



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 11:38 AM UTC

PDB ID : 8SEO / pdb_00008seo
EMDB ID : EMD-40423
Title : Cryo-EM Structure of RyR1 + ATP-gamma-S
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 : 3.92 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:

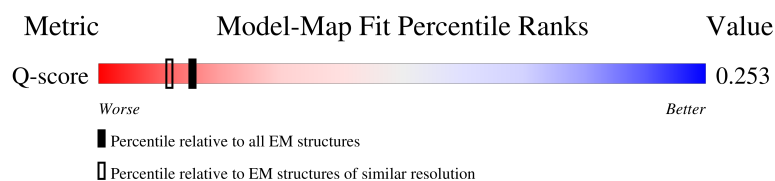
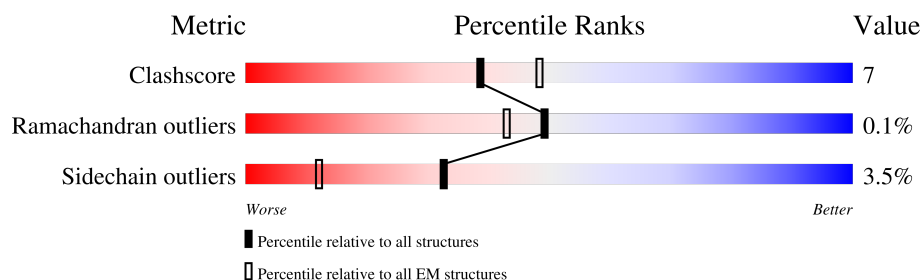
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.92 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7862 (3.42 - 4.42)

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	 13% 68% 18% • 13%
1	B	5037	 13% 68% 18% • 13%
1	C	5037	 13% 68% 19% • 13%
1	D	5037	 13% 68% 18% • 13%

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Mol	Chain	Length	Quality of chain
2	E	350	27% 69%
2	F	350	27% 69%
2	G	350	26% 69%
2	H	350	27% 69%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 143016 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
			34904	22206	6023	6439	236		
1	B	4376	Total	C	N	O	S	9	0
			34904	22206	6023	6439	236		
1	C	4376	Total	C	N	O	S	9	0
			34904	22206	6023	6439	236		
1	D	4376	Total	C	N	O	S	9	0
			34904	22206	6023	6439	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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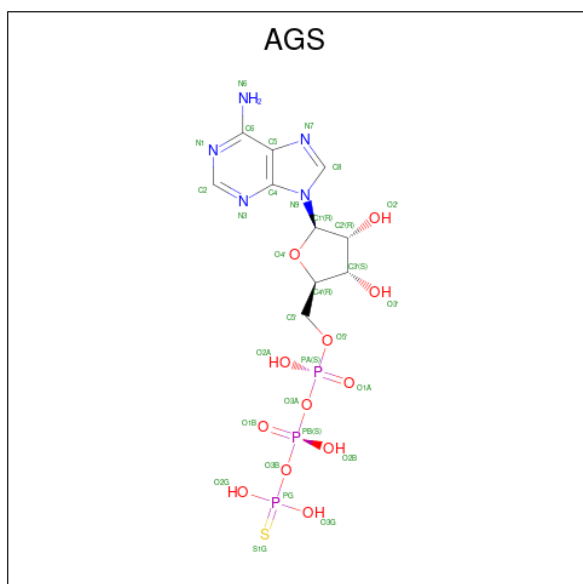
Chain	Residue	Modelled	Actual	Comment	Reference
G	-242	MET	-	expression tag	UNP P08515
G	-241	LYS	-	expression tag	UNP P08515
G	-240	SER	-	expression tag	UNP P08515
G	-239	SER	-	expression tag	UNP P08515
G	-238	HIS	-	expression tag	UNP P08515
G	-237	HIS	-	expression tag	UNP P08515
G	-236	HIS	-	expression 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 PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	C	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

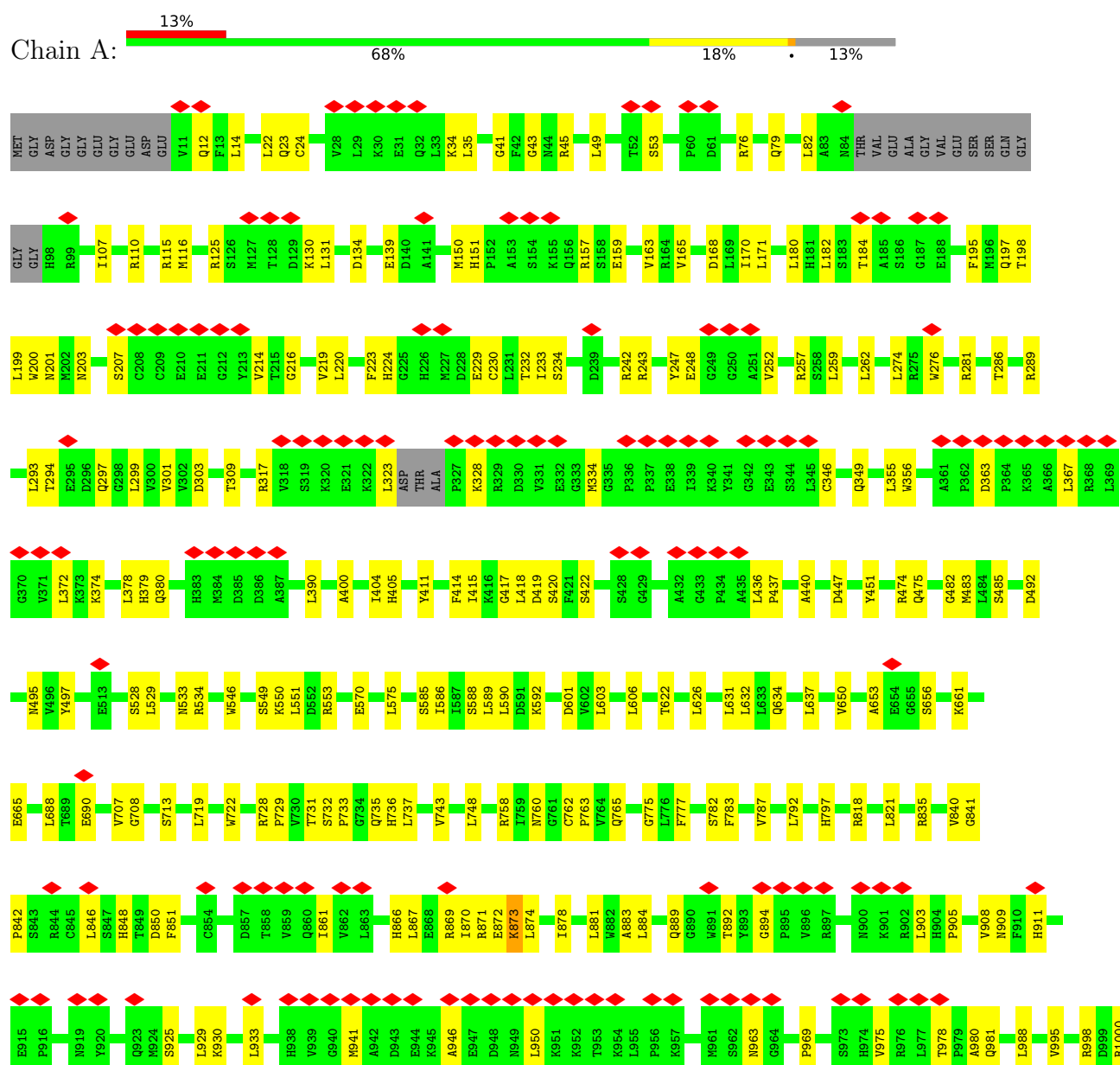
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

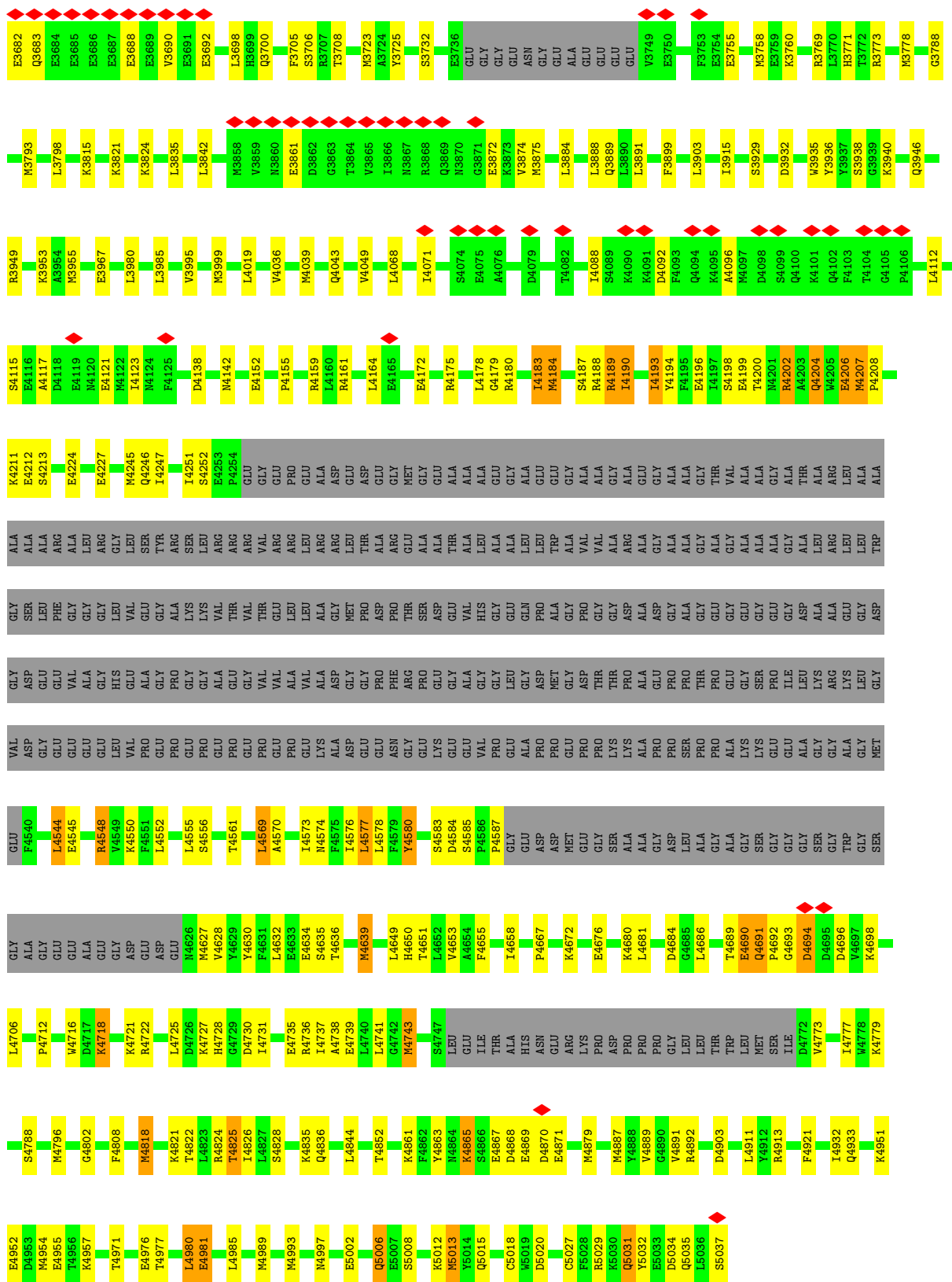
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

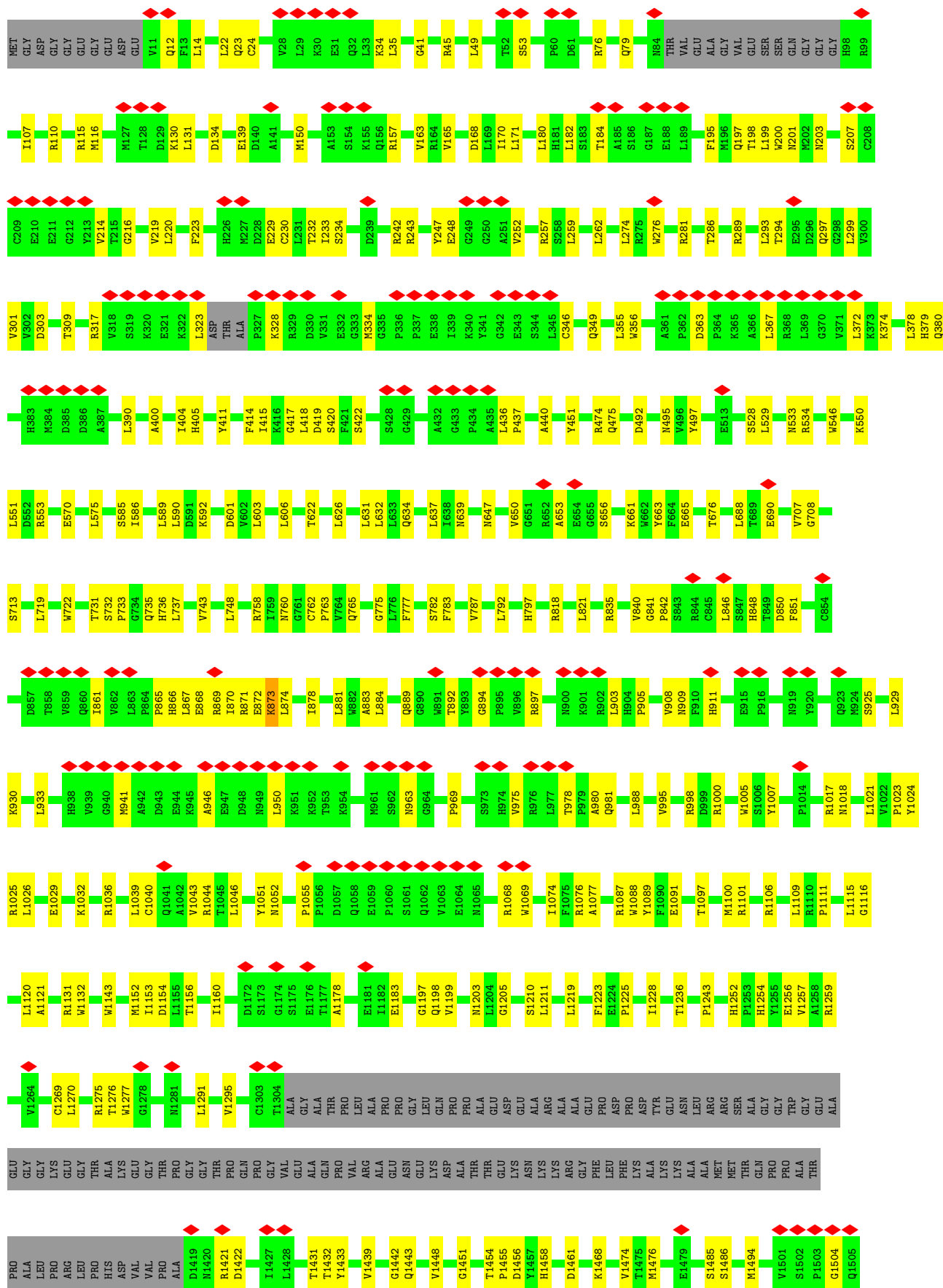
• Molecule 1: Ryanodine receptor 1





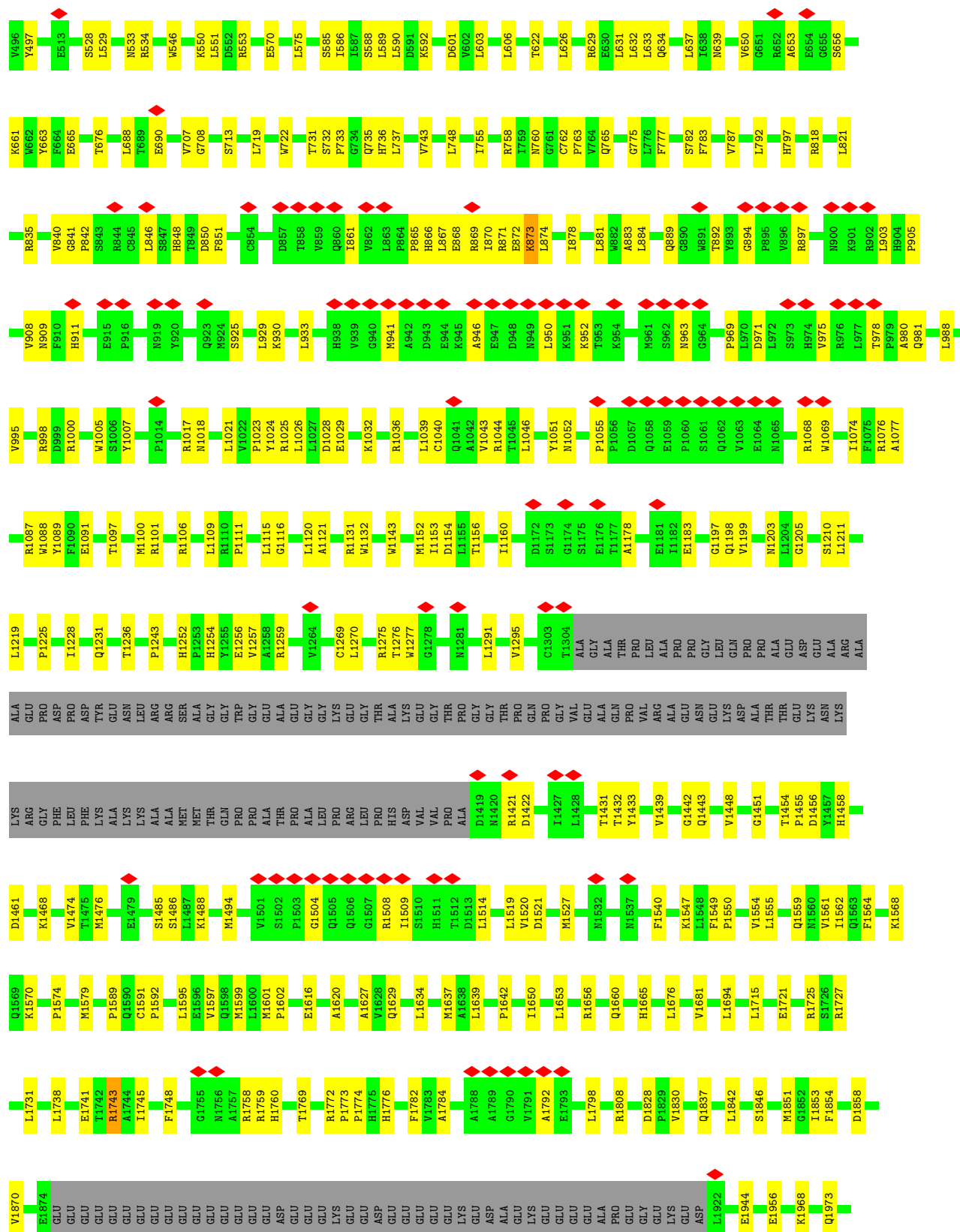
D3587	D3588	P3589	I3592	R3499	Y3415	V3416	R3420	W3423	L3424	F3435	R3436	K3437	T3443	Y3444	W3445	F3451	E3454	N3457	F3458	V3459	V3460	Q3461	N3465	N3466	M3467	S3468	F3469	L3470	T3471	A3472	D3473	S3474	K3475	S3476	L3477	K3478	A3479	LYS	ALA	GLY	ASP	ALA	GLN	SER	GLY	GLY	SER	ASP	GLN	GLU	ARG	THR	LYS	LYS	L3498	R3499	G3500	D3501	R3502	Y3503	S3504	V3505	Q3506	R3507	S3508	L3509	I3510	V3511	K3515	K3516	M3517	N3523	M3524	D3531	L3532	I3533	M3534	K3537	T3538	A3541	L3542	R3543	D3544	N3555	N3556	L3557	H3558	L3559	Q3560	G3561	V3562	V3563	E3564	G3565	S3566	L3569	L3575	V3576	R3577	P3580	G3581	E3582	E3583	E3584	D3585	A3586																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
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E2870	L2871	Q2872	A2873	K2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884	T2885	K2886	G2887	R2888	K2889	K2890	K2891	K2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	V2908	D2909	T2910	L2911	T2912	A2913	E2915	K2916	A2917	K2918	D2919	K2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929																																																																																																																																																																																																																																																																																																																																																																																																																																		
K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	A2818	V2819	E2820	V2821	L2822	L2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	GLU	ARG	THR	GLU	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	T2866	Y2867	S2868	R2869																																																																																																																																																																																																																																																																																																																																																																																																																																		
R2624	V2627	F2628	L2643	P2658	V2666	T2667	S2668	L2674	K2677	L2678	H2688	L2695	A2699	L2703	V2715	D2716	Y2719	S2720	S2721	K2722	A2723	E2724	K2725	LYS	ALA	THR	VAL	ASP	ALA	GLU	GLY	N2734	F2735	D2736	P2737	R2738	P2739	V2740	E2741	T2742	L2743	N2744	V2745	I2746	I2747	P2748	E2749																																																																																																																																																																																																																																																																																																																																																																																																																																													
K2750	L2751	D2752	S2753	F2754	I2755	N2756	K2757	F2758	A2759	E2760	Y2761	T2762	H2763	E2764	K2765	N2766	A2767	F2768	D2769	K2770	L2771	Q2772	N2773	L2774	N2775	S2776	Y2777	G2778	E2779	N2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	N2790	L2791	R2792	P2793	Y2794	K2795	T2796	T2797	S2798	E2799	K2800	D2801	K2802	E2803	I2804	R2805	N2806	N2807	P2808	I2809																																																																																																																																																																																																																																																																																																																																																																																																																																	
G2419	H2420	M2423	I2430	D2431	R2435	C2436	A2437	I2443	R2454	L2457	R2458	S2459	L2460	D2464	D2465	L2466	V2467	G2468	L2469	I2470	S2471	L2472	P2473	T2478	L2479	G2480	K2481	D2482	Q2483	A2484	L2485	P2488	K2499	A2500	S2501	M2502	R2508	V2509	Y2510	G2511	T2512	E2513	D2516	F2517	L2518	L2519	H2520																																																																																																																																																																																																																																																																																																																																																																																																																																													
V2299	L2307	Q2308	L2313	L2314	D2320	I2321	R2336	V2339	V2363	R2369	G2370	E2371	G2372	A2383	S2387	E2388	D2389	P2390	A2391	P2395	G2396	V2397	ARG	ARG	ARG	ARG	ARG	GLU	HIS	PHE	GLY	GLU	P2410	P2411	E2412	E2413	N2414	R2415	V2416																																																																																																																																																																																																																																																																																																																																																																																																																																																					
K2089	L2097	Q2107	Y2110	L2123	P2146	E2157	Q2161	T2167	Q2173	V2190	Q2193	G2202	K2203	H2204	K2208	K2211	V2214	L2215	G2216	G2217	G2218	E2219	T2220	K2221	R2244	Q2245	R2248	L2254	L2258	T2263	N2283	L2286	A2287	L2290	E2296																																																																																																																																																																																																																																																																																																																																																																																																																																																									
E2015	E2018	E2019	D2020	C2021	R2028	Q2029	D2030	L2031	Q2032	L2039	I2044	Q2045	L2046	GLU	GLY	GLU	GLU	GLU	GLU	PRO	GLU	GLU	GLY	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	E2088																																																																																																																																																																																																																																																																																																																																																																																																																																										
GLU	ASP	GLU	GLU	GLU	GLU	LYS	GLU	ALA	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	ASP	L1922	E1944	E1956	K1968	Q1973	L1980	A1983	F1984	T1985	M1986	S1987	A1988	A1989	E1990	R1994	T1995	R1996	S2000	Q2003	E2004	Q2005	ALA	N2007	K2013	D2014																																																																																																																																																																																																																																																																																																																																																																																																																																															
F1782	V1783	A1784	A1788	A1789	G1790	V1791	A1792	E1793	L1798	R1808	D1828	P1829	V1830	Q1837	L1842	S1846	L1849	V1850	M1851	G1852	I1853	F1854	D1858	V1870	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

S4213	A4117	L3965	L3844	Q3700	H3611	K3515	Y3444	A3306	T3220	ARG	S3019	L2930
E4224	D4116	L3966	M3858	F3705	P3612	K3516	M3445	V3324	T3221	THR	A3022	Q2931
E4227	E4119	E3967	V3859	S3706	Y3613	M3517	F3451	I3329	K3222	GLN	K3023	M2932
M4245	N4120	L3980	N3860	T3707	K3614	M3523	E3454	D3330	S3223	VAL	V3024	N2933
Q4246	E4121	L3985	E3861	R3708	S3615	M3524	N3457	F3331	P3224	K3123	L3025	G2934
I4247	M4122	V3995	D3862	M3723	K3616	D3531	F3457	A3332	R3225	G3124	G3026	G2935
I4251	N4123	M3999	G3863	M3729	K3617	L3532	F3458	V3340	P3226	Y3131	S3027	A2936
S4252	N4124	K4002	T3864	S3732	V3619	M3533	V3460	F3341	R3227	T3132	G3028	V2937
E4253	E4125	E3736	I3866	E3736	M3620	M3534	Q3461	A3342	A3228	L3136		T2938
P4254	D4138	GLU	N3867	GLU	H3621	T3538	N3465		I3229	L3137	A3031	T2939
GLY	E4152	GLY	K3867	GLY	K3622	K3538	N3466	I3345	L3230	GLY	S3032	
GLY	P4155	GLY	L3868	GLY	L3623	GLY	N3467	V3346	G3231	LYS	N3033	LEU
PRO	R4159	GLU	Q3869	GLU	L3624	A3541	M3467	F3347	L3232	ASP	K3034	LYS
ALA	M4039	ASN	N3870	ASN	L3625	L3542	S3468	S3347	P3233	ASP	E3035	ASP
ALA	Q4043	GLY	G3871	GLY	S3626	K3543	F3469	L3354	N3234	GLU	K3036	GLU
ASP	R4161	ALA	K3872	ALA	K3627	K3544	L3470	F3358	S3235	Q3151	E3037	L2946
ASP	V4049	ALA	E3873	ALA	R3628	D3544	T3471		V3236	F3152	M3038	D2947
GLY	L4164	GLU	N3555		R3629	N3556	A3472	T3356	E3237	D3155	A3048	T2948
GLY	E4165	GLU	L3557		K3630	N3557	S3474	T3361	E3238	V3156	R3051	S2949
NET	E4172	GLU	H3558		A3631	L3559	K3475	I3362	M3239	I3157	H3052	S2950
GLY	R4175	ALA	K3559		V3632	K3560	S3476	G3363	P3244	L3158	R3053	L2960
ALA	L4178	ALA	V3633		Q3633	Q3561	K3477	E3377	V3245	V3163	F3056	Q2971
ALA	Q4179	ALA	A3634		K3635	K3562	M3478	R3380	D3247		L3057	T2974
GLU	R4180	ALA	F3636		K3637	V3563	A3479	L3381	T3248	S3171	G3058	L2977
ALA	I4183	ALA	P3640			E3564	LYS	E3382	T3256	Y3173	T3059	L2978
GLU	M4184	ALA	M3640			S3566	GLY	A3383	L3256	S3174	P3062	A2979
GLY	S4187	ALA	M3652			L3569	ALA	K3384	S3259	L3175	V3065	V2980
ALA	R4188	ALA	L3652			L3575	GLN	A3385	A3261	N3180	L3075	V2981
GLY	R4189	ALA	A3659			Y3576	SER	E3386	T3264	T3181	D3076	S2982
ALA	I4190	ALA	V3661			R3577	GLY	E3387	E3265	Y3182	S2983	S2983
GLY	I4193	ALA	L3663			P3580	SER	E3388	M3266	E3184	A3077	G2984
ALA	Y4194	ALA	L3663			R3581	ASP	E3389	T3273	K3185	T3079	R2985
ALA	E4195	ALA	E3670			R3582	GLN	E3391			V3080	V2986
GLY	E4196	ALA	L3674			E3583	GLU	L3392	W3284		M3081	E2987
THR	S4198	ALA	D3675			E3584	THR	R3403	G3288	K3201	K3082	R2988
VAL	E4199	ALA	D3676			E3584	LYS	Y3409	P3289	P3202	V3088	S2989
ALA	T4200	ALA	S3678			A3586	LYS	R3414	L3292	V3203	D3102	P2990
GLY	M4201	ALA	E3682			D3587	LYS	Y3415	P3292	L3206	I3103	H2991
ALA	R4202	ALA	Q3683			P3589	R3498	Y3416	P3293	E3207	E3104	E2992
ALA	Q4203	ALA	E3684			P3589	K3499	W3423	P3294	L3208	V3107	F2997
THR	R4203	ALA	E3685			I3592	G3500	L3424	A3295	L3210	L3110	F2998
ALA	Q4204	ALA	E3686			L3592	D3501	P3427	L3296	N3214	R3111	I3001
ARG	E4205	ALA	E3687			R3595	R3498	P3427	P3297	A3215	L3112	L3002
LEU	M4207	ALA	E3688			V3596	G3500	F3435	P3298	C3216	G3113	L3003
ALA	P4208	ALA	E3689			A3601	D3501	M3437	A3298	G3217	L3005	L3004
ALA	E4211	ALA	V3690			E3607	T3507	I3443	A3300	V3218	N3007	L3006
ALA	E4212	ALA	E3691			E3610	S3508		P3301	Y3219	S3115	N3007
			E3692				V3510		P3302		S3116	T3011
			L3698				V3511		G3303		GLN	L3015
			H3699						G3304		ALA	



N3180	T3181	T3182	V3183	E3184	K3185	L3190	K3201	P3202	V3203	L3206	E3207	K3208	V3209	L3210	N3214	A3215	C3216	S3217	N3218	N3219	N3220	T3221	K3222	S3223	P3224	R3225	E3226	R3227	A3228	L3229	L3230	G3231	L3232	P3233	N3234	S3235	V3236	E3237	E3238	M3239	P3244	Y3245	L3246	B3247	R3248	L3253	L3256	S3259	G3260	A3261								
L3075	D3076	A3077	R3078	T3079	N3080	M3081	K3082	V3088	D3102	L3103	E3104	V3107	L3110	R3111	L3112	G3113	C3114	V3115	S3116	ALA	ARG	THR	GLN	VAL	K3123	G3124	T3130	Y3131	T3132	T3133	L3136	H3146	I3147	Q3151	F3152	G3153	D3154	L3155	V3156	I3157	L3158	V3163	S3171	T3172	Y3173	G3174	L3175											
V2980	V2981	S2982	S2983	G2984	R2985	V2986	E2987	K2988	S2989	P2990	H2991	E2992	F2997	F2998	L3001	L3002	L3003	P3004	L3005	L3006	N3007	T3011	L3015	S3019	A3022	K3023	V3024	L3025	G3026	S3027	G3028	N3033	K3034	E3035	K3036	E3037	M3038	A3048	R3051	H3052	R3053	L3056	F3057	G3058	T3059	P3062	V3065											
T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933	Q2934	Y2935	A2936	V2937	T2938	R2939	GLY	LEU	ASP	MET	GLU	L2946	D2947	T2948	S2949	S2950	L2960	Q2971	I2974	L2977	E2978	A2979				
V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	M2790	L2791	R2792	V2793	Y2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	L2802	E2803	L2804	Y2805	R2806	W2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	A2818	W2819	E2820	W2821	T2822	L2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	GLU	ARG	THR	GLU	LYS	LYS	THR	ARG
S2721	K2722	A2723	E2724	K2725	LYS	ALA	THR	VAL	ASP	ALA	GLY	N2734	F2735	D2736	P2737	R2738	P2739	V2740	E2741	T2742	L2743	N2744	V2745	L2746	F2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	I2755	N2756	K2757	F2758	A2759	E2760	Y2761	T2762	H2763	E2764	K2765	W2766	A2767	F2768	D2769	K2770	I2771	T2772	N2773	N2774	W2775	S2776	Y2777	G2778	E2779	N2780
K2576	I2577	W2578	W2582	L2583	T2584	W2585	V2586	W2587	R2588	S2593	S2594	L2595	R2600	M2608	C2611	T2614	R2615	M2618	L2619	Q2620	R2624	V2627	F2628	L2643	P2658	V2666	T2667	S2668	L2674	K2677	L2678	H2688	L2695	A2699	Y2653	L2703	V2715	D2716	Y2719	S2720																		
I2469	I2470	S2471	L2472	P2473	T2476	L2479	Q2480	K2481	D2482	G2483	A2484	L2485	P2488	K2499	A2500	S2501	M2502	Y2510	G2511	L2512	E2513	D2516	F2517	L2519	H2520	V2521	L2522	D2523	V2524	G2525	F2526	D2529	M2530	R2531	S2535	A2539	M2546	Y2553	I2562	C2565	G2571	T2572	H2574	R2575														
G2370	E2371	G2372	A2383	E2387	S2388	D2389	P2390	A2391	P2395	G2396	V2397	ARG	ARG	ASP	ARG	ARG	ARG	GLU	HLIS	PHE	GLY	GLU	P2410	P2411	E2412	E2413	H2420	G2419	H2420	M2423	L2430	D2430	D2431	R2435	I2443	R2454	L2457	R2458	S2459	L2460	V2461	D2464	D2465	L2466	V2467	G2468												
V2214	L2215	G2216	G2217	E2218	E2219	T2220	K2221	R2244	Q2245	Q2246	Q2247	M2250	L2254	L2258	I2263	S2279	N2283	L2286	A2287	L2290	E2296	V2299	L2307	Q2308	L2313	L2314	D2320	I2321	R2336	V2339	N2349	V2353	R2359	G2365	P2366	A2367	L2368	R2369																				
ARG	SER	LEU	GLU	THR	VAL	ARG	LEU	LYS	LYS	GLU	LYS	PRO	GLU	GLU	LEU	GLU	LEU	LEU	PRO	ALA	ALA	E2088	K2089	L2094	L2097	V2098	Q2107	L2123	P2146	E2157	Q2161	I2162	R2163	L2166	I2167	Q2173	V2190	Q2193	G2202	M2203	H2204	M2208	M2211															
L1980	A1983	F1984	T1985	H1986	S1987	A1988	A1989	F1990	R1994	T1995	R1996	S2000	Q2003	E2004	Q2005	T2006	N2007	K2013	D2014	E2015	E2018	E2019	D2020	C2021	R2028	Q2029	D2030	L2031	Q2032	L2039	I2044	Q2045	L2046	GLU	GLY	GLU	GLU	GLU	PRO	GLU	GLU	THR	SER	LEU	SER	ARG	LEU											





V3511	T3443	T3305	S3217	V3115	N3007	E2925	V2865	V2745	R2615	G2511	F2410
K3515	T3444	A3306	V3218	S3116	T3011	L2926	T2866	I2746	M2618	I2512	P2411
K3516	W3445	V3324	T3219	G1N	L3015	L2927	L2867	I2747	L2619	E2413	E2412
N3517	F3451	T3329	T3220	ALA	K2928	K2928	S2868	P2748	Q2620	R2415	R2414
N3523	E3454	D3330	T3221	THR	F2929	F2929	E2870	E2749	R2624	L2518	V2416
D3531	N3457	K3332	K3222	G1N	S3019	L2930	E2871	K2750	G2419	L2519	H2420
L3532	F3458	E3331	S3223	VAL	A3022	Q2931	Q2872	L2751	V2627	H2520	H2423
L3533	V3459	A3332	R3224	K3123	K3023	M2932	Q2873	D2752	F2628	V2521	G2419
N3534	V3460	V3340	E3226	G3124	V3024	N2933	M2874	E2753	L2643	L2522	H2420
K3537	Q3461	F3341	R3227	T3130	L3025	Y2935	A2875	S2754	M2423	V2524	I2430
T3538	N3465	A3342	A3228	Y3131	S3027	A2936	E2876	F2755	P2658	G2525	D2431
A3541	N3466	T3345	L3230	T3132	G3028	T2937	Q2877	N2756	V2666	F2526	R2435
L3542	M3467	V3346	L3231	Y3132	N3033	T2938	L2878	K2757	T2667	R2529	C2436
K3543	S3468	S3347	G3231	L3136	K3034	R2939	L2879	F2758	S2668	M2530	A2437
D3544	F3469	L3354	L3232	H3146	F3035	LEU	E2880	A2759	L2674	R2531	I2443
N3555	T3471	F3358	L3233	Q3151	K3036	ASP	T2881	A2760	L2678	S2535	R2454
N3556	A3472	T3361	S3234	F3152	M3038	MEI	Y2882	Y2761	L2678	A2539	L2457
L3557	A3473	T3362	V3236	G3153	A3048	L2946	T2885	K2766	L2695	M2546	R2458
H3558	S3474	T3363	E3237	D3154	R3051	D2947	W2886	A2767	A2699	Y2553	L2460
R3564	K3475	G3363	M3239	V3155	H3052	T2948	G2887	F2768	L2703	I2562	V2461
L3559	S3476	R3364	P3244	I3157	R3053	S2943	K2888	D2769	V2715	C2565	D2464
Q3560	K3477	E3377	V3245	L3158	L3056	S2960	K2889	K2770	D2716	G2571	D2465
G3561	M3478	R3380	R3247	V3163	F3057	L2960	K2890	I2771	G2576	T2572	L2466
K3562	A3479	L3381	T3248	S3171	Q3059	Q2971	Q2891	Q2772	R2719	S2573	V2467
V3563	ALA	E3382	I3253	I3172	G3058	L2974	E2893	N2773	S2720	H2574	G2468
G3564	GLY	A3383	L3256	Y3173	T3059	E2978	L2894	N2774	K2721	R2575	I2470
S3566	ALA	K3384	L3261	S3174	P3062	E2978	E2895	W2775	A2723	L2576	S2471
L3569	GLN	A3385	A3261	L3175	V3065	E2978	K2897	S2776	E2724	I2577	P2473
L3575	GLY	E3386	T3264	N3180	L3075	A2979	K2897	Y2777	K2725	M2578	T2478
Y3576	GLY	A3387	E3265	T3181	D3076	V2980	G2898	G2778	LYS	M2582	L2479
R3577	ASP	E3388	M3266	T3182	R3078	V2981	G2898	ARG	ALA	L2583	G2480
P3580	GLN	E3389	T3273	V3183	A3077	S2982	G2899	LYS	THR	H2584	K2481
G3581	GLU	G3390	W3284	E3184	R3079	S2983	G2900	THR	VAL	T2585	D2482
E3582	THR	F3391	G3288	K3185	M3081	V2986	L2904	GLN	ALA	V2586	G2483
E3583	LYS	L3392	P3289	L3190	K3082	E2987	L2905	THR	GLY	T2587	A2484
E3584	LYS	R3403	P3292	M3201	V3088	K2988	V2906	TYR	N2734	R2588	L2485
A3586	LYS	Y3409	P3293	V3203	V3088	K2988	V2906	ASP	F2735	R2593	P2488
D3587	R3414	T3415	P3293	L3206	D3102	S2989	P2907	K2786	P2735	S2594	K2499
D3588	V3416	E3207	P3294	F3208	E3104	P2990	V2908	ARG	D2736	L2595	A2500
P3589	R3501	A3295	A3295	P3208	E3104	H2991	D2909	GLY	P2737	R2600	S2501
Y3593	R3502	W3423	L3296	Q3209	V3107	E2992	T2910	P2789	R2738	M2608	M2502
S3594	S3504	L3424	L3210	L3210	L3110	K2996	T2911	M2790	P2739	C2611	R2508
V3595	V3505	N3214	A3298	N3214	R3111	F2997	T2912	L2791	V2740	I2614	Y2510
V3596	Q3506	A3215	G3299	A3215	L3112	F2998	A2913	P2792	E2741		
T3597	T3507	G3113	A3300	G3216	G3113		K2914	P2793	L2742		
S3598	S3508	P3301	P3302		K3114		E2915	Y2794	L2743		
L3599	L3509	P3302	P3303				K2916	K2795	N2744		
Y3604	T3510	C3304					A2917	T2796			
							R2918	F2797			
							D2919	S2798			
							E2920	E2799			
							E2921	D2800			
							K2922	K2801			
							A2923	E2803			
							Q2924	I2804			



- [illegible]



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55892	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	1.268	Depositor
Minimum map value	-0.637	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.064	Depositor
Recommended contour level	0.287	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: ZN, AGS

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	0.26	0/35721	0.61	4/48375 (0.0%)
1	B	0.26	0/35721	0.61	4/48375 (0.0%)
1	C	0.26	0/35721	0.61	4/48375 (0.0%)
1	D	0.26	0/35721	0.61	4/48375 (0.0%)
2	E	0.23	0/834	0.58	0/1123
2	F	0.23	0/834	0.58	0/1123
2	G	0.23	0/834	0.58	0/1123
2	H	0.23	0/834	0.58	0/1123
All	All	0.26	0/146220	0.61	16/197992 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4693	GLY	CA-C-N	6.34	133.66	121.54
1	B	4693	GLY	C-N-CA	6.34	133.66	121.54
1	C	4693	GLY	CA-C-N	6.34	133.66	121.54
1	C	4693	GLY	C-N-CA	6.34	133.66	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4693	GLY	CA-C-N	6.34	133.66	121.54
1	D	4693	GLY	C-N-CA	6.34	133.66	121.54
1	A	4693	GLY	CA-C-N	6.33	133.62	121.54
1	A	4693	GLY	C-N-CA	6.33	133.62	121.54
1	A	3615	SER	CA-C-N	5.91	132.82	121.54
1	A	3615	SER	C-N-CA	5.91	132.82	121.54
1	D	3615	SER	CA-C-N	5.87	132.75	121.54
1	D	3615	SER	C-N-CA	5.87	132.75	121.54
1	B	3615	SER	CA-C-N	5.87	132.74	121.54
1	B	3615	SER	C-N-CA	5.87	132.74	121.54
1	C	3615	SER	CA-C-N	5.87	132.74	121.54
1	C	3615	SER	C-N-CA	5.87	132.74	121.54

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	841	GLY	Mainchain
1	B	841	GLY	Mainchain
1	C	841	GLY	Mainchain
1	D	841	GLY	Mainchain

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	34904	0	34524	523	0
1	B	34904	0	34524	515	0
1	C	34904	0	34524	528	0
1	D	34904	0	34524	521	0
2	E	818	0	824	6	0
2	F	818	0	824	8	0
2	G	818	0	824	11	0
2	H	818	0	824	7	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
3	C	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	31	0	12	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	143016	0	141440	2085	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (2085) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2283:ASN:HD22	1:C:2286:LEU:HG	1.56	0.71
1:B:2283:ASN:HD22	1:B:2286:LEU:HG	1.56	0.70
1:D:2283:ASN:HD22	1:D:2286:LEU:HG	1.56	0.70
1:B:1561:VAL:HG12	1:B:1562:ILE:HG13	1.74	0.69
1:C:317:ARG:NH2	1:C:349:GLN:OE1	2.25	0.69
1:A:2283:ASN:HD22	1:A:2286:LEU:HG	1.56	0.69
1:D:1561:VAL:HG12	1:D:1562:ILE:HG13	1.74	0.69
1:A:3577:ARG:HH21	1:A:3582:ARG:HB3	1.58	0.69
1:D:3577:ARG:HH21	1:D:3582:ARG:HB3	1.58	0.69
1:C:3577:ARG:HH21	1:C:3582:ARG:HB3	1.58	0.68
1:A:1561:VAL:HG12	1:A:1562:ILE:HG13	1.74	0.68
1:B:3577:ARG:HH21	1:B:3582:ARG:HB3	1.58	0.68
1:C:1561:VAL:HG12	1:C:1562:ILE:HG13	1.74	0.68
1:A:317:ARG:NH2	1:A:349:GLN:OE1	2.25	0.68
1:D:317:ARG:NH2	1:D:349:GLN:OE1	2.25	0.68
1:A:2530:MET:SD	1:A:2531:ARG:NH1	2.68	0.67
1:B:2530:MET:SD	1:B:2531:ARG:NH1	2.68	0.67
1:D:2530:MET:SD	1:D:2531:ARG:NH1	2.68	0.67
1:C:2530:MET:SD	1:C:2531:ARG:NH1	2.68	0.67
1:D:946:ALA:O	1:D:950:LEU:HB2	1.95	0.67
1:A:946:ALA:O	1:A:950:LEU:HB2	1.95	0.66
1:C:946:ALA:O	1:C:950:LEU:HB2	1.95	0.66
1:B:317:ARG:NH2	1:B:349:GLN:OE1	2.25	0.66
1:A:3980:LEU:HD12	1:A:3985:LEU:HD22	1.77	0.66
1:C:3980:LEU:HD12	1:C:3985:LEU:HD22	1.77	0.66
1:B:475:GLN:NE2	1:B:528:SER:O	2.29	0.65
1:C:4138:ASP:O	1:C:4142:ASN:ND2	2.29	0.65
1:B:946:ALA:O	1:B:950:LEU:HB2	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3769:ARG:O	1:C:3773:ARG:NH1	2.30	0.65
1:A:475:GLN:NE2	1:A:528:SER:O	2.29	0.65
1:A:2430:ILE:HD13	1:A:2502:MET:HG3	1.79	0.65
1:D:2430:ILE:HD13	1:D:2502:MET:HG3	1.79	0.65
1:D:4138:ASP:O	1:D:4142:ASN:ND2	2.29	0.65
1:A:3769:ARG:O	1:A:3773:ARG:NH1	2.29	0.65
1:B:3980:LEU:HD12	1:B:3985:LEU:HD22	1.77	0.65
1:D:3980:LEU:HD12	1:D:3985:LEU:HD22	1.77	0.65
1:B:1116:GLY:HA3	1:B:1132:TRP:HB3	1.79	0.65
1:D:3932:ASP:HA	1:D:3935:TRP:HB2	1.78	0.65
1:C:3932:ASP:HA	1:C:3935:TRP:HB2	1.78	0.64
1:A:1116:GLY:HA3	1:A:1132:TRP:HB3	1.79	0.64
1:C:1116:GLY:HA3	1:C:1132:TRP:HB3	1.79	0.64
1:C:2430:ILE:HD13	1:C:2502:MET:HG3	1.79	0.64
1:D:1116:GLY:HA3	1:D:1132:TRP:HB3	1.79	0.64
1:B:3769:ARG:O	1:B:3773:ARG:NH1	2.30	0.64
1:D:1476:MET:HB3	1:D:1485:SER:HB3	1.80	0.64
1:B:247:TYR:HB2	1:B:374:LYS:HB3	1.80	0.64
1:D:3769:ARG:O	1:D:3773:ARG:NH1	2.30	0.64
1:B:2430:ILE:HD13	1:B:2502:MET:HG3	1.79	0.64
1:D:475:GLN:NE2	1:D:528:SER:O	2.29	0.64
1:C:1476:MET:HB3	1:C:1485:SER:HB3	1.80	0.64
1:A:1476:MET:HB3	1:A:1485:SER:HB3	1.80	0.63
1:C:475:GLN:NE2	1:C:528:SER:O	2.29	0.63
1:A:1023:PRO:HD2	1:A:1026:LEU:HD12	1.80	0.63
1:A:3932:ASP:HA	1:A:3935:TRP:HB2	1.78	0.63
1:C:842:PRO:O	1:C:1197:GLY:N	2.26	0.63
1:B:3932:ASP:HA	1:B:3935:TRP:HB2	1.78	0.63
1:B:1023:PRO:HD2	1:B:1026:LEU:HD12	1.81	0.63
1:B:1476:MET:HB3	1:B:1485:SER:HB3	1.80	0.63
1:C:247:TYR:HB2	1:C:374:LYS:HB3	1.80	0.63
1:C:1023:PRO:HD2	1:C:1026:LEU:HD12	1.81	0.63
1:D:247:TYR:HB2	1:D:374:LYS:HB3	1.80	0.63
1:D:1029:GLU:HA	1:D:1032:LYS:HB2	1.81	0.62
1:A:247:TYR:HB2	1:A:374:LYS:HB3	1.80	0.62
1:B:842:PRO:O	1:B:1197:GLY:N	2.26	0.62
1:C:1029:GLU:HA	1:C:1032:LYS:HB2	1.81	0.62
1:A:2431:ASP:HB2	1:A:2501:SER:HB3	1.82	0.62
1:C:3377:GLU:HA	1:C:3380:ARG:HG2	1.82	0.62
1:C:2998:PHE:HA	1:C:3002:LEU:HD13	1.82	0.62
1:D:3377:GLU:HA	1:D:3380:ARG:HG2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2608:MET:HE1	1:B:2643:LEU:HB2	1.82	0.62
1:D:1023:PRO:HD2	1:D:1026:LEU:HD12	1.81	0.62
1:B:3114:LYS:HD3	1:B:3116:SER:H	1.65	0.61
1:D:2608:MET:HE1	1:D:2643:LEU:HB2	1.82	0.61
1:D:4152:GLU:OE2	1:D:4180:ARG:NH2	2.33	0.61
1:B:286:THR:HA	1:B:405:HIS:HB2	1.81	0.61
1:C:3114:LYS:HD3	1:C:3116:SER:H	1.65	0.61
1:B:4138:ASP:O	1:B:4142:ASN:ND2	2.29	0.61
1:C:1808:ARG:NH1	1:C:1853:ILE:O	2.33	0.61
1:C:4152:GLU:OE2	1:C:4180:ARG:NH2	2.33	0.61
1:D:3688:GLU:HG3	1:D:3690:VAL:HG12	1.82	0.61
1:A:286:THR:HA	1:A:405:HIS:HB2	1.81	0.61
1:B:2431:ASP:HB2	1:B:2501:SER:HB3	1.82	0.61
1:B:2998:PHE:HA	1:B:3002:LEU:HD13	1.82	0.61
1:C:286:THR:HA	1:C:405:HIS:HB2	1.81	0.61
1:D:2998:PHE:HA	1:D:3002:LEU:HD13	1.82	0.61
1:A:3377:GLU:HA	1:A:3380:ARG:HG2	1.82	0.61
1:A:3688:GLU:HG3	1:A:3690:VAL:HG12	1.82	0.61
1:B:1029:GLU:HA	1:B:1032:LYS:HB2	1.81	0.61
1:A:4152:GLU:OE2	1:A:4180:ARG:NH2	2.33	0.61
1:B:1808:ARG:NH1	1:B:1853:ILE:O	2.33	0.61
1:B:3048:ALA:O	1:B:3053:ARG:NH2	2.34	0.61
1:C:2431:ASP:HB2	1:C:2501:SER:HB3	1.82	0.61
1:D:286:THR:HA	1:D:405:HIS:HB2	1.81	0.61
1:D:3048:ALA:O	1:D:3053:ARG:NH2	2.34	0.61
1:C:1259:ARG:NH2	1:C:1591:CYS:SG	2.74	0.61
1:D:1259:ARG:NH2	1:D:1591:CYS:SG	2.74	0.61
1:A:1259:ARG:NH2	1:A:1591:CYS:SG	2.74	0.61
1:B:866:HIS:HA	1:B:869:ARG:HE	1.66	0.61
1:B:3377:GLU:HA	1:B:3380:ARG:HG2	1.82	0.61
1:B:4152:GLU:OE2	1:B:4180:ARG:NH2	2.33	0.61
1:A:842:PRO:O	1:A:1197:GLY:N	2.26	0.61
1:A:866:HIS:HA	1:A:869:ARG:HE	1.66	0.61
1:A:1029:GLU:HA	1:A:1032:LYS:HB2	1.81	0.61
1:A:4138:ASP:O	1:A:4142:ASN:ND2	2.29	0.61
1:C:3048:ALA:O	1:C:3053:ARG:NH2	2.34	0.61
1:A:2978:GLU:OE2	1:A:3053:ARG:NH1	2.34	0.60
1:B:1738:LEU:HB2	1:B:2146:PRO:HD3	1.83	0.60
1:C:1738:LEU:HB2	1:C:2146:PRO:HD3	1.83	0.60
1:C:3688:GLU:HG3	1:C:3690:VAL:HG12	1.82	0.60
1:D:1520:VAL:HG12	1:D:1527:MET:HG3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3688:GLU:HG3	1:B:3690:VAL:HG12	1.82	0.60
1:A:2608:MET:HE1	1:A:2643:LEU:HB2	1.82	0.60
1:B:35:LEU:HD13	1:B:49:LEU:HD13	1.83	0.60
1:A:35:LEU:HD13	1:A:49:LEU:HD13	1.83	0.60
1:A:975:VAL:O	1:A:1044:ARG:NH1	2.35	0.60
1:A:1808:ARG:NH1	1:A:1853:ILE:O	2.33	0.60
1:B:3454:GLU:HA	1:B:3457:ASN:HB2	1.83	0.60
1:C:2978:GLU:OE2	1:C:3053:ARG:NH1	2.34	0.60
1:A:2998:PHE:HA	1:A:3002:LEU:HD13	1.82	0.60
1:B:1259:ARG:NH2	1:B:1591:CYS:SG	2.74	0.60
1:C:866:HIS:HA	1:C:869:ARG:HE	1.66	0.60
1:D:35:LEU:HD13	1:D:49:LEU:HD13	1.83	0.60
1:A:1520:VAL:HG12	1:A:1527:MET:HG3	1.83	0.60
1:A:1738:LEU:HB2	1:A:2146:PRO:HD3	1.83	0.60
1:C:2608:MET:HE1	1:C:2643:LEU:HB2	1.82	0.60
1:D:866:HIS:HA	1:D:869:ARG:HE	1.66	0.60
1:D:1738:LEU:HB2	1:D:2146:PRO:HD3	1.83	0.60
1:D:3114:LYS:HD3	1:D:3116:SER:H	1.65	0.60
1:D:363:ASP:OD1	1:D:374:LYS:NZ	2.35	0.60
1:D:1808:ARG:NH1	1:D:1853:ILE:O	2.33	0.60
1:D:2431:ASP:HB2	1:D:2501:SER:HB3	1.82	0.60
1:A:3114:LYS:HD3	1:A:3116:SER:H	1.65	0.60
1:B:2003:GLN:OE1	1:B:2007:ASN:ND2	2.35	0.60
1:B:2978:GLU:OE2	1:B:3053:ARG:NH1	2.34	0.60
1:C:3454:GLU:HA	1:C:3457:ASN:HB2	1.83	0.60
1:D:2978:GLU:OE2	1:D:3053:ARG:NH1	2.34	0.60
1:D:3454:GLU:HA	1:D:3457:ASN:HB2	1.83	0.60
1:A:978:THR:OG1	1:A:981:GLN:OE1	2.20	0.60
1:B:975:VAL:O	1:B:1044:ARG:NH1	2.35	0.60
1:B:1520:VAL:HG12	1:B:1527:MET:HG3	1.83	0.60
1:D:975:VAL:O	1:D:1044:ARG:NH1	2.35	0.60
1:D:2003:GLN:OE1	1:D:2007:ASN:ND2	2.35	0.60
1:A:107:ILE:HD13	1:A:150:MET:HG2	1.84	0.60
1:A:276:TRP:NE1	1:A:346:CYS:SG	2.75	0.59
1:C:622:THR:HA	1:C:626:LEU:HD23	1.84	0.59
1:D:622:THR:HA	1:D:626:LEU:HD23	1.84	0.59
1:A:363:ASP:OD1	1:A:374:LYS:NZ	2.35	0.59
1:A:3048:ALA:O	1:A:3053:ARG:NH2	2.34	0.59
1:B:363:ASP:OD1	1:B:374:LYS:NZ	2.35	0.59
1:C:1520:VAL:HG12	1:C:1527:MET:HG3	1.83	0.59
1:D:107:ILE:HD13	1:D:150:MET:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:363:ASP:OD1	1:C:374:LYS:NZ	2.35	0.59
1:D:248:GLU:OE1	1:D:257:ARG:NH2	2.36	0.59
1:B:276:TRP:NE1	1:B:346:CYS:SG	2.75	0.59
1:C:248:GLU:OE1	1:C:257:ARG:NH2	2.36	0.59
1:C:975:VAL:O	1:C:1044:ARG:NH1	2.35	0.59
1:C:2003:GLN:OE1	1:C:2007:ASN:ND2	2.35	0.59
1:A:4179:GLY:O	1:A:4194:TYR:HA	2.03	0.59
1:B:24:CYS:HB2	1:B:35:LEU:HB2	1.84	0.59
1:B:4179:GLY:O	1:B:4194:TYR:HA	2.03	0.59
1:C:276:TRP:NE1	1:C:346:CYS:SG	2.75	0.59
1:C:818:ARG:NH2	1:C:1025:ARG:O	2.36	0.59
1:D:978:THR:OG1	1:D:981:GLN:OE1	2.20	0.59
1:A:2003:GLN:OE1	1:A:2007:ASN:ND2	2.35	0.59
1:C:107:ILE:HD13	1:C:150:MET:HG2	1.84	0.59
1:C:5013:MET:HE1	1:C:5020:ASP:HB2	1.85	0.59
1:D:276:TRP:O	1:D:328:LYS:NZ	2.34	0.59
1:D:2499:LYS:NZ	1:D:2529:ASP:OD2	2.33	0.59
1:A:3946:GLN:OE1	1:A:3949:ARG:NH2	2.36	0.59
1:B:818:ARG:NH2	1:B:1025:ARG:O	2.36	0.59
1:B:1101:ARG:NH1	1:B:1115:LEU:O	2.36	0.59
1:D:276:TRP:NE1	1:D:346:CYS:SG	2.75	0.59
1:A:3454:GLU:HA	1:A:3457:ASN:HB2	1.83	0.59
1:A:5013:MET:HE1	1:A:5020:ASP:HB2	1.85	0.59
1:B:248:GLU:OE1	1:B:257:ARG:NH2	2.36	0.59
1:B:978:THR:OG1	1:B:981:GLN:OE1	2.20	0.59
1:B:3946:GLN:OE1	1:B:3949:ARG:NH2	2.36	0.59
1:D:818:ARG:NH2	1:D:1025:ARG:O	2.36	0.59
1:A:248:GLU:OE1	1:A:257:ARG:NH2	2.36	0.58
1:A:622:THR:HA	1:A:626:LEU:HD23	1.84	0.58
1:B:622:THR:HA	1:B:626:LEU:HD23	1.84	0.58
1:B:5013:MET:HE1	1:B:5020:ASP:HB2	1.85	0.58
1:C:35:LEU:HD13	1:C:49:LEU:HD13	1.83	0.58
1:C:3946:GLN:OE1	1:C:3949:ARG:NH2	2.36	0.58
1:D:1101:ARG:NH1	1:D:1115:LEU:O	2.36	0.58
1:D:5013:MET:HE1	1:D:5020:ASP:HB2	1.85	0.58
1:A:157:ARG:HH12	1:A:163:VAL:HA	1.68	0.58
1:B:157:ARG:HH12	1:B:163:VAL:HA	1.68	0.58
1:A:818:ARG:NH2	1:A:1025:ARG:O	2.36	0.58
1:A:2499:LYS:NZ	1:A:2529:ASP:OD2	2.33	0.58
1:B:3459:VAL:HG11	1:B:3503:TYR:HB2	1.85	0.58
1:C:157:ARG:HH12	1:C:163:VAL:HA	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3459:VAL:HG11	1:C:3503:TYR:HB2	1.85	0.58
1:C:4179:GLY:O	1:C:4194:TYR:HA	2.03	0.58
1:D:157:ARG:HH12	1:D:163:VAL:HA	1.68	0.58
1:A:1101:ARG:NH1	1:A:1115:LEU:O	2.36	0.58
1:B:22:LEU:HD11	1:B:200:TRP:HB3	1.85	0.58
1:B:1259:ARG:NH1	1:B:1595:LEU:O	2.37	0.58
1:C:24:CYS:HB2	1:C:35:LEU:HB2	1.84	0.58
1:D:4570:ALA:O	1:D:4574:ASN:ND2	2.36	0.58
1:A:276:TRP:O	1:A:328:LYS:NZ	2.35	0.58
1:D:3459:VAL:HG11	1:D:3503:TYR:HB2	1.85	0.58
1:B:4570:ALA:O	1:B:4574:ASN:ND2	2.36	0.58
1:C:34:LYS:H	1:C:53:SER:HB3	1.69	0.58
1:C:197:GLN:NE2	1:C:198:THR:O	2.37	0.58
1:C:978:THR:OG1	1:C:981:GLN:OE1	2.20	0.58
1:D:4179:GLY:O	1:D:4194:TYR:HA	2.03	0.58
1:A:24:CYS:HB2	1:A:35:LEU:HB2	1.84	0.58
1:A:1259:ARG:NH1	1:A:1595:LEU:O	2.37	0.58
1:A:2443:ILE:HD12	1:A:2454:ARG:HH21	1.69	0.58
1:A:3459:VAL:HG11	1:A:3503:TYR:HB2	1.85	0.58
1:B:107:ILE:HD13	1:B:150:MET:HG2	1.84	0.58
1:C:276:TRP:O	1:C:328:LYS:NZ	2.34	0.58
1:C:3244:PRO:HA	1:C:3248:ARG:HH21	1.69	0.58
1:D:3946:GLN:OE1	1:D:3949:ARG:NH2	2.36	0.58
1:A:2470:ILE:HG22	1:A:2525:GLY:HA3	1.86	0.58
1:C:534:ARG:HH11	1:C:570:GLU:HG3	1.69	0.58
1:D:2470:ILE:HA	1:D:2499:LYS:HE3	1.86	0.58
1:B:3675:ASP:OD1	1:B:3769:ARG:NH1	2.37	0.58
1:C:22:LEU:HD11	1:C:200:TRP:HB3	1.85	0.58
1:C:3675:ASP:OD1	1:C:3769:ARG:NH1	2.37	0.58
1:A:197:GLN:NE2	1:A:198:THR:O	2.37	0.57
1:A:2107:GLN:O	1:A:3683:GLN:NE2	2.37	0.57
1:C:1259:ARG:NH1	1:C:1595:LEU:O	2.37	0.57
1:C:4570:ALA:O	1:C:4574:ASN:ND2	2.36	0.57
1:D:34:LYS:H	1:D:53:SER:HB3	1.69	0.57
1:D:878:ILE:HD11	1:D:925:SER:HB2	1.86	0.57
1:D:2470:ILE:HG22	1:D:2525:GLY:HA3	1.86	0.57
1:D:3244:PRO:HA	1:D:3248:ARG:HH21	1.69	0.57
1:A:2470:ILE:HA	1:A:2499:LYS:HE3	1.86	0.57
1:B:197:GLN:NE2	1:B:198:THR:O	2.37	0.57
1:C:1101:ARG:NH1	1:C:1115:LEU:O	2.36	0.57
1:C:2365:GLY:O	1:C:2369[B]:ARG:NH2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2470:ILE:HG22	1:C:2525:GLY:HA3	1.86	0.57
1:A:878:ILE:HD11	1:A:925:SER:HB2	1.86	0.57
1:A:3244:PRO:HA	1:A:3248:ARG:HH21	1.69	0.57
1:B:34:LYS:H	1:B:53:SER:HB3	1.69	0.57
1:B:1748:PHE:HB2	1:B:1758:ARG:HH21	1.69	0.57
1:C:2107:GLN:O	1:C:3683:GLN:NE2	2.37	0.57
1:D:534:ARG:HH11	1:D:570:GLU:HG3	1.69	0.57
1:D:2107:GLN:O	1:D:3683:GLN:NE2	2.37	0.57
1:A:22:LEU:HD11	1:A:200:TRP:HB3	1.85	0.57
1:A:4570:ALA:O	1:A:4574:ASN:ND2	2.36	0.57
1:D:1259:ARG:NH1	1:D:1595:LEU:O	2.37	0.57
1:D:3107:VAL:HG21	1:D:3171:SER:HB2	1.86	0.57
1:D:22:LEU:HD11	1:D:200:TRP:HB3	1.85	0.57
1:D:197:GLN:NE2	1:D:198:THR:O	2.37	0.57
1:A:1694:LEU:HB3	1:A:1715:LEU:HD12	1.87	0.57
1:A:2018:GLU:OE1	1:A:2028:ARG:NH1	2.38	0.57
1:A:3523:ASN:O	1:A:3582:ARG:NH2	2.38	0.57
1:B:534:ARG:HH11	1:B:570:GLU:HG3	1.69	0.57
1:B:941:MET:SD	1:B:1052:ASN:ND2	2.78	0.57
1:B:2107:GLN:O	1:B:3683:GLN:NE2	2.37	0.57
1:C:878:ILE:HD11	1:C:925:SER:HB2	1.86	0.57
1:D:24:CYS:HB2	1:D:35:LEU:HB2	1.84	0.57
1:D:2365:GLY:O	1:D:2369[B]:ARG:NH2	2.37	0.57
1:A:34:LYS:H	1:A:53:SER:HB3	1.69	0.57
1:A:2365:GLY:O	1:A:2369[B]:ARG:NH2	2.38	0.57
1:B:276:TRP:O	1:B:328:LYS:NZ	2.34	0.57
1:B:2443:ILE:HD12	1:B:2454:ARG:HH21	1.69	0.57
1:B:3244:PRO:HA	1:B:3248:ARG:HH21	1.69	0.57
1:A:1748:PHE:HB2	1:A:1758:ARG:HH21	1.70	0.57
1:A:2021:CYS:O	1:A:2028:ARG:NH2	2.38	0.57
1:A:3675:ASP:OD1	1:A:3769:ARG:NH1	2.37	0.57
1:B:632:LEU:O	1:B:634:GLN:NE2	2.38	0.57
1:B:2021:CYS:O	1:B:2028:ARG:NH2	2.38	0.57
1:C:941:MET:SD	1:C:1052:ASN:ND2	2.78	0.57
1:D:2013:LYS:NZ	1:D:3661:TRP:O	2.38	0.57
1:D:2021:CYS:O	1:D:2028:ARG:NH2	2.38	0.57
1:A:941:MET:SD	1:A:1052:ASN:ND2	2.78	0.57
1:B:289:ARG:HB3	1:B:301:VAL:HB	1.87	0.57
1:B:3706:SER:HB2	1:B:3778:MET:HE1	1.87	0.57
1:D:941:MET:SD	1:D:1052:ASN:ND2	2.78	0.57
1:D:3675:ASP:OD1	1:D:3769:ARG:NH1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:ARG:HH11	1:A:570:GLU:HG3	1.69	0.57
1:A:632:LEU:O	1:A:634:GLN:NE2	2.38	0.57
1:A:1504:GLY:O	1:A:1508:ARG:NH2	2.38	0.57
1:B:2365:GLY:O	1:B:2369[B]:ARG:NH2	2.38	0.57
1:B:2470:ILE:HG22	1:B:2525:GLY:HA3	1.86	0.57
1:B:3107:VAL:HG21	1:B:3171:SER:HB2	1.86	0.57
1:C:1748:PHE:HB2	1:C:1758:ARG:HH21	1.69	0.57
1:C:2499:LYS:NZ	1:C:2529:ASP:OD2	2.33	0.57
1:C:3107:VAL:HG21	1:C:3171:SER:HB2	1.86	0.57
1:D:2443:ILE:HD12	1:D:2454:ARG:HH21	1.69	0.57
1:D:3706:SER:HB2	1:D:3778:MET:HE1	1.87	0.57
1:A:3107:VAL:HG21	1:A:3171:SER:HB2	1.86	0.56
1:B:878:ILE:HD11	1:B:925:SER:HB2	1.86	0.56
1:B:2595:LEU:O	1:B:2600:ARG:NH2	2.38	0.56
1:B:4738:ALA:HA	1:B:4743:MET:HG3	1.87	0.56
1:C:3523:ASN:O	1:C:3582:ARG:NH2	2.38	0.56
1:C:3706:SER:HB2	1:C:3778:MET:HE1	1.87	0.56
1:D:289:ARG:HB3	1:D:301:VAL:HB	1.87	0.56
1:D:1243:PRO:O	1:D:1458:HIS:ND1	2.38	0.56
1:D:2018:GLU:OE1	1:D:2028:ARG:NH1	2.38	0.56
1:A:2595:LEU:O	1:A:2600:ARG:NH2	2.38	0.56
1:B:2470:ILE:HA	1:B:2499:LYS:HE3	1.86	0.56
1:C:2021:CYS:O	1:C:2028:ARG:NH2	2.38	0.56
1:D:1694:LEU:HB3	1:D:1715:LEU:HD12	1.87	0.56
1:A:289:ARG:HB3	1:A:301:VAL:HB	1.87	0.56
1:A:3706:SER:HB2	1:A:3778:MET:HE1	1.87	0.56
1:A:4738:ALA:HA	1:A:4743:MET:HG3	1.87	0.56
1:B:884:LEU:HD13	1:B:969:PRO:HD2	1.87	0.56
1:C:289:ARG:HB3	1:C:301:VAL:HB	1.87	0.56
1:C:632:LEU:O	1:C:634:GLN:NE2	2.38	0.56
1:C:1504:GLY:O	1:C:1508:ARG:NH2	2.38	0.56
1:C:3051:ARG:O	1:C:3053:ARG:NE	2.38	0.56
1:D:1504:GLY:O	1:D:1508:ARG:NH2	2.38	0.56
1:C:2443:ILE:HD12	1:C:2454:ARG:HH21	1.69	0.56
1:D:3236:VAL:HA	1:D:3239:MET:HG2	1.88	0.56
1:B:1504:GLY:O	1:B:1508:ARG:NH2	2.38	0.56
1:B:3288:GLY:HA2	1:B:3303:PRO:HB3	1.88	0.56
1:C:2470:ILE:HA	1:C:2499:LYS:HE3	1.86	0.56
1:C:3236:VAL:HA	1:C:3239:MET:HG2	1.88	0.56
1:C:3256:LEU:HB3	1:C:3266:MET:HE2	1.88	0.56
1:D:884:LEU:HD13	1:D:969:PRO:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1243:PRO:O	1:A:1458:HIS:ND1	2.38	0.56
1:B:869:ARG:NH1	1:B:1051:TYR:OH	2.39	0.56
1:C:2018:GLU:OE1	1:C:2028:ARG:NH1	2.38	0.56
1:C:2595:LEU:O	1:C:2600:ARG:NH2	2.38	0.56
1:D:688:LEU:HD23	1:D:690:GLU:H	1.71	0.56
1:D:1748:PHE:HB2	1:D:1758:ARG:HH21	1.69	0.56
1:A:688:LEU:HD23	1:A:690:GLU:H	1.71	0.56
1:B:3051:ARG:O	1:B:3053:ARG:NE	2.38	0.56
1:C:884:LEU:HD13	1:C:969:PRO:HD2	1.87	0.56
1:D:632:LEU:O	1:D:634:GLN:NE2	2.38	0.56
1:D:2595:LEU:O	1:D:2600:ARG:NH2	2.38	0.56
1:D:3051:ARG:O	1:D:3053:ARG:NE	2.38	0.56
1:A:3288:GLY:HA2	1:A:3303:PRO:HB3	1.88	0.56
1:A:3788:GLY:HA2	1:A:3835:LEU:HG	1.88	0.56
1:B:3788:GLY:HA2	1:B:3835:LEU:HG	1.88	0.56
1:D:451:TYR:O	1:D:474:ARG:NH1	2.39	0.56
1:D:3256:LEU:HB3	1:D:3266:MET:HE2	1.88	0.56
1:A:3051:ARG:O	1:A:3053:ARG:NE	2.38	0.56
1:C:1694:LEU:HB3	1:C:1715:LEU:HD12	1.87	0.56
1:C:2620:GLN:HE22	1:C:2674:LEU:HD22	1.71	0.56
1:A:869:ARG:NH1	1:A:1051:TYR:OH	2.39	0.56
1:A:1731:LEU:HD13	1:A:1772:ARG:HH21	1.72	0.56
1:B:234:SER:HB2	1:B:242:ARG:HA	1.88	0.56
1:B:2620:GLN:HE22	1:B:2674:LEU:HD22	1.71	0.56
1:B:3236:VAL:HA	1:B:3239:MET:HG2	1.88	0.56
1:C:451:TYR:O	1:C:474:ARG:NH1	2.39	0.56
1:D:869:ARG:NH1	1:D:1051:TYR:OH	2.39	0.56
1:A:229:GLU:HB3	1:A:247:TYR:HB3	1.88	0.55
1:B:229:GLU:HB3	1:B:247:TYR:HB3	1.88	0.55
1:B:2215:LEU:O	1:B:2219:GLU:HA	2.05	0.55
1:C:1005:TRP:HB3	1:C:1021:LEU:HD11	1.88	0.55
1:C:1243:PRO:O	1:C:1458:HIS:ND1	2.38	0.55
1:C:2215:LEU:O	1:C:2219:GLU:HA	2.05	0.55
1:D:229:GLU:HB3	1:D:247:TYR:HB3	1.88	0.55
1:D:861:ILE:O	1:D:930:LYS:NZ	2.39	0.55
1:B:1731:LEU:HD13	1:B:1772:ARG:HH21	1.72	0.55
1:C:3288:GLY:HA2	1:C:3303:PRO:HB3	1.88	0.55
1:A:1005:TRP:HB3	1:A:1021:LEU:HD11	1.88	0.55
1:A:2215:LEU:O	1:A:2219:GLU:HA	2.06	0.55
1:B:1694:LEU:HB3	1:B:1715:LEU:HD12	1.87	0.55
1:C:229:GLU:HB3	1:C:247:TYR:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:869:ARG:NH1	1:C:1051:TYR:OH	2.39	0.55
1:C:2013:LYS:NZ	1:C:3661:TRP:O	2.38	0.55
1:C:2715:VAL:HG21	1:C:2950:SER:HB2	1.88	0.55
1:C:4738:ALA:HA	1:C:4743:MET:HG3	1.87	0.55
1:D:2715:VAL:HG21	1:D:2950:SER:HB2	1.88	0.55
1:A:861:ILE:O	1:A:930:LYS:NZ	2.39	0.55
1:A:884:LEU:HD13	1:A:969:PRO:HD2	1.87	0.55
1:A:451:TYR:O	1:A:474:ARG:NH1	2.39	0.55
1:C:861:ILE:O	1:C:930:LYS:NZ	2.39	0.55
1:D:2215:LEU:O	1:D:2219:GLU:HA	2.05	0.55
1:A:234:SER:HB2	1:A:242:ARG:HA	1.88	0.55
1:C:234:SER:HB2	1:C:242:ARG:HA	1.88	0.55
1:C:3227:ARG:NH1	1:C:3234:ASN:OD1	2.40	0.55
1:D:842:PRO:O	1:D:1197:GLY:N	2.26	0.55
1:D:4738:ALA:HA	1:D:4743:MET:HG3	1.87	0.55
2:E:24:VAL:HG12	2:E:103:LEU:HA	1.88	0.55
1:A:2827:ARG:HE	1:A:2933:ASN:HB3	1.71	0.55
1:A:3206:LEU:HB3	1:A:3246:LEU:HB2	1.88	0.55
1:A:3227:ARG:NH1	1:A:3234:ASN:OD1	2.40	0.55
1:C:2827:ARG:HE	1:C:2933:ASN:HB3	1.71	0.55
1:D:2827:ARG:HE	1:D:2933:ASN:HB3	1.71	0.55
1:D:3218:VAL:O	1:D:3222:LYS:HB2	2.07	0.55
1:A:3236:VAL:HA	1:A:3239:MET:HG2	1.88	0.55
1:A:3256:LEU:HB3	1:A:3266:MET:HE2	1.88	0.55
1:C:688:LEU:HD23	1:C:690:GLU:H	1.71	0.55
1:D:883:ALA:HB1	1:D:905:PRO:HA	1.89	0.55
1:A:2715:VAL:HG21	1:A:2950:SER:HB2	1.88	0.55
1:A:3218:VAL:O	1:A:3222:LYS:HB2	2.07	0.55
1:B:1243:PRO:O	1:B:1458:HIS:ND1	2.38	0.55
1:B:1527:MET:HB2	1:B:1540:PHE:HB2	1.89	0.55
1:B:3324:VAL:HG11	1:B:3361:THR:HB	1.89	0.55
1:C:3206:LEU:HB3	1:C:3246:LEU:HB2	1.89	0.55
1:C:3324:VAL:HG11	1:C:3361:THR:HB	1.89	0.55
1:D:1527:MET:HB2	1:D:1540:PHE:HB2	1.89	0.55
1:D:1731:LEU:HD13	1:D:1772:ARG:HH21	1.72	0.55
1:D:3288:GLY:HA2	1:D:3303:PRO:HB3	1.88	0.55
1:B:451:TYR:O	1:B:474:ARG:NH1	2.39	0.55
1:B:688:LEU:HD23	1:B:690:GLU:H	1.71	0.55
1:B:883:ALA:HB1	1:B:905:PRO:HA	1.89	0.55
1:B:988:LEU:HG	1:B:1039:LEU:HD13	1.89	0.55
1:C:988:LEU:HG	1:C:1039:LEU:HD13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3218:VAL:O	1:C:3222:LYS:HB2	2.07	0.55
1:D:3227:ARG:NH1	1:D:3234:ASN:OD1	2.40	0.55
1:A:883:ALA:HB1	1:A:905:PRO:HA	1.89	0.54
1:B:861:ILE:O	1:B:930:LYS:NZ	2.39	0.54
1:B:3523:ASN:O	1:B:3582:ARG:NH2	2.38	0.54
1:B:2749:GLU:HG3	1:B:2752:ASP:HB2	1.90	0.54
1:B:3227:ARG:NH1	1:B:3234:ASN:OD1	2.40	0.54
1:C:3788:GLY:HA2	1:C:3835:LEU:HG	1.88	0.54
1:D:3523:ASN:O	1:D:3582:ARG:NH2	2.38	0.54
1:D:3788:GLY:HA2	1:D:3835:LEU:HG	1.88	0.54
1:C:3821:LYS:O	1:C:3824:LYS:NZ	2.39	0.54
1:D:1005:TRP:HB3	1:D:1021:LEU:HD11	1.88	0.54
1:D:2620:GLN:HE22	1:D:2674:LEU:HD22	1.71	0.54
2:F:24:VAL:HG12	2:F:103:LEU:HA	1.88	0.54
1:A:2749:GLU:HG3	1:A:2752:ASP:HB2	1.89	0.54
1:B:1005:TRP:HB3	1:B:1021:LEU:HD11	1.88	0.54
1:B:2827:ARG:HE	1:B:2933:ASN:HB3	1.71	0.54
1:B:3151:GLN:NE2	1:B:3154:ASP:OD2	2.41	0.54
1:B:3256:LEU:HB3	1:B:3266:MET:HE2	1.88	0.54
1:C:883:ALA:HB1	1:C:905:PRO:HA	1.89	0.54
1:A:1527:MET:HB2	1:A:1540:PHE:HB2	1.89	0.54
1:A:3151:GLN:NE2	1:A:3154:ASP:OD2	2.41	0.54
1:A:3207:GLU:OE1	1:A:3305:THR:OG1	2.26	0.54
1:B:846:LEU:HD22	1:B:851:PHE:HE1	1.73	0.54
1:B:1097:THR:HA	1:B:1143:TRP:HE1	1.73	0.54
1:B:2420:HIS:HA	1:B:2423:MET:HE2	1.89	0.54
1:B:2715:VAL:HG21	1:B:2950:SER:HB2	1.88	0.54
1:C:1097:THR:HA	1:C:1143:TRP:HE1	1.73	0.54
1:C:3151:GLN:NE2	1:C:3154:ASP:OD2	2.41	0.54
2:G:24:VAL:HG12	2:G:103:LEU:HA	1.88	0.54
1:A:988:LEU:HG	1:A:1039:LEU:HD13	1.89	0.54
1:B:3218:VAL:O	1:B:3222:LYS:HB2	2.07	0.54
1:D:846:LEU:HD22	1:D:851:PHE:HE1	1.73	0.54
1:D:3172:ILE:HD11	1:D:3190:LEU:HB3	1.90	0.54
1:A:1074:ILE:HD11	1:A:1111:PRO:HA	1.89	0.54
1:A:2519:LEU:HD12	1:A:2578:MET:HE3	1.90	0.54
1:A:2620:GLN:HE22	1:A:2674:LEU:HD22	1.71	0.54
1:C:1074:ILE:HD11	1:C:1111:PRO:HA	1.89	0.54
1:C:1527:MET:HB2	1:C:1540:PHE:HB2	1.89	0.54
1:C:3172:ILE:HD11	1:C:3190:LEU:HB3	1.90	0.54
1:D:234:SER:HB2	1:D:242:ARG:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3771:HIS:O	1:D:3815:LYS:NZ	2.40	0.54
1:A:731:THR:O	1:A:765:GLN:NE2	2.41	0.54
1:A:846:LEU:HD22	1:A:851:PHE:HE1	1.73	0.54
1:B:2519:LEU:HD12	1:B:2578:MET:HE3	1.90	0.54
1:C:2749:GLU:HG3	1:C:2752:ASP:HB2	1.90	0.54
1:D:988:LEU:HG	1:D:1039:LEU:HD13	1.89	0.54
1:D:2287:ALA:HA	1:D:2290:LEU:HB2	1.90	0.54
1:D:2749:GLU:HG3	1:D:2752:ASP:HB2	1.90	0.54
1:D:3324:VAL:HG11	1:D:3361:THR:HB	1.89	0.54
1:A:2420:HIS:HA	1:A:2423:MET:HE2	1.89	0.54
1:A:2792:ARG:NH2	1:A:2798:SER:OG	2.41	0.54
1:B:219:VAL:HG12	1:B:259:LEU:HD12	1.90	0.54
1:B:2499:LYS:NZ	1:B:2529:ASP:OD2	2.33	0.54
1:D:2519:LEU:HD12	1:D:2578:MET:HE3	1.90	0.54
2:H:24:VAL:HG12	2:H:103:LEU:HA	1.88	0.54
1:A:2287:ALA:HA	1:A:2290:LEU:HB2	1.90	0.54
1:B:3206:LEU:HB3	1:B:3246:LEU:HB2	1.89	0.54
1:D:650:VAL:O	1:D:777:PHE:N	2.41	0.54
1:D:2792:ARG:NH2	1:D:2798:SER:OG	2.41	0.54
1:D:3151:GLN:NE2	1:D:3154:ASP:OD2	2.41	0.54
1:B:2018:GLU:OE1	1:B:2028:ARG:NH1	2.38	0.53
1:C:1731:LEU:HD13	1:C:1772:ARG:HH21	1.72	0.53
1:D:1074:ILE:HD11	1:D:1111:PRO:HA	1.89	0.53
1:D:1776:HIS:HB3	1:D:1798:LEU:HD13	1.90	0.53
1:D:3206:LEU:HB3	1:D:3246:LEU:HB2	1.89	0.53
1:A:4721:LYS:NZ	1:A:4741:LEU:O	2.41	0.53
1:B:2792:ARG:NH2	1:B:2798:SER:OG	2.41	0.53
1:C:2519:LEU:HD12	1:C:2578:MET:HE3	1.90	0.53
1:A:3324:VAL:HG11	1:A:3361:THR:HB	1.89	0.53
1:B:41:GLY:O	1:B:45:ARG:NH1	2.41	0.53
1:B:731:THR:O	1:B:765:GLN:NE2	2.41	0.53
1:C:2287:ALA:HA	1:C:2290:LEU:HB2	1.90	0.53
1:A:4088:ILE:O	1:A:4123:ILE:N	2.42	0.53
1:B:1295:VAL:HG12	1:B:1579:MET:HB3	1.90	0.53
1:B:4088:ILE:O	1:B:4123:ILE:N	2.42	0.53
1:C:650:VAL:O	1:C:777:PHE:N	2.41	0.53
1:D:1097:THR:HA	1:D:1143:TRP:HE1	1.73	0.53
1:D:1295:VAL:HG12	1:D:1579:MET:HB3	1.90	0.53
1:D:2420:HIS:HA	1:D:2423:MET:HE2	1.89	0.53
1:D:3821:LYS:O	1:D:3824:LYS:NZ	2.39	0.53
1:A:1097:THR:HA	1:A:1143:TRP:HE1	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:731:THR:O	1:C:765:GLN:NE2	2.41	0.53
1:D:3207:GLU:OE1	1:D:3305:THR:OG1	2.26	0.53
1:D:4117:ALA:HB1	1:D:4121:GLU:HA	1.91	0.53
1:A:3172:ILE:HD11	1:A:3190:LEU:HB3	1.90	0.53
1:C:219:VAL:HG12	1:C:259:LEU:HD12	1.90	0.53
1:C:889:GLN:O	1:C:892:THR:OG1	2.25	0.53
1:A:3821:LYS:O	1:A:3824:LYS:NZ	2.40	0.53
1:B:1830:VAL:HB	1:B:1837:GLN:HG3	1.91	0.53
1:C:1574:PRO:HG3	1:C:1589:PRO:HG3	1.91	0.53
1:A:1295:VAL:HG12	1:A:1579:MET:HB3	1.90	0.53
1:A:2500:ALA:HB2	1:A:2553:TYR:HD1	1.74	0.53
1:B:1074:ILE:HD11	1:B:1111:PRO:HA	1.89	0.53
1:C:846:LEU:HD22	1:C:851:PHE:HE1	1.73	0.53
1:C:2420:HIS:HA	1:C:2423:MET:HE2	1.89	0.53
1:D:731:THR:O	1:D:765:GLN:NE2	2.41	0.53
1:A:219:VAL:HG12	1:A:259:LEU:HD12	1.90	0.53
1:A:650:VAL:O	1:A:777:PHE:N	2.41	0.53
1:A:1776:HIS:HB3	1:A:1798:LEU:HD13	1.91	0.53
1:B:2287:ALA:HA	1:B:2290:LEU:HB2	1.90	0.53
1:B:3172:ILE:HD11	1:B:3190:LEU:HB3	1.90	0.53
1:B:3771:HIS:O	1:B:3815:LYS:NZ	2.40	0.53
1:C:3955:MET:HB2	1:C:4019:LEU:HD22	1.91	0.53
1:A:1448:VAL:HG22	1:A:1554:VAL:HG23	1.91	0.53
1:A:3955:MET:HB2	1:A:4019:LEU:HD22	1.91	0.53
1:B:743:VAL:HB	1:B:760:ASN:HA	1.91	0.53
1:B:3955:MET:HB2	1:B:4019:LEU:HD22	1.91	0.53
1:D:355:LEU:HD22	1:D:380:GLN:HA	1.91	0.53
1:D:1432:THR:HA	1:D:1520:VAL:O	2.09	0.53
1:D:2500:ALA:HB2	1:D:2553:TYR:HD1	1.74	0.53
1:A:3075:LEU:O	1:A:3146:HIS:NE2	2.43	0.52
1:B:650:VAL:O	1:B:777:PHE:N	2.41	0.52
1:B:1432:THR:HA	1:B:1520:VAL:O	2.09	0.52
1:C:732:SER:HB2	1:C:735:GLN:HB3	1.91	0.52
1:C:3207:GLU:OE1	1:C:3305:THR:OG1	2.26	0.52
1:C:3575:LEU:HD23	1:D:1219:LEU:HD22	1.91	0.52
1:D:603:LEU:HD23	1:D:606:LEU:HD12	1.91	0.52
1:B:2500:ALA:HB2	1:B:2553:TYR:HD1	1.74	0.52
1:C:603:LEU:HD23	1:C:606:LEU:HD12	1.91	0.52
1:C:1295:VAL:HG12	1:C:1579:MET:HB3	1.90	0.52
1:C:3075:LEU:O	1:C:3146:HIS:NE2	2.43	0.52
1:C:4117:ALA:HB1	1:C:4121:GLU:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:VAL:HG12	1:B:274:LEU:HD12	1.92	0.52
1:B:603:LEU:HD23	1:B:606:LEU:HD12	1.91	0.52
1:B:995:VAL:HG22	1:B:998:ARG:HH21	1.74	0.52
1:B:1574:PRO:HG3	1:B:1589:PRO:HG3	1.91	0.52
1:B:2107:GLN:NE2	1:B:3682:GLU:OE1	2.43	0.52
1:C:214:VAL:HG12	1:C:274:LEU:HD12	1.92	0.52
1:C:2792:ARG:NH2	1:C:2798:SER:OG	2.41	0.52
1:C:4088:ILE:O	1:C:4123:ILE:N	2.42	0.52
1:D:3955:MET:HB2	1:D:4019:LEU:HD22	1.91	0.52
1:D:4088:ILE:O	1:D:4123:ILE:N	2.42	0.52
1:A:1830:VAL:HB	1:A:1837:GLN:HG3	1.91	0.52
1:A:2107:GLN:NE2	1:A:3682:GLU:OE1	2.43	0.52
1:B:2488:PRO:HD2	1:B:2546:MET:HE3	1.92	0.52
1:B:3075:LEU:O	1:B:3146:HIS:NE2	2.43	0.52
1:C:1432:THR:HA	1:C:1520:VAL:O	2.09	0.52
1:C:3051:ARG:NH2	1:C:3102:ASP:OD1	2.43	0.52
1:C:4068:LEU:HA	1:C:4071:ILE:HB	1.92	0.52
1:A:4117:ALA:HB1	1:A:4121:GLU:HA	1.91	0.52
1:B:3677:LEU:HB3	1:B:3698:LEU:HB2	1.92	0.52
1:C:3677:LEU:HB3	1:C:3698:LEU:HB2	1.92	0.52
1:D:1830:VAL:HB	1:D:1837:GLN:HG3	1.91	0.52
1:D:3677:LEU:HB3	1:D:3698:LEU:HB2	1.92	0.52
1:B:3330:ASP:O	1:B:3403:ARG:NH2	2.43	0.52
1:D:732:SER:HB2	1:D:735:GLN:HB3	1.91	0.52
1:D:1243:PRO:HA	1:D:1602:PRO:HA	1.92	0.52
1:A:1243:PRO:HA	1:A:1602:PRO:HA	1.92	0.52
1:A:3677:LEU:HB3	1:A:3698:LEU:HB2	1.92	0.52
1:B:1448:VAL:HG22	1:B:1554:VAL:HG23	1.92	0.52
1:B:1776:HIS:HB3	1:B:1798:LEU:HD13	1.90	0.52
1:B:2519:LEU:HD13	1:B:2522:LEU:HD12	1.92	0.52
1:B:3670:GLU:HB3	1:B:3732:SER:HB3	1.92	0.52
1:C:743:VAL:HB	1:C:760:ASN:HA	1.91	0.52
1:C:1106:ARG:NH2	1:C:1183:GLU:O	2.39	0.52
1:C:2500:ALA:HB2	1:C:2553:TYR:HD1	1.74	0.52
1:D:219:VAL:HG12	1:D:259:LEU:HD12	1.90	0.52
1:D:2519:LEU:HD13	1:D:2522:LEU:HD12	1.92	0.52
1:A:214:VAL:HG12	1:A:274:LEU:HD12	1.92	0.52
1:A:355:LEU:HD22	1:A:380:GLN:HA	1.91	0.52
1:A:878:ILE:HG22	1:A:881:LEU:HD13	1.92	0.52
1:A:1432:THR:HA	1:A:1520:VAL:O	2.09	0.52
1:A:1574:PRO:HG3	1:A:1589:PRO:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1808:ARG:HD3	1:B:1853:ILE:HG22	1.92	0.52
1:C:1243:PRO:HA	1:C:1602:PRO:HA	1.92	0.52
1:D:214:VAL:HG12	1:D:274:LEU:HD12	1.92	0.52
1:D:2488:PRO:HD2	1:D:2546:MET:HE3	1.91	0.52
1:D:3051:ARG:NH2	1:D:3102:ASP:OD1	2.43	0.52
1:A:41:GLY:O	1:A:45:ARG:NH1	2.41	0.52
1:A:743:VAL:HB	1:A:760:ASN:HA	1.91	0.52
1:A:2013:LYS:NZ	1:A:3661:TRP:O	2.38	0.52
1:A:2519:LEU:HD13	1:A:2522:LEU:HD12	1.92	0.52
1:A:3051:ARG:NH2	1:A:3102:ASP:OD1	2.43	0.52
1:B:4068:LEU:HA	1:B:4071:ILE:HB	1.92	0.52
1:C:1043:VAL:HA	1:C:1046:LEU:HD12	1.92	0.52
1:C:1474:VAL:O	1:C:1486:SER:HA	2.10	0.52
1:C:3330:ASP:O	1:C:3403:ARG:NH2	2.43	0.52
1:C:3670:GLU:HB3	1:C:3732:SER:HB3	1.92	0.52
1:D:3330:ASP:O	1:D:3403:ARG:NH2	2.43	0.52
1:A:3330:ASP:O	1:A:3403:ARG:NH2	2.43	0.52
1:C:1808:ARG:HD3	1:C:1853:ILE:HG22	1.92	0.52
1:C:2107:GLN:NE2	1:C:3682:GLU:OE1	2.43	0.52
1:C:2519:LEU:HD13	1:C:2522:LEU:HD12	1.92	0.52
1:A:3007:ASN:O	1:A:3011:THR:OG1	2.26	0.51
1:B:1106:ARG:NH2	1:B:1183:GLU:O	2.39	0.51
1:D:1036:ARG:O	1:D:1040:CYS:HB2	2.10	0.51
1:D:1474:VAL:O	1:D:1486:SER:HA	2.10	0.51
1:D:2107:GLN:NE2	1:D:3682:GLU:OE1	2.43	0.51
1:A:1036:ARG:O	1:A:1040:CYS:HB2	2.10	0.51
1:B:3051:ARG:NH2	1:B:3102:ASP:OD1	2.43	0.51
1:C:76:ARG:HA	1:C:79:GLN:HG2	1.92	0.51
1:C:707:VAL:HG23	1:C:782:SER:HB3	1.92	0.51
1:C:1422:ASP:OD2	1:C:1568:LYS:NZ	2.38	0.51
1:C:1448:VAL:HG22	1:C:1554:VAL:HG23	1.92	0.51
1:D:1043:VAL:HA	1:D:1046:LEU:HD12	1.92	0.51
1:D:1448:VAL:HG22	1:D:1554:VAL:HG23	1.92	0.51
1:D:3075:LEU:O	1:D:3146:HIS:NE2	2.43	0.51
1:A:995:VAL:HG22	1:A:998:ARG:HH21	1.74	0.51
1:A:1252:HIS:O	1:A:1275:ARG:NH1	2.43	0.51
1:A:3443:ILE:HD11	1:A:3601:ALA:HB1	1.93	0.51
1:B:732:SER:HB2	1:B:735:GLN:HB3	1.91	0.51
1:B:4117:ALA:HB1	1:B:4121:GLU:HA	1.91	0.51
1:C:1776:HIS:HB3	1:C:1798:LEU:HD13	1.90	0.51
1:C:3771:HIS:O	1:C:3815:LYS:NZ	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4721:LYS:NZ	1:C:4741:LEU:O	2.41	0.51
1:D:1574:PRO:HG3	1:D:1589:PRO:HG3	1.91	0.51
1:D:2997:PHE:O	1:D:3001:ILE:HB	2.10	0.51
1:D:3443:ILE:HD11	1:D:3601:ALA:HB1	1.93	0.51
1:D:4721:LYS:NZ	1:D:4741:LEU:O	2.41	0.51
1:A:2997:PHE:O	1:A:3001:ILE:HB	2.10	0.51
1:A:4068:LEU:HA	1:A:4071:ILE:HB	1.92	0.51
1:B:76:ARG:HA	1:B:79:GLN:HG2	1.92	0.51
1:B:130:LYS:HD3	1:B:131:LEU:HG	1.93	0.51
1:B:3888:LEU:HD23	1:B:3891:LEU:HD21	1.92	0.51
1:C:2997:PHE:O	1:C:3001:ILE:HB	2.10	0.51
1:C:3842:LEU:HB2	1:C:3929:SER:HB2	1.93	0.51
1:D:1808:ARG:HD3	1:D:1853:ILE:HG22	1.92	0.51
1:A:1225:PRO:HG2	1:A:1228:ILE:HD13	1.93	0.51
1:A:1808:ARG:HD3	1:A:1853:ILE:HG22	1.92	0.51
1:A:3888:LEU:HD23	1:A:3891:LEU:HD21	1.92	0.51
1:B:1243:PRO:HA	1:B:1602:PRO:HA	1.92	0.51
1:B:1252:HIS:O	1:B:1275:ARG:NH1	2.43	0.51
1:C:130:LYS:HD3	1:C:131:LEU:HG	1.93	0.51
1:D:3670:GLU:HB3	1:D:3732:SER:HB3	1.92	0.51
1:A:529:LEU:O	1:A:533:ASN:ND2	2.44	0.51
1:A:603:LEU:HD23	1:A:606:LEU:HD12	1.91	0.51
1:A:732:SER:HB2	1:A:735:GLN:HB3	1.91	0.51
1:A:2469:ILE:HG21	1:A:2502:MET:HE3	1.93	0.51
1:B:355:LEU:HD22	1:B:380:GLN:HA	1.91	0.51
1:B:878:ILE:HG22	1:B:881:LEU:HD13	1.92	0.51
1:D:707:VAL:HG23	1:D:782:SER:HB3	1.92	0.51
1:D:995:VAL:HG22	1:D:998:ARG:HH21	1.74	0.51
1:A:3670:GLU:HB3	1:A:3732:SER:HB3	1.92	0.51
1:A:3842:LEU:HB2	1:A:3929:SER:HB2	1.93	0.51
1:B:1225:PRO:HG2	1:B:1228:ILE:HD13	1.93	0.51
1:B:1443:GLN:NE2	1:B:1555:LEU:O	2.35	0.51
1:B:3575:LEU:HD23	1:C:1219:LEU:HD22	1.91	0.51
1:B:3842:LEU:HB2	1:B:3929:SER:HB2	1.93	0.51
1:C:355:LEU:HD22	1:C:380:GLN:HA	1.91	0.51
1:C:1007:TYR:O	1:C:1017:ARG:NH2	2.39	0.51
1:C:1036:ARG:O	1:C:1040:CYS:HB2	2.10	0.51
1:C:1830:VAL:HB	1:C:1837:GLN:HG3	1.91	0.51
1:C:2488:PRO:HD2	1:C:2546:MET:HE3	1.92	0.51
1:D:878:ILE:HG22	1:D:881:LEU:HD13	1.92	0.51
1:A:2488:PRO:HD2	1:A:2546:MET:HE3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2522:LEU:HB3	1:A:2582:MET:HE1	1.93	0.51
1:B:1043:VAL:HA	1:B:1046:LEU:HD12	1.92	0.51
1:B:1474:VAL:O	1:B:1486:SER:HA	2.10	0.51
1:C:529:LEU:O	1:C:533:ASN:ND2	2.44	0.51
1:D:743:VAL:HB	1:D:760:ASN:HA	1.91	0.51
1:D:2522:LEU:HB3	1:D:2582:MET:HE1	1.93	0.51
1:A:2517:PHE:HA	1:A:2520:HIS:HB3	1.93	0.51
1:A:3771:HIS:O	1:A:3815:LYS:NZ	2.40	0.51
1:B:3443:ILE:HD11	1:B:3601:ALA:HB1	1.93	0.51
1:C:1968:LYS:NZ	1:C:2030:ASP:OD2	2.44	0.51
1:C:2522:LEU:HB3	1:C:2582:MET:HE1	1.93	0.51
1:D:76:ARG:HA	1:D:79:GLN:HG2	1.92	0.51
1:A:707:VAL:HG23	1:A:782:SER:HB3	1.92	0.51
1:A:1256:GLU:HB3	1:A:1275:ARG:HD2	1.93	0.51
1:C:995:VAL:HG22	1:C:998:ARG:HH21	1.74	0.51
1:C:1225:PRO:HG2	1:C:1228:ILE:HD13	1.93	0.51
1:D:835:ARG:NH2	1:D:1210:SER:O	2.44	0.51
1:D:1252:HIS:O	1:D:1275:ARG:NH1	2.43	0.51
1:D:1968:LYS:NZ	1:D:2030:ASP:OD2	2.44	0.51
1:D:2469:ILE:HG21	1:D:2502:MET:HE3	1.93	0.51
1:D:2517:PHE:HA	1:D:2520:HIS:HB3	1.93	0.51
1:D:4068:LEU:HA	1:D:4071:ILE:HB	1.92	0.51
1:A:417:GLY:HA3	1:A:436:LEU:HD21	1.93	0.50
1:A:835:ARG:NH2	1:A:1210:SER:O	2.44	0.50
1:A:1007:TYR:O	1:A:1017:ARG:NH2	2.39	0.50
1:A:3203:VAL:HG12	1:A:3214:ASN:HD22	1.76	0.50
1:A:4686:LEU:HA	1:A:4690:GLU:HG3	1.92	0.50
1:C:4686:LEU:HA	1:C:4690:GLU:HG3	1.92	0.50
1:D:3842:LEU:HB2	1:D:3929:SER:HB2	1.93	0.50
1:A:76:ARG:NH1	1:D:3938:SER:OG	2.44	0.50
1:A:3690:VAL:HG13	1:A:3692:GLU:H	1.75	0.50
1:A:4544:LEU:O	1:A:4548:ARG:HB2	2.12	0.50
1:B:529:LEU:O	1:B:533:ASN:ND2	2.44	0.50
1:B:1131:ARG:NH1	1:B:1178:ALA:O	2.45	0.50
1:B:2469:ILE:HG21	1:B:2502:MET:HE3	1.93	0.50
1:B:2522:LEU:HB3	1:B:2582:MET:HE1	1.93	0.50
1:C:835:ARG:NH2	1:C:1210:SER:O	2.44	0.50
1:C:1256:GLU:HB3	1:C:1275:ARG:HD2	1.93	0.50
1:C:1443:GLN:NE2	1:C:1555:LEU:O	2.35	0.50
1:C:3007:ASN:O	1:C:3011:THR:OG1	2.26	0.50
1:D:41:GLY:O	1:D:45:ARG:NH1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3007:ASN:O	1:D:3011:THR:OG1	2.26	0.50
1:D:4544:LEU:O	1:D:4548:ARG:HB2	2.12	0.50
1:A:1474:VAL:O	1:A:1486:SER:HA	2.10	0.50
1:B:1036:ARG:O	1:B:1040:CYS:HB2	2.10	0.50
1:B:1870:VAL:HG11	1:B:2097:LEU:HD22	1.93	0.50
1:B:2000:SER:O	1:B:2005:GLN:NE2	2.34	0.50
1:C:878:ILE:HG22	1:C:881:LEU:HD13	1.92	0.50
1:C:2611:CYS:HA	1:C:2614:ILE:HG22	1.94	0.50
1:C:2755:ILE:HD12	1:C:2813:LEU:HG	1.93	0.50
1:D:1851:MET:HB2	1:D:1853:ILE:HG12	1.93	0.50
1:D:3592:ILE:HG13	1:D:3595:ARG:HE	1.76	0.50
1:D:4686:LEU:HA	1:D:4690:GLU:HG3	1.92	0.50
1:A:1968:LYS:NZ	1:A:2030:ASP:OD2	2.44	0.50
1:A:3592:ILE:HG13	1:A:3595:ARG:HE	1.76	0.50
1:D:529:LEU:O	1:D:533:ASN:ND2	2.44	0.50
1:B:1944:GLU:HB3	1:B:2123:LEU:HD21	1.94	0.50
1:B:2997:PHE:O	1:B:3001:ILE:HB	2.10	0.50
1:C:417:GLY:HA3	1:C:436:LEU:HD21	1.94	0.50
1:C:1870:VAL:HG11	1:C:2097:LEU:HD22	1.93	0.50
1:D:417:GLY:HA3	1:D:436:LEU:HD21	1.94	0.50
1:D:1721:GLU:OE1	1:D:1725:ARG:NH2	2.45	0.50
1:D:3218:VAL:HB	1:D:3227:ARG:HD3	1.93	0.50
1:A:1043:VAL:HA	1:A:1046:LEU:HD12	1.92	0.50
1:A:1851:MET:HB2	1:A:1853:ILE:HG12	1.94	0.50
1:B:417:GLY:HA3	1:B:436:LEU:HD21	1.94	0.50
1:B:707:VAL:HG23	1:B:782:SER:HB3	1.92	0.50
1:B:835:ARG:NH2	1:B:1210:SER:O	2.44	0.50
1:B:2517:PHE:HA	1:B:2520:HIS:HB3	1.93	0.50
1:B:3207:GLU:OE1	1:B:3305:THR:OG1	2.26	0.50
1:B:3690:VAL:HG13	1:B:3692:GLU:H	1.75	0.50
1:B:4721:LYS:NZ	1:B:4741:LEU:O	2.41	0.50
1:C:1721:GLU:OE1	1:C:1725:ARG:NH2	2.45	0.50
1:C:3443:ILE:HD11	1:C:3601:ALA:HB1	1.93	0.50
1:C:3888:LEU:HD23	1:C:3891:LEU:HD21	1.92	0.50
1:D:3690:VAL:HG13	1:D:3692:GLU:H	1.75	0.50
1:D:4155:PRO:O	1:D:4161:ARG:NH1	2.45	0.50
1:A:76:ARG:HA	1:A:79:GLN:HG2	1.92	0.50
1:A:1870:VAL:HG11	1:A:2097:LEU:HD22	1.93	0.50
1:A:3607:GLU:HA	1:A:3610:GLU:HG2	1.94	0.50
1:B:1851:MET:HB2	1:B:1853:ILE:HG12	1.94	0.50
1:B:2755:ILE:HD12	1:B:2813:LEU:HG	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1131:ARG:NH1	1:C:1178:ALA:O	2.45	0.50
1:D:1131:ARG:NH1	1:D:1178:ALA:O	2.45	0.50
1:D:1225:PRO:HG2	1:D:1228:ILE:HD13	1.93	0.50
1:D:2695:LEU:O	1:D:2699:ALA:HB2	2.12	0.50
1:A:653:ALA:HB3	1:A:656:SER:HB2	1.94	0.50
1:A:2755:ILE:HD12	1:A:2813:LEU:HG	1.93	0.50
1:B:1257:VAL:HG21	1:B:1597:VAL:HG11	1.94	0.50
1:C:4161:ARG:HE	1:C:4164:LEU:HD21	1.77	0.50
1:D:492:ASP:OD1	1:D:546:TRP:NE1	2.36	0.50
1:D:1422:ASP:OD2	1:D:1568:LYS:NZ	2.38	0.50
1:D:3203:VAL:HG12	1:D:3214:ASN:HD22	1.76	0.50
1:A:130:LYS:HD3	1:A:131:LEU:HG	1.93	0.50
1:A:168:ASP:OD1	1:A:201:ASN:ND2	2.45	0.50
1:A:1547:LYS:NZ	1:A:1642:PRO:O	2.45	0.50
1:A:3226:GLU:HA	1:A:3229:ILE:HG12	1.94	0.50
1:B:110:ARG:NH1	1:B:115:ARG:O	2.45	0.50
1:B:1256:GLU:HB3	1:B:1275:ARG:HD2	1.93	0.50
1:B:1721:GLU:OE1	1:B:1725:ARG:NH2	2.45	0.50
1:B:2211:MET:HA	1:B:2214:VAL:HG12	1.94	0.50
1:B:4686:LEU:HA	1:B:4690:GLU:HG3	1.92	0.50
1:C:1461:ASP:OD2	1:C:1468:LYS:NZ	2.40	0.50
1:C:2469:ILE:HG21	1:C:2502:MET:HE3	1.93	0.50
1:C:3607:GLU:HA	1:C:3610:GLU:HG2	1.93	0.50
1:C:4155:PRO:O	1:C:4161:ARG:NH1	2.45	0.50
1:D:110:ARG:NH1	1:D:115:ARG:O	2.45	0.50
1:D:2015:GLU:OE2	1:D:2032:GLN:NE2	2.45	0.50
1:D:2611:CYS:HA	1:D:2614:ILE:HG22	1.94	0.50
1:A:1106:ARG:NH2	1:A:1183:GLU:O	2.39	0.49
1:B:3007:ASN:O	1:B:3011:THR:OG1	2.26	0.49
1:B:3592:ILE:HG13	1:B:3595:ARG:HE	1.76	0.49
1:C:1851:MET:HB2	1:C:1853:ILE:HG12	1.94	0.49
1:C:3690:VAL:HG13	1:C:3692:GLU:H	1.75	0.49
1:D:870:ILE:HG13	1:D:874:LEU:HD23	1.94	0.49
1:D:3888:LEU:HD23	1:D:3891:LEU:HD21	1.92	0.49
1:D:4161:ARG:HE	1:D:4164:LEU:HD21	1.77	0.49
1:A:1131:ARG:NH1	1:A:1178:ALA:O	2.45	0.49
1:A:1257:VAL:HG21	1:A:1597:VAL:HG11	1.94	0.49
1:A:2211:MET:HA	1:A:2214:VAL:HG12	1.94	0.49
1:C:1547:LYS:NZ	1:C:1642:PRO:O	2.45	0.49
1:C:2517:PHE:HA	1:C:2520:HIS:HB3	1.93	0.49
1:C:2627:VAL:HG22	1:C:2678:LEU:HG	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2695:LEU:O	1:C:2699:ALA:HB2	2.12	0.49
1:D:1257:VAL:HG21	1:D:1597:VAL:HG11	1.94	0.49
1:A:1721:GLU:OE1	1:A:1725:ARG:NH2	2.45	0.49
1:A:2695:LEU:O	1:A:2699:ALA:HB2	2.12	0.49
1:B:1225:PRO:HB2	1:B:1228:ILE:HB	1.94	0.49
1:B:3218:VAL:HB	1:B:3227:ARG:HD3	1.93	0.49
1:B:4161:ARG:HE	1:B:4164:LEU:HD21	1.77	0.49
1:C:110:ARG:NH1	1:C:115:ARG:O	2.45	0.49
1:C:870:ILE:HG13	1:C:874:LEU:HD23	1.94	0.49
1:C:1116:GLY:H	1:C:1121:ALA:HB3	1.77	0.49
1:C:1225:PRO:HB2	1:C:1228:ILE:HB	1.94	0.49
1:C:3206:LEU:HD13	1:C:3246:LEU:HD13	1.94	0.49
1:C:3226:GLU:HA	1:C:3229:ILE:HG12	1.94	0.49
1:C:3891:LEU:HD13	1:C:3899:PHE:HE1	1.77	0.49
1:C:4544:LEU:O	1:C:4548:ARG:HB2	2.12	0.49
1:D:653:ALA:HB3	1:D:656:SER:HB2	1.94	0.49
1:D:1547:LYS:NZ	1:D:1642:PRO:O	2.45	0.49
1:D:1870:VAL:HG11	1:D:2097:LEU:HD22	1.93	0.49
1:D:2755:ILE:HD12	1:D:2813:LEU:HG	1.93	0.49
1:A:2015:GLU:OE2	1:A:2032:GLN:NE2	2.45	0.49
1:A:3218:VAL:HB	1:A:3227:ARG:HD3	1.93	0.49
1:A:3435:PHE:HA	1:A:3517:MET:HE1	1.94	0.49
1:B:14:LEU:HB2	1:B:163:VAL:HG13	1.94	0.49
1:C:168:ASP:OD1	1:C:201:ASN:ND2	2.45	0.49
1:C:653:ALA:HB3	1:C:656:SER:HB2	1.94	0.49
1:C:1944:GLU:HB3	1:C:2123:LEU:HD21	1.94	0.49
1:D:130:LYS:HD3	1:D:131:LEU:HG	1.93	0.49
1:D:551:LEU:HD21	1:D:585:SER:HB3	1.95	0.49
1:D:2627:VAL:HG22	1:D:2678:LEU:HG	1.95	0.49
1:D:2716:ASP:N	1:D:2716:ASP:OD1	2.46	0.49
2:G:78:PRO:HA	2:G:81:ALA:HB3	1.95	0.49
1:A:551:LEU:HD21	1:A:585:SER:HB3	1.94	0.49
1:A:1421:ARG:O	1:A:1570:LYS:NZ	2.42	0.49
1:B:653:ALA:HB3	1:B:656:SER:HB2	1.94	0.49
1:B:1547:LYS:NZ	1:B:1642:PRO:O	2.45	0.49
1:B:1968:LYS:NZ	1:B:2030:ASP:OD2	2.44	0.49
1:B:2611:CYS:HA	1:B:2614:ILE:HG22	1.94	0.49
1:B:2695:LEU:O	1:B:2699:ALA:HB2	2.12	0.49
1:B:3203:VAL:HG12	1:B:3214:ASN:HD22	1.76	0.49
1:C:2015:GLU:OE2	1:C:2032:GLN:NE2	2.45	0.49
1:D:1116:GLY:H	1:D:1121:ALA:HB3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1443:GLN:NE2	1:D:1555:LEU:O	2.35	0.49
1:A:168:ASP:HB3	1:A:199:LEU:HD11	1.94	0.49
1:A:1650:ILE:HA	1:A:1653:LEU:HD13	1.95	0.49
1:B:3607:GLU:HA	1:B:3610:GLU:HG2	1.93	0.49
1:D:1225:PRO:HB2	1:D:1228:ILE:HB	1.94	0.49
1:D:2927:LEU:HD12	1:D:2930:LEU:HD12	1.94	0.49
2:H:78:PRO:HA	2:H:81:ALA:HB3	1.95	0.49
1:A:492:ASP:OD1	1:A:546:TRP:NE1	2.36	0.49
1:A:1461:ASP:OD2	1:A:1468:LYS:NZ	2.40	0.49
1:A:2927:LEU:HD12	1:A:2930:LEU:HD12	1.95	0.49
1:B:4544:LEU:O	1:B:4548:ARG:HB2	2.12	0.49
1:C:3218:VAL:HB	1:C:3227:ARG:HD3	1.93	0.49
1:D:1650:ILE:HA	1:D:1653:LEU:HD13	1.95	0.49
1:D:1944:GLU:HB3	1:D:2123:LEU:HD21	1.94	0.49
1:D:3872:GLU:HG3	1:D:3874:VAL:H	1.78	0.49
1:D:3891:LEU:HD13	1:D:3899:PHE:HE1	1.77	0.49
2:F:78:PRO:HA	2:F:81:ALA:HB3	1.95	0.49
1:A:110:ARG:NH1	1:A:115:ARG:O	2.45	0.49
1:A:1944:GLU:HB3	1:A:2123:LEU:HD21	1.94	0.49
1:A:3019:SER:O	1:A:3036:LYS:NZ	2.46	0.49
1:A:3206:LEU:HD13	1:A:3246:LEU:HD13	1.94	0.49
1:B:3111:ARG:NH2	1:B:3174:SER:OG	2.46	0.49
1:B:3821:LYS:O	1:B:3824:LYS:NZ	2.39	0.49
1:B:4155:PRO:O	1:B:4161:ARG:NH1	2.45	0.49
1:C:3284:TRP:HB3	1:C:3305:THR:HG21	1.95	0.49
1:C:3435:PHE:HA	1:C:3517:MET:HE1	1.94	0.49
1:D:3284:TRP:HB3	1:D:3305:THR:HG21	1.95	0.49
1:A:14:LEU:HB2	1:A:163:VAL:HG13	1.94	0.49
1:A:867:LEU:HB3	1:A:929:LEU:HD13	1.94	0.49
1:A:2611:CYS:HA	1:A:2614:ILE:HG22	1.94	0.49
1:A:3284:TRP:HB3	1:A:3305:THR:HG21	1.95	0.49
1:B:1650:ILE:HA	1:B:1653:LEU:HD13	1.95	0.49
1:B:2015:GLU:OE2	1:B:2032:GLN:NE2	2.45	0.49
1:B:2627:VAL:HG22	1:B:2678:LEU:HG	1.95	0.49
1:C:2211:MET:HA	1:C:2214:VAL:HG12	1.94	0.49
1:C:3037:GLU:HB3	1:C:3088:VAL:HG21	1.95	0.49
1:C:3203:VAL:HG12	1:C:3214:ASN:HD22	1.76	0.49
1:D:1106:ARG:NH2	1:D:1183:GLU:O	2.39	0.49
1:D:3111:ARG:NH2	1:D:3174:SER:OG	2.46	0.49
2:E:78:PRO:HA	2:E:81:ALA:HB3	1.95	0.49
1:A:195:PHE:O	1:D:2359:ARG:NH1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:TYR:O	1:A:553:ARG:NH2	2.41	0.49
1:A:3111:ARG:NH2	1:A:3174:SER:OG	2.46	0.49
1:A:3575:LEU:HD23	1:B:1219:LEU:HD22	1.94	0.49
1:A:4155:PRO:O	1:A:4161:ARG:NH1	2.45	0.49
1:A:4161:ARG:HE	1:A:4164:LEU:HD21	1.77	0.49
1:B:870:ILE:HG13	1:B:874:LEU:HD23	1.94	0.49
1:B:1007:TYR:O	1:B:1017:ARG:NH2	2.39	0.49
1:B:2013:LYS:NZ	1:B:3661:TRP:O	2.38	0.49
1:B:2971:GLN:HA	1:B:2974:ILE:HG12	1.95	0.49
1:C:1650:ILE:HA	1:C:1653:LEU:HD13	1.95	0.49
1:D:14:LEU:HB2	1:D:163:VAL:HG13	1.94	0.49
1:D:168:ASP:OD1	1:D:201:ASN:ND2	2.45	0.49
1:D:1454:THR:OG1	1:D:1456:ASP:OD1	2.30	0.49
1:D:3202:PRO:O	1:D:3214:ASN:ND2	2.46	0.49
1:D:3206:LEU:HD13	1:D:3246:LEU:HD13	1.94	0.49
1:A:1225:PRO:HB2	1:A:1228:ILE:HB	1.94	0.48
1:A:2627:VAL:HG22	1:A:2678:LEU:HG	1.94	0.48
1:A:2971:GLN:HA	1:A:2974:ILE:HG12	1.95	0.48
1:B:168:ASP:OD1	1:B:201:ASN:ND2	2.45	0.48
1:C:14:LEU:HB2	1:C:163:VAL:HG13	1.94	0.48
1:C:637:LEU:HD13	1:C:1637:MET:HB3	1.95	0.48
1:C:1257:VAL:HG21	1:C:1597:VAL:HG11	1.94	0.48
1:C:3592:ILE:HG13	1:C:3595:ARG:HE	1.76	0.48
1:D:586:ILE:HA	1:D:589:LEU:HD23	1.96	0.48
1:D:1256:GLU:HB3	1:D:1275:ARG:HD2	1.93	0.48
1:D:2739:PRO:HG3	1:D:2888:ARG:HG2	1.95	0.48
1:C:3202:PRO:O	1:C:3214:ASN:ND2	2.46	0.48
1:D:2871:LEU:HG	1:D:2927:LEU:HD21	1.95	0.48
1:D:3226:GLU:HA	1:D:3229:ILE:HG12	1.94	0.48
1:A:586:ILE:HA	1:A:589:LEU:HD23	1.96	0.48
1:A:870:ILE:HG13	1:A:874:LEU:HD23	1.94	0.48
1:A:2871:LEU:HG	1:A:2927:LEU:HD21	1.95	0.48
1:A:3256:LEU:O	1:A:3259:SER:OG	2.30	0.48
1:B:3015:LEU:HD12	1:B:3025:LEU:HB3	1.95	0.48
1:B:3435:PHE:HA	1:B:3517:MET:HE1	1.94	0.48
1:C:2927:LEU:HD12	1:C:2930:LEU:HD12	1.94	0.48
1:C:3755:GLU:HA	1:C:3758:MET:HE3	1.95	0.48
1:C:3798:LEU:HD11	1:C:3884:LEU:HA	1.95	0.48
1:C:3872:GLU:HG3	1:C:3874:VAL:H	1.78	0.48
1:D:1024:TYR:O	1:D:1032:LYS:NZ	2.46	0.48
1:D:2211:MET:HA	1:D:2214:VAL:HG12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1068:ARG:HG2	1:A:1069:TRP:CD1	2.48	0.48
1:A:3566:SER:HB3	1:A:3569:LEU:HG	1.96	0.48
1:B:1068:ARG:HG2	1:B:1069:TRP:CD1	2.48	0.48
1:B:1116:GLY:H	1:B:1121:ALA:HB3	1.77	0.48
1:B:3053:ARG:HG3	1:B:3056:LEU:HD13	1.96	0.48
1:B:3206:LEU:HD13	1:B:3246:LEU:HD13	1.94	0.48
1:B:3226:GLU:HA	1:B:3229:ILE:HG12	1.94	0.48
1:C:168:ASP:HB3	1:C:199:LEU:HD11	1.94	0.48
1:C:586:ILE:HA	1:C:589:LEU:HD23	1.96	0.48
1:D:1077:ALA:HA	1:D:1236:THR:HG22	1.95	0.48
1:D:3607:GLU:HA	1:D:3610:GLU:HG2	1.93	0.48
1:A:1077:ALA:HA	1:A:1236:THR:HG22	1.95	0.48
1:A:3414:ARG:NH1	1:A:3469:PHE:O	2.45	0.48
1:A:3872:GLU:HG3	1:A:3874:VAL:H	1.78	0.48
1:A:3891:LEU:HD13	1:A:3899:PHE:HE1	1.78	0.48
1:B:3037:GLU:HB3	1:B:3088:VAL:HG21	1.95	0.48
1:C:497:TYR:O	1:C:553:ARG:NH2	2.41	0.48
1:C:2460:LEU:HA	1:D:131:LEU:HD21	1.96	0.48
1:C:3566:SER:HB3	1:C:3569:LEU:HG	1.96	0.48
1:D:867:LEU:HB3	1:D:929:LEU:HD13	1.94	0.48
1:D:3019:SER:O	1:D:3036:LYS:NZ	2.46	0.48
1:D:3566:SER:HB3	1:D:3569:LEU:HG	1.96	0.48
1:D:3798:LEU:HD11	1:D:3884:LEU:HA	1.95	0.48
1:A:637:LEU:HD13	1:A:1637:MET:HB3	1.95	0.48
1:A:3202:PRO:O	1:A:3214:ASN:ND2	2.46	0.48
1:B:168:ASP:HB3	1:B:199:LEU:HD11	1.94	0.48
1:B:551:LEU:HD21	1:B:585:SER:HB3	1.95	0.48
1:B:637:LEU:HD13	1:B:1637:MET:HB3	1.95	0.48
1:B:867:LEU:HB3	1:B:929:LEU:HD13	1.94	0.48
1:C:639:ASN:HD21	1:C:676:THR:HG1	1.56	0.48
1:C:867:LEU:HB3	1:C:929:LEU:HD13	1.94	0.48
1:C:4865:LYS:HA	1:C:4865:LYS:HD2	1.66	0.48
1:D:775:GLY:H	1:D:848:HIS:CG	2.32	0.48
1:A:2677:LYS:HB3	1:A:2677:LYS:HE2	1.67	0.48
1:A:3533:ILE:HD13	1:A:3596:VAL:HG13	1.95	0.48
1:B:2460:LEU:HA	1:C:131:LEU:HD21	1.96	0.48
1:B:2927:LEU:HD12	1:B:2930:LEU:HD12	1.94	0.48
1:B:3755:GLU:HA	1:B:3758:MET:HE3	1.95	0.48
1:B:3891:LEU:HD13	1:B:3899:PHE:HE1	1.77	0.48
1:D:2971:GLN:HA	1:D:2974:ILE:HG12	1.95	0.48
1:D:3755:GLU:HA	1:D:3758:MET:HE3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:MET:HE3	1:A:139:GLU:HG3	1.96	0.48
1:A:1116:GLY:H	1:A:1121:ALA:HB3	1.77	0.48
1:A:3015:LEU:HD12	1:A:3025:LEU:HB3	1.95	0.48
1:B:1431:THR:OG1	1:B:1521:ASP:OD1	2.31	0.48
1:B:3409:TYR:HE2	1:B:3510:ILE:HG12	1.78	0.48
1:C:2871:LEU:HG	1:C:2927:LEU:HD21	1.95	0.48
1:C:3111:ARG:NH2	1:C:3174:SER:OG	2.46	0.48
1:D:182:LEU:HG	1:D:184:THR:HG23	1.96	0.48
1:A:2000:SER:O	1:A:2005:GLN:NE2	2.34	0.48
1:B:116:MET:HE3	1:B:139:GLU:HG3	1.96	0.48
1:B:1422:ASP:OD2	1:B:1568:LYS:NZ	2.38	0.48
1:B:3872:GLU:HG3	1:B:3874:VAL:H	1.78	0.48
1:C:116:MET:HE3	1:C:139:GLU:HG3	1.96	0.48
1:C:551:LEU:HD21	1:C:585:SER:HB3	1.95	0.48
1:C:775:GLY:H	1:C:848:HIS:CG	2.32	0.48
1:C:2971:GLN:HA	1:C:2974:ILE:HG12	1.95	0.48
1:C:3110:LEU:HB3	1:C:3175:LEU:HD11	1.96	0.48
1:D:497:TYR:O	1:D:553:ARG:NH2	2.41	0.48
1:D:637:LEU:HD13	1:D:1637:MET:HB3	1.95	0.48
1:D:758:ARG:HG2	1:D:763:PRO:HA	1.96	0.48
1:D:3435:PHE:HA	1:D:3517:MET:HE1	1.94	0.48
1:A:2739:PRO:HG3	1:A:2888:ARG:HG2	1.95	0.48
1:B:861:ILE:HG23	1:B:933:LEU:HD22	1.96	0.48
1:B:2465:ASP:O	1:B:2469:ILE:HG13	2.14	0.48
1:B:2467:VAL:HG23	1:B:2521:VAL:HG13	1.96	0.48
1:B:3566:SER:HB3	1:B:3569:LEU:HG	1.96	0.48
1:C:665:GLU:HB2	1:C:792:LEU:HB2	1.96	0.48
1:C:3015:LEU:HD12	1:C:3025:LEU:HB3	1.95	0.48
1:D:116:MET:HE3	1:D:139:GLU:HG3	1.96	0.48
1:D:861:ILE:HG23	1:D:933:LEU:HD22	1.96	0.48
1:D:3053:ARG:HG3	1:D:3056:LEU:HD13	1.96	0.48
1:A:2465:ASP:O	1:A:2469:ILE:HG13	2.14	0.47
1:B:586:ILE:HA	1:B:589:LEU:HD23	1.96	0.47
1:B:775:GLY:H	1:B:848:HIS:CG	2.32	0.47
1:B:1421:ARG:O	1:B:1570:LYS:NZ	2.42	0.47
1:B:3798:LEU:HD11	1:B:3884:LEU:HA	1.95	0.47
1:B:4183:ILE:HG12	1:B:4193:ILE:HD11	1.96	0.47
1:C:1842:LEU:O	1:C:1846:SER:OG	2.30	0.47
1:C:2739:PRO:HG3	1:C:2888:ARG:HG2	1.95	0.47
1:D:1068:ARG:HG2	1:D:1069:TRP:CD1	2.48	0.47
1:D:2039:LEU:HD23	1:D:2044:ILE:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2465:ASP:O	1:D:2469:ILE:HG13	2.14	0.47
1:D:3037:GLU:HB3	1:D:3088:VAL:HG21	1.95	0.47
1:D:3409:TYR:HE2	1:D:3510:ILE:HG12	1.78	0.47
1:D:4189:ARG:HG2	1:D:5031:GLN:HE22	1.79	0.47
1:A:878:ILE:HA	1:A:881:LEU:HB2	1.96	0.47
1:B:3284:TRP:HB3	1:B:3305:THR:HG21	1.95	0.47
1:B:4861:LYS:H	1:B:4861:LYS:HG3	1.47	0.47
1:C:293:LEU:HD12	1:C:378:LEU:HD23	1.96	0.47
1:C:758:ARG:HG2	1:C:763:PRO:HA	1.96	0.47
1:C:861:ILE:HG23	1:C:933:LEU:HD22	1.96	0.47
1:C:1077:ALA:HA	1:C:1236:THR:HG22	1.95	0.47
1:C:2863:SER:HA	1:C:2928:LYS:HG3	1.96	0.47
1:C:4189:ARG:HG2	1:C:5031:GLN:HE22	1.79	0.47
1:D:168:ASP:HB3	1:D:199:LEU:HD11	1.94	0.47
1:D:2461:VAL:O	1:D:2510:TYR:OH	2.32	0.47
1:D:3110:LEU:HB3	1:D:3175:LEU:HD11	1.96	0.47
1:A:775:GLY:H	1:A:848:HIS:CG	2.32	0.47
1:A:3037:GLU:HB3	1:A:3088:VAL:HG21	1.95	0.47
1:A:3209:GLN:HG2	1:A:3210:LEU:HG	1.96	0.47
1:B:1076:ARG:HD3	1:B:1109:LEU:HD21	1.96	0.47
1:B:2739:PRO:HG3	1:B:2888:ARG:HG2	1.95	0.47
1:B:3264:THR:OG1	1:B:3265:GLU:OE1	2.32	0.47
1:B:3903:LEU:HB3	1:B:3915:ILE:HD11	1.96	0.47
1:C:2339:VAL:HG11	1:C:2353:VAL:HG11	1.96	0.47
1:C:2588:ARG:HE	1:C:2900:GLY:HA2	1.80	0.47
1:C:4183:ILE:HG12	1:C:4193:ILE:HD11	1.96	0.47
1:D:2624:ARG:HG3	1:D:2910:THR:HB	1.96	0.47
1:D:3015:LEU:HD12	1:D:3025:LEU:HB3	1.95	0.47
1:A:861:ILE:HG23	1:A:933:LEU:HD22	1.97	0.47
1:A:2457:LEU:HA	1:A:2460:LEU:HD12	1.97	0.47
1:B:2296:GLU:HA	1:B:2299:VAL:HG22	1.97	0.47
1:B:2457:LEU:HA	1:B:2460:LEU:HD12	1.97	0.47
1:C:1252:HIS:O	1:C:1275:ARG:NH1	2.43	0.47
1:C:2467:VAL:HG23	1:C:2521:VAL:HG13	1.96	0.47
1:C:3209:GLN:HG2	1:C:3210:LEU:HG	1.97	0.47
1:A:850:ASP:O	1:A:1025:ARG:NH2	2.45	0.47
1:A:1076:ARG:HD3	1:A:1109:LEU:HD21	1.96	0.47
1:A:3053:ARG:HG3	1:A:3056:LEU:HD13	1.96	0.47
1:B:2190:VAL:HA	1:B:2193:GLN:HB2	1.97	0.47
1:B:2863:SER:HA	1:B:2928:LYS:HG3	1.96	0.47
1:D:878:ILE:HA	1:D:881:LEU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1743[A]:ARG:HE	1:D:1743[A]:ARG:HB2	1.47	0.47
1:D:3533:ILE:HD13	1:D:3596:VAL:HG13	1.95	0.47
1:A:2460:LEU:HA	1:B:131:LEU:HD21	1.96	0.47
1:A:4183:ILE:HG12	1:A:4193:ILE:HD11	1.96	0.47
1:B:182:LEU:HG	1:B:184:THR:HG23	1.96	0.47
1:B:1077:ALA:HA	1:B:1236:THR:HG22	1.95	0.47
1:B:2339:VAL:HG11	1:B:2353:VAL:HG11	1.96	0.47
1:B:3110:LEU:HB3	1:B:3175:LEU:HD11	1.96	0.47
1:B:3202:PRO:O	1:B:3214:ASN:ND2	2.46	0.47
1:B:3729:MET:HE2	1:B:3729:MET:HB2	1.67	0.47
1:C:41:GLY:O	1:C:45:ARG:NH1	2.41	0.47
1:C:1068:ARG:HG2	1:C:1069:TRP:CD1	2.48	0.47
1:C:2457:LEU:HA	1:C:2460:LEU:HD12	1.97	0.47
1:C:2465:ASP:O	1:C:2469:ILE:HG13	2.14	0.47
1:C:3533:ILE:HD13	1:C:3596:VAL:HG13	1.95	0.47
1:D:2457:LEU:HA	1:D:2460:LEU:HD12	1.97	0.47
2:H:55:VAL:HG21	2:H:59:PHE:HD2	1.80	0.47
1:A:293:LEU:HD12	1:A:378:LEU:HD23	1.96	0.47
1:A:2190:VAL:HA	1:A:2193:GLN:HB2	1.97	0.47
1:A:3110:LEU:HB3	1:A:3175:LEU:HD11	1.96	0.47
1:A:3755:GLU:HA	1:A:3758:MET:HE3	1.95	0.47
1:B:497:TYR:O	1:B:553:ARG:NH2	2.41	0.47
1:B:665:GLU:HB2	1:B:792:LEU:HB2	1.96	0.47
1:B:2039:LEU:HD23	1:B:2044:ILE:HG21	1.96	0.47
1:B:2871:LEU:HG	1:B:2927:LEU:HD21	1.95	0.47
1:B:3209:GLN:HG2	1:B:3210:LEU:HG	1.97	0.47
1:C:232:THR:HG21	1:C:252:VAL:HG12	1.96	0.47
1:C:3409:TYR:HE2	1:C:3510:ILE:HG12	1.78	0.47
1:C:3889:GLN:HG3	1:C:3967:GLU:HG3	1.97	0.47
1:C:3903:LEU:HB3	1:C:3915:ILE:HD11	1.96	0.47
1:C:4184:MET:HE2	1:C:4184:MET:HB2	1.79	0.47
1:D:232:THR:HG21	1:D:252:VAL:HG12	1.96	0.47
1:D:2977:LEU:HG	1:D:3056:LEU:HD23	1.97	0.47
1:A:2039:LEU:HD23	1:A:2044:ILE:HG21	1.96	0.47
1:A:3003:LEU:O	1:A:3007:ASN:HB2	2.15	0.47
1:B:232:THR:HG21	1:B:252:VAL:HG12	1.96	0.47
1:B:639:ASN:HD21	1:B:676:THR:HG1	1.56	0.47
1:C:1024:TYR:O	1:C:1032:LYS:NZ	2.46	0.47
1:C:2716:ASP:OD1	1:C:2716:ASP:N	2.46	0.47
1:C:3019:SER:O	1:C:3036:LYS:NZ	2.46	0.47
1:C:3053:ARG:HG3	1:C:3056:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:850:ASP:O	1:D:1025:ARG:NH2	2.45	0.47
1:D:1455:PRO:HB3	1:D:1549:PHE:HE1	1.80	0.47
1:D:1653:LEU:HA	1:D:1656:ARG:HB2	1.97	0.47
2:G:55:VAL:HG21	2:G:59:PHE:HD2	1.80	0.47
1:A:131:LEU:HD21	1:D:2460:LEU:HA	1.97	0.47
1:A:232:THR:HG21	1:A:252:VAL:HG12	1.96	0.47
1:A:2737:PRO:HB2	1:A:2884:ASN:HB2	1.97	0.47
1:A:3889:GLN:HG3	1:A:3967:GLU:HG3	1.97	0.47
1:B:3889:GLN:HG3	1:B:3967:GLU:HG3	1.97	0.47
1:C:417:GLY:O	1:C:420:SER:OG	2.32	0.47
1:D:2588:ARG:HE	1:D:2900:GLY:HA2	1.80	0.47
1:D:3903:LEU:HB3	1:D:3915:ILE:HD11	1.96	0.47
1:A:294:THR:HG23	1:A:297:GLN:H	1.80	0.47
1:A:758:ARG:HG2	1:A:763:PRO:HA	1.96	0.47
1:A:1454:THR:OG1	1:A:1456:ASP:OD1	2.30	0.47
1:A:2296:GLU:HA	1:A:2299:VAL:HG22	1.96	0.47
1:A:3214:ASN:HB3	1:A:3217:SER:HB2	1.97	0.47
1:A:3409:TYR:HE2	1:A:3510:ILE:HG12	1.78	0.47
1:B:758:ARG:HG2	1:B:763:PRO:HA	1.96	0.47
1:B:783:PHE:HB2	1:B:787:VAL:HG21	1.97	0.47
1:B:2977:LEU:HG	1:B:3056:LEU:HD23	1.97	0.47
1:C:1076:ARG:HD3	1:C:1109:LEU:HD21	1.96	0.47
1:D:293:LEU:HD12	1:D:378:LEU:HD23	1.96	0.47
1:D:1983:ALA:O	1:D:1987:SER:OG	2.30	0.47
1:D:2863:SER:HA	1:D:2928:LYS:HG3	1.96	0.47
1:D:3003:LEU:O	1:D:3007:ASN:HB2	2.15	0.47
1:A:76:ARG:HD2	1:D:3935:TRP:O	2.15	0.46
1:A:1091:GLU:HB2	1:A:1203:ASN:HB3	1.97	0.46
1:A:2624:ARG:HG3	1:A:2910:THR:HB	1.96	0.46
1:A:2863:SER:HA	1:A:2928:LYS:HG3	1.96	0.46
1:A:3261:ALA:HB3	1:A:3266:MET:HE3	1.97	0.46
1:B:878:ILE:HA	1:B:881:LEU:HB2	1.97	0.46
1:B:2677:LYS:HE2	1:B:2677:LYS:HB3	1.67	0.46
1:B:2737:PRO:HB2	1:B:2884:ASN:HB2	1.97	0.46
1:C:294:THR:HG23	1:C:297:GLN:H	1.80	0.46
1:C:783:PHE:HB2	1:C:787:VAL:HG21	1.97	0.46
1:C:1091:GLU:HB2	1:C:1203:ASN:HB3	1.97	0.46
1:C:1421:ARG:O	1:C:1570:LYS:NZ	2.42	0.46
1:C:1454:THR:OG1	1:C:1456:ASP:OD1	2.30	0.46
1:C:2039:LEU:HD23	1:C:2044:ILE:HG21	1.96	0.46
1:D:889:GLN:O	1:D:892:THR:OG1	2.25	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1091:GLU:HB2	1:D:1203:ASN:HB3	1.97	0.46
1:A:76:ARG:HH12	1:D:3938:SER:N	2.14	0.46
1:B:1996:ARG:O	1:B:2000:SER:OG	2.31	0.46
1:C:182:LEU:HG	1:C:184:THR:HG23	1.96	0.46
1:C:873:LYS:H	1:C:873:LYS:HG2	1.48	0.46
1:C:878:ILE:HA	1:C:881:LEU:HB2	1.97	0.46
1:C:1270:LEU:HB2	1:C:1564:PHE:HB2	1.98	0.46
1:C:2190:VAL:HA	1:C:2193:GLN:HB2	1.97	0.46
1:D:294:THR:HG23	1:D:297:GLN:H	1.80	0.46
1:D:665:GLU:HB2	1:D:792:LEU:HB2	1.96	0.46
1:D:783:PHE:HB2	1:D:787:VAL:HG21	1.97	0.46
1:D:1076:ARG:HD3	1:D:1109:LEU:HD21	1.96	0.46
1:D:2467:VAL:HG23	1:D:2521:VAL:HG13	1.96	0.46
1:D:3589:PRO:HA	1:D:3592:ILE:HG22	1.98	0.46
1:D:3889:GLN:HG3	1:D:3967:GLU:HG3	1.97	0.46
1:A:182:LEU:HG	1:A:184:THR:HG23	1.96	0.46
1:A:3264:THR:OG1	1:A:3265:GLU:OE1	2.31	0.46
1:A:3589:PRO:HA	1:A:3592:ILE:HG22	1.98	0.46
1:B:4188:ARG:HA	1:B:4188:ARG:HD2	1.57	0.46
1:B:4189:ARG:HG2	1:B:5031:GLN:HE22	1.79	0.46
1:C:2624:ARG:HG3	1:C:2910:THR:HB	1.96	0.46
1:D:2190:VAL:HA	1:D:2193:GLN:HB2	1.97	0.46
1:A:1433:TYR:O	1:A:1519:LEU:HA	2.15	0.46
1:A:1653:LEU:HA	1:A:1656:ARG:HB2	1.97	0.46
1:A:2467:VAL:HG23	1:A:2521:VAL:HG13	1.96	0.46
1:A:2588:ARG:HE	1:A:2900:GLY:HA2	1.80	0.46
1:A:3798:LEU:HD11	1:A:3884:LEU:HA	1.96	0.46
1:A:4189:ARG:HG2	1:A:5031:GLN:HE22	1.79	0.46
1:A:4202:ARG:O	1:A:4206:GLU:HG2	2.16	0.46
1:B:3533:ILE:HD13	1:B:3596:VAL:HG13	1.95	0.46
1:B:3938:SER:OG	1:C:76:ARG:NH1	2.48	0.46
1:C:2737:PRO:HB2	1:C:2884:ASN:HB2	1.97	0.46
1:C:3003:LEU:O	1:C:3007:ASN:HB2	2.15	0.46
1:C:3938:SER:OG	1:D:76:ARG:NH1	2.48	0.46
1:D:233:ILE:HD12	1:D:242:ARG:HB3	1.97	0.46
1:D:1676:LEU:HD22	1:D:2167:ILE:HD12	1.97	0.46
1:D:3209:GLN:HG2	1:D:3210:LEU:HG	1.97	0.46
1:D:3214:ASN:HB3	1:D:3217:SER:HB2	1.97	0.46
1:B:1089:TYR:HD2	1:B:1152:MET:HE1	1.81	0.46
1:B:1091:GLU:HB2	1:B:1203:ASN:HB3	1.97	0.46
1:B:4865:LYS:HA	1:B:4865:LYS:HD2	1.66	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:736:HIS:ND1	1:C:737:LEU:O	2.42	0.46
1:C:1455:PRO:HB3	1:C:1549:PHE:HE1	1.80	0.46
1:C:1653:LEU:HA	1:C:1656:ARG:HB2	1.97	0.46
1:C:1980:LEU:HD11	1:C:1994:ARG:HB3	1.98	0.46
1:C:2296:GLU:HA	1:C:2299:VAL:HG22	1.97	0.46
1:D:1154:ASP:OD1	1:D:1156:THR:OG1	2.34	0.46
1:D:2339:VAL:HG11	1:D:2353:VAL:HG11	1.96	0.46
1:A:783:PHE:HB2	1:A:787:VAL:HG21	1.97	0.46
1:A:946:ALA:O	1:A:950:LEU:CB	2.64	0.46
1:A:1018:ASN:H	1:A:1021:LEU:HD12	1.81	0.46
1:A:1154:ASP:OD1	1:A:1156:THR:OG1	2.34	0.46
1:A:1455:PRO:HB3	1:A:1549:PHE:HE1	1.80	0.46
1:A:2339:VAL:HG11	1:A:2353:VAL:HG11	1.96	0.46
1:A:2583:LEU:HA	1:A:2586:VAL:HG22	1.98	0.46
1:A:3903:LEU:HB3	1:A:3915:ILE:HD11	1.96	0.46
1:B:1433:TYR:O	1:B:1519:LEU:HA	2.15	0.46
1:B:1769:THR:N	1:B:1956:GLU:OE2	2.49	0.46
1:B:2624:ARG:HG3	1:B:2910:THR:HB	1.96	0.46
1:B:3003:LEU:O	1:B:3007:ASN:HB2	2.15	0.46
1:C:1291:LEU:HD12	1:C:1550:PRO:HG2	1.97	0.46
1:C:1769:THR:N	1:C:1956:GLU:OE2	2.49	0.46
1:D:2296:GLU:HA	1:D:2299:VAL:HG22	1.97	0.46
1:D:4183:ILE:HG12	1:D:4193:ILE:HD11	1.96	0.46
1:A:585:SER:O	1:A:588:SER:OG	2.27	0.46
1:A:2977:LEU:HG	1:A:3056:LEU:HD23	1.97	0.46
1:B:207:SER:H	1:B:334:MET:HE1	1.81	0.46
1:B:233:ILE:HD12	1:B:242:ARG:HB3	1.97	0.46
1:B:1291:LEU:HD12	1:B:1550:PRO:HG2	1.97	0.46
1:B:1980:LEU:HD11	1:B:1994:ARG:HB3	1.98	0.46
1:B:2583:LEU:HA	1:B:2586:VAL:HG22	1.98	0.46
1:B:3589:PRO:HA	1:B:3592:ILE:HG22	1.98	0.46
1:B:3705:PHE:HA	1:B:3708:THR:HG22	1.97	0.46
1:B:4204:GLN:HA	1:B:4207:MET:HG3	1.98	0.46
1:C:3214:ASN:HB3	1:C:3217:SER:HB2	1.97	0.46
1:D:2867:LEU:HB2	1:D:2928:LYS:HZ3	1.81	0.46
1:A:207:SER:H	1:A:334:MET:HE1	1.81	0.46
1:A:4204:GLN:HA	1:A:4207:MET:HG3	1.98	0.46
1:B:1154:ASP:OD1	1:B:1156:THR:OG1	2.34	0.46
1:B:1270:LEU:HB2	1:B:1564:PHE:HB2	1.98	0.46
1:B:4202:ARG:O	1:B:4206:GLU:HG2	2.16	0.46
1:C:719:LEU:HD23	1:C:735:GLN:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2977:LEU:HG	1:C:3056:LEU:HD23	1.97	0.46
1:D:1018:ASN:H	1:D:1021:LEU:HD12	1.81	0.46
1:A:665:GLU:HB2	1:A:792:LEU:HB2	1.96	0.46
1:B:1454:THR:OG1	1:B:1456:ASP:OD1	2.30	0.46
1:C:207:SER:H	1:C:334:MET:HE1	1.81	0.46
1:C:3051:ARG:HA	1:C:3131:TYR:CZ	2.51	0.46
1:C:4718:LYS:H	1:C:4718:LYS:HG2	1.43	0.46
1:D:207:SER:H	1:D:334:MET:HE1	1.81	0.46
1:D:2703:LEU:HG	1:D:3005:LEU:HD13	1.98	0.46
1:D:3261:ALA:HB3	1:D:3266:MET:HE3	1.97	0.46
1:D:3705:PHE:HA	1:D:3708:THR:HG22	1.97	0.46
1:D:4202:ARG:O	1:D:4206:GLU:HG2	2.16	0.46
1:A:299:LEU:HD22	1:A:378:LEU:HB2	1.98	0.46
1:A:1451:GLY:HA3	1:A:1494:MET:HA	1.98	0.46
1:A:3705:PHE:HA	1:A:3708:THR:HG22	1.97	0.46
1:B:719:LEU:HD23	1:B:735:GLN:HB2	1.98	0.46
1:B:1973:GLN:HE22	1:B:3640:PRO:HB2	1.81	0.46
1:B:2003:GLN:O	1:B:2007:ASN:ND2	2.49	0.46
1:B:3214:ASN:HB3	1:B:3217:SER:HB2	1.97	0.46
1:C:1676:LEU:HD22	1:C:2167:ILE:HD12	1.97	0.46
1:C:2003:GLN:O	1:C:2007:ASN:ND2	2.49	0.46
1:C:3589:PRO:HA	1:C:3592:ILE:HG22	1.98	0.46
1:C:4202:ARG:O	1:C:4206:GLU:HG2	2.16	0.46
1:D:719:LEU:HD23	1:D:735:GLN:HB2	1.98	0.46
1:D:1433:TYR:O	1:D:1519:LEU:HA	2.15	0.46
1:D:1842:LEU:O	1:D:1846:SER:OG	2.30	0.46
1:A:873:LYS:HE3	1:A:873:LYS:HB3	1.85	0.45
1:A:1694:LEU:HD12	1:A:1715:LEU:HB2	1.98	0.45
1:A:1828:ASP:OD1	1:A:1828:ASP:N	2.49	0.45
1:A:3523:ASN:OD1	1:A:3582:ARG:NH2	2.50	0.45
1:A:3659:ALA:HA	1:A:3663:LEU:HD12	1.99	0.45
1:B:889:GLN:O	1:B:892:THR:OG1	2.25	0.45
1:B:1455:PRO:HB3	1:B:1549:PHE:HE1	1.80	0.45
1:B:1676:LEU:HD22	1:B:2167:ILE:HD12	1.97	0.45
1:B:2588:ARG:HE	1:B:2900:GLY:HA2	1.80	0.45
1:B:3329:ILE:HD11	1:B:3332:ALA:HB2	1.98	0.45
1:C:1089:TYR:HD2	1:C:1152:MET:HE1	1.81	0.45
1:C:1154:ASP:OD1	1:C:1156:THR:OG1	2.34	0.45
1:C:1451:GLY:HA3	1:C:1494:MET:HA	1.98	0.45
1:C:1694:LEU:HD12	1:C:1715:LEU:HB2	1.98	0.45
1:D:299:LEU:HD22	1:D:378:LEU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1109:LEU:HA	1:D:1120:LEU:HD13	1.98	0.45
1:D:1270:LEU:HB2	1:D:1564:PHE:HB2	1.98	0.45
1:D:3051:ARG:HA	1:D:3131:TYR:CZ	2.51	0.45
1:D:3264:THR:OG1	1:D:3265:GLU:OE1	2.32	0.45
1:D:4112:LEU:O	1:D:4115:SER:OG	2.34	0.45
2:E:55:VAL:HG21	2:E:59:PHE:HD2	1.80	0.45
1:A:2615:ARG:HD3	1:A:2618:MET:HE1	1.98	0.45
1:B:3261:ALA:HB3	1:B:3266:MET:HE3	1.97	0.45
1:C:629:ARG:NH1	2:G:90:VAL:O	2.44	0.45
1:C:1018:ASN:H	1:C:1021:LEU:HD12	1.81	0.45
1:C:3705:PHE:HA	1:C:3708:THR:HG22	1.97	0.45
1:D:1291:LEU:HD12	1:D:1550:PRO:HG2	1.97	0.45
1:D:4188:ARG:HD2	1:D:4188:ARG:HA	1.57	0.45
1:A:1089:TYR:HD2	1:A:1152:MET:HE1	1.81	0.45
1:B:299:LEU:HD22	1:B:378:LEU:HB2	1.98	0.45
1:C:492:ASP:OD1	1:C:546:TRP:NE1	2.36	0.45
1:C:1433:TYR:O	1:C:1519:LEU:HA	2.15	0.45
1:D:1782:PHE:O	2:H:82:TYR:OH	2.35	0.45
1:D:2737:PRO:HB2	1:D:2884:ASN:HB2	1.97	0.45
1:D:3132:THR:HG23	1:D:3136:LEU:HD23	1.98	0.45
1:D:3659:ALA:HA	1:D:3663:LEU:HD12	1.99	0.45
2:G:2:VAL:HA	2:G:75:THR:O	2.17	0.45
1:A:233:ILE:HD12	1:A:242:ARG:HB3	1.97	0.45
1:A:719:LEU:HD23	1:A:735:GLN:HB2	1.98	0.45
1:A:1291:LEU:HD12	1:A:1550:PRO:HG2	1.97	0.45
1:B:293:LEU:HD12	1:B:378:LEU:HD23	1.96	0.45
1:B:294:THR:HG23	1:B:297:GLN:H	1.80	0.45
1:B:946:ALA:O	1:B:950:LEU:CB	2.64	0.45
1:B:1018:ASN:H	1:B:1021:LEU:HD12	1.81	0.45
1:B:1653:LEU:HA	1:B:1656:ARG:HB2	1.97	0.45
1:B:1694:LEU:HD12	1:B:1715:LEU:HB2	1.98	0.45
1:B:2765:LYS:HA	1:B:2765:LYS:HD3	1.71	0.45
1:B:3019:SER:O	1:B:3036:LYS:NZ	2.46	0.45
1:B:3659:ALA:HA	1:B:3663:LEU:HD12	1.99	0.45
1:C:873:LYS:HE3	1:C:873:LYS:HB3	1.85	0.45
1:C:2703:LEU:HG	1:C:3005:LEU:HD13	1.98	0.45
1:C:3659:ALA:HA	1:C:3663:LEU:HD12	1.99	0.45
1:D:2003:GLN:O	1:D:2007:ASN:ND2	2.49	0.45
1:D:2583:LEU:HA	1:D:2586:VAL:HG22	1.98	0.45
1:D:3062:PRO:HA	1:D:3065:VAL:HG22	1.99	0.45
2:F:55:VAL:HG21	2:F:59:PHE:HD2	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1109:LEU:HA	1:A:1120:LEU:HD13	1.98	0.45
1:A:3051:ARG:HA	1:A:3131:TYR:CZ	2.51	0.45
1:A:3938:SER:OG	1:B:76:ARG:NH1	2.49	0.45
1:B:1828:ASP:N	1:B:1828:ASP:OD1	2.49	0.45
1:B:3062:PRO:HA	1:B:3065:VAL:HG22	1.99	0.45
1:B:4680:LYS:HB2	1:B:4680:LYS:HE3	1.72	0.45
1:C:233:ILE:HD12	1:C:242:ARG:HB3	1.97	0.45
1:C:1973:GLN:HE22	1:C:3640:PRO:HB2	1.81	0.45
1:C:4569:LEU:HD23	1:C:4650:HIS:HA	1.99	0.45
1:D:2615:ARG:HD3	1:D:2618:MET:HE1	1.99	0.45
1:A:1024:TYR:O	1:A:1032:LYS:NZ	2.46	0.45
1:A:1422:ASP:OD2	1:A:1568:LYS:NZ	2.38	0.45
1:A:2003:GLN:O	1:A:2007:ASN:ND2	2.49	0.45
1:B:171:LEU:HD21	1:B:180:LEU:HB2	1.98	0.45
1:B:736:HIS:ND1	1:B:737:LEU:O	2.42	0.45
1:B:2703:LEU:HG	1:B:3005:LEU:HD13	1.98	0.45
1:B:3147:ILE:HG23	1:B:3152:PHE:HB2	1.99	0.45
1:B:3414:ARG:NH1	1:B:3469:PHE:O	2.45	0.45
1:C:400:ALA:O	1:C:404:ILE:HD12	2.17	0.45
1:C:3132:THR:HG23	1:C:3136:LEU:HD23	1.98	0.45
1:C:3523:ASN:OD1	1:C:3582:ARG:NH2	2.50	0.45
1:D:1089:TYR:HD2	1:D:1152:MET:HE1	1.81	0.45
1:D:1451:GLY:HA3	1:D:1494:MET:HA	1.98	0.45
1:D:3523:ASN:OD1	1:D:3582:ARG:NH2	2.50	0.45
1:D:4204:GLN:HA	1:D:4207:MET:HG3	1.98	0.45
1:A:1676:LEU:HD22	1:A:2167:ILE:HD12	1.97	0.45
1:A:1973:GLN:HE22	1:A:3640:PRO:HB2	1.81	0.45
1:A:1980:LEU:HD11	1:A:1994:ARG:HB3	1.98	0.45
1:A:3062:PRO:HA	1:A:3065:VAL:HG22	1.99	0.45
1:B:3051:ARG:HA	1:B:3131:TYR:CZ	2.51	0.45
1:C:707:VAL:HG13	1:C:713:SER:HB2	1.99	0.45
1:C:1109:LEU:HA	1:C:1120:LEU:HD13	1.98	0.45
1:D:1461:ASP:OD2	1:D:1468:LYS:NZ	2.40	0.45
1:D:1828:ASP:OD1	1:D:1828:ASP:N	2.49	0.45
1:D:3414:ARG:NH1	1:D:3469:PHE:O	2.45	0.45
1:A:400:ALA:O	1:A:404:ILE:HD12	2.17	0.45
1:A:1270:LEU:HB2	1:A:1564:PHE:HB2	1.97	0.45
1:A:2461:VAL:O	1:A:2510:TYR:OH	2.32	0.45
1:A:3132:THR:HG23	1:A:3136:LEU:HD23	1.98	0.45
1:A:4690:GLU:H	1:A:4690:GLU:HG2	1.53	0.45
1:B:1109:LEU:HA	1:B:1120:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2615:ARG:HD3	1:B:2618:MET:HE1	1.99	0.45
1:C:590:LEU:HG	1:C:631:LEU:HD22	1.99	0.45
1:C:3062:PRO:HA	1:C:3065:VAL:HG22	1.99	0.45
1:C:3414:ARG:NH1	1:C:3469:PHE:O	2.45	0.45
1:D:1980:LEU:HD11	1:D:1994:ARG:HB3	1.98	0.45
1:D:3329:ILE:HD11	1:D:3332:ALA:HB2	1.98	0.45
1:A:873:LYS:H	1:A:873:LYS:HG2	1.47	0.45
1:B:1842:LEU:O	1:B:1846:SER:OG	2.30	0.45
1:C:171:LEU:HD21	1:C:180:LEU:HB2	1.98	0.45
1:C:299:LEU:HD13	1:C:378:LEU:HD22	1.99	0.45
1:C:1254:HIS:HA	1:C:1276:THR:HG22	1.99	0.45
1:C:1828:ASP:OD1	1:C:1828:ASP:N	2.49	0.45
1:C:2583:LEU:HA	1:C:2586:VAL:HG22	1.98	0.45
1:C:2765:LYS:HD3	1:C:2765:LYS:HA	1.71	0.45
1:C:4092:ASP:O	1:C:4096:ALA:HB2	2.17	0.45
1:D:134:ASP:OD1	1:D:134:ASP:N	2.50	0.45
1:D:1254:HIS:HA	1:D:1276:THR:HG22	1.99	0.45
1:D:2004:GLU:HA	1:D:2007:ASN:HB2	1.99	0.45
1:A:3329:ILE:HD11	1:A:3332:ALA:HB2	1.98	0.45
1:B:590:LEU:HG	1:B:631:LEU:HD22	1.99	0.45
1:B:707:VAL:HG13	1:B:713:SER:HB2	1.99	0.45
1:B:3523:ASN:OD1	1:B:3582:ARG:NH2	2.50	0.45
1:C:946:ALA:O	1:C:950:LEU:CB	2.64	0.45
1:C:1743[A]:ARG:HE	1:C:1743[A]:ARG:HB2	1.47	0.45
1:C:1782:PHE:O	2:G:82:TYR:OH	2.35	0.45
1:C:3147:ILE:HG23	1:C:3152:PHE:HB2	1.99	0.45
1:C:3261:ALA:HB3	1:C:3266:MET:HE3	1.97	0.45
1:C:3264:THR:OG1	1:C:3265:GLU:OE1	2.32	0.45
1:C:4204:GLN:HA	1:C:4207:MET:HG3	1.98	0.45
1:C:4823:LEU:HD23	1:C:4823:LEU:HA	1.82	0.45
1:C:4848:VAL:O	1:C:4852:THR:OG1	2.34	0.45
1:D:171:LEU:HD21	1:D:180:LEU:HB2	1.98	0.45
2:F:2:VAL:HA	2:F:75:THR:O	2.17	0.45
1:A:590:LEU:HG	1:A:631:LEU:HD22	1.99	0.44
1:A:3556:ASN:HB3	1:A:3559:LEU:HD13	1.98	0.44
1:B:134:ASP:OD1	1:B:134:ASP:N	2.50	0.44
1:B:1451:GLY:HA3	1:B:1494:MET:HA	1.98	0.44
1:B:3132:THR:HG23	1:B:3136:LEU:HD23	1.98	0.44
1:B:4092:ASP:O	1:B:4096:ALA:HB2	2.17	0.44
1:C:2313:LEU:HG	1:C:2416:VAL:HG21	2.00	0.44
1:C:3329:ILE:HD11	1:C:3332:ALA:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3995:VAL:O	1:C:3999:MET:HG2	2.17	0.44
1:D:2458:ARG:NH2	1:D:2510:TYR:O	2.50	0.44
1:D:2960:LEU:HB3	1:D:3038:MET:HE3	1.98	0.44
1:D:4569:LEU:HD23	1:D:4650:HIS:HA	1.99	0.44
2:H:2:VAL:HA	2:H:75:THR:O	2.17	0.44
1:A:889:GLN:O	1:A:892:THR:OG1	2.25	0.44
1:A:1769:THR:N	1:A:1956:GLU:OE2	2.49	0.44
1:A:2867:LEU:HB2	1:A:2928:LYS:HZ3	1.83	0.44
1:A:4921:PHE:HE2	1:D:4891:VAL:HG12	1.81	0.44
1:B:299:LEU:HD13	1:B:378:LEU:HD22	1.99	0.44
1:B:400:ALA:O	1:B:404:ILE:HD12	2.17	0.44
1:B:873:LYS:HE3	1:B:873:LYS:HB3	1.85	0.44
1:B:1087:ARG:HA	1:B:1153:ILE:O	2.17	0.44
1:B:1727:ARG:NH2	1:B:1773:PRO:O	2.50	0.44
1:B:2313:LEU:HG	1:B:2416:VAL:HG21	2.00	0.44
1:C:294:THR:N	1:C:298:GLY:O	2.49	0.44
1:C:733:PRO:HG2	1:C:762:CYS:HB3	2.00	0.44
1:C:1087:ARG:HA	1:C:1153:ILE:O	2.17	0.44
1:D:629:ARG:NH1	2:H:90:VAL:O	2.44	0.44
1:D:733:PRO:HG2	1:D:762:CYS:HB3	2.00	0.44
1:D:1973:GLN:HE22	1:D:3640:PRO:HB2	1.81	0.44
1:D:2395:PRO:HG2	1:D:2397:VAL:HG12	2.00	0.44
2:E:2:VAL:HA	2:E:75:THR:O	2.17	0.44
1:A:1219:LEU:HD22	1:D:3575:LEU:HD23	1.98	0.44
1:A:1727:ARG:NH2	1:A:1773:PRO:O	2.50	0.44
1:A:3147:ILE:HG23	1:A:3152:PHE:HB2	1.99	0.44
1:A:3995:VAL:O	1:A:3999:MET:HG2	2.17	0.44
1:B:733:PRO:HG2	1:B:762:CYS:HB3	2.00	0.44
1:B:3556:ASN:HB3	1:B:3559:LEU:HD13	1.98	0.44
1:C:299:LEU:HD22	1:C:378:LEU:HB2	1.98	0.44
1:C:2004:GLU:HA	1:C:2007:ASN:HB2	1.99	0.44
1:C:2458:ARG:NH2	1:C:2510:TYR:O	2.50	0.44
1:D:3995:VAL:O	1:D:3999:MET:HG2	2.17	0.44
1:A:171:LEU:HD21	1:A:180:LEU:HB2	1.98	0.44
1:A:2458:ARG:NH2	1:A:2510:TYR:O	2.51	0.44
1:A:2960:LEU:HB3	1:A:3038:MET:HE3	1.99	0.44
1:B:3031:ALA:HB3	1:B:3036:LYS:HZ3	1.83	0.44
1:B:4207:MET:HE2	1:B:4208:PRO:HD2	2.00	0.44
1:C:4112:LEU:O	1:C:4115:SER:OG	2.34	0.44
1:C:4207:MET:HE2	1:C:4208:PRO:HD2	2.00	0.44
1:D:1028:ASP:OD1	1:D:1028:ASP:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1087:ARG:HA	1:D:1153:ILE:O	2.17	0.44
1:D:1088:TRP:HB2	1:D:1153:ILE:HG22	1.99	0.44
1:A:733:PRO:HG2	1:A:762:CYS:HB3	2.00	0.44
1:A:1088:TRP:HB2	1:A:1153:ILE:HG22	1.99	0.44
1:A:1443:GLN:NE2	1:A:1555:LEU:O	2.35	0.44
1:A:2395:PRO:HG2	1:A:2397:VAL:HG12	2.00	0.44
1:A:2703:LEU:HG	1:A:3005:LEU:HD13	1.98	0.44
1:A:3616:LYS:HD3	1:A:3616:LYS:HA	1.83	0.44
1:A:4092:ASP:O	1:A:4096:ALA:HB2	2.17	0.44
1:B:850:ASP:O	1:B:1025:ARG:NH2	2.45	0.44
1:B:1782:PHE:O	2:F:82:TYR:OH	2.35	0.44
1:B:2359:ARG:NH1	1:C:195:PHE:O	2.50	0.44
1:B:2867:LEU:HB2	1:B:2928:LYS:HZ3	1.82	0.44
1:B:3078:ARG:NH2	1:B:3151:GLN:O	2.51	0.44
1:C:3556:ASN:HB3	1:C:3559:LEU:HD13	1.98	0.44
1:D:707:VAL:HG13	1:D:713:SER:HB2	1.99	0.44
1:D:1421:ARG:O	1:D:1570:LYS:NZ	2.42	0.44
1:D:3652:MET:HE3	1:D:3652:MET:HB3	1.87	0.44
1:A:707:VAL:HG13	1:A:713:SER:HB2	1.99	0.44
1:A:3935:TRP:O	1:B:76:ARG:HD2	2.17	0.44
1:A:4569:LEU:HD23	1:A:4650:HIS:HA	1.99	0.44
1:B:3587:ASP:OD1	1:B:3595:ARG:NH2	2.51	0.44
1:B:4112:LEU:O	1:B:4115:SER:OG	2.34	0.44
1:C:2960:LEU:HB3	1:C:3038:MET:HE3	1.98	0.44
1:C:3104:GLU:HA	1:C:3107:VAL:HG22	2.00	0.44
1:D:1769:THR:N	1:D:1956:GLU:OE2	2.49	0.44
2:G:19:GLY:C	2:G:49:ARG:HH12	2.26	0.44
1:A:495:ASN:HD21	1:A:550:LYS:HG2	1.83	0.44
1:A:1254:HIS:HA	1:A:1276:THR:HG22	1.99	0.44
1:A:1431:THR:OG1	1:A:1521:ASP:OD1	2.31	0.44
1:A:2121:PHE:O	1:A:3725:TYR:OH	2.28	0.44
1:A:2313:LEU:HG	1:A:2416:VAL:HG21	2.00	0.44
1:A:2359:ARG:NH1	1:B:195:PHE:O	2.51	0.44
1:B:2395:PRO:HG2	1:B:2397:VAL:HG12	2.00	0.44
1:B:2960:LEU:HB3	1:B:3038:MET:HE3	1.98	0.44
1:B:4569:LEU:HD23	1:B:4650:HIS:HA	1.99	0.44
1:C:2336:ARG:HG2	1:C:2435:ARG:HD2	2.00	0.44
1:D:894:GLY:H	1:D:903:LEU:HD13	1.83	0.44
1:D:1694:LEU:HD12	1:D:1715:LEU:HB2	1.98	0.44
1:D:3147:ILE:HG23	1:D:3152:PHE:HB2	1.99	0.44
1:D:3769:ARG:HG3	1:D:3773:ARG:HH12	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4092:ASP:O	1:D:4096:ALA:HB2	2.17	0.44
1:A:299:LEU:HD13	1:A:378:LEU:HD22	1.99	0.44
1:A:708:GLY:HA3	1:A:722:TRP:HB3	2.00	0.44
1:A:2530:MET:HE2	1:A:2530:MET:HB2	1.91	0.44
1:A:3760:LYS:HA	1:A:3760:LYS:HD3	1.88	0.44
1:A:4207:MET:HE2	1:A:4208:PRO:HD2	2.00	0.44
1:B:894:GLY:H	1:B:903:LEU:HD13	1.83	0.44
1:B:3508:SER:HB3	1:B:3511:VAL:HG22	2.00	0.44
1:B:4580:TYR:HE2	1:B:4630:TYR:HB3	1.82	0.44
1:C:850:ASP:O	1:C:1025:ARG:NH2	2.45	0.44
1:C:894:GLY:H	1:C:903:LEU:HD13	1.83	0.44
1:C:3769:ARG:HG3	1:C:3773:ARG:HH12	1.83	0.44
1:D:436:LEU:HD23	1:D:436:LEU:HA	1.91	0.44
1:D:3508:SER:HB3	1:D:3511:VAL:HG22	2.00	0.44
2:H:19:GLY:C	2:H:49:ARG:HH12	2.26	0.44
1:A:1089:TYR:HE1	1:A:1211:LEU:HD22	1.83	0.44
1:A:4681:LEU:HD11	1:A:4706:LEU:HD22	2.00	0.44
1:B:871:ARG:HA	1:B:874:LEU:HB2	2.00	0.44
1:B:2336:ARG:HG2	1:B:2435:ARG:HD2	2.00	0.44
1:B:3844:LEU:HD23	1:B:3844:LEU:HA	1.85	0.44
1:C:1088:TRP:HB2	1:C:1153:ILE:HG22	1.99	0.44
1:C:2000:SER:O	1:C:2005:GLN:NE2	2.34	0.44
1:C:2615:ARG:HD3	1:C:2618:MET:HE1	1.99	0.44
1:C:3157:ILE:HB	1:C:3202:PRO:HG3	2.00	0.44
1:C:4680:LYS:HB2	1:C:4680:LYS:HE3	1.72	0.44
1:D:590:LEU:HG	1:D:631:LEU:HD22	1.99	0.44
1:D:2336:ARG:HG2	1:D:2435:ARG:HD2	2.00	0.44
1:A:894:GLY:H	1:A:903:LEU:HD13	1.83	0.43
1:A:2336:ARG:HG2	1:A:2435:ARG:HD2	2.00	0.43
1:A:3587:ASP:OD1	1:A:3595:ARG:NH2	2.51	0.43
1:B:1792:ALA:HA	1:B:2173:GLN:HA	2.00	0.43
1:B:3940:LYS:O	1:B:4002:LYS:NZ	2.50	0.43
1:B:3995:VAL:O	1:B:3999:MET:HG2	2.17	0.43
1:B:4247:ILE:HD11	1:B:4667:PRO:HB2	2.00	0.43
1:B:4823:LEU:HD23	1:B:4823:LEU:HA	1.82	0.43
1:C:585:SER:O	1:C:588:SER:OG	2.27	0.43
1:C:663:TYR:OH	1:C:665:GLU:OE2	2.29	0.43
1:C:3301:PRO:HA	1:C:3302:PRO:HD3	1.92	0.43
1:C:3628:ARG:HG3	1:C:3631:ALA:HB3	2.00	0.43
1:C:4580:TYR:HE2	1:C:4630:TYR:HB3	1.82	0.43
1:D:3104:GLU:HA	1:D:3107:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3301:PRO:HA	1:D:3302:PRO:HD3	1.92	0.43
1:D:3760:LYS:HA	1:D:3760:LYS:HD3	1.88	0.43
1:D:4580:TYR:HE2	1:D:4630:TYR:HB3	1.82	0.43
1:D:4681:LEU:HD11	1:D:4706:LEU:HD22	2.00	0.43
2:F:19:GLY:C	2:F:49:ARG:HH12	2.26	0.43
1:A:49:LEU:HD23	1:A:49:LEU:HA	1.89	0.43
1:A:223:PHE:HD1	1:A:230:CYS:HB3	1.83	0.43
1:A:1008:SER:OG	1:A:1010:VAL:O	2.33	0.43
1:B:873:LYS:H	1:B:873:LYS:HG2	1.48	0.43
1:B:1254:HIS:HA	1:B:1276:THR:HG22	1.99	0.43
1:B:2245:GLN:NE2	1:B:3861:GLU:OE1	2.51	0.43
1:B:3628:ARG:HG3	1:B:3631:ALA:HB3	2.00	0.43
1:C:3587:ASP:OD1	1:C:3595:ARG:NH2	2.51	0.43
1:D:400:ALA:O	1:D:404:ILE:HD12	2.17	0.43
1:D:2245:GLN:NE2	1:D:3861:GLU:OE1	2.51	0.43
1:D:3556:ASN:HB3	1:D:3559:LEU:HD13	1.98	0.43
1:D:3587:ASP:OD1	1:D:3595:ARG:NH2	2.51	0.43
1:A:1087:ARG:HA	1:A:1153:ILE:O	2.17	0.43
1:A:3936:TYR:O	1:A:3940:LYS:NZ	2.48	0.43
1:B:223:PHE:HD1	1:B:230:CYS:HB3	1.83	0.43
1:B:417:GLY:O	1:B:420:SER:OG	2.32	0.43
1:B:647:ASN:OD1	1:B:647:ASN:N	2.51	0.43
1:B:2716:ASP:OD1	1:B:2716:ASP:N	2.46	0.43
1:C:415:ILE:HA	1:C:418:LEU:HD12	2.01	0.43
1:C:419:ASP:HA	1:C:422:SER:HB3	2.00	0.43
1:C:1089:TYR:HE1	1:C:1211:LEU:HD22	1.83	0.43
1:C:1792:ALA:HA	1:C:2173:GLN:HA	2.00	0.43
1:C:2395:PRO:HG2	1:C:2397:VAL:HG12	2.00	0.43
1:C:2461:VAL:O	1:C:2510:TYR:OH	2.32	0.43
1:C:3078:ARG:NH2	1:C:3151:GLN:O	2.51	0.43
1:C:3844:LEU:HD23	1:C:3844:LEU:HA	1.85	0.43
1:C:4188:ARG:HA	1:C:4188:ARG:HD2	1.57	0.43
1:D:495:ASN:HD21	1:D:550:LYS:HG2	1.83	0.43
1:D:708:GLY:HA3	1:D:722:TRP:HB3	2.00	0.43
1:D:2313:LEU:HG	1:D:2416:VAL:HG21	2.00	0.43
1:D:3729:MET:HE2	1:D:3729:MET:HB2	1.67	0.43
1:D:4680:LYS:HB2	1:D:4680:LYS:HE3	1.72	0.43
1:A:1254:HIS:O	1:A:1275:ARG:N	2.43	0.43
1:A:1295:VAL:O	1:A:1547:LYS:HA	2.19	0.43
1:A:2245:GLN:NE2	1:A:3861:GLU:OE1	2.51	0.43
1:A:2911:LEU:HB2	1:A:2915:GLU:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3078:ARG:NH2	1:A:3151:GLN:O	2.51	0.43
1:A:3875:MET:HB2	1:A:3953:LYS:HD3	2.01	0.43
1:A:4977:THR:O	1:A:4981:GLU:HB3	2.19	0.43
1:B:419:ASP:HA	1:B:422:SER:HB3	2.00	0.43
1:B:2559:LEU:O	1:B:2563:THR:OG1	2.32	0.43
1:B:3915:ILE:O	1:B:3919:THR:OG1	2.34	0.43
1:B:3965:LEU:HD23	1:B:3965:LEU:HA	1.90	0.43
1:C:1431:THR:OG1	1:C:1521:ASP:OD1	2.31	0.43
1:C:1983:ALA:O	1:C:1987:SER:OG	2.30	0.43
1:C:3508:SER:HB3	1:C:3511:VAL:HG22	2.00	0.43
1:D:299:LEU:HD13	1:D:378:LEU:HD22	1.99	0.43
1:D:601:ASP:OD1	1:D:1665:HIS:ND1	2.45	0.43
1:D:4207:MET:HE2	1:D:4208:PRO:HD2	2.00	0.43
1:A:3157:ILE:HB	1:A:3202:PRO:HG3	2.00	0.43
1:B:1089:TYR:HE1	1:B:1211:LEU:HD22	1.83	0.43
1:B:3769:ARG:HG3	1:B:3773:ARG:HH12	1.83	0.43
1:C:495:ASN:HD21	1:C:550:LYS:HG2	1.83	0.43
1:C:661:LYS:HA	1:C:748:LEU:O	2.19	0.43
1:C:708:GLY:HA3	1:C:722:TRP:HB3	2.00	0.43
1:C:871:ARG:HA	1:C:874:LEU:HB2	2.00	0.43
1:C:1269:CYS:HA	1:C:1564:PHE:O	2.19	0.43
1:C:3256:LEU:O	1:C:3259:SER:OG	2.30	0.43
1:C:4247:ILE:HD11	1:C:4667:PRO:HB2	2.00	0.43
1:D:585:SER:O	1:D:588:SER:OG	2.27	0.43
1:D:2000:SER:O	1:D:2005:GLN:NE2	2.34	0.43
1:D:4977:THR:O	1:D:4981:GLU:HB3	2.19	0.43
1:A:2411:PRO:HD2	1:A:2415:ARG:HD2	2.00	0.43
1:B:1088:TRP:HB2	1:B:1153:ILE:HG22	1.99	0.43
1:B:2314:LEU:HD12	1:B:2314:LEU:HA	1.85	0.43
1:C:1028:ASP:OD1	1:C:1028:ASP:N	2.51	0.43
1:C:1295:VAL:O	1:C:1547:LYS:HA	2.19	0.43
1:C:2245:GLN:NE2	1:C:3861:GLU:OE1	2.51	0.43
1:C:2411:PRO:HD2	1:C:2415:ARG:HD2	2.00	0.43
1:C:3390:GLY:H	1:C:3392:LEU:HD23	1.84	0.43
1:D:946:ALA:O	1:D:950:LEU:CB	2.64	0.43
1:D:1089:TYR:HE1	1:D:1211:LEU:HD22	1.83	0.43
1:D:3354:LEU:O	1:D:3358:PHE:HB2	2.19	0.43
1:D:4718:LYS:H	1:D:4718:LYS:HG2	1.43	0.43
1:A:23:GLN:OE1	1:A:203:ASN:ND2	2.52	0.43
1:A:1743[A]:ARG:HE	1:A:1743[A]:ARG:HB2	1.46	0.43
1:A:3508:SER:HB3	1:A:3511:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4639:MET:HE3	1:A:4639:MET:HB3	1.85	0.43
1:B:495:ASN:HD21	1:B:550:LYS:HG2	1.83	0.43
1:B:708:GLY:HA3	1:B:722:TRP:HB3	2.00	0.43
1:B:2004:GLU:HA	1:B:2007:ASN:HB2	1.99	0.43
1:B:2458:ARG:NH2	1:B:2510:TYR:O	2.50	0.43
1:B:3354:LEU:O	1:B:3358:PHE:HB2	2.19	0.43
1:C:403:MET:O	1:C:407:THR:OG1	2.24	0.43
1:C:2911:LEU:HB2	1:C:2915:GLU:HG3	2.01	0.43
1:D:2121:PHE:O	1:D:3725:TYR:OH	2.28	0.43
1:D:3915:ILE:O	1:D:3919:THR:OG1	2.34	0.43
1:D:4247:ILE:HD11	1:D:4667:PRO:HB2	2.00	0.43
1:A:482:GLY:O	1:A:485:SER:OG	2.36	0.43
1:B:415:ILE:HA	1:B:418:LEU:HD12	2.01	0.43
1:B:1269:CYS:HA	1:B:1564:PHE:O	2.19	0.43
1:B:3104:GLU:HA	1:B:3107:VAL:HG22	2.00	0.43
1:B:3390:GLY:H	1:B:3392:LEU:HD23	1.84	0.43
1:B:4801:LEU:HD23	1:B:4801:LEU:HA	1.87	0.43
1:B:4977:THR:O	1:B:4981:GLU:HB3	2.19	0.43
1:C:2359:ARG:NH1	1:D:195:PHE:O	2.50	0.43
1:C:2387:SER:HB2	1:C:2419:GLY:HA3	2.00	0.43
1:C:2499:LYS:HA	1:C:2502:MET:HE2	2.01	0.43
1:C:3875:MET:HB2	1:C:3953:LYS:HD3	2.01	0.43
1:C:4977:THR:O	1:C:4981:GLU:HB3	2.19	0.43
1:D:415:ILE:HA	1:D:418:LEU:HD12	2.00	0.43
1:D:1254:HIS:O	1:D:1275:ARG:N	2.43	0.43
1:D:1269:CYS:HA	1:D:1564:PHE:O	2.19	0.43
1:D:3390:GLY:H	1:D:3392:LEU:HD23	1.84	0.43
1:A:134:ASP:OD1	1:A:134:ASP:N	2.50	0.43
1:A:871:ARG:HA	1:A:874:LEU:HB2	2.00	0.43
1:A:4247:ILE:HD11	1:A:4667:PRO:HB2	2.00	0.43
1:B:436:LEU:HD23	1:B:436:LEU:HA	1.91	0.43
1:B:1024:TYR:O	1:B:1032:LYS:NZ	2.46	0.43
1:B:4681:LEU:HD11	1:B:4706:LEU:HD22	2.00	0.43
1:C:1727:ARG:NH2	1:C:1773:PRO:O	2.50	0.43
1:C:3180:ASN:HB2	1:C:3183:VAL:HG23	2.01	0.43
1:C:3935:TRP:O	1:D:76:ARG:HD2	2.19	0.43
1:D:1263:THR:OG1	1:D:1265:ASP:OD1	2.31	0.43
1:D:2411:PRO:HD2	1:D:2415:ARG:HD2	2.00	0.43
1:D:2911:LEU:HB2	1:D:2915:GLU:HG3	2.01	0.43
1:A:840:VAL:HG22	1:A:1199:VAL:HG22	2.01	0.43
1:A:1996:ARG:NH2	1:A:1999:ARG:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2202:GLY:HA2	1:A:2204:HIS:CE1	2.54	0.43
1:A:2521:VAL:HG12	1:A:2526:PHE:HE2	1.84	0.43
1:C:1160:ILE:O	1:C:1178:ALA:N	2.52	0.43
1:C:1277:TRP:HD1	1:C:1559:GLN:HG3	1.84	0.43
1:C:3445:TRP:HA	1:C:3451:PHE:HD2	1.84	0.43
1:C:4861:LYS:H	1:C:4861:LYS:HG3	1.47	0.43
1:D:417:GLY:O	1:D:420:SER:OG	2.32	0.43
1:D:661:LYS:HA	1:D:748:LEU:O	2.19	0.43
1:D:1685:LEU:HD23	1:D:1685:LEU:HA	1.91	0.43
1:D:1792:ALA:HA	1:D:2173:GLN:HA	2.00	0.43
1:D:2499:LYS:HA	1:D:2502:MET:HE2	2.01	0.43
1:D:3157:ILE:HB	1:D:3202:PRO:HG3	2.00	0.43
1:A:82:LEU:HD23	1:A:82:LEU:HA	1.91	0.42
1:A:1160:ILE:O	1:A:1178:ALA:N	2.52	0.42
1:A:4580:TYR:HE2	1:A:4630:TYR:HB3	1.83	0.42
1:B:23:GLN:OE1	1:B:203:ASN:ND2	2.52	0.42
1:B:663:TYR:OH	1:B:665:GLU:OE2	2.29	0.42
1:B:3157:ILE:HB	1:B:3202:PRO:HG3	2.00	0.42
1:B:3652:MET:HE3	1:B:3652:MET:HB3	1.87	0.42
1:C:23:GLN:OE1	1:C:203:ASN:ND2	2.52	0.42
1:C:436:LEU:HD23	1:C:436:LEU:HA	1.91	0.42
1:C:4039:MET:SD	1:C:4043:GLN:NE2	2.92	0.42
1:C:4681:LEU:HD11	1:C:4706:LEU:HD22	2.00	0.42
1:D:2521:VAL:HG12	1:D:2526:PHE:HE2	1.84	0.42
1:D:3078:ARG:NH2	1:D:3151:GLN:O	2.51	0.42
1:D:4821:LYS:H	1:D:4821:LYS:HG2	1.53	0.42
2:E:19:GLY:C	2:E:49:ARG:HH12	2.26	0.42
1:A:417:GLY:O	1:A:420:SER:OG	2.32	0.42
1:A:1028:ASP:OD1	1:A:1028:ASP:N	2.51	0.42
1:A:1100:MET:HE3	1:A:1198:GLN:HB3	2.00	0.42
1:A:1842:LEU:O	1:A:1846:SER:OG	2.30	0.42
1:A:2499:LYS:HA	1:A:2502:MET:HE2	2.01	0.42
1:A:3104:GLU:HA	1:A:3107:VAL:HG22	2.00	0.42
1:A:3390:GLY:H	1:A:3392:LEU:HD23	1.84	0.42
1:B:1254:HIS:O	1:B:1275:ARG:N	2.43	0.42
1:B:3445:TRP:HA	1:B:3451:PHE:HD2	1.84	0.42
1:B:3935:TRP:O	1:C:76:ARG:HD2	2.19	0.42
1:B:4039:MET:SD	1:B:4043:GLN:NE2	2.92	0.42
1:B:4690:GLU:H	1:B:4690:GLU:HG2	1.54	0.42
1:D:23:GLN:OE1	1:D:203:ASN:ND2	2.52	0.42
1:D:243:ARG:NH2	1:D:303:ASP:OD1	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1100:MET:HE3	1:D:1198:GLN:HB3	2.00	0.42
1:D:1295:VAL:O	1:D:1547:LYS:HA	2.19	0.42
1:D:3180:ASN:HB2	1:D:3183:VAL:HG23	2.01	0.42
1:D:3752:SER:OG	1:D:3755:GLU:OE1	2.33	0.42
1:A:736:HIS:ND1	1:A:737:LEU:O	2.42	0.42
1:A:872:GLU:HG2	1:A:873:LYS:HG2	2.01	0.42
1:A:1996:ARG:O	1:A:2000:SER:OG	2.31	0.42
1:A:2244:ARG:NH2	1:A:3861:GLU:OE2	2.53	0.42
1:B:411:TYR:HA	1:B:414:PHE:HB3	2.02	0.42
1:B:661:LYS:HA	1:B:748:LEU:O	2.19	0.42
1:B:2202:GLY:HA2	1:B:2204:HIS:CE1	2.54	0.42
1:B:2387:SER:HB2	1:B:2419:GLY:HA3	2.00	0.42
1:B:2499:LYS:HA	1:B:2502:MET:HE2	2.01	0.42
1:B:4049:VAL:HG21	1:B:4159:ARG:HD2	2.02	0.42
1:C:12:GLN:HG3	1:C:165:VAL:HG22	2.02	0.42
1:C:2244:ARG:NH2	1:C:3861:GLU:OE2	2.53	0.42
1:D:223:PHE:HD1	1:D:230:CYS:HB3	1.83	0.42
1:D:1008:SER:OG	1:D:1010:VAL:O	2.33	0.42
1:A:1792:ALA:HA	1:A:2173:GLN:HA	2.00	0.42
1:A:2004:GLU:HA	1:A:2007:ASN:HB2	1.99	0.42
1:A:3354:LEU:O	1:A:3358:PHE:HB2	2.19	0.42
1:B:216:GLY:HA2	1:B:262:LEU:HD11	2.02	0.42
1:B:2244:ARG:NH2	1:B:3861:GLU:OE2	2.53	0.42
1:B:2254:LEU:O	1:B:2258:LEU:N	2.53	0.42
1:B:2411:PRO:HD2	1:B:2415:ARG:HD2	2.00	0.42
1:B:2575:ARG:HB3	1:B:2578:MET:HE2	2.00	0.42
1:B:2810:LYS:HA	1:B:2810:LYS:HD3	1.89	0.42
1:B:3137:LEU:O	1:B:3141:THR:OG1	2.30	0.42
1:B:3171:SER:O	1:B:3174:SER:OG	2.38	0.42
1:D:1205:GLY:HA2	1:D:1211:LEU:HD21	2.02	0.42
1:D:2765:LYS:HD3	1:D:2765:LYS:HA	1.71	0.42
1:D:3628:ARG:HG3	1:D:3631:ALA:HB3	2.00	0.42
1:D:4681:LEU:HD23	1:D:4681:LEU:HA	1.90	0.42
2:E:73:LYS:HZ3	2:E:75:THR:HG1	1.60	0.42
1:A:130:LYS:NZ	1:D:2460:LEU:O	2.52	0.42
1:A:661:LYS:HA	1:A:748:LEU:O	2.19	0.42
1:A:1653:LEU:HD23	1:A:1660:GLN:HA	2.02	0.42
1:A:3769:ARG:HG3	1:A:3773:ARG:HH12	1.83	0.42
1:B:840:VAL:HG22	1:B:1199:VAL:HG22	2.01	0.42
1:B:1295:VAL:O	1:B:1547:LYS:HA	2.19	0.42
1:B:4190:ILE:H	1:B:4190:ILE:HG12	1.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4227:GLU:H	1:B:4227:GLU:HG3	1.53	0.42
1:C:216:GLY:HA2	1:C:262:LEU:HD11	2.02	0.42
1:C:872:GLU:HG2	1:C:873:LYS:HG2	2.01	0.42
1:C:3354:LEU:O	1:C:3358:PHE:HB2	2.19	0.42
1:C:3670:GLU:OE1	1:C:3670:GLU:N	2.53	0.42
1:C:4049:VAL:HG21	1:C:4159:ARG:HD2	2.02	0.42
1:D:411:TYR:HA	1:D:414:PHE:HB3	2.02	0.42
1:D:871:ARG:HA	1:D:874:LEU:HB2	2.00	0.42
1:D:2387:SER:HB2	1:D:2419:GLY:HA3	2.00	0.42
1:D:2472:LEU:HD23	1:D:2472:LEU:HA	1.91	0.42
1:D:4049:VAL:HG21	1:D:4159:ARG:HD2	2.02	0.42
1:A:1269:CYS:HA	1:A:1564:PHE:O	2.19	0.42
1:A:2110:TYR:HA	1:A:3700:GLN:HE21	1.85	0.42
1:A:3628:ARG:HG3	1:A:3631:ALA:HB3	2.00	0.42
1:A:3652:MET:HE3	1:A:3652:MET:HB3	1.87	0.42
1:A:4049:VAL:HG21	1:A:4159:ARG:HD2	2.02	0.42
1:A:4184:MET:HE2	1:A:4184:MET:HB2	1.79	0.42
1:B:12:GLN:HG3	1:B:165:VAL:HG22	2.02	0.42
1:B:1100:MET:HE3	1:B:1198:GLN:HB3	2.00	0.42
1:B:1277:TRP:HD1	1:B:1559:GLN:HG3	1.84	0.42
1:B:1849:LEU:HD23	1:B:1849:LEU:HA	1.88	0.42
1:B:2521:VAL:HG12	1:B:2526:PHE:HE2	1.84	0.42
1:B:3875:MET:HB2	1:B:3953:LYS:HD3	2.01	0.42
1:C:1205:GLY:HA2	1:C:1211:LEU:HD21	2.02	0.42
1:C:2208:MET:HA	1:C:2211:MET:HE2	2.02	0.42
1:D:12:GLN:HG3	1:D:165:VAL:HG22	2.02	0.42
1:D:419:ASP:HA	1:D:422:SER:HB3	2.00	0.42
1:D:575:LEU:HD11	1:D:606:LEU:HA	2.02	0.42
1:D:2202:GLY:HA2	1:D:2204:HIS:CE1	2.54	0.42
1:D:2254:LEU:O	1:D:2258:LEU:N	2.53	0.42
1:D:2546:MET:N	1:D:2546:MET:SD	2.93	0.42
1:D:2575:ARG:HB3	1:D:2578:MET:HE2	2.00	0.42
1:D:3875:MET:HB2	1:D:3953:LYS:HD3	2.01	0.42
1:A:216:GLY:HA2	1:A:262:LEU:HD11	2.02	0.42
1:A:419:ASP:HA	1:A:422:SER:HB3	2.00	0.42
1:A:1439:VAL:HB	1:A:1514:LEU:HB3	2.02	0.42
1:A:2387:SER:HB2	1:A:2419:GLY:HA3	2.00	0.42
1:A:2575:ARG:HB3	1:A:2578:MET:HE2	2.00	0.42
1:A:3670:GLU:OE1	1:A:3670:GLU:N	2.53	0.42
1:A:4039:MET:SD	1:A:4043:GLN:NE2	2.92	0.42
1:B:2788:HIS:HB3	1:B:2791:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2911:LEU:HB2	1:B:2915:GLU:HG3	2.01	0.42
1:C:223:PHE:HD1	1:C:230:CYS:HB3	1.83	0.42
1:C:1488:LYS:HE3	1:C:1488:LYS:HB2	1.85	0.42
1:C:2677:LYS:HE2	1:C:2677:LYS:HB3	1.67	0.42
1:C:4639:MET:HB3	1:C:4639:MET:HE3	1.85	0.42
1:D:2740:VAL:HG21	1:D:2819:TRP:HE1	1.85	0.42
1:D:3445:TRP:HA	1:D:3451:PHE:HD2	1.84	0.42
1:D:3723:MET:HE1	1:D:3793:MET:HA	2.01	0.42
1:D:4865:LYS:HA	1:D:4865:LYS:HD2	1.66	0.42
1:A:415:ILE:HA	1:A:418:LEU:HD12	2.01	0.42
1:A:2208:MET:HA	1:A:2211:MET:HE2	2.02	0.42
1:A:3723:MET:HE1	1:A:3793:MET:HA	2.01	0.42
1:B:1205:GLY:HA2	1:B:1211:LEU:HD21	2.02	0.42
1:B:2208:MET:HA	1:B:2211:MET:HE2	2.02	0.42
1:B:2628:PHE:HE1	1:B:2725:LYS:HE3	1.85	0.42
1:B:3180:ASN:HB2	1:B:3183:VAL:HG23	2.01	0.42
1:B:3670:GLU:OE1	1:B:3670:GLU:N	2.53	0.42
1:C:411:TYR:HA	1:C:414:PHE:HB3	2.02	0.42
1:C:575:LEU:HD11	1:C:606:LEU:HA	2.02	0.42
1:C:1620:ALA:HB2	1:C:1627:ALA:HB2	2.02	0.42
1:C:2740:VAL:HG21	1:C:2819:TRP:HE1	1.85	0.42
1:D:736:HIS:ND1	1:D:737:LEU:O	2.42	0.42
1:A:411:TYR:HA	1:A:414:PHE:HB3	2.02	0.42
1:A:1205:GLY:HA2	1:A:1211:LEU:HD21	2.02	0.42
1:A:1277:TRP:HD1	1:A:1559:GLN:HG3	1.84	0.42
1:B:220:LEU:HD12	1:B:390:LEU:HB3	2.02	0.42
1:B:492:ASP:OD1	1:B:546:TRP:NE1	2.36	0.42
1:B:980:ALA:HB1	1:B:1055:PRO:HB3	2.02	0.42
1:B:2110:TYR:HA	1:B:3700:GLN:HE21	1.85	0.42
1:B:3995:VAL:HG13	1:B:3999:MET:HE3	2.02	0.42
1:C:317:ARG:HG2	1:C:323:LEU:HG	2.01	0.42
1:C:909:ASN:OD1	1:C:911:HIS:ND1	2.53	0.42
1:C:2202:GLY:HA2	1:C:2204:HIS:CE1	2.54	0.42
1:C:2521:VAL:HG12	1:C:2526:PHE:HE2	1.84	0.42
1:C:2546:MET:N	1:C:2546:MET:SD	2.93	0.42
1:C:2575:ARG:HB3	1:C:2578:MET:HE2	2.00	0.42
1:D:220:LEU:HD12	1:D:390:LEU:HB3	2.02	0.42
1:D:1277:TRP:HD1	1:D:1559:GLN:HG3	1.84	0.42
1:D:2208:MET:HA	1:D:2211:MET:HE2	2.02	0.42
1:D:2244:ARG:NH2	1:D:3861:GLU:OE2	2.53	0.42
1:D:4039:MET:SD	1:D:4043:GLN:NE2	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4639:MET:HE3	1:D:4639:MET:HB3	1.85	0.42
1:A:908:VAL:HG13	1:A:963:ASN:HB3	2.02	0.42
1:A:980:ALA:HB1	1:A:1055:PRO:HB3	2.02	0.42
1:A:2546:MET:N	1:A:2546:MET:SD	2.93	0.42
1:A:4578:LEU:HD23	1:A:4578:LEU:HA	1.89	0.42
1:B:281:ARG:NH1	1:B:309:THR:OG1	2.53	0.42
1:B:872:GLU:HG2	1:B:873:LYS:HG2	2.01	0.42
1:B:4802:GLY:HA2	1:B:4808:PHE:HB2	2.02	0.42
1:C:49:LEU:HD23	1:C:49:LEU:HA	1.89	0.42
1:C:601:ASP:OD1	1:C:1665:HIS:ND1	2.45	0.42
1:C:797:HIS:CE1	1:C:821:LEU:HD23	2.55	0.42
1:C:980:ALA:HB1	1:C:1055:PRO:HB3	2.02	0.42
1:C:1100:MET:HE3	1:C:1198:GLN:HB3	2.00	0.42
1:C:4802:GLY:HA2	1:C:4808:PHE:HB2	2.02	0.42
1:D:216:GLY:HA2	1:D:262:LEU:HD11	2.02	0.42
1:D:872:GLU:HG2	1:D:873:LYS:HG2	2.01	0.42
1:D:1653:LEU:HD23	1:D:1660:GLN:HA	2.02	0.42
1:D:3253:ILE:HD11	1:D:3273:THR:HG22	2.02	0.42
1:D:5006:GLN:H	1:D:5006:GLN:HG3	1.65	0.42
1:A:367:LEU:HD22	1:A:372:LEU:HA	2.02	0.41
1:A:3163:VAL:HG22	1:A:3232:LEU:HD21	2.02	0.41
1:A:3253:ILE:HD11	1:A:3273:THR:HG22	2.02	0.41
1:B:797:HIS:CE1	1:B:821:LEU:HD23	2.55	0.41
1:B:2437:ALA:O	1:B:2508:ARG:NH2	2.53	0.41
1:B:3256:LEU:O	1:B:3259:SER:OG	2.30	0.41
1:C:281:ARG:NH1	1:C:309:THR:OG1	2.53	0.41
1:C:356:TRP:N	1:C:379:HIS:O	2.53	0.41
1:C:2939:ARG:H	1:C:2939:ARG:HG3	1.70	0.41
1:C:3253:ILE:HD11	1:C:3273:THR:HG22	2.02	0.41
1:C:3936:TYR:O	1:C:3940:LYS:NZ	2.48	0.41
1:C:3949:ARG:O	1:C:3953:LYS:HG2	2.21	0.41
1:D:1727:ARG:NH2	1:D:1773:PRO:O	2.50	0.41
1:D:3844:LEU:HD23	1:D:3844:LEU:HA	1.85	0.41
1:D:4036:VAL:HG22	1:D:5032:TYR:HD2	1.86	0.41
1:A:243:ARG:NH2	1:A:303:ASP:OD1	2.51	0.41
1:A:317:ARG:HG2	1:A:323:LEU:HG	2.01	0.41
1:A:909:ASN:OD1	1:A:911:HIS:ND1	2.53	0.41
1:A:2314:LEU:HD12	1:A:2314:LEU:HA	1.85	0.41
1:A:2628:PHE:HE1	1:A:2725:LYS:HE3	1.85	0.41
1:A:3180:ASN:HB2	1:A:3183:VAL:HG23	2.01	0.41
1:B:170:ILE:HG23	1:B:197:GLN:HE21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1000:ARG:HD3	1:B:1000:ARG:HA	1.94	0.41
1:B:1653:LEU:HD23	1:B:1660:GLN:HA	2.02	0.41
1:C:367:LEU:HD22	1:C:372:LEU:HA	2.02	0.41
1:C:1773:PRO:HA	1:C:1774:PRO:HD3	1.91	0.41
1:C:3420:ARG:NH1	1:C:3516:LYS:O	2.43	0.41
1:C:3729:MET:HE2	1:C:3729:MET:HB2	1.67	0.41
1:D:786:GLY:N	1:D:1630:CYS:O	2.48	0.41
1:D:1160:ILE:O	1:D:1178:ALA:N	2.52	0.41
1:D:1599:MET:HG3	1:D:1601:MET:HE3	2.02	0.41
1:A:12:GLN:HG3	1:A:165:VAL:HG22	2.02	0.41
1:A:2090:LYS:HD3	1:A:2090:LYS:HA	1.96	0.41
1:A:2307:LEU:HD12	1:A:2308:GLN:HB3	2.02	0.41
1:A:3445:TRP:HA	1:A:3451:PHE:HD2	1.84	0.41
1:A:4036:VAL:HG22	1:A:5032:TYR:HD2	1.85	0.41
1:A:4802:GLY:HA2	1:A:4808:PHE:HB2	2.02	0.41
1:B:1160:ILE:O	1:B:1178:ALA:N	2.52	0.41
1:B:1461:ASP:OD2	1:B:1468:LYS:NZ	2.40	0.41
1:C:2254:LEU:O	1:C:2258:LEU:N	2.53	0.41
1:C:3163:VAL:HG22	1:C:3232:LEU:HD21	2.03	0.41
1:C:4036:VAL:HG22	1:C:5032:TYR:HD2	1.86	0.41
1:C:4150:LEU:HD23	1:C:4150:LEU:HA	1.89	0.41
1:D:170:ILE:HG23	1:D:197:GLN:HE21	1.85	0.41
1:D:367:LEU:HD22	1:D:372:LEU:HA	2.02	0.41
1:D:840:VAL:HG22	1:D:1199:VAL:HG22	2.01	0.41
1:D:1439:VAL:HB	1:D:1514:LEU:HB3	2.02	0.41
1:D:1759:ARG:HE	1:D:1760:HIS:H	1.69	0.41
1:D:2307:LEU:HD12	1:D:2308:GLN:HB3	2.02	0.41
1:D:3362:ILE:HG22	1:D:3437:MET:HE1	2.03	0.41
1:A:592:LYS:HB3	1:A:1592:PRO:HB3	2.02	0.41
1:A:728:ARG:HA	1:A:729:PRO:HD3	1.96	0.41
1:A:2004:GLU:HA	1:A:2007:ASN:HD22	1.85	0.41
1:A:3207:GLU:HG2	1:A:3209:GLN:HE22	1.86	0.41
1:A:3362:ILE:HG22	1:A:3437:MET:HE1	2.03	0.41
1:B:909:ASN:OD1	1:B:911:HIS:ND1	2.53	0.41
1:B:1439:VAL:HB	1:B:1514:LEU:HB3	2.02	0.41
1:B:2004:GLU:HA	1:B:2007:ASN:HD22	1.85	0.41
1:C:82:LEU:HD23	1:C:82:LEU:HA	1.91	0.41
1:C:134:ASP:OD1	1:C:134:ASP:N	2.50	0.41
1:C:840:VAL:HG22	1:C:1199:VAL:HG22	2.01	0.41
1:C:1599:MET:HG3	1:C:1601:MET:HE3	2.03	0.41
1:C:1759:ARG:HE	1:C:1760:HIS:H	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2314:LEU:HD12	1:C:2314:LEU:HA	1.85	0.41
1:C:2365:GLY:H	1:C:2369[B]:ARG:HH21	1.69	0.41
1:D:49:LEU:HD23	1:D:49:LEU:HA	1.89	0.41
1:D:294:THR:N	1:D:298:GLY:O	2.49	0.41
1:D:317:ARG:HG2	1:D:323:LEU:HG	2.01	0.41
1:D:797:HIS:CE1	1:D:821:LEU:HD23	2.55	0.41
1:D:2810:LYS:HA	1:D:2810:LYS:HD3	1.89	0.41
1:D:4690:GLU:H	1:D:4690:GLU:HG2	1.54	0.41
1:A:437:PRO:HB2	1:A:440:ALA:HB3	2.02	0.41
1:A:1599:MET:HG3	1:A:1601:MET:HE3	2.03	0.41
1:A:2365:GLY:H	1:A:2369[B]:ARG:HH21	1.69	0.41
1:A:2740:VAL:HG21	1:A:2819:TRP:HE1	1.85	0.41
1:A:2788:HIS:HB3	1:A:2791:LEU:HB2	2.02	0.41
1:A:3130:THR:HA	1:A:3133:THR:HG22	2.02	0.41
1:A:4172:GLU:HA	1:A:4175:ARG:HD3	2.03	0.41
1:A:4892:ARG:NH2	1:B:4899:ASP:OD1	2.54	0.41
1:B:592:LYS:HB3	1:B:1592:PRO:HB3	2.03	0.41
1:B:601:ASP:OD1	1:B:1665:HIS:ND1	2.45	0.41
1:B:622:THR:HG21	1:B:1681:VAL:HG22	2.03	0.41
1:B:908:VAL:HG13	1:B:963:ASN:HB3	2.02	0.41
1:B:1599:MET:HG3	1:B:1601:MET:HE3	2.03	0.41
1:B:3163:VAL:HG22	1:B:3232:LEU:HD21	2.03	0.41
1:B:3207:GLU:HG2	1:B:3209:GLN:HE22	1.86	0.41
1:C:592:LYS:HB3	1:C:1592:PRO:HB3	2.03	0.41
1:C:1254:HIS:O	1:C:1275:ARG:N	2.43	0.41
1:C:3171:SER:O	1:C:3174:SER:OG	2.38	0.41
1:C:3723:MET:HE1	1:C:3793:MET:HA	2.01	0.41
1:C:3878:ASP:OD1	1:C:3878:ASP:N	2.53	0.41
1:D:592:LYS:HB3	1:D:1592:PRO:HB3	2.03	0.41
1:D:909:ASN:OD1	1:D:911:HIS:ND1	2.53	0.41
1:D:1620:ALA:HB2	1:D:1627:ALA:HB2	2.02	0.41
1:D:3163:VAL:HG22	1:D:3232:LEU:HD21	2.03	0.41
1:D:3945:GLU:OE1	1:D:3949:ARG:NH1	2.54	0.41
1:A:356:TRP:N	1:A:379:HIS:O	2.53	0.41
1:A:622:THR:HG21	1:A:1681:VAL:HG22	2.03	0.41
1:A:2559:LEU:O	1:A:2563:THR:OG1	2.32	0.41
1:A:3949:ARG:O	1:A:3953:LYS:HG2	2.20	0.41
1:A:3995:VAL:HG13	1:A:3999:MET:HE3	2.02	0.41
1:A:4548:ARG:HE	1:A:4548:ARG:HB3	1.53	0.41
1:A:4573:ILE:HG22	1:A:4577:LEU:HD22	2.03	0.41
1:B:317:ARG:HG2	1:B:323:LEU:HG	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1854:PHE:HB3	1:B:1858:ASP:HB2	2.03	0.41
1:B:2546:MET:N	1:B:2546:MET:SD	2.93	0.41
1:B:3437:MET:HE2	1:B:3437:MET:HB2	1.94	0.41
1:C:622:THR:HG21	1:C:1681:VAL:HG22	2.03	0.41
1:C:2788:HIS:HB3	1:C:2791:LEU:HB2	2.02	0.41
1:C:3915:ILE:O	1:C:3919:THR:OG1	2.34	0.41
1:C:4172:GLU:HA	1:C:4175:ARG:HD3	2.03	0.41
1:D:1616:GLU:HB2	1:D:1629:GLN:HB3	2.03	0.41
1:D:1854:PHE:HB3	1:D:1858:ASP:HB2	2.03	0.41
1:D:1996:ARG:NH2	1:D:1999:ARG:O	2.52	0.41
1:D:3949:ARG:O	1:D:3953:LYS:HG2	2.20	0.41
1:A:575:LEU:HD11	1:A:606:LEU:HA	2.02	0.41
1:A:2254:LEU:O	1:A:2258:LEU:N	2.53	0.41
1:A:3171:SER:O	1:A:3174:SER:OG	2.38	0.41
1:A:4891:VAL:HG12	1:B:4921:PHE:HE2	1.85	0.41
1:B:865:PRO:HA	1:B:868:GLU:HG2	2.03	0.41
1:B:1784:ALA:HA	2:F:55:VAL:HA	2.03	0.41
1:B:2365:GLY:H	1:B:2369[B]:ARG:HH21	1.69	0.41
1:B:2816:MET:HG3	1:B:2878:LEU:HD22	2.03	0.41
1:B:3253:ILE:HD11	1:B:3273:THR:HG22	2.02	0.41
1:B:3362:ILE:HG22	1:B:3437:MET:HE1	2.03	0.41
1:B:3723:MET:HE1	1:B:3793:MET:HA	2.01	0.41
1:B:4172:GLU:HA	1:B:4175:ARG:HD3	2.03	0.41
1:B:4548:ARG:HE	1:B:4548:ARG:HB3	1.53	0.41
1:C:111:HIS:ND1	1:C:114:SER:OG	2.35	0.41
1:C:170:ILE:HG23	1:C:197:GLN:HE21	1.85	0.41
1:C:3112:LEU:HG	1:C:3180:ASN:HD21	1.86	0.41
1:C:3130:THR:HA	1:C:3133:THR:HG22	2.02	0.41
1:C:3537:LYS:HE2	1:C:3604:TYR:HB2	2.02	0.41
1:D:748:LEU:HD13	1:D:755:ILE:HG12	2.03	0.41
1:D:980:ALA:HB1	1:D:1055:PRO:HB3	2.02	0.41
1:D:2365:GLY:H	1:D:2369[B]:ARG:HH21	1.69	0.41
1:D:3416:VAL:HG23	1:D:3423:TRP:HZ3	1.86	0.41
1:D:3878:ASP:OD1	1:D:3878:ASP:N	2.53	0.41
1:D:3995:VAL:HG13	1:D:3999:MET:HE3	2.02	0.41
1:D:4957:LYS:HB2	1:D:4957:LYS:HE2	1.82	0.41
2:F:38:SER:O	2:F:42:ARG:NH2	2.54	0.41
1:A:1759:ARG:HE	1:A:1760:HIS:H	1.69	0.41
1:A:2410:PRO:HA	1:A:2411:PRO:HD3	1.99	0.41
1:A:2437:ALA:O	1:A:2508:ARG:NH2	2.53	0.41
1:A:3420:ARG:NH1	1:A:3516:LYS:O	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:575:LEU:HD11	1:B:606:LEU:HA	2.02	0.41
1:B:1620:ALA:HB2	1:B:1627:ALA:HB2	2.02	0.41
1:B:2740:VAL:HG21	1:B:2819:TRP:HE1	1.85	0.41
1:C:1231[B]:GLN:H	1:C:1231[B]:GLN:HG3	1.74	0.41
1:C:1784:ALA:HA	2:G:55:VAL:HA	2.03	0.41
1:C:2004:GLU:HA	1:C:2007:ASN:HD22	1.85	0.41
1:C:2816:MET:HG3	1:C:2878:LEU:HD22	2.03	0.41
1:C:3362:ILE:HG22	1:C:3437:MET:HE1	2.03	0.41
1:D:437:PRO:HB2	1:D:440:ALA:HB3	2.02	0.41
1:D:622:THR:HG21	1:D:1681:VAL:HG22	2.03	0.41
1:D:2628:PHE:HE1	1:D:2725:LYS:HE3	1.85	0.41
1:D:3537:LYS:HE2	1:D:3604:TYR:HB2	2.02	0.41
1:A:43:GLY:N	1:A:447:ASP:OD2	2.54	0.41
1:A:195:PHE:HA	1:D:2359:ARG:HH22	1.85	0.41
1:A:220:LEU:HD12	1:A:390:LEU:HB3	2.02	0.41
1:A:404:ILE:HG23	1:A:483:MET:HE2	2.03	0.41
1:A:601:ASP:OD1	1:A:1665:HIS:ND1	2.45	0.41
1:A:1000:ARG:HA	1:A:1000:ARG:HD3	1.94	0.41
1:A:1153:ILE:H	1:A:1223:PHE:HE2	1.69	0.41
1:A:1620:ALA:HB2	1:A:1627:ALA:HB2	2.01	0.41
1:A:2203:MET:SD	1:A:2203:MET:N	2.92	0.41
1:A:2816:MET:HG3	1:A:2878:LEU:HD22	2.03	0.41
1:A:3416:VAL:HG23	1:A:3423:TRP:HZ3	1.86	0.41
1:A:3524:MET:O	1:A:3595:ARG:NH1	2.54	0.41
1:A:4718:LYS:H	1:A:4718:LYS:HG2	1.43	0.41
1:A:4725:LEU:HD12	1:A:4725:LEU:HA	1.95	0.41
1:A:4865:LYS:HD2	1:A:4865:LYS:HA	1.66	0.41
1:A:5006:GLN:H	1:A:5006:GLN:HG3	1.65	0.41
1:B:1442:GLY:H	1:B:1509:ILE:HG23	1.86	0.41
1:B:2585:THR:HG22	1:B:2588:ARG:HH22	1.86	0.41
1:B:2779:GLU:HG3	1:B:2792:ARG:HG2	2.03	0.41
1:B:3112:LEU:HG	1:B:3180:ASN:HD21	1.86	0.41
1:B:3949:ARG:O	1:B:3953:LYS:HG2	2.21	0.41
1:B:4036:VAL:HG22	1:B:5032:TYR:HD2	1.86	0.41
1:B:4184:MET:HE2	1:B:4184:MET:HB2	1.79	0.41
1:B:5006:GLN:H	1:B:5006:GLN:HG3	1.65	0.41
1:C:437:PRO:HB2	1:C:440:ALA:HB3	2.02	0.41
1:C:748:LEU:HD13	1:C:755:ILE:HG12	2.03	0.41
1:C:908:VAL:HG13	1:C:963:ASN:HB3	2.02	0.41
1:C:1442:GLY:H	1:C:1509:ILE:HG23	1.86	0.41
1:C:1616:GLU:HB2	1:C:1629:GLN:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1653:LEU:HD23	1:C:1660:GLN:HA	2.02	0.41
1:C:1854:PHE:HB3	1:C:1858:ASP:HB2	2.03	0.41
1:C:2287:ALA:O	1:C:2349:ASN:ND2	2.48	0.41
1:C:2307:LEU:HD12	1:C:2308:GLN:HB3	2.02	0.41
1:C:2585:THR:HG22	1:C:2588:ARG:HH22	1.86	0.41
1:C:3207:GLU:HG2	1:C:3209:GLN:HE22	1.86	0.41
1:C:3995:VAL:HG13	1:C:3999:MET:HE3	2.02	0.41
1:C:4573:ILE:HG22	1:C:4577:LEU:HD22	2.03	0.41
1:D:281:ARG:NH1	1:D:309:THR:OG1	2.53	0.41
1:D:356:TRP:N	1:D:379:HIS:O	2.53	0.41
1:D:873:LYS:HE3	1:D:873:LYS:HB3	1.85	0.41
1:D:952:LYS:HA	1:D:971:ASP:HB3	2.03	0.41
1:D:2090:LYS:HD3	1:D:2090:LYS:HA	1.96	0.41
1:D:2110:TYR:HA	1:D:3700:GLN:HE21	1.85	0.41
1:D:2816:MET:HG3	1:D:2878:LEU:HD22	2.03	0.41
1:D:2905:LEU:HD23	1:D:2905:LEU:HA	1.95	0.41
1:D:3171:SER:O	1:D:3174:SER:OG	2.38	0.41
1:D:3936:TYR:O	1:D:3940:LYS:NZ	2.48	0.41
1:D:3965:LEU:HD23	1:D:3965:LEU:HA	1.90	0.41
1:D:4172:GLU:HA	1:D:4175:ARG:HD3	2.03	0.41
1:D:4802:GLY:HA2	1:D:4808:PHE:HB2	2.02	0.41
1:A:170:ILE:HG23	1:A:197:GLN:HE21	1.85	0.41
1:A:2094:LEU:O	1:A:2098:VAL:HG12	2.22	0.41
1:A:3537:LYS:HE2	1:A:3604:TYR:HB2	2.02	0.41
1:B:356:TRP:N	1:B:379:HIS:O	2.53	0.41
1:B:367:LEU:HD22	1:B:372:LEU:HA	2.02	0.41
1:B:437:PRO:HB2	1:B:440:ALA:HB3	2.02	0.41
1:B:3562:LYS:HA	1:B:3562:LYS:HD3	1.87	0.41
1:B:3945:GLU:OE1	1:B:3949:ARG:NH1	2.54	0.41
1:C:243:ARG:NH2	1:C:303:ASP:OD1	2.51	0.41
1:C:865:PRO:HA	1:C:868:GLU:HG2	2.03	0.41
1:C:897:ARG:HD2	1:C:897:ARG:HA	1.96	0.41
1:C:1439:VAL:HB	1:C:1514:LEU:HB3	2.02	0.41
1:C:2779:GLU:HG3	1:C:2792:ARG:HG2	2.03	0.41
1:C:5006:GLN:H	1:C:5006:GLN:HG3	1.65	0.41
1:D:2247:GLN:HG3	1:D:2279:SER:HA	2.03	0.41
1:D:4190:ILE:H	1:D:4190:ILE:HG12	1.48	0.41
2:G:73:LYS:NZ	2:G:75:THR:OG1	2.47	0.41
1:A:2716:ASP:N	1:A:2716:ASP:OD1	2.46	0.40
1:A:3037:GLU:HG2	1:A:3080:VAL:HG13	2.03	0.40
1:B:1153:ILE:H	1:B:1223:PHE:HE2	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1759:ARG:HE	1:B:1760:HIS:H	1.69	0.40
1:B:3416:VAL:HG23	1:B:3423:TRP:HZ3	1.86	0.40
1:C:220:LEU:HD12	1:C:390:LEU:HB3	2.02	0.40
1:C:1634:LEU:HD23	1:C:1634:LEU:HA	1.87	0.40
1:C:1996:ARG:O	1:C:2000:SER:OG	2.31	0.40
1:C:3524:MET:O	1:C:3595:ARG:NH1	2.54	0.40
1:D:43:GLY:N	1:D:447:ASP:OD2	2.54	0.40
1:D:144:GLU:HG3	1:D:175:SER:HB3	2.03	0.40
1:D:2094:LEU:O	1:D:2098:VAL:HG12	2.22	0.40
1:D:2437:ALA:O	1:D:2508:ARG:NH2	2.53	0.40
1:D:3112:LEU:HG	1:D:3180:ASN:HD21	1.86	0.40
1:D:3670:GLU:OE1	1:D:3670:GLU:N	2.53	0.40
1:A:546:TRP:O	1:A:549:SER:OG	2.39	0.40
1:A:2585:THR:HG22	1:A:2588:ARG:HH22	1.86	0.40
1:A:4112:LEU:O	1:A:4115:SER:OG	2.34	0.40
1:A:4681:LEU:HD23	1:A:4681:LEU:HA	1.90	0.40
1:A:4825:THR:O	1:A:4828:SER:OG	2.39	0.40
1:B:2307:LEU:HD12	1:B:2308:GLN:HB3	2.02	0.40
1:B:4869:GLU:H	1:B:4869:GLU:HG2	1.59	0.40
1:C:43:GLY:N	1:C:447:ASP:OD2	2.54	0.40
1:C:952:LYS:HA	1:C:971:ASP:HB3	2.03	0.40
1:C:1000:ARG:HD3	1:C:1000:ARG:HA	1.94	0.40
1:C:2094:LEU:O	1:C:2098:VAL:HG12	2.22	0.40
1:C:3652:MET:HE3	1:C:3652:MET:HB3	1.87	0.40
1:D:1007:TYR:O	1:D:1017:ARG:NH2	2.39	0.40
1:D:2996:LYS:HA	1:D:2996:LYS:HD3	1.91	0.40
1:D:3207:GLU:HG2	1:D:3209:GLN:HE22	1.86	0.40
1:D:4976:GLU:O	1:D:4980:LEU:HB2	2.22	0.40
1:A:125:ARG:H	1:A:125:ARG:HD3	1.86	0.40
1:A:1442:GLY:H	1:A:1509:ILE:HG23	1.86	0.40
1:A:1616:GLU:HB2	1:A:1629:GLN:HB3	2.03	0.40
1:A:4190:ILE:H	1:A:4190:ILE:HG12	1.48	0.40
1:A:4976:GLU:O	1:A:4980:LEU:HB2	2.21	0.40
1:B:897:ARG:HD2	1:B:897:ARG:HA	1.96	0.40
1:B:1685:LEU:HD23	1:B:1685:LEU:HA	1.91	0.40
1:B:2244:ARG:O	1:B:2248:ARG:N	2.46	0.40
1:B:3524:MET:O	1:B:3595:ARG:NH1	2.54	0.40
1:B:3936:TYR:O	1:B:3940:LYS:NZ	2.48	0.40
1:C:1741:GLU:O	1:C:1745:ILE:HG13	2.22	0.40
1:C:2247:GLN:HG3	1:C:2279:SER:HA	2.03	0.40
1:C:2410:PRO:HA	1:C:2411:PRO:HD3	1.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2628:PHE:HE1	1:C:2725:LYS:HE3	1.85	0.40
1:C:3752:SER:OG	1:C:3755:GLU:OE1	2.32	0.40
1:D:2788:HIS:HB3	1:D:2791:LEU:HB2	2.02	0.40
1:D:3780:LEU:HD22	1:D:3820:LEU:HD21	2.03	0.40
1:D:4184:MET:HE2	1:D:4184:MET:HB2	1.79	0.40
1:D:4818:MET:H	1:D:4818:MET:HG2	1.67	0.40
1:A:151:HIS:HB2	1:A:170:ILE:HB	2.03	0.40
1:A:224:HIS:HB2	1:A:229:GLU:HB2	2.04	0.40
1:A:797:HIS:CE1	1:A:821:LEU:HD23	2.55	0.40
1:A:1249:PRO:HA	1:A:1250:PRO:HD3	2.00	0.40
1:A:1685:LEU:HD23	1:A:1685:LEU:HA	1.91	0.40
1:A:1741:GLU:O	1:A:1745:ILE:HG13	2.22	0.40
1:A:1854:PHE:HB3	1:A:1858:ASP:HB2	2.03	0.40
1:A:4818:MET:H	1:A:4818:MET:HG2	1.67	0.40
1:B:243:ARG:NH2	1:B:303:ASP:OD1	2.51	0.40
1:B:1634:LEU:HD23	1:B:1634:LEU:HA	1.87	0.40
1:B:1741:GLU:O	1:B:1745:ILE:HG13	2.22	0.40
1:B:2157:GLU:O	1:B:2161:GLN:HG2	2.21	0.40
1:B:3674:ILE:O	1:B:3678:SER:OG	2.36	0.40
1:B:3862:ASP:OD1	1:B:3862:ASP:N	2.55	0.40
1:B:3878:ASP:OD1	1:B:3878:ASP:N	2.53	0.40
1:B:3924:LEU:HD12	1:B:3924:LEU:HA	1.94	0.40
1:C:151:HIS:ND1	1:C:159:GLU:OE2	2.55	0.40
1:C:633:LEU:HD12	1:C:1639:LEU:HG	2.03	0.40
1:C:1784:ALA:O	2:G:82:TYR:OH	2.33	0.40
1:C:2157:GLU:O	1:C:2161:GLN:HG2	2.21	0.40
1:C:2204:HIS:HB2	1:C:2250:MET:HE1	2.04	0.40
1:C:2867:LEU:HB2	1:C:2928:LYS:HZ3	1.85	0.40
1:C:3828:PHE:O	1:C:3831:SER:OG	2.38	0.40
1:C:4567:LEU:HD12	1:C:4567:LEU:HA	1.94	0.40
1:C:4878:ASP:OD1	1:C:4879:MET:N	2.55	0.40
1:D:728:ARG:HA	1:D:729:PRO:HD3	1.96	0.40
1:D:2004:GLU:HA	1:D:2007:ASN:HD22	1.85	0.40
1:D:3037:GLU:HG2	1:D:3080:VAL:HG13	2.03	0.40
1:D:3130:THR:HA	1:D:3133:THR:HG22	2.02	0.40
1:D:4573:ILE:HG22	1:D:4577:LEU:HD22	2.03	0.40
1:D:4578:LEU:HD23	1:D:4578:LEU:HA	1.89	0.40
1:A:151:HIS:ND1	1:A:159:GLU:OE2	2.55	0.40
1:A:281:ARG:NH1	1:A:309:THR:OG1	2.53	0.40
1:A:2443:ILE:HD13	1:A:2443:ILE:HA	1.94	0.40
1:A:3112:LEU:HG	1:A:3180:ASN:HD21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3752:SER:OG	1:B:3755:GLU:OE1	2.32	0.40
1:C:2163:ARG:HA	1:C:2166:LEU:HD13	2.04	0.40
1:C:3945:GLU:OE1	1:C:3949:ARG:NH1	2.54	0.40
1:D:908:VAL:HG13	1:D:963:ASN:HB3	2.02	0.40
1:D:2585:THR:HG22	1:D:2588:ARG:HH22	1.86	0.40
1:D:4582:VAL:HA	1:D:4629:TYR:O	2.22	0.40
2:G:38:SER:O	2:G:42:ARG:NH2	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4353/5037 (86%)	4217 (97%)	131 (3%)	5 (0%)	48	81
1	B	4353/5037 (86%)	4216 (97%)	132 (3%)	5 (0%)	48	81
1	C	4353/5037 (86%)	4216 (97%)	132 (3%)	5 (0%)	48	81
1	D	4353/5037 (86%)	4217 (97%)	131 (3%)	5 (0%)	48	81
2	E	105/350 (30%)	100 (95%)	5 (5%)	0	100	100
2	F	105/350 (30%)	100 (95%)	5 (5%)	0	100	100
2	G	105/350 (30%)	100 (95%)	5 (5%)	0	100	100
2	H	105/350 (30%)	100 (95%)	5 (5%)	0	100	100
All	All	17832/21548 (83%)	17266 (97%)	546 (3%)	20 (0%)	49	81

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3616	LYS
1	B	3616	LYS
1	C	3616	LYS

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Mol	Chain	Res	Type
1	D	3616	LYS
1	A	4694	ASP
1	B	4694	ASP
1	C	4694	ASP
1	D	4694	ASP
1	A	4691	GLN
1	B	4691	GLN
1	C	4691	GLN
1	D	4691	GLN
1	A	4712	PRO
1	B	4712	PRO
1	C	4712	PRO
1	D	4712	PRO
1	A	3612	PRO
1	B	3612	PRO
1	C	3612	PRO
1	D	3612	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3805/4276 (89%)	3666 (96%)	139 (4%)	30	52
1	B	3805/4276 (89%)	3665 (96%)	140 (4%)	30	52
1	C	3805/4276 (89%)	3665 (96%)	140 (4%)	30	52
1	D	3805/4276 (89%)	3666 (96%)	139 (4%)	30	52
2	E	88/304 (29%)	88 (100%)	0	100	100
2	F	88/304 (29%)	88 (100%)	0	100	100
2	G	88/304 (29%)	88 (100%)	0	100	100
2	H	88/304 (29%)	88 (100%)	0	100	100
All	All	15572/18320 (85%)	15014 (96%)	558 (4%)	32	53

All (558) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	873	LYS
1	A	1743[A]	ARG
1	A	1743[B]	ARG
1	A	2369[A]	ARG
1	A	2369[B]	ARG
1	A	2584[A]	HIS
1	A	2584[B]	HIS
1	A	4178	LEU
1	A	4183	ILE
1	A	4184	MET
1	A	4187	SER
1	A	4188	ARG
1	A	4189	ARG
1	A	4190	ILE
1	A	4193	ILE
1	A	4196	GLU
1	A	4198	SER
1	A	4199	GLU
1	A	4200	THR
1	A	4202	ARG
1	A	4204	GLN
1	A	4206	GLU
1	A	4207	MET
1	A	4211	LYS
1	A	4212	GLU
1	A	4213	SER
1	A	4224	GLU
1	A	4227	GLU
1	A	4245	MET
1	A	4246	GLN
1	A	4251	ILE
1	A	4252	SER
1	A	4544	LEU
1	A	4545	GLU
1	A	4548	ARG
1	A	4550	LYS
1	A	4552	LEU
1	A	4555	LEU
1	A	4556	SER
1	A	4561	THR
1	A	4569	LEU
1	A	4576	ILE
1	A	4577	LEU

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Mol	Chain	Res	Type
1	A	4580	TYR
1	A	4583	SER
1	A	4584	ASP
1	A	4585	SER
1	A	4587	PRO
1	A	4627	MET
1	A	4628	VAL
1	A	4632	LEU
1	A	4634	GLU
1	A	4635	SER
1	A	4636	THR
1	A	4639	MET
1	A	4649	LEU
1	A	4651	THR
1	A	4653	VAL
1	A	4655	PHE
1	A	4658	ILE
1	A	4672	LYS
1	A	4676	GLU
1	A	4680	LYS
1	A	4684	ASP
1	A	4689	THR
1	A	4690	GLU
1	A	4691	GLN
1	A	4692	PRO
1	A	4694	ASP
1	A	4696	ASP
1	A	4698	LYS
1	A	4716	TRP
1	A	4718	LYS
1	A	4722	ARG
1	A	4727	LYS
1	A	4728	HIS
1	A	4730	ASP
1	A	4731	ILE
1	A	4735	GLU
1	A	4736	ARG
1	A	4737	ILE
1	A	4739	GLU
1	A	4743	MET
1	A	4773	VAL
1	A	4777	ILE

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Mol	Chain	Res	Type
1	A	4779	LYS
1	A	4788	SER
1	A	4796	MET
1	A	4818	MET
1	A	4821	LYS
1	A	4822	THR
1	A	4824	ARG
1	A	4825	THR
1	A	4826	ILE
1	A	4835	LYS
1	A	4836	GLN
1	A	4844	LEU
1	A	4852	THR
1	A	4861	LYS
1	A	4863	TYR
1	A	4865	LYS
1	A	4867	GLU
1	A	4868	ASP
1	A	4869	GLU
1	A	4870	ASP
1	A	4871	GLU
1	A	4879	MET
1	A	4887	MET
1	A	4889	VAL
1	A	4903	ASP
1	A	4911	LEU
1	A	4913	ARG
1	A	4932	ILE
1	A	4933	GLN
1	A	4951	LYS
1	A	4952	GLU
1	A	4954	MET
1	A	4955	GLU
1	A	4957	LYS
1	A	4971	THR
1	A	4980	LEU
1	A	4981	GLU
1	A	4985	LEU
1	A	4989	MET
1	A	4993	MET
1	A	4997	ASN
1	A	5002	GLU

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Mol	Chain	Res	Type
1	A	5006	GLN
1	A	5008	SER
1	A	5012	LYS
1	A	5013	MET
1	A	5015	GLN
1	A	5018	CYS
1	A	5027	CYS
1	A	5029	ARG
1	A	5031	GLN
1	A	5034	ASP
1	A	5035	GLN
1	A	5037	SER
1	B	873	LYS
1	B	1743[A]	ARG
1	B	1743[B]	ARG
1	B	2369[A]	ARG
1	B	2369[B]	ARG
1	B	2584[A]	HIS
1	B	2584[B]	HIS
1	B	3690	VAL
1	B	4178	LEU
1	B	4183	ILE
1	B	4184	MET
1	B	4187	SER
1	B	4188	ARG
1	B	4189	ARG
1	B	4190	ILE
1	B	4193	ILE
1	B	4196	GLU
1	B	4198	SER
1	B	4199	GLU
1	B	4200	THR
1	B	4202	ARG
1	B	4204	GLN
1	B	4206	GLU
1	B	4207	MET
1	B	4211	LYS
1	B	4212	GLU
1	B	4213	SER
1	B	4224	GLU
1	B	4227	GLU
1	B	4245	MET

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Mol	Chain	Res	Type
1	B	4246	GLN
1	B	4251	ILE
1	B	4252	SER
1	B	4544	LEU
1	B	4545	GLU
1	B	4548	ARG
1	B	4550	LYS
1	B	4552	LEU
1	B	4555	LEU
1	B	4556	SER
1	B	4561	THR
1	B	4569	LEU
1	B	4576	ILE
1	B	4577	LEU
1	B	4580	TYR
1	B	4583	SER
1	B	4584	ASP
1	B	4585	SER
1	B	4587	PRO
1	B	4627	MET
1	B	4628	VAL
1	B	4632	LEU
1	B	4634	GLU
1	B	4635	SER
1	B	4636	THR
1	B	4639	MET
1	B	4649	LEU
1	B	4651	THR
1	B	4653	VAL
1	B	4655	PHE
1	B	4658	ILE
1	B	4672	LYS
1	B	4676	GLU
1	B	4680	LYS
1	B	4684	ASP
1	B	4689	THR
1	B	4690	GLU
1	B	4691	GLN
1	B	4692	PRO
1	B	4694	ASP
1	B	4696	ASP
1	B	4698	LYS

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Mol	Chain	Res	Type
1	B	4716	TRP
1	B	4718	LYS
1	B	4722	ARG
1	B	4727	LYS
1	B	4728	HIS
1	B	4730	ASP
1	B	4731	ILE
1	B	4735	GLU
1	B	4736	ARG
1	B	4737	ILE
1	B	4739	GLU
1	B	4743	MET
1	B	4773	VAL
1	B	4777	ILE
1	B	4779	LYS
1	B	4788	SER
1	B	4796	MET
1	B	4818	MET
1	B	4821	LYS
1	B	4822	THR
1	B	4824	ARG
1	B	4825	THR
1	B	4826	ILE
1	B	4835	LYS
1	B	4836	GLN
1	B	4844	LEU
1	B	4852	THR
1	B	4861	LYS
1	B	4863	TYR
1	B	4865	LYS
1	B	4867	GLU
1	B	4868	ASP
1	B	4869	GLU
1	B	4870	ASP
1	B	4871	GLU
1	B	4879	MET
1	B	4887	MET
1	B	4889	VAL
1	B	4903	ASP
1	B	4911	LEU
1	B	4913	ARG
1	B	4932	ILE

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Mol	Chain	Res	Type
1	B	4933	GLN
1	B	4951	LYS
1	B	4952	GLU
1	B	4954	MET
1	B	4955	GLU
1	B	4957	LYS
1	B	4971	THR
1	B	4980	LEU
1	B	4981	GLU
1	B	4985	LEU
1	B	4989	MET
1	B	4993	MET
1	B	4997	ASN
1	B	5002	GLU
1	B	5006	GLN
1	B	5008	SER
1	B	5012	LYS
1	B	5013	MET
1	B	5015	GLN
1	B	5018	CYS
1	B	5027	CYS
1	B	5029	ARG
1	B	5031	GLN
1	B	5034	ASP
1	B	5035	GLN
1	B	5037	SER
1	C	873	LYS
1	C	1743[A]	ARG
1	C	1743[B]	ARG
1	C	2369[A]	ARG
1	C	2369[B]	ARG
1	C	2584[A]	HIS
1	C	2584[B]	HIS
1	C	3690	VAL
1	C	4178	LEU
1	C	4183	ILE
1	C	4184	MET
1	C	4187	SER
1	C	4188	ARG
1	C	4189	ARG
1	C	4190	ILE
1	C	4193	ILE

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Mol	Chain	Res	Type
1	C	4196	GLU
1	C	4198	SER
1	C	4199	GLU
1	C	4200	THR
1	C	4202	ARG
1	C	4204	GLN
1	C	4206	GLU
1	C	4207	MET
1	C	4211	LYS
1	C	4212	GLU
1	C	4213	SER
1	C	4224	GLU
1	C	4227	GLU
1	C	4245	MET
1	C	4246	GLN
1	C	4251	ILE
1	C	4252	SER
1	C	4544	LEU
1	C	4545	GLU
1	C	4548	ARG
1	C	4550	LYS
1	C	4552	LEU
1	C	4555	LEU
1	C	4556	SER
1	C	4561	THR
1	C	4569	LEU
1	C	4576	ILE
1	C	4577	LEU
1	C	4580	TYR
1	C	4583	SER
1	C	4584	ASP
1	C	4585	SER
1	C	4587	PRO
1	C	4627	MET
1	C	4628	VAL
1	C	4632	LEU
1	C	4634	GLU
1	C	4635	SER
1	C	4636	THR
1	C	4639	MET
1	C	4649	LEU
1	C	4651	THR

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Mol	Chain	Res	Type
1	C	4653	VAL
1	C	4655	PHE
1	C	4658	ILE
1	C	4672	LYS
1	C	4676	GLU
1	C	4680	LYS
1	C	4684	ASP
1	C	4689	THR
1	C	4690	GLU
1	C	4691	GLN
1	C	4692	PRO
1	C	4694	ASP
1	C	4696	ASP
1	C	4698	LYS
1	C	4716	TRP
1	C	4718	LYS
1	C	4722	ARG
1	C	4727	LYS
1	C	4728	HIS
1	C	4730	ASP
1	C	4731	ILE
1	C	4735	GLU
1	C	4736	ARG
1	C	4737	ILE
1	C	4739	GLU
1	C	4743	MET
1	C	4773	VAL
1	C	4777	ILE
1	C	4779	LYS
1	C	4788	SER
1	C	4796	MET
1	C	4818	MET
1	C	4821	LYS
1	C	4822	THR
1	C	4824	ARG
1	C	4825	THR
1	C	4826	ILE
1	C	4835	LYS
1	C	4836	GLN
1	C	4844	LEU
1	C	4852	THR
1	C	4861	LYS

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Mol	Chain	Res	Type
1	C	4863	TYR
1	C	4865	LYS
1	C	4867	GLU
1	C	4868	ASP
1	C	4869	GLU
1	C	4870	ASP
1	C	4871	GLU
1	C	4879	MET
1	C	4887	MET
1	C	4889	VAL
1	C	4903	ASP
1	C	4911	LEU
1	C	4913	ARG
1	C	4932	ILE
1	C	4933	GLN
1	C	4951	LYS
1	C	4952	GLU
1	C	4954	MET
1	C	4955	GLU
1	C	4957	LYS
1	C	4971	THR
1	C	4980	LEU
1	C	4981	GLU
1	C	4985	LEU
1	C	4989	MET
1	C	4993	MET
1	C	4997	ASN
1	C	5002	GLU
1	C	5006	GLN
1	C	5008	SER
1	C	5012	LYS
1	C	5013	MET
1	C	5015	GLN
1	C	5018	CYS
1	C	5027	CYS
1	C	5029	ARG
1	C	5031	GLN
1	C	5034	ASP
1	C	5035	GLN
1	C	5037	SER
1	D	873	LYS
1	D	1743[A]	ARG

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Mol	Chain	Res	Type
1	D	1743[B]	ARG
1	D	2369[A]	ARG
1	D	2369[B]	ARG
1	D	2584[A]	HIS
1	D	2584[B]	HIS
1	D	4178	LEU
1	D	4183	ILE
1	D	4184	MET
1	D	4187	SER
1	D	4188	ARG
1	D	4189	ARG
1	D	4190	ILE
1	D	4193	ILE
1	D	4196	GLU
1	D	4198	SER
1	D	4199	GLU
1	D	4200	THR
1	D	4202	ARG
1	D	4204	GLN
1	D	4206	GLU
1	D	4207	MET
1	D	4211	LYS
1	D	4212	GLU
1	D	4213	SER
1	D	4224	GLU
1	D	4227	GLU
1	D	4245	MET
1	D	4246	GLN
1	D	4251	ILE
1	D	4252	SER
1	D	4544	LEU
1	D	4545	GLU
1	D	4548	ARG
1	D	4550	LYS
1	D	4552	LEU
1	D	4555	LEU
1	D	4556	SER
1	D	4561	THR
1	D	4569	LEU
1	D	4576	ILE
1	D	4577	LEU
1	D	4580	TYR

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Mol	Chain	Res	Type
1	D	4583	SER
1	D	4584	ASP
1	D	4585	SER
1	D	4587	PRO
1	D	4627	MET
1	D	4628	VAL
1	D	4632	LEU
1	D	4634	GLU
1	D	4635	SER
1	D	4636	THR
1	D	4639	MET
1	D	4649	LEU
1	D	4651	THR
1	D	4653	VAL
1	D	4655	PHE
1	D	4658	ILE
1	D	4672	LYS
1	D	4676	GLU
1	D	4680	LYS
1	D	4684	ASP
1	D	4689	THR
1	D	4690	GLU
1	D	4691	GLN
1	D	4692	PRO
1	D	4694	ASP
1	D	4696	ASP
1	D	4698	LYS
1	D	4716	TRP
1	D	4718	LYS
1	D	4722	ARG
1	D	4727	LYS
1	D	4728	HIS
1	D	4730	ASP
1	D	4731	ILE
1	D	4735	GLU
1	D	4736	ARG
1	D	4737	ILE
1	D	4739	GLU
1	D	4743	MET
1	D	4773	VAL
1	D	4777	ILE
1	D	4779	LYS

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Mol	Chain	Res	Type
1	D	4788	SER
1	D	4796	MET
1	D	4818	MET
1	D	4821	LYS
1	D	4822	THR
1	D	4824	ARG
1	D	4825	THR
1	D	4826	ILE
1	D	4835	LYS
1	D	4836	GLN
1	D	4844	LEU
1	D	4852	THR
1	D	4861	LYS
1	D	4863	TYR
1	D	4865	LYS
1	D	4867	GLU
1	D	4868	ASP
1	D	4869	GLU
1	D	4870	ASP
1	D	4871	GLU
1	D	4879	MET
1	D	4887	MET
1	D	4889	VAL
1	D	4903	ASP
1	D	4911	LEU
1	D	4913	ARG
1	D	4932	ILE
1	D	4933	GLN
1	D	4951	LYS
1	D	4952	GLU
1	D	4954	MET
1	D	4955	GLU
1	D	4957	LYS
1	D	4971	THR
1	D	4980	LEU
1	D	4981	GLU
1	D	4985	LEU
1	D	4989	MET
1	D	4993	MET
1	D	4997	ASN
1	D	5002	GLU
1	D	5006	GLN

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Mol	Chain	Res	Type
1	D	5008	SER
1	D	5012	LYS
1	D	5013	MET
1	D	5015	GLN
1	D	5018	CYS
1	D	5027	CYS
1	D	5029	ARG
1	D	5031	GLN
1	D	5034	ASP
1	D	5035	GLN
1	D	5037	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (185) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	GLN
1	A	201	ASN
1	A	226	HIS
1	A	241	GLN
1	A	255	HIS
1	A	460	GLN
1	A	489	ASN
1	A	495	ASN
1	A	533	ASN
1	A	581	ASN
1	A	705	ASN
1	A	725	HIS
1	A	860	GLN
1	A	1052	ASN
1	A	1229	ASN
1	A	1281	ASN
1	A	1563	GLN
1	A	1611	HIS
1	A	1631	GLN
1	A	1702	HIS
1	A	2003	GLN
1	A	2007	ASN
1	A	2029	GLN
1	A	2095	GLN
1	A	2127	GLN
1	A	2283	ASN
1	A	2551	ASN

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Mol	Chain	Res	Type
1	A	2620	GLN
1	A	2734	ASN
1	A	2881	ASN
1	A	2883	HIS
1	A	2924	GLN
1	A	2933	ASN
1	A	2976	HIS
1	A	3180	ASN
1	A	3214	ASN
1	A	3555	ASN
1	A	3897	ASN
1	A	3963	ASN
1	A	4109	GLN
1	A	4120	ASN
1	A	4558	ASN
1	A	4691	GLN
1	A	4886	HIS
1	A	5003	HIS
1	A	5031	GLN
1	B	54	ASN
1	B	197	GLN
1	B	201	ASN
1	B	226	HIS
1	B	241	GLN
1	B	460	GLN
1	B	489	ASN
1	B	495	ASN
1	B	533	ASN
1	B	581	ASN
1	B	860	GLN
1	B	1052	ASN
1	B	1229	ASN
1	B	1281	ASN
1	B	1541	GLN
1	B	1563	GLN
1	B	1611	HIS
1	B	1631	GLN
1	B	1702	HIS
1	B	2003	GLN
1	B	2007	ASN
1	B	2095	GLN
1	B	2127	GLN

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Mol	Chain	Res	Type
1	B	2283	ASN
1	B	2551	ASN
1	B	2620	GLN
1	B	2734	ASN
1	B	2881	ASN
1	B	2883	HIS
1	B	2924	GLN
1	B	2933	ASN
1	B	2976	HIS
1	B	3180	ASN
1	B	3214	ASN
1	B	3466	ASN
1	B	3814	GLN
1	B	3897	ASN
1	B	3963	ASN
1	B	4109	GLN
1	B	4120	ASN
1	B	4156	HIS
1	B	4558	ASN
1	B	4691	GLN
1	B	5003	HIS
1	B	5031	GLN
1	C	197	GLN
1	C	201	ASN
1	C	226	HIS
1	C	241	GLN
1	C	255	HIS
1	C	460	GLN
1	C	489	ASN
1	C	495	ASN
1	C	533	ASN
1	C	581	ASN
1	C	705	ASN
1	C	725	HIS
1	C	860	GLN
1	C	1035	ASN
1	C	1052	ASN
1	C	1229	ASN
1	C	1281	ASN
1	C	1563	GLN
1	C	1611	HIS
1	C	1631	GLN

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Mol	Chain	Res	Type
1	C	2003	GLN
1	C	2007	ASN
1	C	2095	GLN
1	C	2127	GLN
1	C	2283	ASN
1	C	2551	ASN
1	C	2620	GLN
1	C	2647	HIS
1	C	2734	ASN
1	C	2881	ASN
1	C	2883	HIS
1	C	2924	GLN
1	C	2933	ASN
1	C	2976	HIS
1	C	2993	GLN
1	C	3180	ASN
1	C	3214	ASN
1	C	3466	ASN
1	C	3555	ASN
1	C	3814	GLN
1	C	3897	ASN
1	C	3963	ASN
1	C	4109	GLN
1	C	4120	ASN
1	C	4558	ASN
1	C	4691	GLN
1	C	5003	HIS
1	C	5031	GLN
1	D	54	ASN
1	D	197	GLN
1	D	201	ASN
1	D	241	GLN
1	D	460	GLN
1	D	489	ASN
1	D	495	ASN
1	D	533	ASN
1	D	581	ASN
1	D	705	ASN
1	D	725	HIS
1	D	860	GLN
1	D	1052	ASN
1	D	1229	ASN

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Mol	Chain	Res	Type
1	D	1281	ASN
1	D	1560	ASN
1	D	1563	GLN
1	D	1611	HIS
1	D	1631	GLN
1	D	2003	GLN
1	D	2007	ASN
1	D	2029	GLN
1	D	2095	GLN
1	D	2127	GLN
1	D	2283	ASN
1	D	2551	ASN
1	D	2620	GLN
1	D	2734	ASN
1	D	2881	ASN
1	D	2883	HIS
1	D	2924	GLN
1	D	2933	ASN
1	D	2976	HIS
1	D	2993	GLN
1	D	3180	ASN
1	D	3214	ASN
1	D	3466	ASN
1	D	3555	ASN
1	D	3897	ASN
1	D	3963	ASN
1	D	4109	GLN
1	D	4120	ASN
1	D	4558	ASN
1	D	4691	GLN
1	D	5003	HIS
1	D	5031	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	AGS	D	5101	-	32,33,33	0.53	1 (3%)	45,52,52	1.11	2 (4%)
3	AGS	C	5101	-	32,33,33	0.53	1 (3%)	45,52,52	1.11	2 (4%)
3	AGS	A	5101	-	32,33,33	0.53	1 (3%)	45,52,52	1.11	2 (4%)
3	AGS	B	5101	-	32,33,33	0.53	1 (3%)	45,52,52	1.11	2 (4%)

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	AGS	D	5101	-	-	7/21/38/38	0/3/3/3
3	AGS	C	5101	-	-	7/21/38/38	0/3/3/3
3	AGS	A	5101	-	-	7/21/38/38	0/3/3/3
3	AGS	B	5101	-	-	7/21/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5101	AGS	PG-S1G	2.09	1.95	1.90
3	D	5101	AGS	PG-S1G	2.09	1.95	1.90
3	B	5101	AGS	PG-S1G	2.09	1.95	1.90
3	C	5101	AGS	PG-S1G	2.09	1.95	1.90

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	5101	AGS	PB-O3B-PG	-3.64	119.86	133.17
3	A	5101	AGS	PB-O3B-PG	-3.64	119.86	133.17
3	B	5101	AGS	PB-O3B-PG	-3.64	119.86	133.17
3	C	5101	AGS	PB-O3B-PG	-3.64	119.86	133.17
3	C	5101	AGS	O5'-C5'-C4'	3.12	119.63	108.99
3	D	5101	AGS	O5'-C5'-C4'	3.12	119.63	108.99
3	A	5101	AGS	O5'-C5'-C4'	3.12	119.62	108.99
3	B	5101	AGS	O5'-C5'-C4'	3.12	119.62	108.99

There are no chirality outliers.

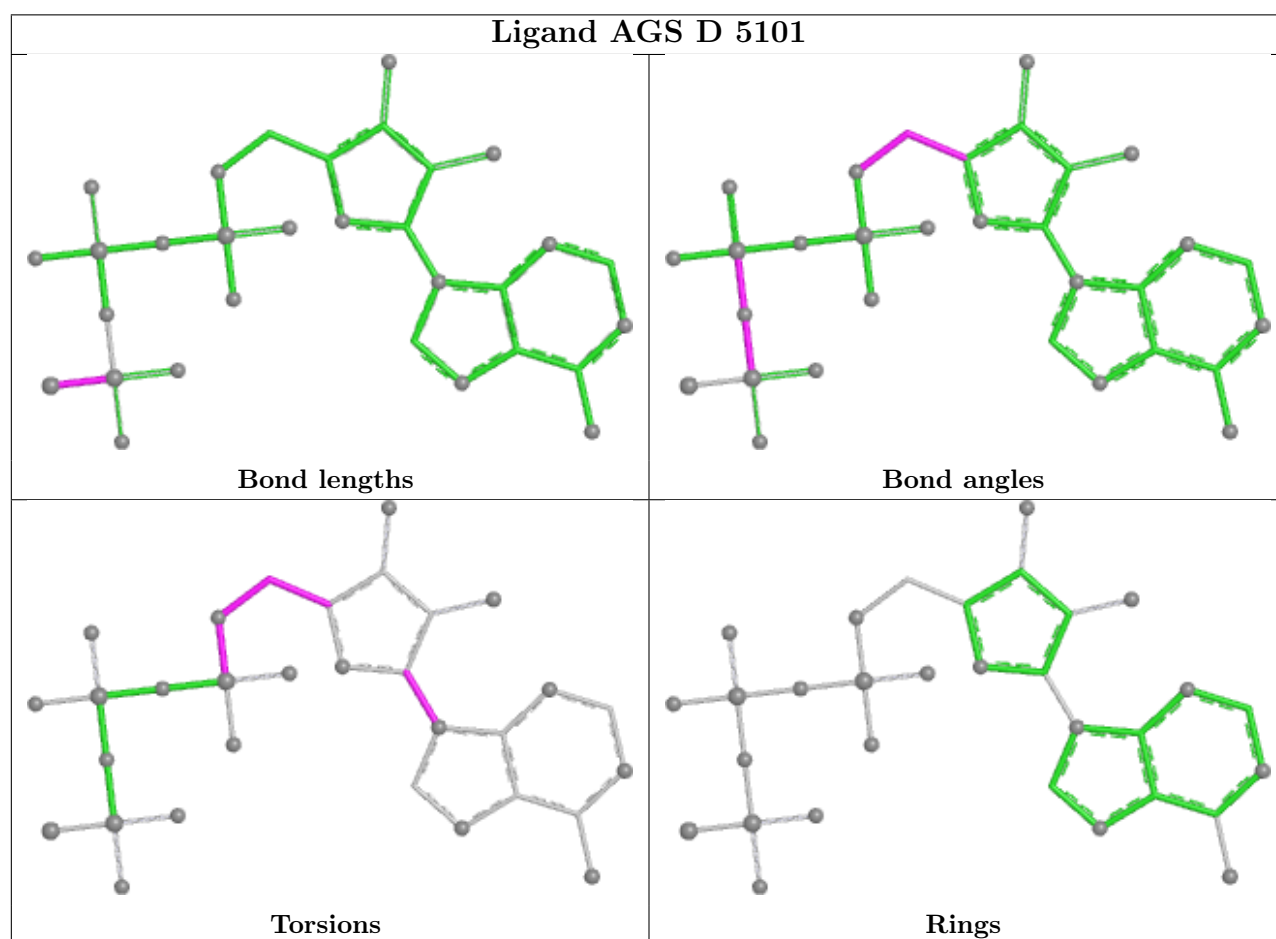
All (28) torsion outliers are listed below:

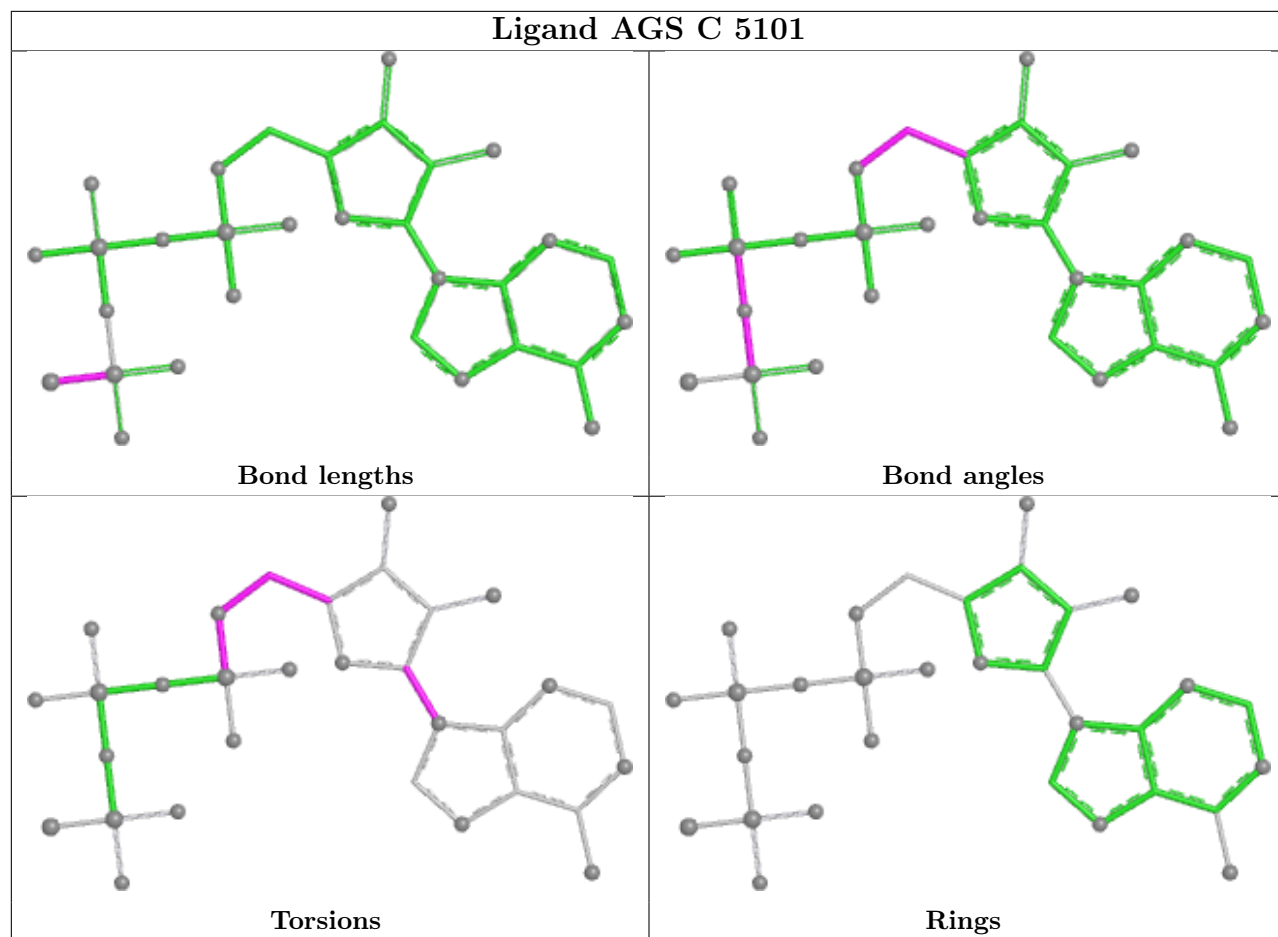
Mol	Chain	Res	Type	Atoms
3	A	5101	AGS	C5'-O5'-PA-O3A
3	A	5101	AGS	C4'-C5'-O5'-PA
3	A	5101	AGS	O4'-C4'-C5'-O5'
3	B	5101	AGS	C5'-O5'-PA-O3A
3	B	5101	AGS	C4'-C5'-O5'-PA
3	B	5101	AGS	O4'-C4'-C5'-O5'
3	C	5101	AGS	C5'-O5'-PA-O3A
3	C	5101	AGS	C4'-C5'-O5'-PA
3	C	5101	AGS	O4'-C4'-C5'-O5'
3	D	5101	AGS	C5'-O5'-PA-O3A
3	D	5101	AGS	C4'-C5'-O5'-PA
3	D	5101	AGS	O4'-C4'-C5'-O5'
3	A	5101	AGS	C3'-C4'-C5'-O5'
3	B	5101	AGS	C3'-C4'-C5'-O5'
3	C	5101	AGS	C3'-C4'-C5'-O5'
3	D	5101	AGS	C3'-C4'-C5'-O5'
3	A	5101	AGS	C5'-O5'-PA-O1A
3	A	5101	AGS	C5'-O5'-PA-O2A
3	B	5101	AGS	C5'-O5'-PA-O1A
3	B	5101	AGS	C5'-O5'-PA-O2A
3	C	5101	AGS	C5'-O5'-PA-O1A
3	C	5101	AGS	C5'-O5'-PA-O2A
3	D	5101	AGS	C5'-O5'-PA-O1A
3	D	5101	AGS	C5'-O5'-PA-O2A
3	A	5101	AGS	O4'-C1'-N9-C8
3	B	5101	AGS	O4'-C1'-N9-C8
3	C	5101	AGS	O4'-C1'-N9-C8
3	D	5101	AGS	O4'-C1'-N9-C8

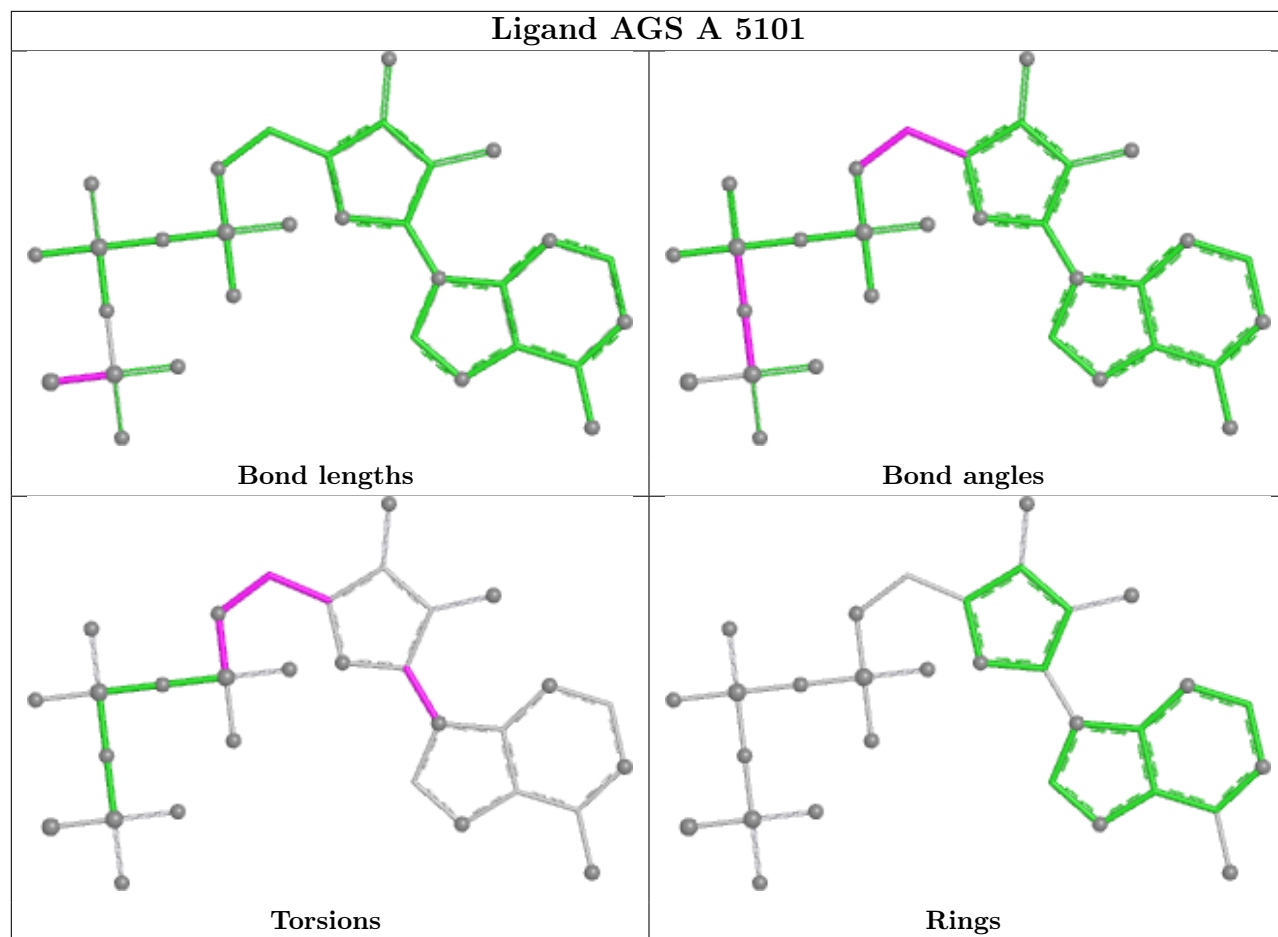
There are no ring outliers.

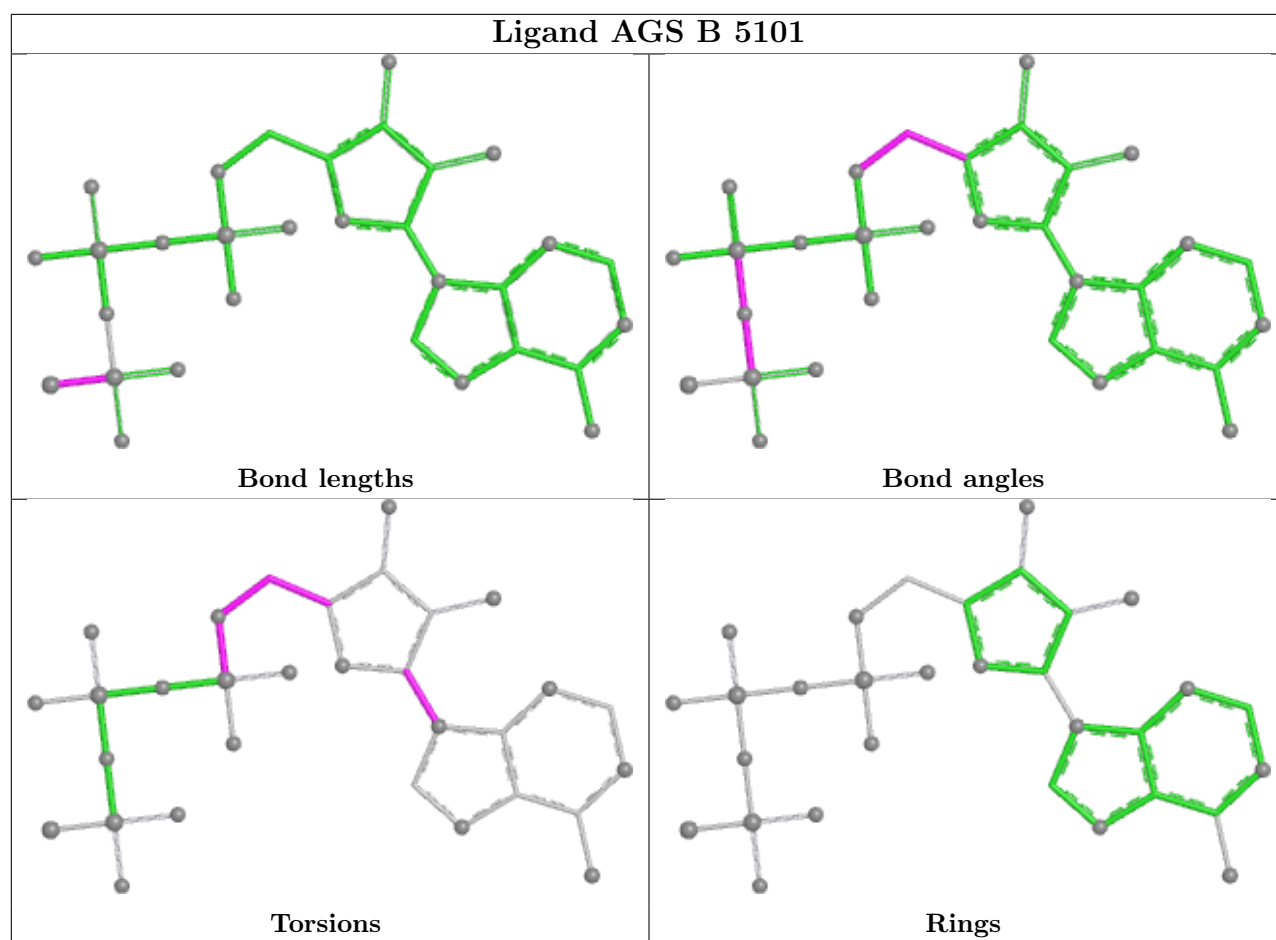
No monomer is involved in short contacts.

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.

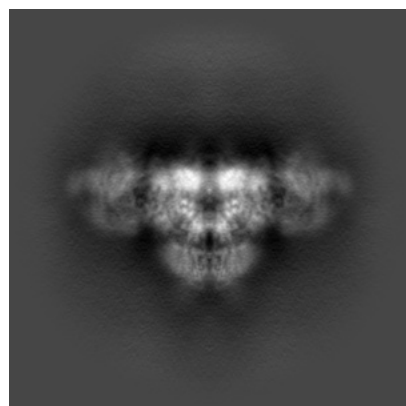
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40423. These allow visual inspection of the internal detail of the map and identification of artifacts.

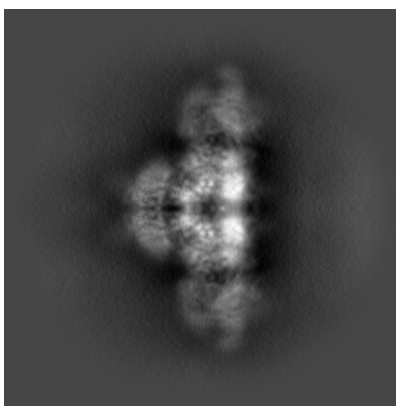
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

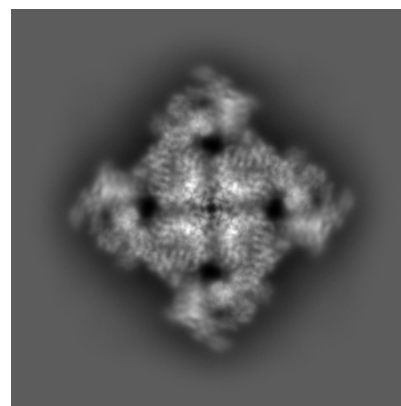
6.1.1 Primary map



X

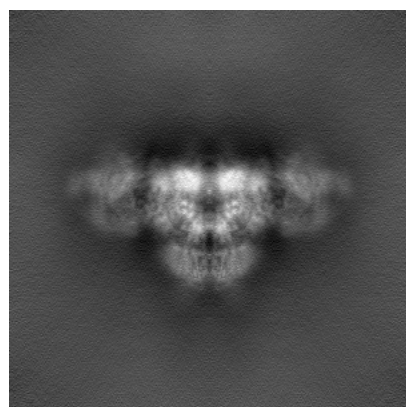


Y

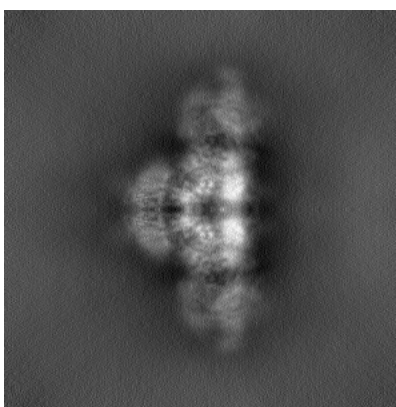


Z

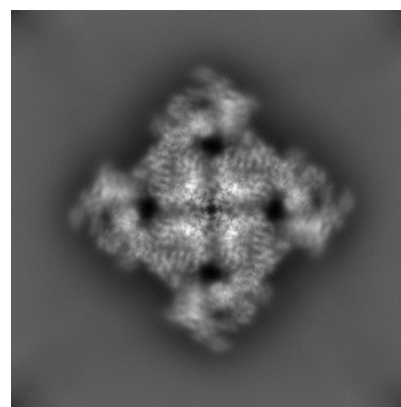
6.1.2 Raw map



X



Y

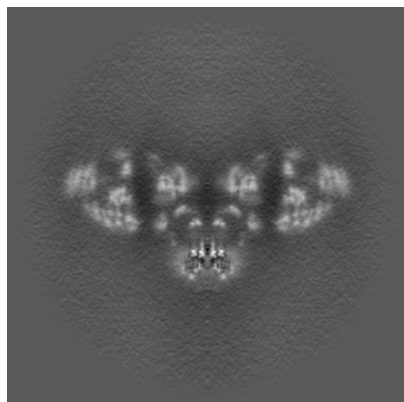


Z

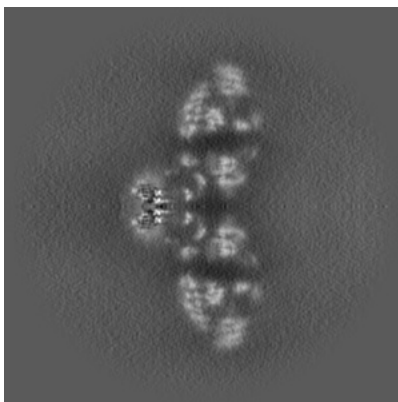
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

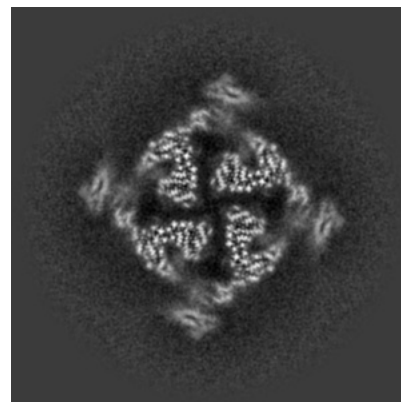
6.2.1 Primary map



X Index: 200

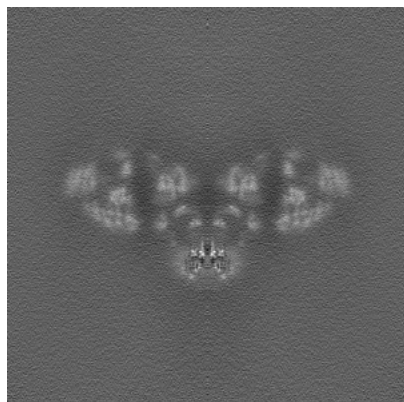


Y Index: 200

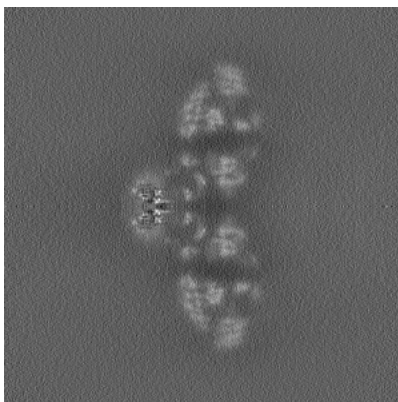


Z Index: 200

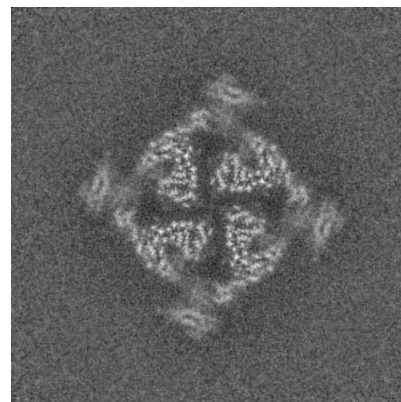
6.2.2 Raw map



X Index: 200



Y Index: 200

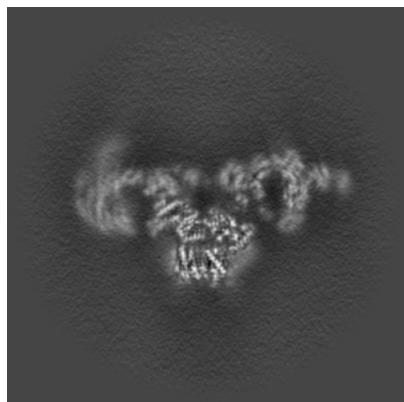


Z Index: 200

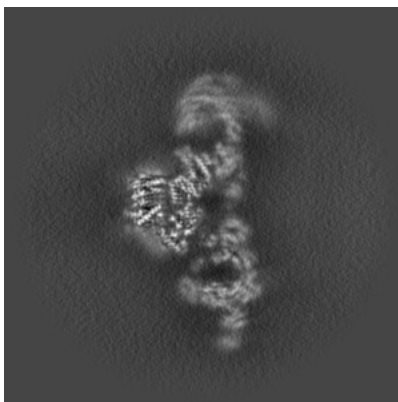
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

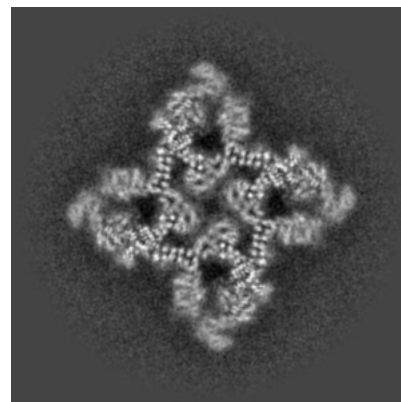
6.3.1 Primary map



X Index: 186

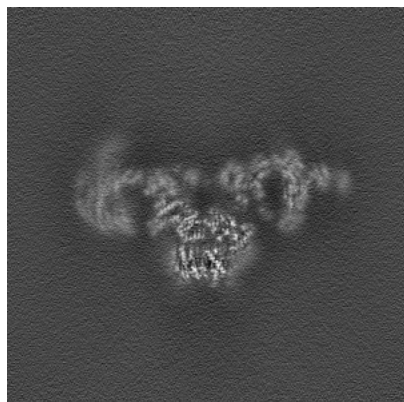


Y Index: 186

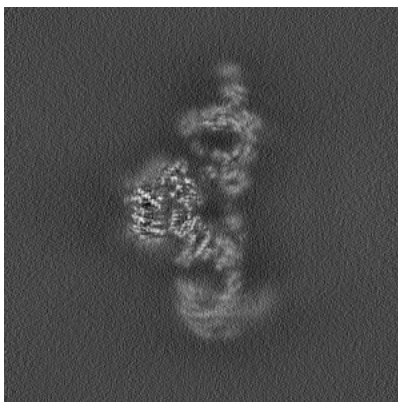


Z Index: 225

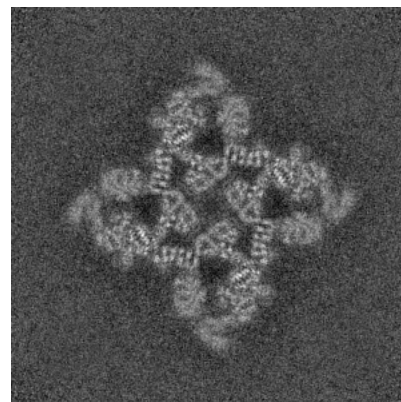
6.3.2 Raw map



X Index: 186



Y Index: 214

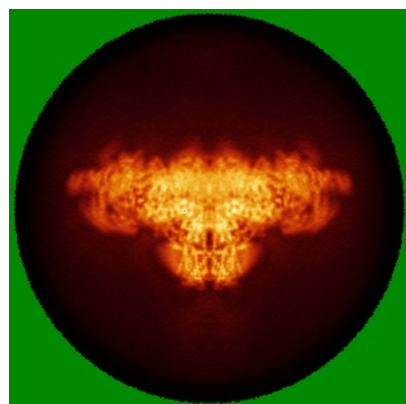


Z Index: 223

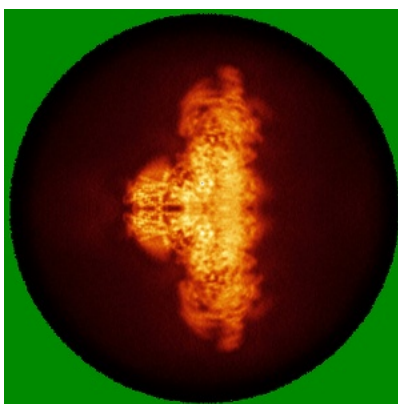
The images above show the largest variance slices of the map in three orthogonal directions.

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

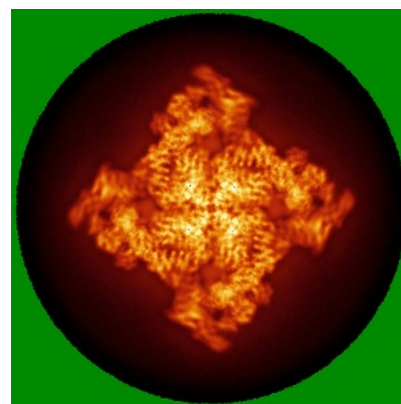
6.4.1 Primary map



X

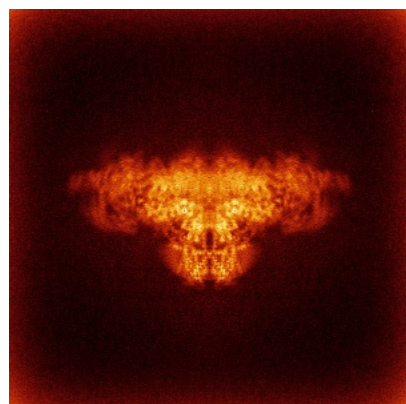


Y

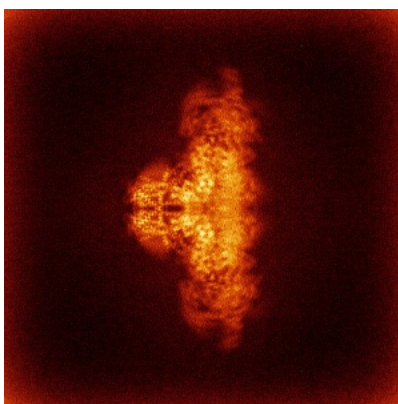


Z

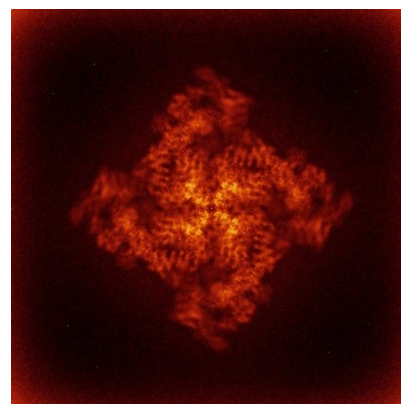
6.4.2 Raw map



X



Y

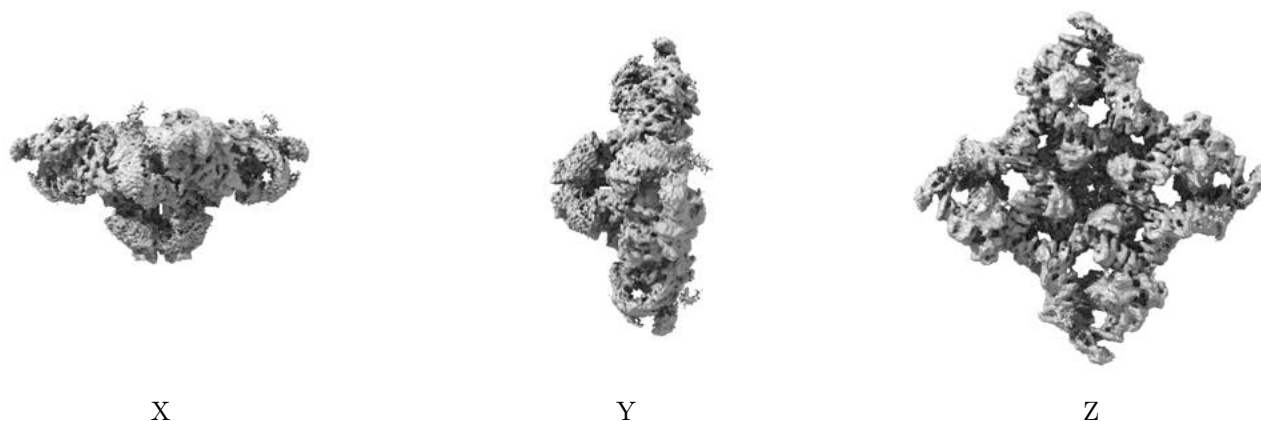


Z

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

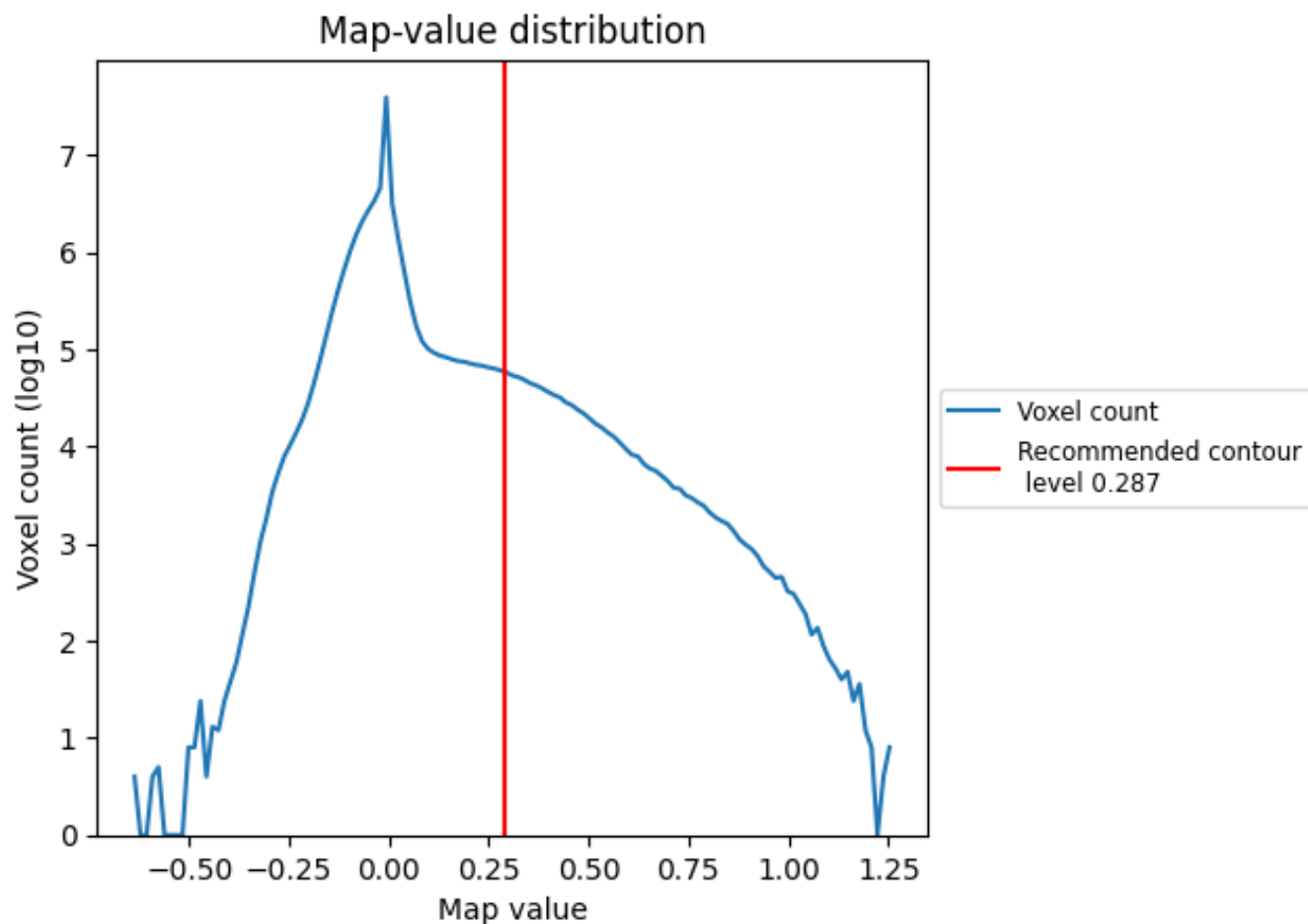
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

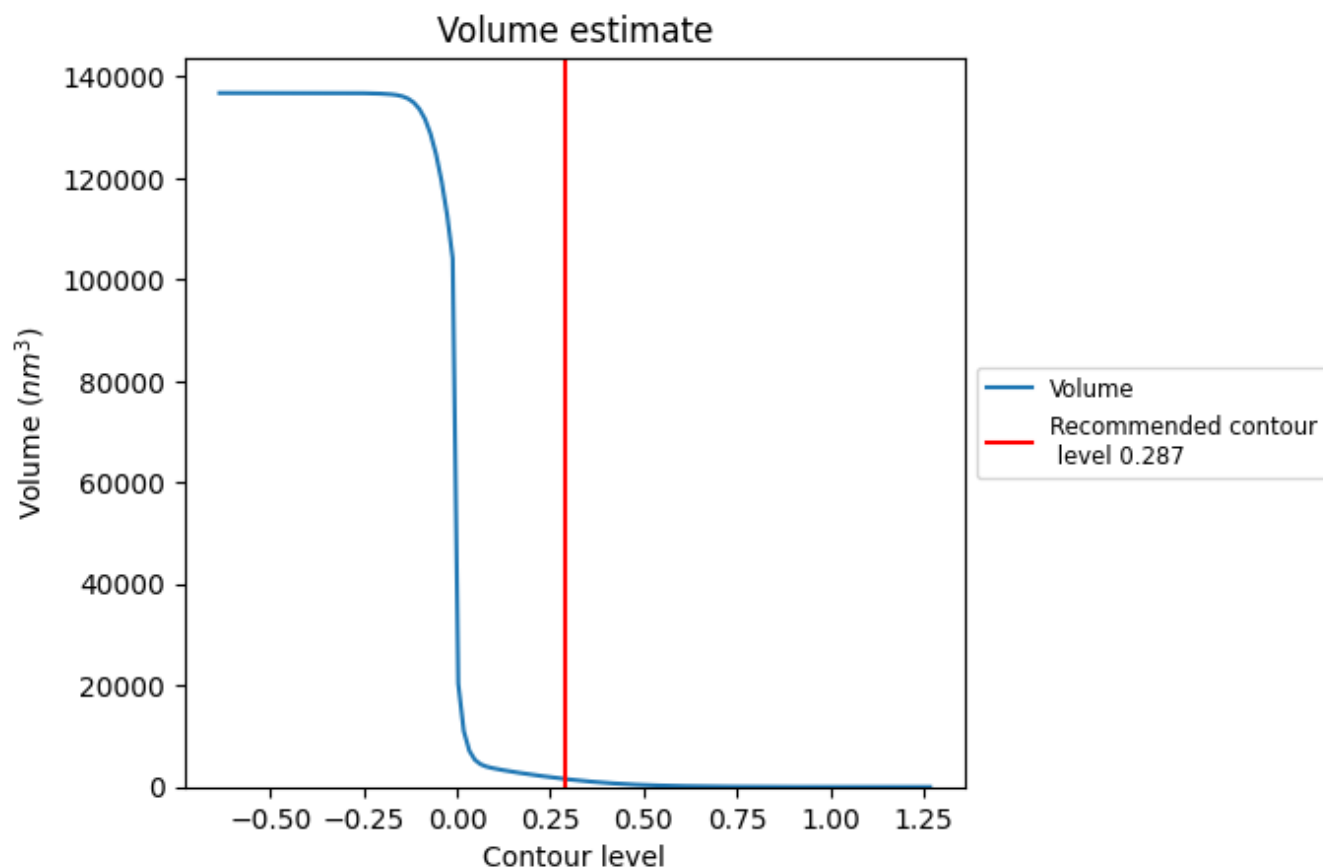
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

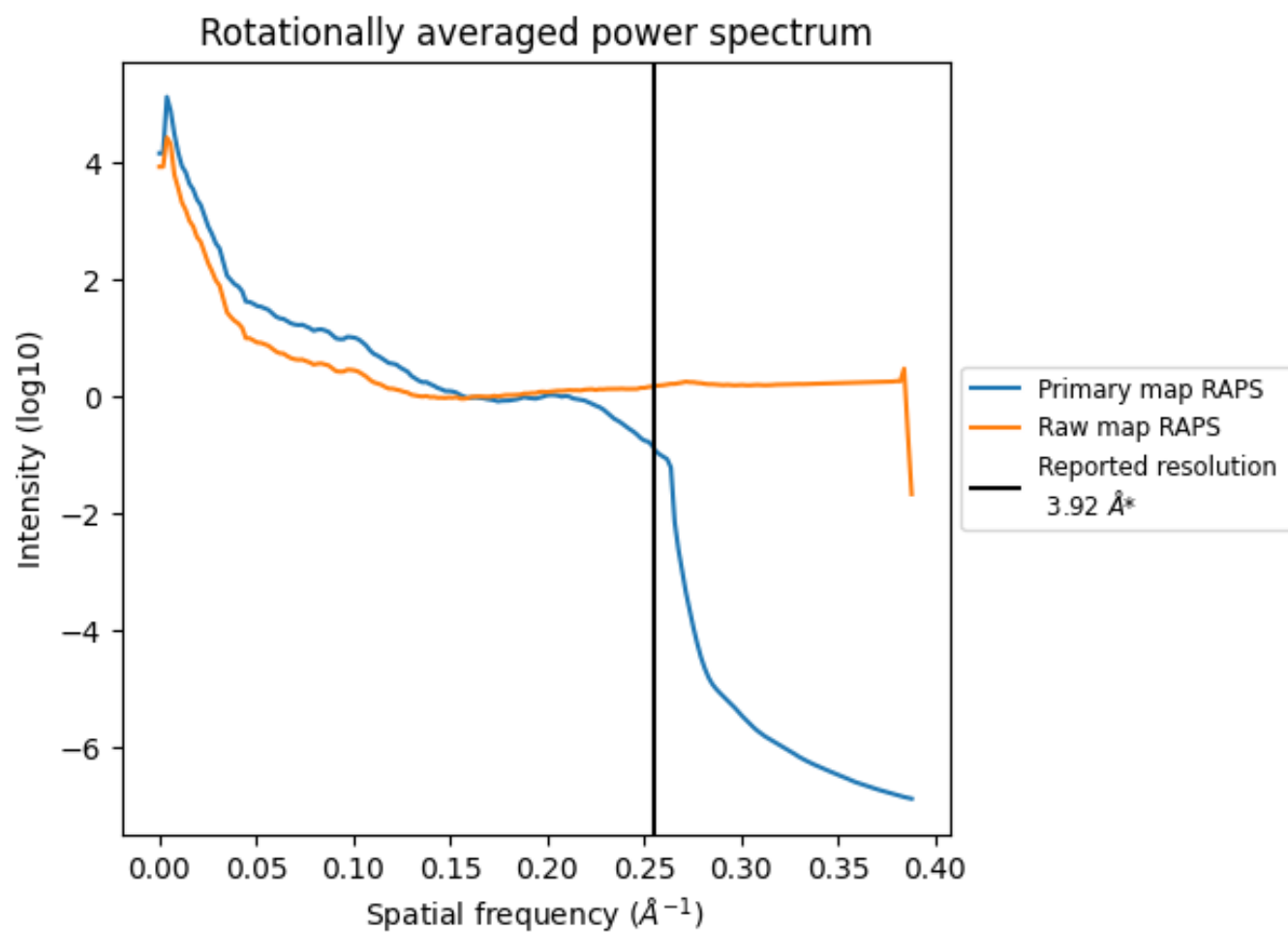
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1594 nm^3 ; this corresponds to an approximate mass of 1440 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 ⓘ

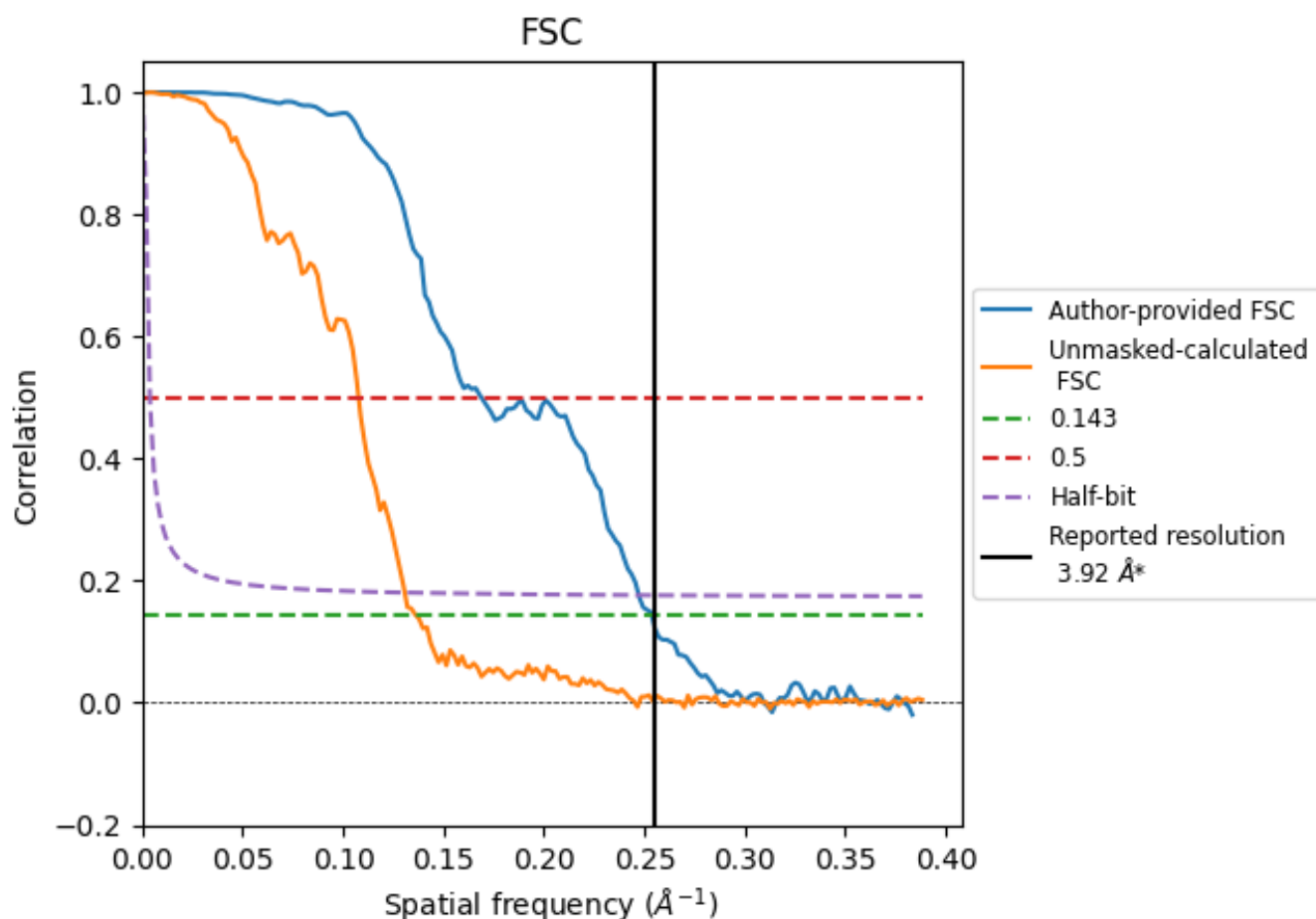


*Reported resolution corresponds to spatial frequency of 0.255 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.255 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.92	-	-
Author-provided FSC curve	3.94	5.92	4.05
Unmasked-calculated*	7.34	9.29	7.65

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.34 differs from the reported value 3.92 by more than 10 %

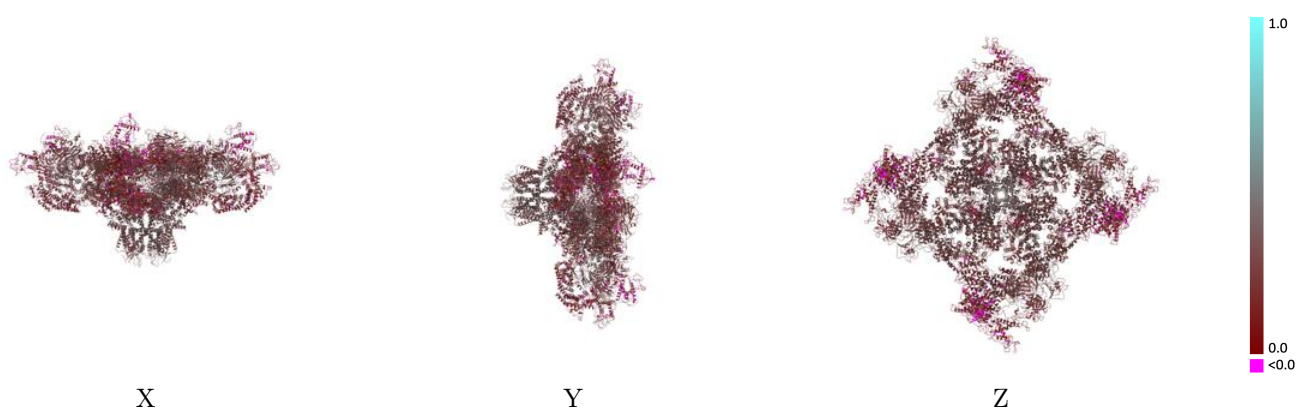
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-40423 and PDB model 8SEO. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

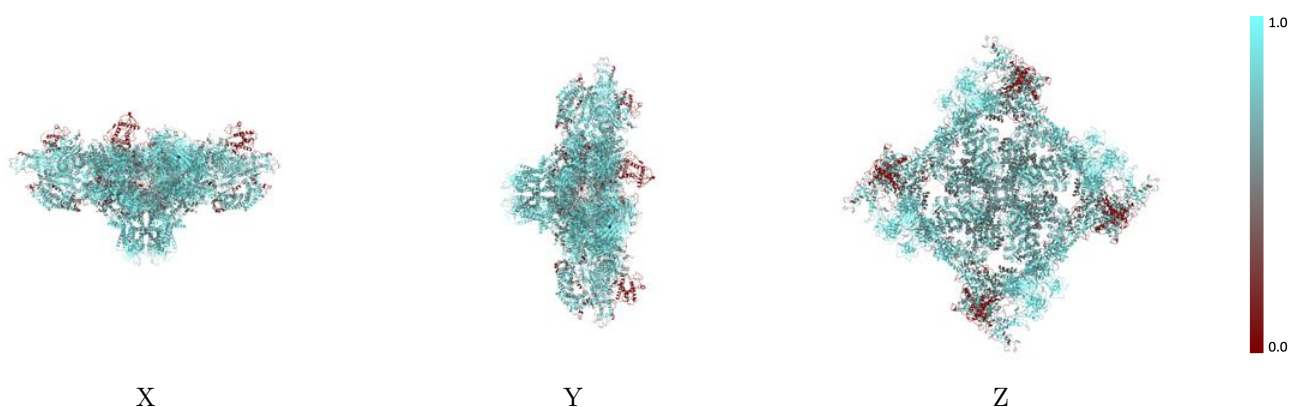
This section was not generated.

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



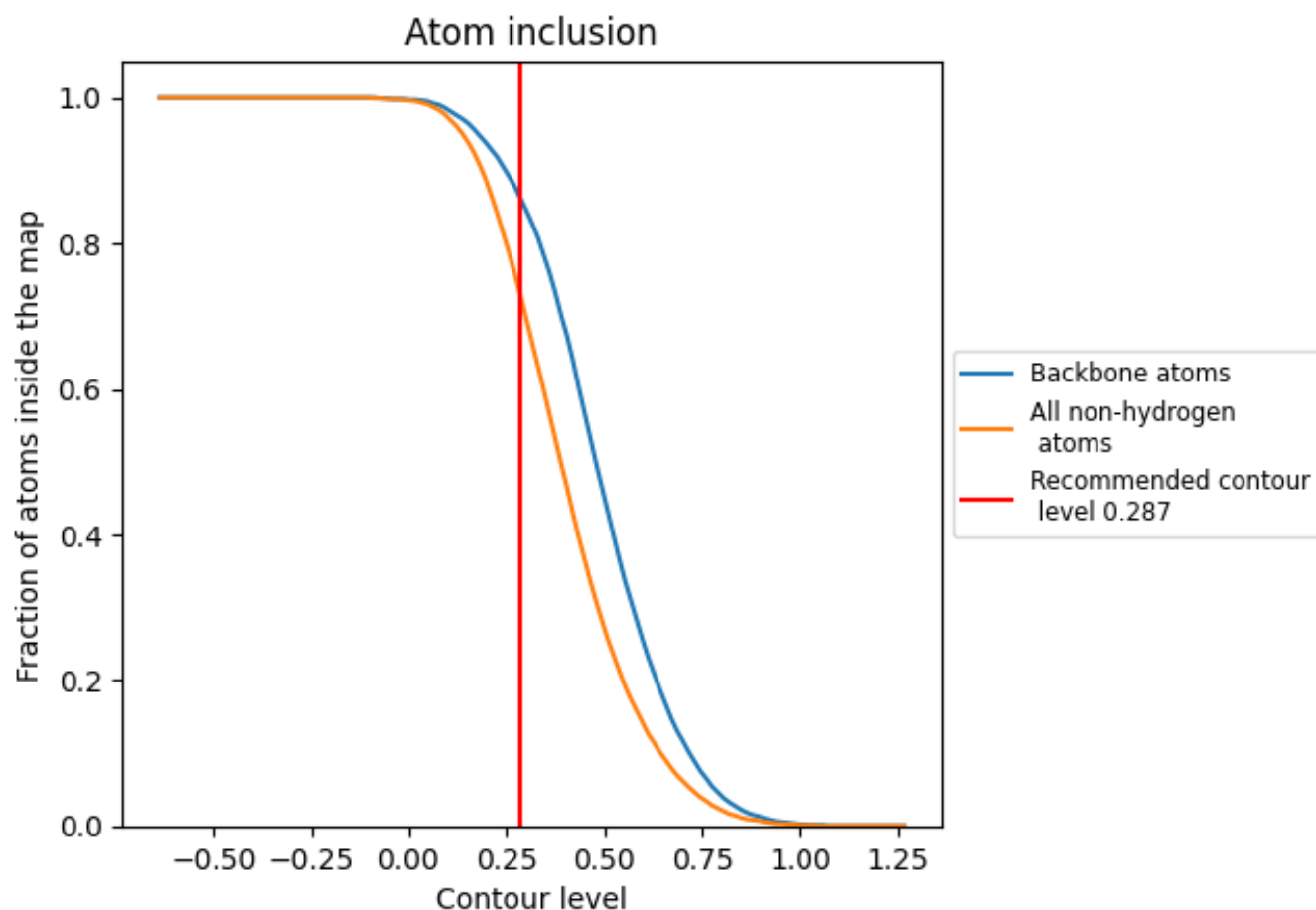
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.287).

9.4 Atom inclusion ⓘ



At the recommended contour level, 86% of all backbone atoms, 73% 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 (0.287) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7270	0.2530
A	0.7230	0.2520
B	0.7230	0.2530
C	0.7230	0.2520
D	0.7230	0.2520
E	0.8870	0.3060
F	0.8870	0.3060
G	0.8870	0.3060
H	0.8870	0.3080

1.0

0.0

<0.0