:HB3	1.94	0.41
1:D:2109:ASP:N	1:D:2109:ASP:OD1	2.54	0.41
1:D:2781:VAL:HA	1:D:2789:PRO:HB2	2.03	0.41
1:D:2806:ARG:HA	1:D:2809:ILE:HD13	2.03	0.41
1:D:3969:ILE:HD13	1:D:3969:ILE:HA	1.88	0.41
1:D:4710:SER:OG	1:D:4772:ASP:OD2	2.38	0.41
1:A:356:TRP:O	1:A:379:HIS:N	2.54	0.41
1:A:415:ILE:HA	1:A:418:LEU:HD12	2.03	0.41
1:A:863:LEU:HA	1:A:864:PRO:HD3	1.85	0.41
1:A:2542:SER:OG	1:A:2593:ARG:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3271:GLU:OE2	1:A:3337:ARG:NH2	2.44	0.41
1:A:3696:ASP:N	1:A:3696:ASP:OD1	2.53	0.41
1:A:3862:ASP:N	1:A:3862:ASP:OD1	2.52	0.41
1:A:4090:LYS:HE2	1:A:4090:LYS:HB3	1.91	0.41
1:B:1739:THR:O	1:B:1743[B]:ARG:HG3	2.20	0.41
1:B:2790:MET:HE3	1:B:2790:MET:HB3	1.91	0.41
1:B:3272:ILE:O	1:B:3276:MET:HG2	2.21	0.41
1:B:3301:PRO:HA	1:B:3302:PRO:HD3	1.91	0.41
1:B:3696:ASP:N	1:B:3696:ASP:OD1	2.53	0.41
1:B:4821:LYS:O	1:B:4825:THR:HG23	2.21	0.41
1:B:4951:LYS:HE3	1:B:4951:LYS:HB3	1.82	0.41
1:C:265:LEU:HD22	1:C:279:PRO:HB2	2.03	0.41
1:C:348:VAL:HB	1:C:357:LEU:HD22	2.03	0.41
1:C:2736:ASP:N	1:C:2736:ASP:OD1	2.54	0.41
1:C:2781:VAL:HA	1:C:2789:PRO:HB2	2.03	0.41
1:C:2790:MET:HE3	1:C:2790:MET:HB3	1.91	0.41
1:D:415:ILE:HA	1:D:418:LEU:HD12	2.03	0.41
1:D:766:GLY:HA2	1:D:1475:THR:O	2.21	0.41
1:D:1762:LEU:HD12	1:D:1863:LEU:HD13	2.03	0.41
1:D:2538:THR:OG1	1:D:2539:ALA:N	2.53	0.41
1:D:2736:ASP:OD1	1:D:2736:ASP:N	2.54	0.41
1:D:2906:VAL:HG23	1:D:2911:LEU:HD23	2.03	0.41
1:D:3260:GLY:HA2	1:D:3325:ASN:ND2	2.36	0.41
1:D:3261:ALA:HB1	1:D:3265:GLU:HG3	2.03	0.41
1:D:3514:LEU:HD11	1:D:3602:VAL:HG13	2.02	0.41
2:G:78:PRO:HA	2:G:81:ALA:HB3	2.03	0.41
1:A:766:GLY:HA2	1:A:1475:THR:O	2.21	0.41
1:A:2757:LYS:HG2	1:A:2929:PHE:HZ	1.86	0.41
1:A:3260:GLY:HA2	1:A:3325:ASN:ND2	2.36	0.41
1:A:3291:ALA:HA	1:A:3292:PRO:HD3	1.88	0.41
1:B:3209:GLN:HG2	1:B:3210:LEU:HG	2.03	0.41
1:B:3713:LYS:HB2	1:B:3713:LYS:HE2	1.93	0.41
1:C:880:GLU:HB3	1:C:883:ALA:HB3	2.02	0.41
1:C:1253:PRO:HG2	1:C:1254:HIS:CD2	2.56	0.41
1:C:3974:THR:O	1:C:3978:GLN:HG2	2.21	0.41
1:C:4821:LYS:O	1:C:4825:THR:HG23	2.21	0.41
1:D:657:THR:HG22	1:D:1001:VAL:HG21	2.02	0.41
1:D:793:LEU:HD12	1:D:821:LEU:HD21	2.03	0.41
1:D:838:HIS:CE1	1:D:1201:HIS:HB2	2.56	0.41
1:D:880:GLU:HB3	1:D:883:ALA:HB3	2.02	0.41
1:D:3068:LEU:HD23	1:D:3139:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1676:LEU:HD22	1:A:2167:ILE:HD12	2.02	0.40
1:A:1808:ARG:HD3	1:A:1853:ILE:HG22	2.01	0.40
1:A:3694:LYS:HA	1:A:3695:PRO:HD3	1.91	0.40
1:A:5006:GLN:O	1:A:5010:VAL:HG12	2.21	0.40
1:B:73:LEU:O	1:B:106:ALA:N	2.40	0.40
1:B:766:GLY:HA2	1:B:1475:THR:O	2.21	0.40
1:B:793:LEU:HD12	1:B:821:LEU:HD21	2.03	0.40
1:B:2781:VAL:HA	1:B:2789:PRO:HB2	2.03	0.40
1:C:283:ARG:NH1	1:C:290:TYR:OH	2.53	0.40
1:C:766:GLY:HA2	1:C:1475:THR:O	2.21	0.40
1:C:3110:LEU:HD23	1:C:3183:VAL:HG22	2.02	0.40
1:D:4801:LEU:HD23	1:D:4801:LEU:HA	1.93	0.40
2:H:78:PRO:HA	2:H:81:ALA:HB3	2.03	0.40
1:A:1948:ASP:OD1	1:A:2126:ARG:NH2	2.42	0.40
1:A:2906:VAL:HG23	1:A:2911:LEU:HD23	2.03	0.40
1:A:3974:THR:O	1:A:3978:GLN:HG2	2.22	0.40
1:A:4066:LEU:HD22	1:A:4133:GLN:HE22	1.86	0.40
1:B:4552:LEU:O	1:B:4556:SER:OG	2.34	0.40
1:C:1084:GLN:NE2	1:C:1186:ASP:O	2.42	0.40
1:C:2236:LEU:HD22	1:C:2250:MET:HE1	2.03	0.40
1:C:2463:LEU:HA	1:C:2466:LEU:HD12	2.03	0.40
1:C:2527:LEU:HA	1:C:2530:MET:HG3	2.03	0.40
1:C:2542:SER:OG	1:C:2593:ARG:O	2.39	0.40
1:C:3272:ILE:O	1:C:3276:MET:HG2	2.21	0.40
1:D:356:TRP:O	1:D:379:HIS:N	2.54	0.40
1:D:1116:GLY:O	1:D:1134:LEU:N	2.52	0.40
1:D:1156:THR:OG1	1:D:1157:GLU:OE1	2.29	0.40
1:D:2781:VAL:HG22	1:D:2790:MET:HB2	2.02	0.40
1:D:3582:ARG:HD3	1:D:3582:ARG:HA	1.87	0.40
1:D:3852:LYS:HE3	1:D:3852:LYS:HB3	1.93	0.40
1:D:4677:LEU:HD12	1:D:4677:LEU:HA	1.85	0.40
1:A:1156:THR:OG1	1:A:1157:GLU:OE1	2.29	0.40
1:A:3116:SER:O	1:A:3182:TYR:OH	2.36	0.40
1:A:4951:LYS:HE3	1:A:4951:LYS:HB3	1.83	0.40
1:B:869:ARG:CZ	1:B:870:ILE:HB	2.51	0.40
1:B:3051:ARG:NH2	1:B:3102:ASP:OD1	2.50	0.40
1:C:838:HIS:CE1	1:C:1201:HIS:HB2	2.56	0.40
1:C:2258:LEU:HD23	1:C:2258:LEU:HA	1.96	0.40
1:C:2905:LEU:HD23	1:C:2905:LEU:HA	1.95	0.40
1:C:3209:GLN:HG2	1:C:3210:LEU:HG	2.03	0.40
1:C:5006:GLN:O	1:C:5010:VAL:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1466:LEU:HD23	1:D:1466:LEU:HA	1.95	0.40
1:A:1253:PRO:HG2	1:A:1254:HIS:CD2	2.56	0.40
1:A:3272:ILE:O	1:A:3276:MET:HG2	2.21	0.40
1:B:1676:LEU:HD22	1:B:2167:ILE:HD12	2.02	0.40
1:B:2109:ASP:OD1	1:B:2109:ASP:N	2.54	0.40
1:B:3974:THR:O	1:B:3978:GLN:HG2	2.21	0.40
1:C:22:LEU:HD12	1:C:37:LEU:HD12	2.03	0.40
1:C:364:PRO:HD2	1:C:367:LEU:HD12	2.04	0.40
1:C:793:LEU:HD12	1:C:821:LEU:HD21	2.03	0.40
1:C:2109:ASP:OD1	1:C:2109:ASP:N	2.54	0.40
1:D:4675:LYS:HE3	1:D:4675:LYS:HB3	1.83	0.40
2:E:78:PRO:HA	2:E:81:ALA:HB3	2.03	0.40
1:A:364:PRO:HD2	1:A:367:LEU:HD12	2.04	0.40
1:A:4934:GLY:HA2	1:D:4937:ILE:HG12	2.04	0.40
1:B:22:LEU:HD12	1:B:37:LEU:HD12	2.03	0.40
1:B:356:TRP:O	1:B:379:HIS:N	2.54	0.40
1:B:2542:SER:OG	1:B:2593:ARG:O	2.39	0.40
1:B:2906:VAL:HG23	1:B:2911:LEU:HD23	2.03	0.40
1:C:1773:PRO:HA	1:C:1774:PRO:HD3	1.93	0.40
1:C:2711:PRO:HA	1:C:2712:PRO:HD3	2.00	0.40
1:C:4066:LEU:HD22	1:C:4133:GLN:HE22	1.86	0.40
1:D:364:PRO:HD2	1:D:367:LEU:HD12	2.04	0.40
1:D:721:LEU:HD23	1:D:721:LEU:HA	1.90	0.40
1:D:2690:LYS:HA	1:D:2690:LYS:HD2	1.92	0.40
1:D:3974:THR:O	1:D:3978:GLN:HG2	2.21	0.40
1:D:4128:PHE:HA	1:D:4131:ARG:HH21	1.85	0.40
2:F:61:GLU:O	2:F:65:GLN:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4353/5037 (86%)	4168 (96%)	182 (4%)	3 (0%)	48	78
1	B	4353/5037 (86%)	4168 (96%)	182 (4%)	3 (0%)	48	78
1	C	4353/5037 (86%)	4167 (96%)	183 (4%)	3 (0%)	48	78
1	D	4353/5037 (86%)	4167 (96%)	183 (4%)	3 (0%)	48	78
2	E	105/350 (30%)	98 (93%)	7 (7%)	0	100	100
2	F	105/350 (30%)	98 (93%)	7 (7%)	0	100	100
2	G	105/350 (30%)	98 (93%)	7 (7%)	0	100	100
2	H	105/350 (30%)	98 (93%)	7 (7%)	0	100	100
All	All	17832/21548 (83%)	17062 (96%)	758 (4%)	12 (0%)	50	78

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3616	LYS
1	A	4712	PRO
1	B	3616	LYS
1	B	4712	PRO
1	C	3616	LYS
1	C	4712	PRO
1	D	3616	LYS
1	D	4712	PRO
1	A	4691	GLN
1	B	4691	GLN
1	C	4691	GLN
1	D	4691	GLN

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	3806/4276 (89%)	3697 (97%)	109 (3%)	37	61
1	B	3806/4276 (89%)	3697 (97%)	109 (3%)	37	61
1	C	3806/4276 (89%)	3697 (97%)	109 (3%)	37	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	3806/4276 (89%)	3697 (97%)	109 (3%)	37	61
2	E	88/304 (29%)	87 (99%)	1 (1%)	70	81
2	F	88/304 (29%)	87 (99%)	1 (1%)	70	81
2	G	88/304 (29%)	87 (99%)	1 (1%)	70	81
2	H	88/304 (29%)	87 (99%)	1 (1%)	70	81
All	All	15576/18320 (85%)	15136 (97%)	440 (3%)	41	62

All (440) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	ARG
1	A	373	LYS
1	A	830	ARG
1	A	846	LEU
1	A	1534	LYS
1	A	1743[A]	ARG
1	A	1743[B]	ARG
1	A	1752	ARG
1	A	2100[A]	HIS
1	A	2100[B]	HIS
1	A	2268[A]	GLN
1	A	2268[B]	GLN
1	A	2336	ARG
1	A	2369[A]	ARG
1	A	2369[B]	ARG
1	A	2738	ARG
1	A	2786	LYS
1	A	2806	ARG
1	A	2827	ARG
1	A	2914	LYS
1	A	3053	ARG
1	A	3225	ARG
1	A	3611	HIS
1	A	3622	LYS
1	A	3692	GLU
1	A	4180	ARG
1	A	4184	MET
1	A	4187	SER
1	A	4189	ARG
1	A	4191	GLU

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Mol	Chain	Res	Type
1	A	4192	ARG
1	A	4200	THR
1	A	4204	GLN
1	A	4221	VAL
1	A	4245	MET
1	A	4246	GLN
1	A	4252	SER
1	A	4543	GLU
1	A	4544	LEU
1	A	4548	ARG
1	A	4556	SER
1	A	4563	ARG
1	A	4565	LEU
1	A	4569	LEU
1	A	4577	LEU
1	A	4580	TYR
1	A	4626	ASN
1	A	4627	MET
1	A	4628	VAL
1	A	4633	GLU
1	A	4634	GLU
1	A	4636	THR
1	A	4651	THR
1	A	4673	ARG
1	A	4675	LYS
1	A	4676	GLU
1	A	4690	GLU
1	A	4697	VAL
1	A	4698	LYS
1	A	4707	ASN
1	A	4710	SER
1	A	4713	SER
1	A	4718	LYS
1	A	4725	LEU
1	A	4730	ASP
1	A	4731	ILE
1	A	4736	ARG
1	A	4737	ILE
1	A	4743	MET
1	A	4747	SER
1	A	4749	GLU
1	A	4750	ILE

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Mol	Chain	Res	Type
1	A	4813	LEU
1	A	4814	LEU
1	A	4818	MET
1	A	4821	LYS
1	A	4822	THR
1	A	4866	SER
1	A	4870	ASP
1	A	4871	GLU
1	A	4876	CYS
1	A	4879	MET
1	A	4880	MET
1	A	4882	CYS
1	A	4889	VAL
1	A	4902	GLU
1	A	4903	ASP
1	A	4907	ASP
1	A	4951	LYS
1	A	4956	THR
1	A	4957	LYS
1	A	4958	CYS
1	A	4971	THR
1	A	4980	LEU
1	A	4981	GLU
1	A	4989	MET
1	A	4992	LEU
1	A	4993	MET
1	A	4995	LEU
1	A	4997	ASN
1	A	4999	ASP
1	A	5001	THR
1	A	5008	SER
1	A	5010	VAL
1	A	5012	LYS
1	A	5027	CYS
1	A	5033	GLU
1	A	5034	ASP
1	A	5035	GLN
1	B	99	ARG
1	B	373	LYS
1	B	830	ARG
1	B	846	LEU
1	B	1534	LYS

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Mol	Chain	Res	Type
1	B	1743[A]	ARG
1	B	1743[B]	ARG
1	B	1752	ARG
1	B	2100[A]	HIS
1	B	2100[B]	HIS
1	B	2268[A]	GLN
1	B	2268[B]	GLN
1	B	2336	ARG
1	B	2369[A]	ARG
1	B	2369[B]	ARG
1	B	2738	ARG
1	B	2786	LYS
1	B	2806	ARG
1	B	2827	ARG
1	B	2914	LYS
1	B	3053	ARG
1	B	3225	ARG
1	B	3611	HIS
1	B	3622	LYS
1	B	3692	GLU
1	B	4180	ARG
1	B	4184	MET
1	B	4187	SER
1	B	4189	ARG
1	B	4191	GLU
1	B	4192	ARG
1	B	4200	THR
1	B	4204	GLN
1	B	4221	VAL
1	B	4245	MET
1	B	4246	GLN
1	B	4252	SER
1	B	4543	GLU
1	B	4544	LEU
1	B	4548	ARG
1	B	4556	SER
1	B	4563	ARG
1	B	4565	LEU
1	B	4569	LEU
1	B	4577	LEU
1	B	4580	TYR
1	B	4626	ASN

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Mol	Chain	Res	Type
1	B	4627	MET
1	B	4628	VAL
1	B	4633	GLU
1	B	4634	GLU
1	B	4636	THR
1	B	4651	THR
1	B	4673	ARG
1	B	4675	LYS
1	B	4676	GLU
1	B	4690	GLU
1	B	4697	VAL
1	B	4698	LYS
1	B	4707	ASN
1	B	4710	SER
1	B	4713	SER
1	B	4718	LYS
1	B	4725	LEU
1	B	4730	ASP
1	B	4731	ILE
1	B	4736	ARG
1	B	4737	ILE
1	B	4743	MET
1	B	4747	SER
1	B	4749	GLU
1	B	4750	ILE
1	B	4813	LEU
1	B	4814	LEU
1	B	4818	MET
1	B	4821	LYS
1	B	4822	THR
1	B	4866	SER
1	B	4870	ASP
1	B	4871	GLU
1	B	4876	CYS
1	B	4879	MET
1	B	4880	MET
1	B	4882	CYS
1	B	4889	VAL
1	B	4902	GLU
1	B	4903	ASP
1	B	4907	ASP
1	B	4951	LYS

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Mol	Chain	Res	Type
1	B	4956	THR
1	B	4957	LYS
1	B	4958	CYS
1	B	4971	THR
1	B	4980	LEU
1	B	4981	GLU
1	B	4989	MET
1	B	4992	LEU
1	B	4993	MET
1	B	4995	LEU
1	B	4997	ASN
1	B	4999	ASP
1	B	5001	THR
1	B	5008	SER
1	B	5010	VAL
1	B	5012	LYS
1	B	5027	CYS
1	B	5033	GLU
1	B	5034	ASP
1	B	5035	GLN
1	C	99	ARG
1	C	373	LYS
1	C	830	ARG
1	C	846	LEU
1	C	1534	LYS
1	C	1743[A]	ARG
1	C	1743[B]	ARG
1	C	1752	ARG
1	C	2100[A]	HIS
1	C	2100[B]	HIS
1	C	2268[A]	GLN
1	C	2268[B]	GLN
1	C	2336	ARG
1	C	2369[A]	ARG
1	C	2369[B]	ARG
1	C	2738	ARG
1	C	2786	LYS
1	C	2806	ARG
1	C	2827	ARG
1	C	2914	LYS
1	C	3053	ARG
1	C	3225	ARG

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Mol	Chain	Res	Type
1	C	3611	HIS
1	C	3622	LYS
1	C	3692	GLU
1	C	4180	ARG
1	C	4184	MET
1	C	4187	SER
1	C	4189	ARG
1	C	4191	GLU
1	C	4192	ARG
1	C	4200	THR
1	C	4204	GLN
1	C	4221	VAL
1	C	4245	MET
1	C	4246	GLN
1	C	4252	SER
1	C	4543	GLU
1	C	4544	LEU
1	C	4548	ARG
1	C	4556	SER
1	C	4563	ARG
1	C	4565	LEU
1	C	4569	LEU
1	C	4577	LEU
1	C	4580	TYR
1	C	4626	ASN
1	C	4627	MET
1	C	4628	VAL
1	C	4633	GLU
1	C	4634	GLU
1	C	4636	THR
1	C	4651	THR
1	C	4673	ARG
1	C	4675	LYS
1	C	4676	GLU
1	C	4690	GLU
1	C	4697	VAL
1	C	4698	LYS
1	C	4707	ASN
1	C	4710	SER
1	C	4713	SER
1	C	4718	LYS
1	C	4725	LEU

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Mol	Chain	Res	Type
1	C	4730	ASP
1	C	4731	ILE
1	C	4736	ARG
1	C	4737	ILE
1	C	4743	MET
1	C	4747	SER
1	C	4749	GLU
1	C	4750	ILE
1	C	4813	LEU
1	C	4814	LEU
1	C	4818	MET
1	C	4821	LYS
1	C	4822	THR
1	C	4866	SER
1	C	4870	ASP
1	C	4871	GLU
1	C	4876	CYS
1	C	4879	MET
1	C	4880	MET
1	C	4882	CYS
1	C	4889	VAL
1	C	4902	GLU
1	C	4903	ASP
1	C	4907	ASP
1	C	4951	LYS
1	C	4956	THR
1	C	4957	LYS
1	C	4958	CYS
1	C	4971	THR
1	C	4980	LEU
1	C	4981	GLU
1	C	4989	MET
1	C	4992	LEU
1	C	4993	MET
1	C	4995	LEU
1	C	4997	ASN
1	C	4999	ASP
1	C	5001	THR
1	C	5008	SER
1	C	5010	VAL
1	C	5012	LYS
1	C	5027	CYS

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Mol	Chain	Res	Type
1	C	5033	GLU
1	C	5034	ASP
1	C	5035	GLN
1	D	99	ARG
1	D	373	LYS
1	D	830	ARG
1	D	846	LEU
1	D	1534	LYS
1	D	1743[A]	ARG
1	D	1743[B]	ARG
1	D	1752	ARG
1	D	2100[A]	HIS
1	D	2100[B]	HIS
1	D	2268[A]	GLN
1	D	2268[B]	GLN
1	D	2336	ARG
1	D	2369[A]	ARG
1	D	2369[B]	ARG
1	D	2738	ARG
1	D	2786	LYS
1	D	2806	ARG
1	D	2827	ARG
1	D	2914	LYS
1	D	3053	ARG
1	D	3225	ARG
1	D	3611	HIS
1	D	3622	LYS
1	D	3692	GLU
1	D	4180	ARG
1	D	4184	MET
1	D	4187	SER
1	D	4189	ARG
1	D	4191	GLU
1	D	4192	ARG
1	D	4200	THR
1	D	4204	GLN
1	D	4221	VAL
1	D	4245	MET
1	D	4246	GLN
1	D	4252	SER
1	D	4543	GLU
1	D	4544	LEU

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Mol	Chain	Res	Type
1	D	4548	ARG
1	D	4556	SER
1	D	4563	ARG
1	D	4565	LEU
1	D	4569	LEU
1	D	4577	LEU
1	D	4580	TYR
1	D	4626	ASN
1	D	4627	MET
1	D	4628	VAL
1	D	4633	GLU
1	D	4634	GLU
1	D	4636	THR
1	D	4651	THR
1	D	4673	ARG
1	D	4675	LYS
1	D	4676	GLU
1	D	4690	GLU
1	D	4697	VAL
1	D	4698	LYS
1	D	4707	ASN
1	D	4710	SER
1	D	4713	SER
1	D	4718	LYS
1	D	4725	LEU
1	D	4730	ASP
1	D	4731	ILE
1	D	4736	ARG
1	D	4737	ILE
1	D	4743	MET
1	D	4747	SER
1	D	4749	GLU
1	D	4750	ILE
1	D	4813	LEU
1	D	4814	LEU
1	D	4818	MET
1	D	4821	LYS
1	D	4822	THR
1	D	4866	SER
1	D	4870	ASP
1	D	4871	GLU
1	D	4876	CYS

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Mol	Chain	Res	Type
1	D	4879	MET
1	D	4880	MET
1	D	4882	CYS
1	D	4889	VAL
1	D	4902	GLU
1	D	4903	ASP
1	D	4907	ASP
1	D	4951	LYS
1	D	4956	THR
1	D	4957	LYS
1	D	4958	CYS
1	D	4971	THR
1	D	4980	LEU
1	D	4981	GLU
1	D	4989	MET
1	D	4992	LEU
1	D	4993	MET
1	D	4995	LEU
1	D	4997	ASN
1	D	4999	ASP
1	D	5001	THR
1	D	5008	SER
1	D	5010	VAL
1	D	5012	LYS
1	D	5027	CYS
1	D	5033	GLU
1	D	5034	ASP
1	D	5035	GLN
2	E	25	HIS
2	F	25	HIS
2	G	25	HIS
2	H	25	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	475	GLN
1	A	533	ASN
1	A	624	ASN
1	A	877	ASN
1	A	2127	GLN
1	A	2247	GLN

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Mol	Chain	Res	Type
1	A	2872	GLN
1	A	2971	GLN
1	A	3052	HIS
1	A	3419	ASN
1	A	3766	GLN
1	A	3895	HIS
1	A	4201	ASN
1	A	4805	ASN
1	A	5003	HIS
1	A	5035	GLN
1	B	475	GLN
1	B	533	ASN
1	B	624	ASN
1	B	877	ASN
1	B	2127	GLN
1	B	2247	GLN
1	B	2872	GLN
1	B	2971	GLN
1	B	3052	HIS
1	B	3419	ASN
1	B	3766	GLN
1	B	3895	HIS
1	B	4201	ASN
1	B	4805	ASN
1	B	5003	HIS
1	B	5035	GLN
1	C	475	GLN
1	C	533	ASN
1	C	624	ASN
1	C	877	ASN
1	C	2127	GLN
1	C	2247	GLN
1	C	2872	GLN
1	C	2971	GLN
1	C	3052	HIS
1	C	3419	ASN
1	C	3766	GLN
1	C	3895	HIS
1	C	4201	ASN
1	C	4805	ASN
1	C	5003	HIS
1	C	5035	GLN

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Mol	Chain	Res	Type
1	D	475	GLN
1	D	533	ASN
1	D	624	ASN
1	D	877	ASN
1	D	2127	GLN
1	D	2247	GLN
1	D	2872	GLN
1	D	2971	GLN
1	D	3052	HIS
1	D	3419	ASN
1	D	3766	GLN
1	D	3895	HIS
1	D	4201	ASN
1	D	4805	ASN
1	D	5003	HIS
1	D	5035	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 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
3	ADN	D	5101	-	17,21,21	0.72	0	17,31,31	0.80	1 (5%)
3	ADN	A	5101	-	17,21,21	0.72	0	17,31,31	0.79	1 (5%)
3	ADN	B	5101	-	17,21,21	0.72	0	17,31,31	0.79	1 (5%)
3	ADN	C	5101	-	17,21,21	0.72	0	17,31,31	0.79	1 (5%)

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
3	ADN	D	5101	-	-	2/2/22/22	0/3/3/3
3	ADN	A	5101	-	-	2/2/22/22	0/3/3/3
3	ADN	B	5101	-	-	2/2/22/22	0/3/3/3
3	ADN	C	5101	-	-	2/2/22/22	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	5101	ADN	C5-C6-N6	2.26	123.75	120.31
3	A	5101	ADN	C5-C6-N6	2.26	123.75	120.31
3	C	5101	ADN	C5-C6-N6	2.26	123.75	120.31
3	B	5101	ADN	C5-C6-N6	2.26	123.75	120.31

There are no chirality outliers.

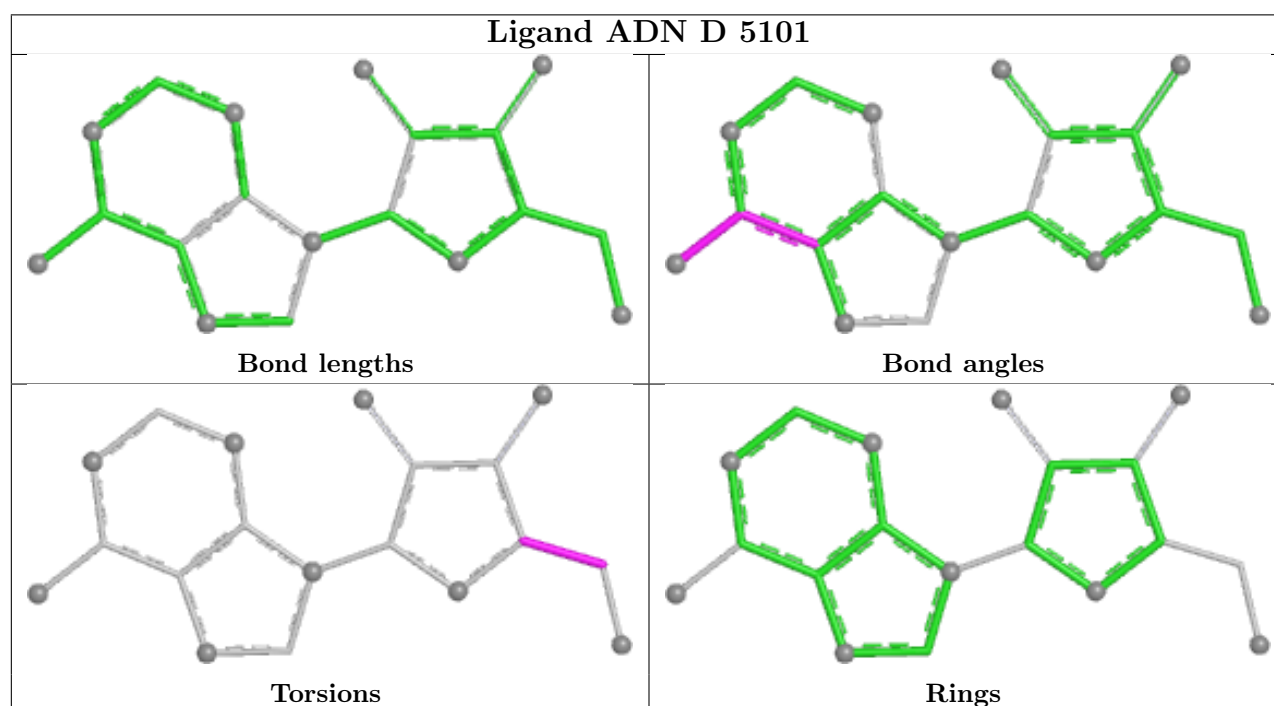
All (8) torsion outliers are listed below:

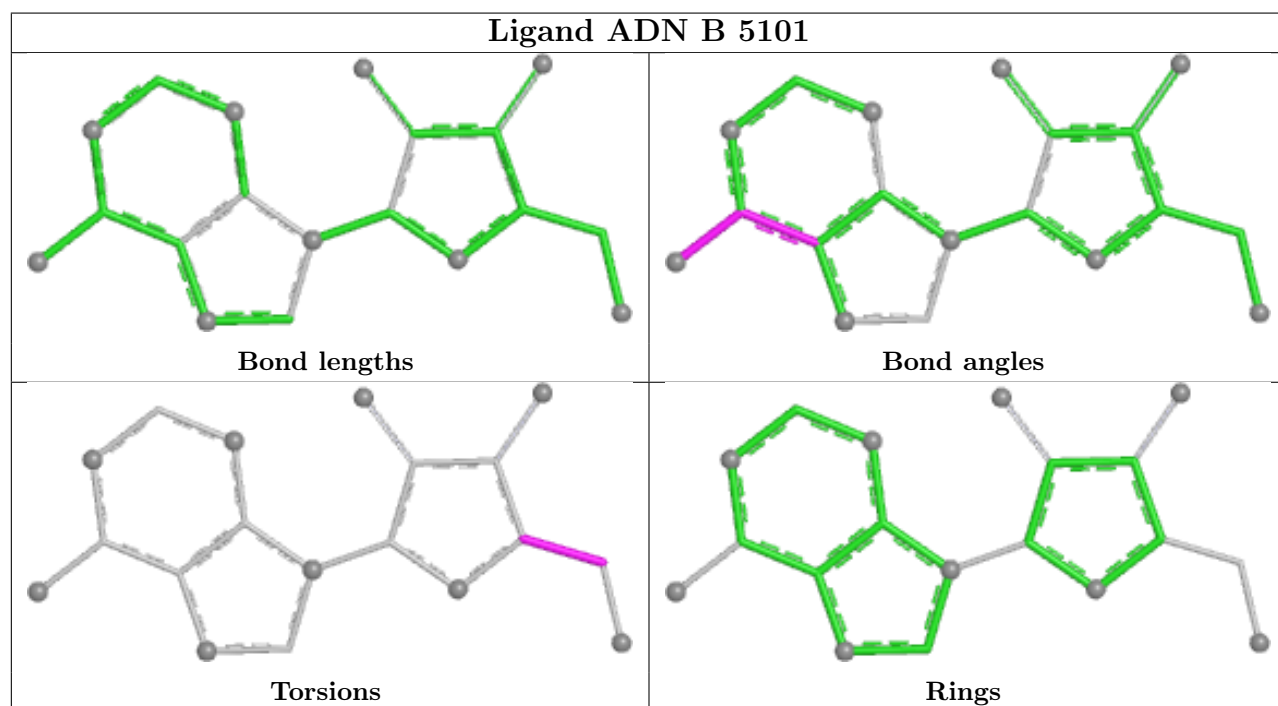
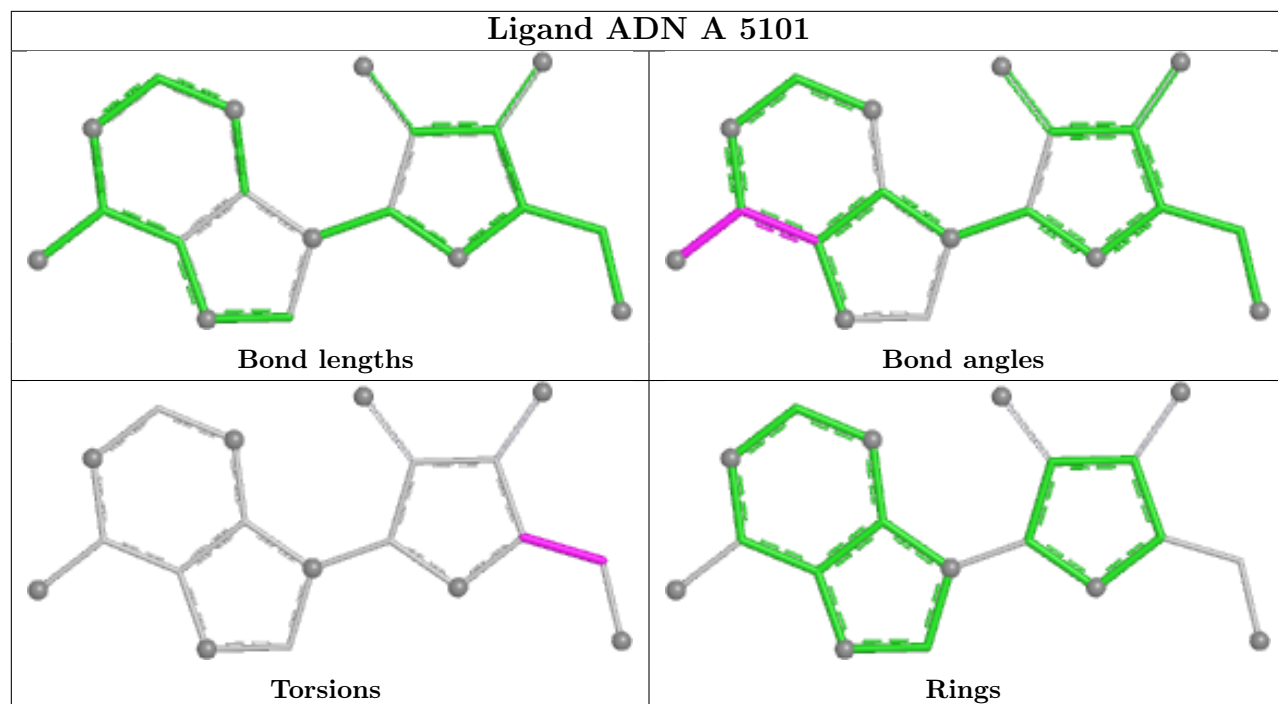
Mol	Chain	Res	Type	Atoms
3	A	5101	ADN	C3'-C4'-C5'-O5'
3	B	5101	ADN	C3'-C4'-C5'-O5'
3	C	5101	ADN	C3'-C4'-C5'-O5'
3	D	5101	ADN	C3'-C4'-C5'-O5'
3	A	5101	ADN	O4'-C4'-C5'-O5'
3	B	5101	ADN	O4'-C4'-C5'-O5'
3	C	5101	ADN	O4'-C4'-C5'-O5'
3	D	5101	ADN	O4'-C4'-C5'-O5'

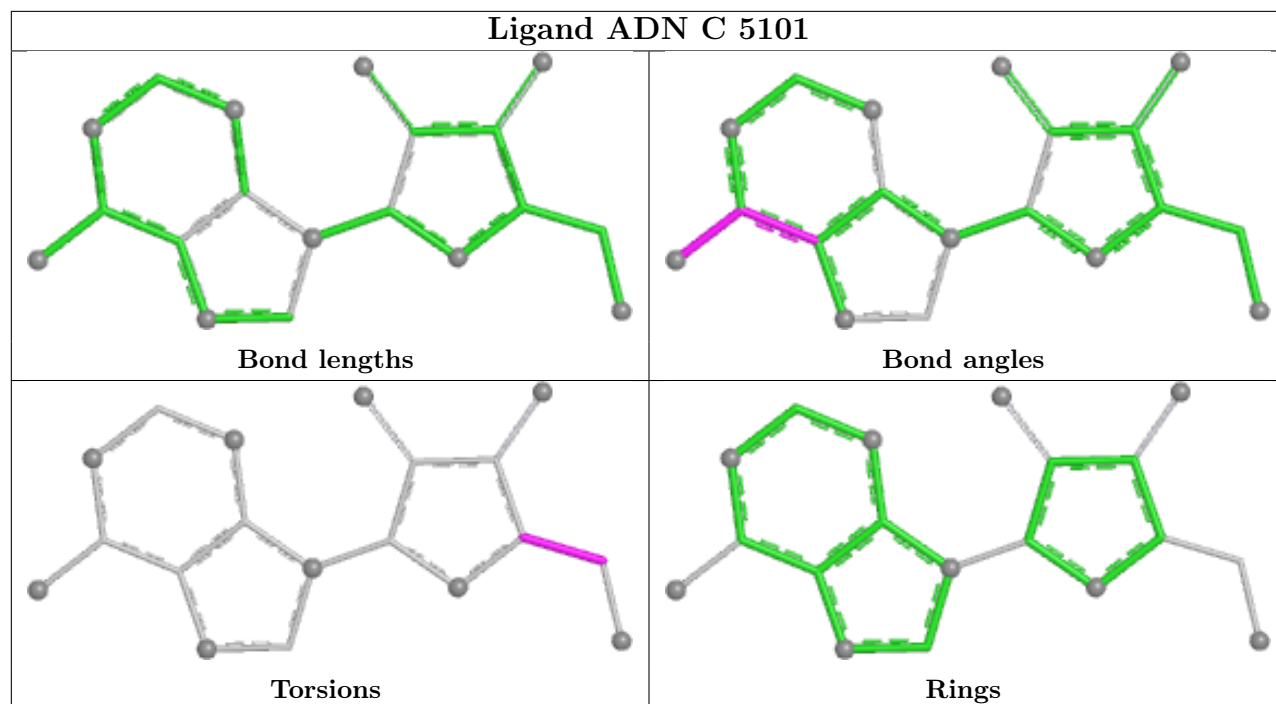
There are no ring outliers.

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.

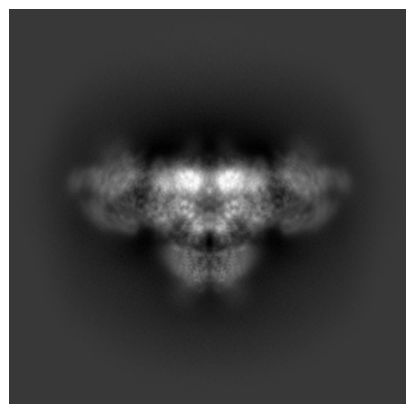
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40426. These allow visual inspection of the internal detail of the map and identification of artifacts.

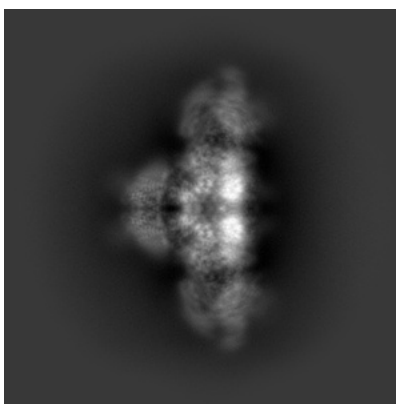
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

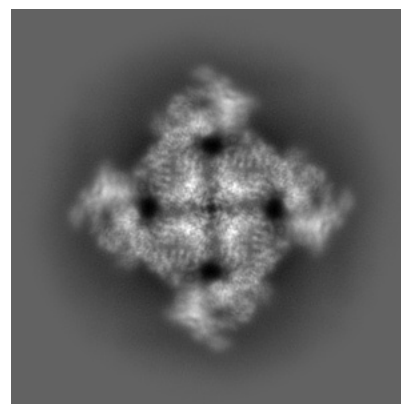
6.1.1 Primary map



X

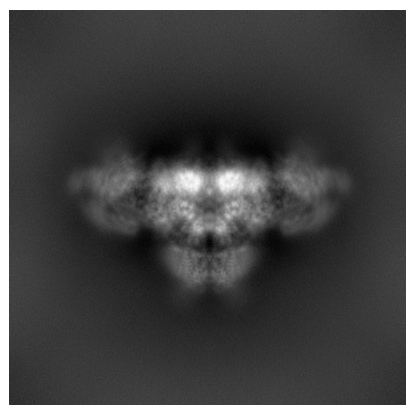


Y

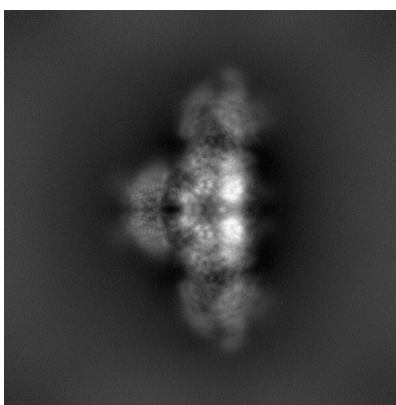


Z

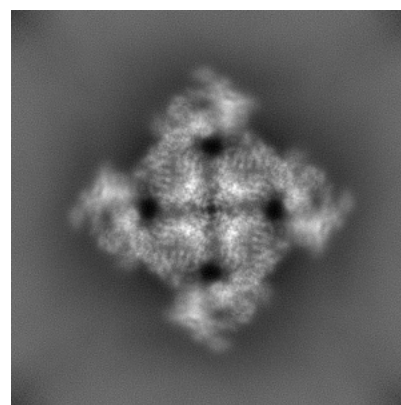
6.1.2 Raw map



X



Y

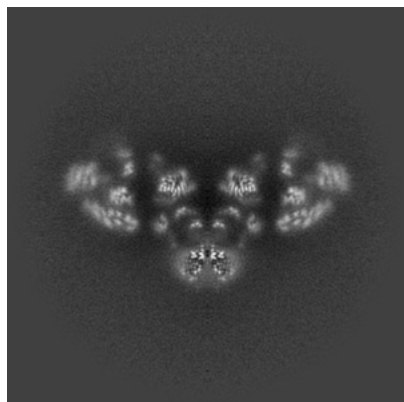


Z

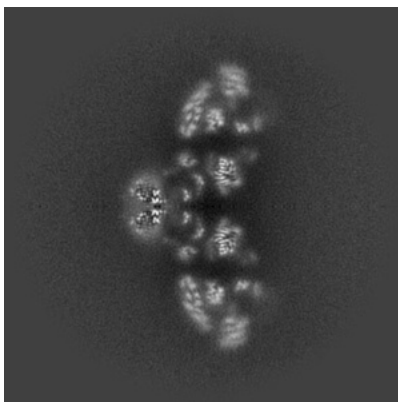
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

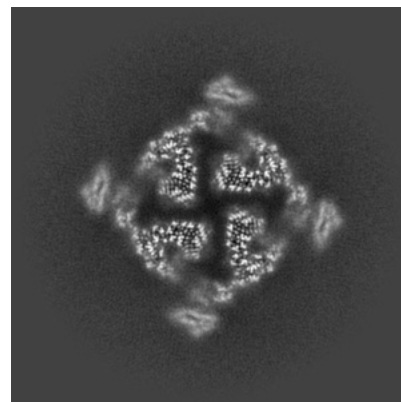
6.2.1 Primary map



X Index: 200

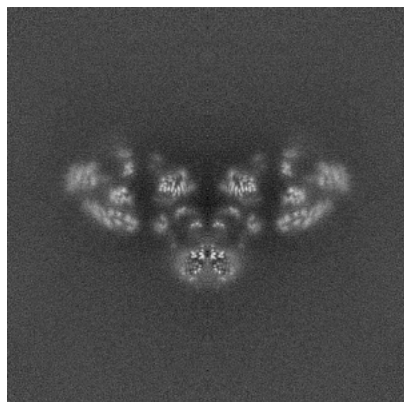


Y Index: 200

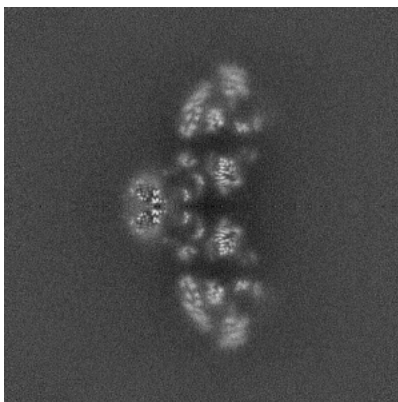


Z Index: 200

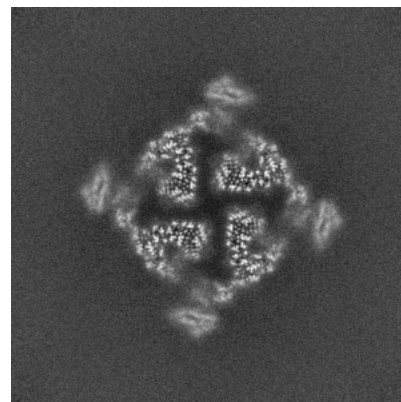
6.2.2 Raw map



X Index: 200



Y Index: 200

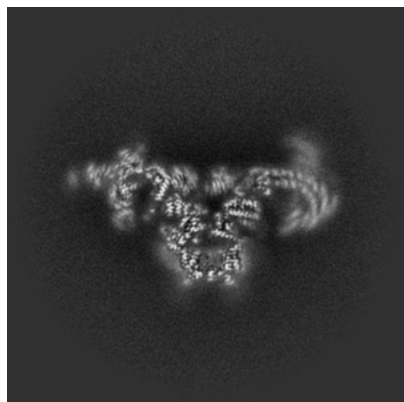


Z Index: 200

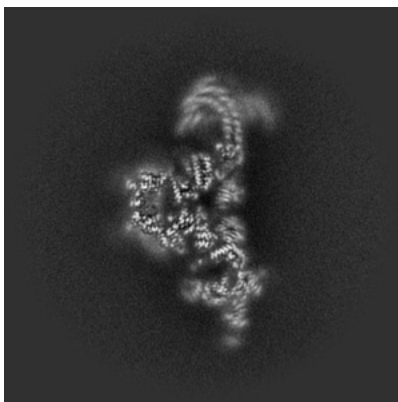
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

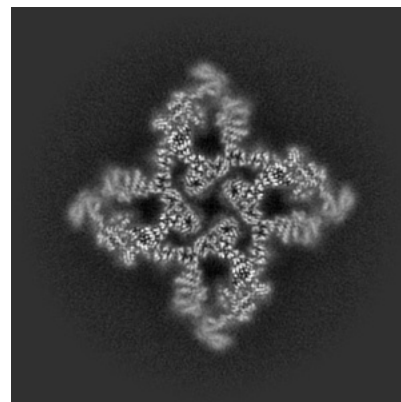
6.3.1 Primary map



X Index: 218

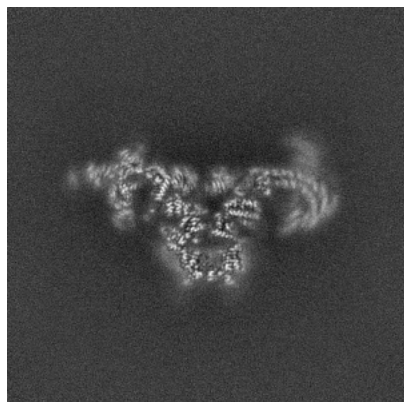


Y Index: 182

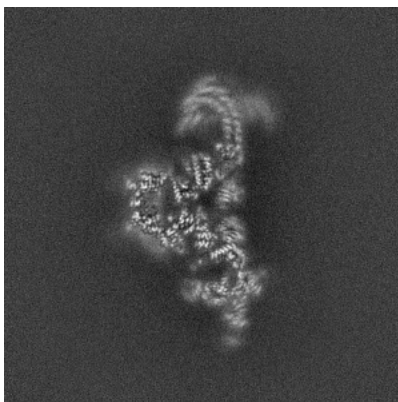


Z Index: 225

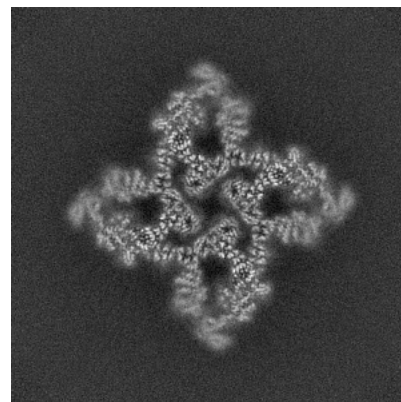
6.3.2 Raw map



X Index: 218



Y Index: 182

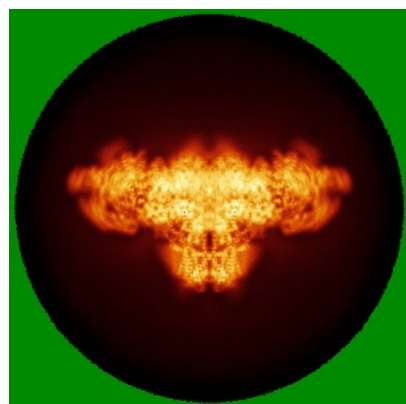


Z Index: 225

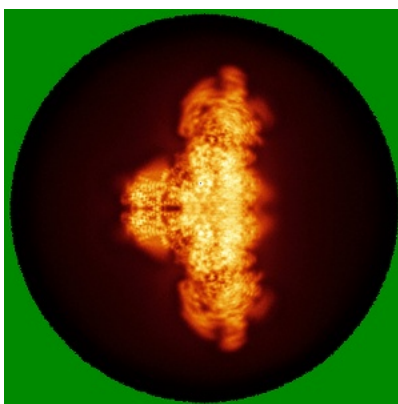
The images above show the largest variance slices of the map in three orthogonal directions.

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

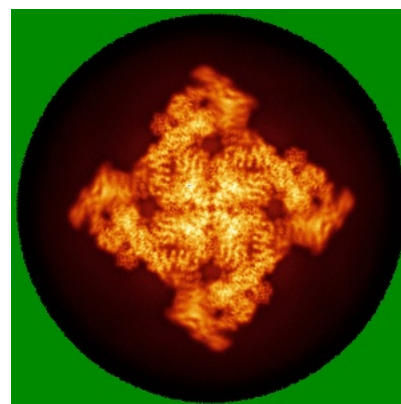
6.4.1 Primary map



X

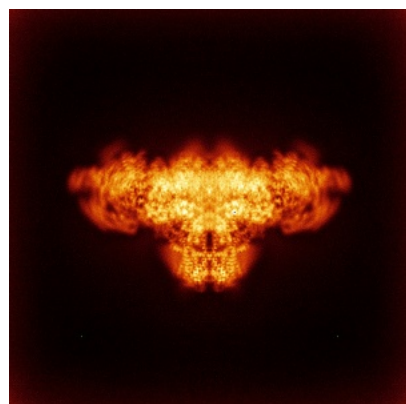


Y

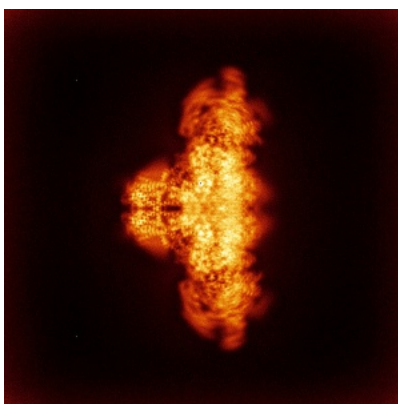


Z

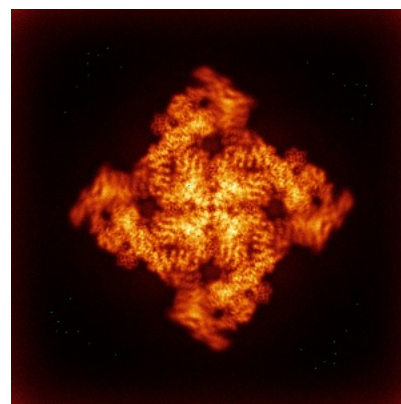
6.4.2 Raw map



X



Y

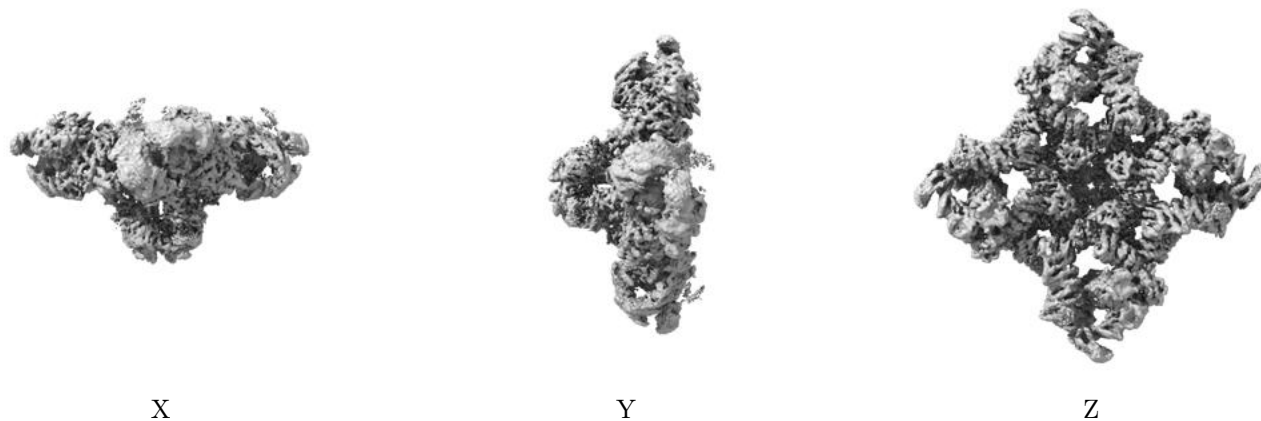


Z

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

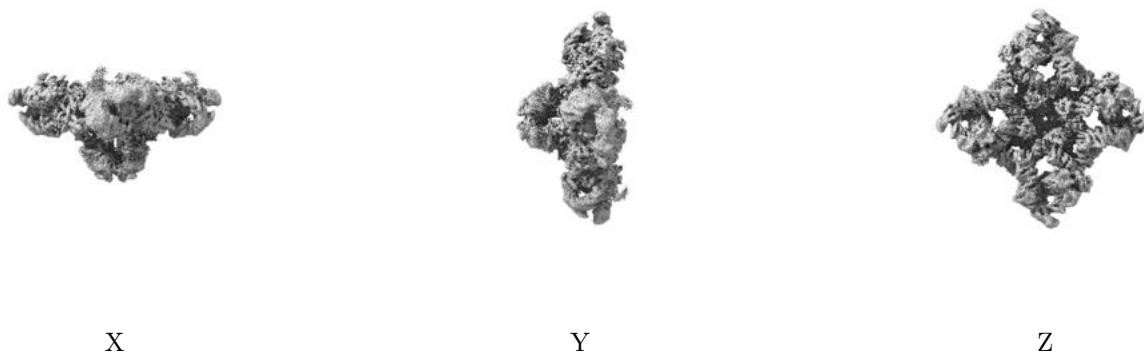
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.387. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

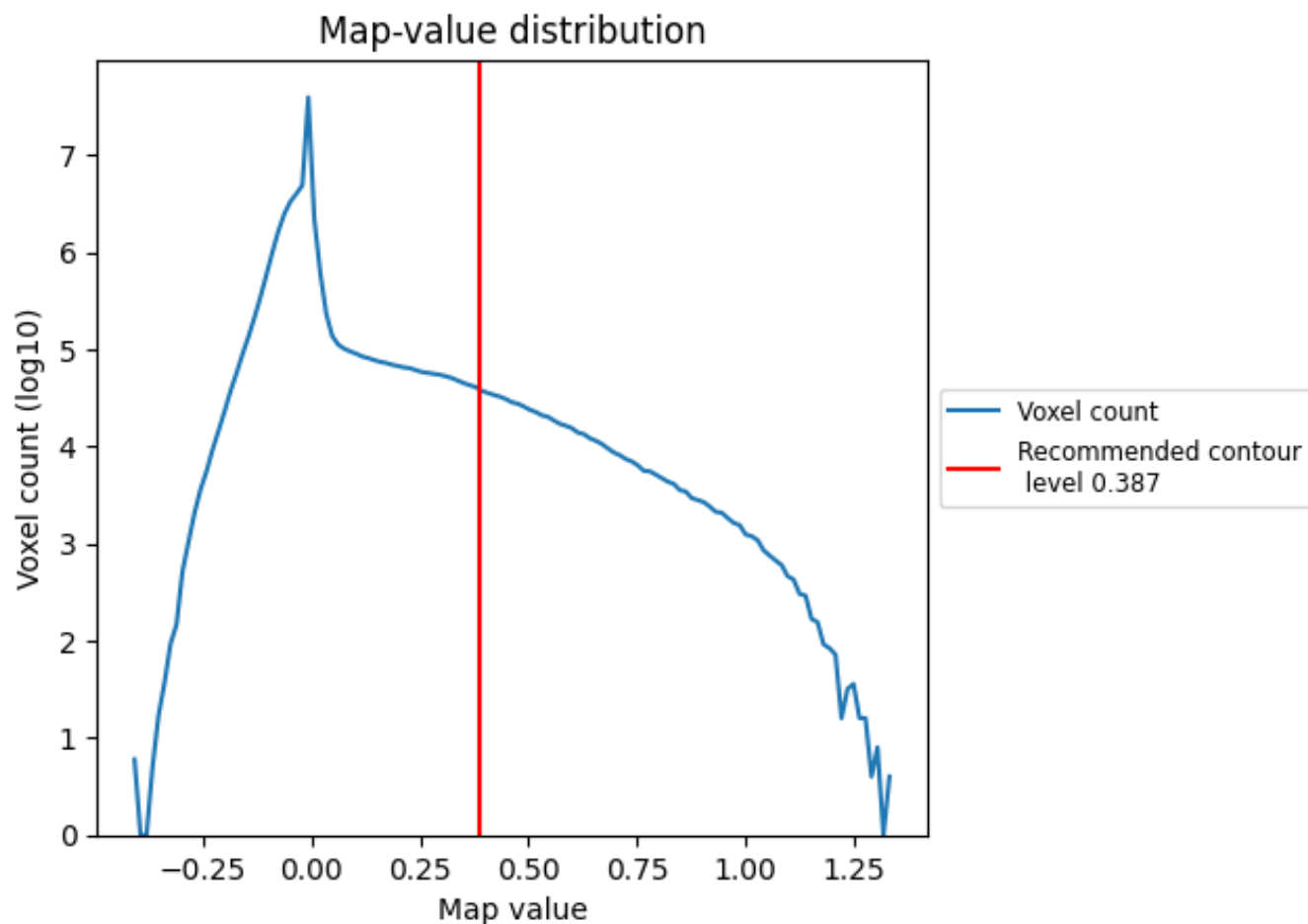
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

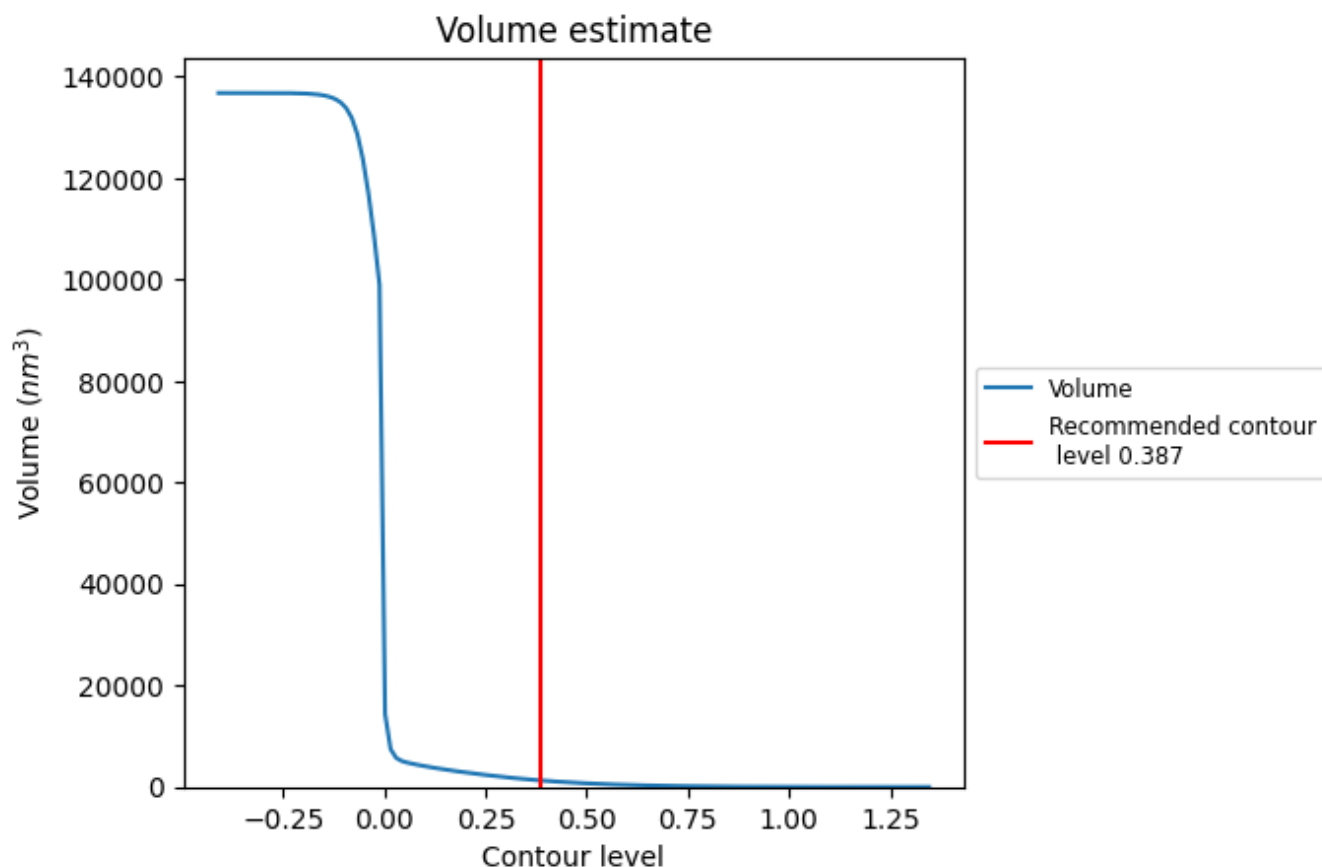
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

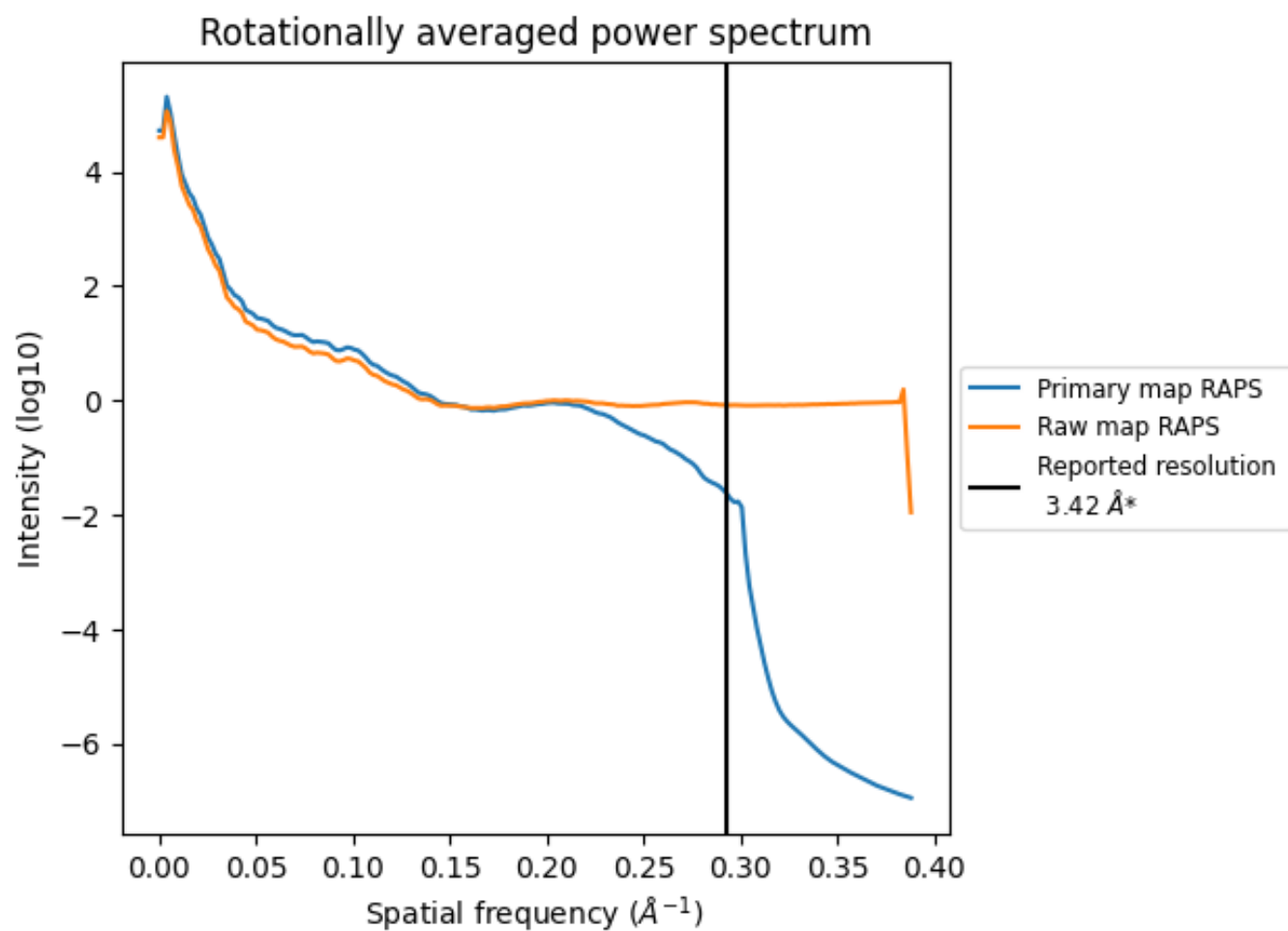
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1280 nm^3 ; this corresponds to an approximate mass of 1156 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 ⓘ

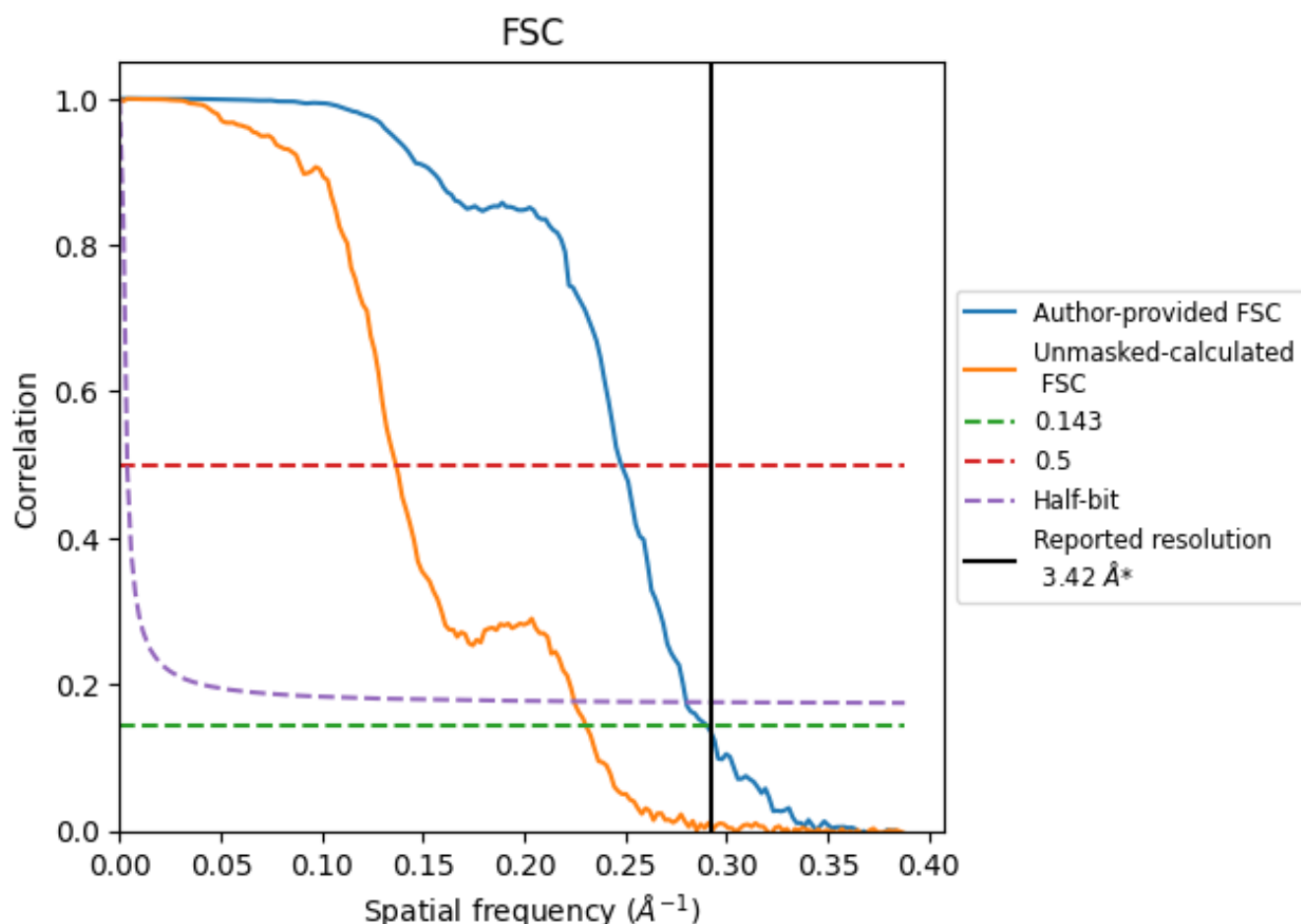


*Reported resolution corresponds to spatial frequency of 0.292 \AA^{-1}

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 0.292 \AA^{-1}

8.2 Resolution estimates [i](#)

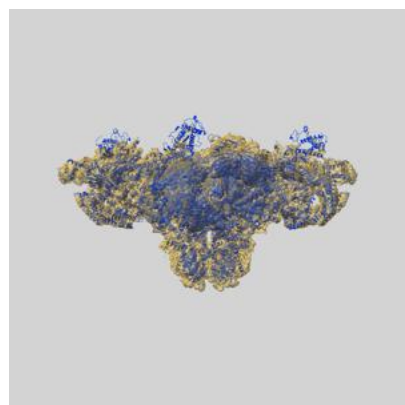
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.42	-	-
Author-provided FSC curve	3.44	4.03	3.57
Unmasked-calculated*	4.33	7.32	4.45

*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 4.33 differs from the reported value 3.42 by more than 10 %

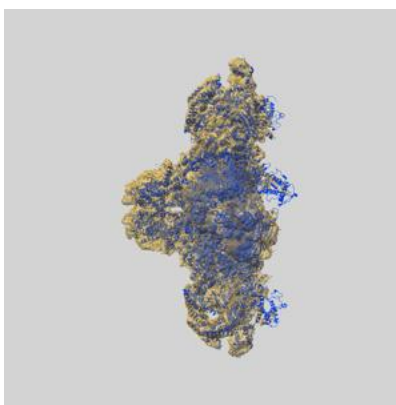
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-40426 and PDB model 8SER. Per-residue inclusion information can be found in section [3](#) on page [8](#).

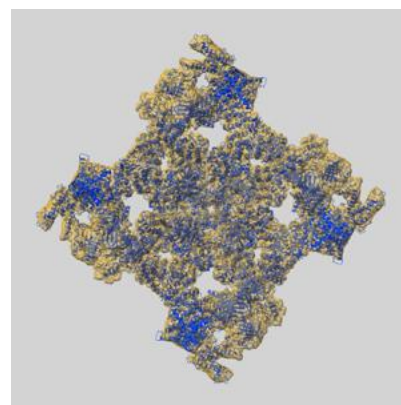
9.1 Map-model overlay [i](#)



X



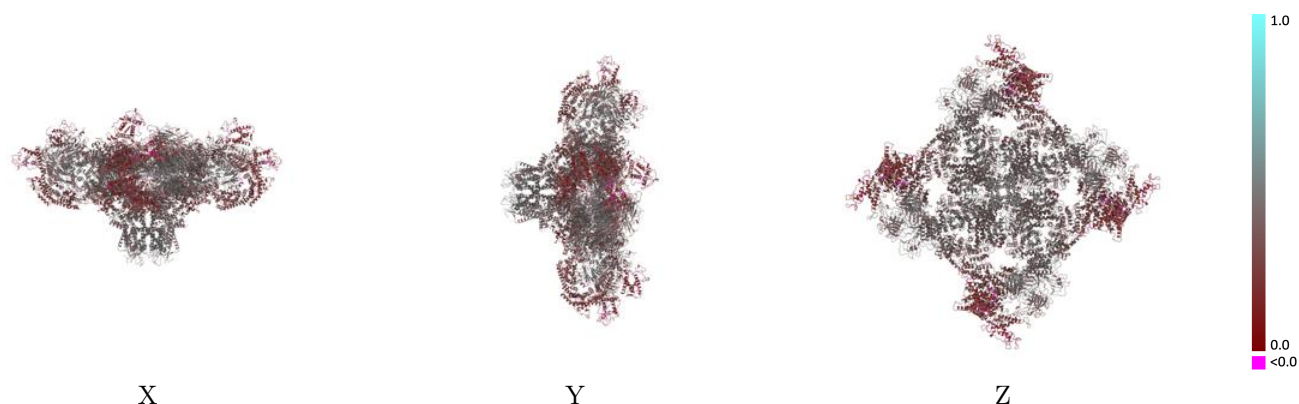
Y



Z

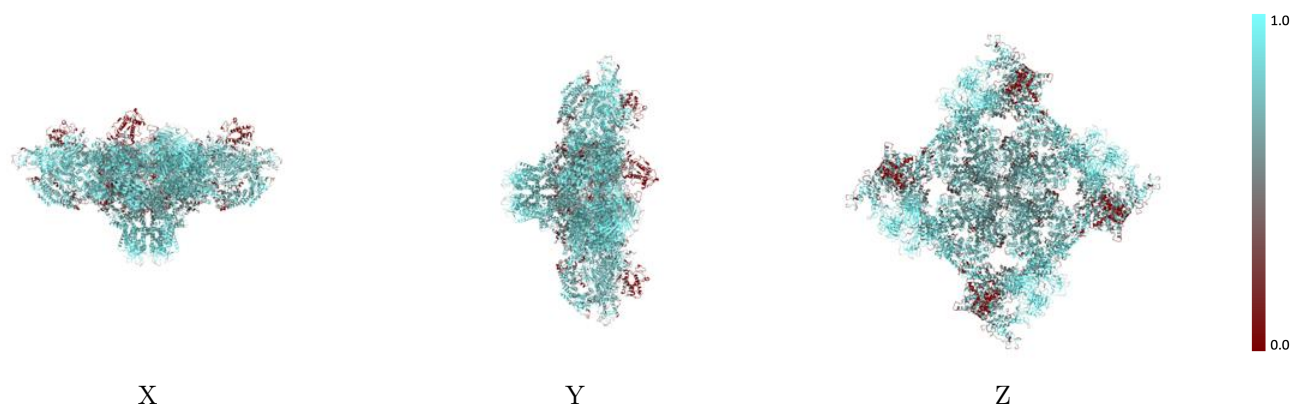
The images above show the 3D surface view of the map at the recommended contour level 0.387 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



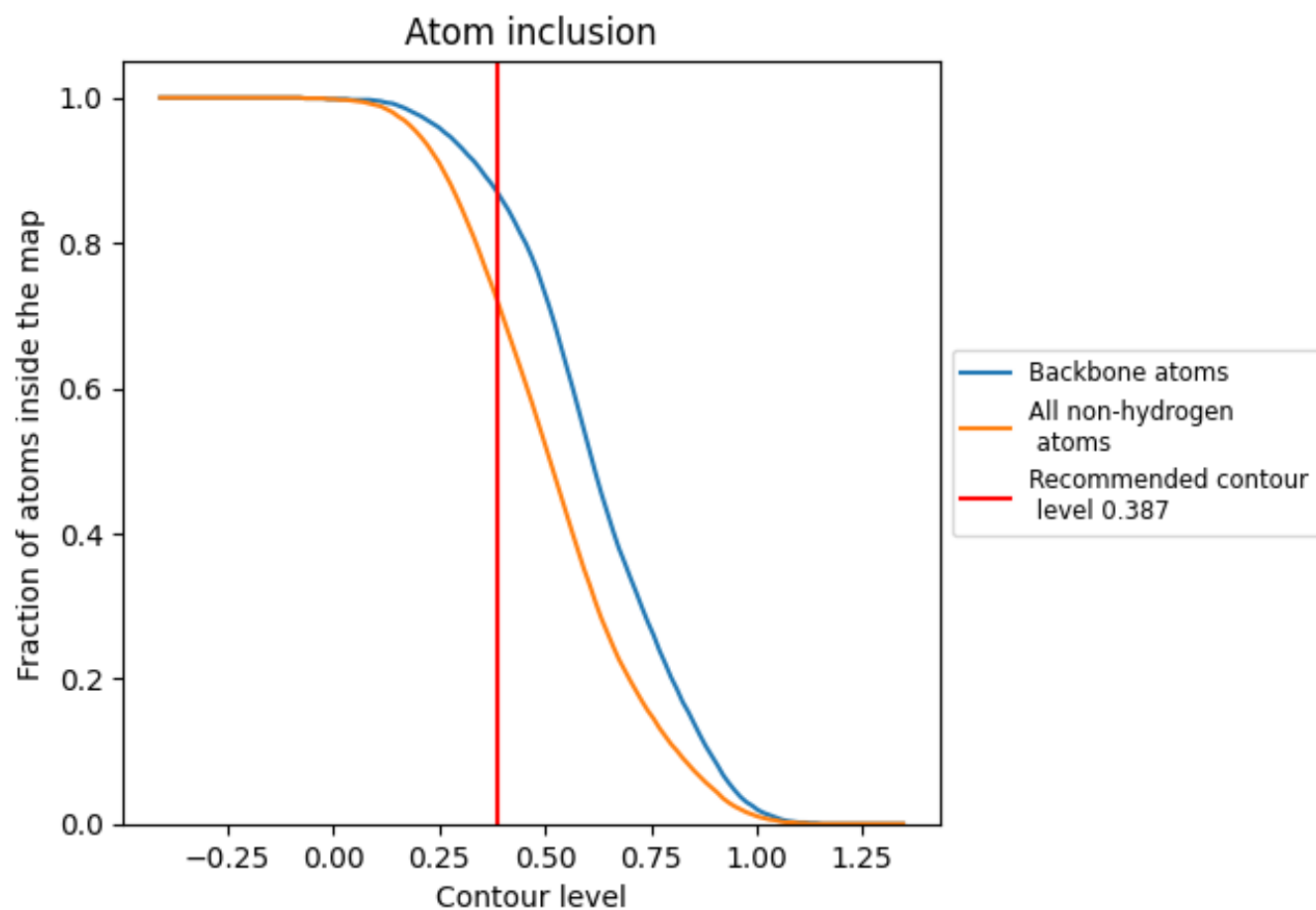
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.387).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 72% 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 (0.387) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7210	<div></div> 0.3530
A	<div></div> 0.7170	<div></div> 0.3510
B	<div></div> 0.7170	<div></div> 0.3510
C	<div></div> 0.7170	<div></div> 0.3510
D	<div></div> 0.7170	<div></div> 0.3520
E	<div></div> 0.8730	<div></div> 0.4230
F	<div></div> 0.8730	<div></div> 0.4230
G	<div></div> 0.8730	<div></div> 0.4240
H	<div></div> 0.8730	<div></div> 0.4250

1.0

0.0

<0.0