



Full wwPDB EM Validation Report ⓘ

Nov 11, 2024 – 05:00 AM EST

PDB ID : 8SEQ
EMDB ID : EMD-40425
Title : Cryo-EM Structure of RyR1 + AMP
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 : 3.40 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

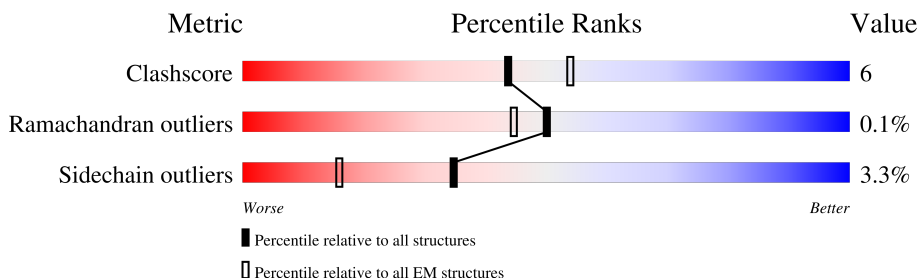
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	5037	<div> <div>18%</div> <div>70%</div> <div>16%</div> <div>13%</div> </div>
1	B	5037	<div> <div>18%</div> <div>70%</div> <div>16%</div> <div>13%</div> </div>
1	C	5037	<div> <div>18%</div> <div>70%</div> <div>17%</div> <div>13%</div> </div>
1	D	5037	<div> <div>18%</div> <div>70%</div> <div>16%</div> <div>13%</div> </div>
2	E	350	<div> <div>26%</div> <div>69%</div> </div>
2	F	350	<div> <div>26%</div> <div>69%</div> </div>
2	G	350	<div> <div>26%</div> <div>69%</div> </div>
2	H	350	<div> <div>26%</div> <div>69%</div> </div>

2 Entry composition [i](#)

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

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

- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4376	Total	C	N	O	S	9	0
			34896	22197	6022	6441	236		
1	B	4376	Total	C	N	O	S	9	0
			34896	22197	6022	6441	236		
1	C	4376	Total	C	N	O	S	9	0
			34896	22197	6022	6441	236		
1	D	4376	Total	C	N	O	S	9	0
			34896	22197	6022	6441	236		

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

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

There are 100 discrepancies between the modelled and reference sequences:

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

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

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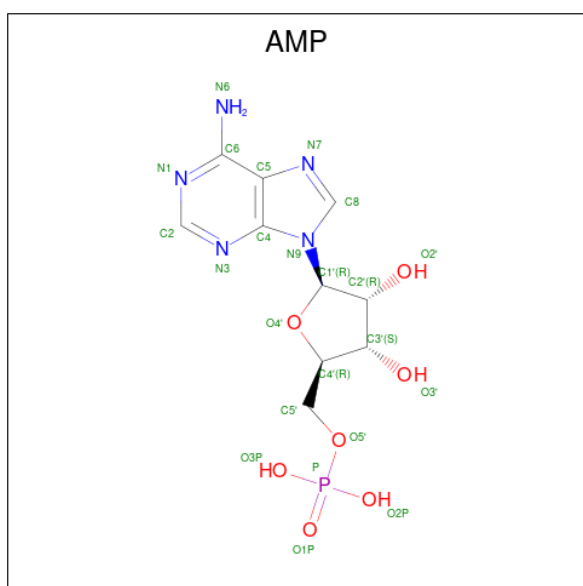
Chain	Residue	Modelled	Actual	Comment	Reference
G	-242	MET	-	expression tag	UNP P08515
G	-241	LYS	-	expression tag	UNP P08515
G	-240	SER	-	expression tag	UNP P08515
G	-239	SER	-	expression tag	UNP P08515
G	-238	HIS	-	expression tag	UNP P08515
G	-237	HIS	-	expression tag	UNP P08515
G	-236	HIS	-	expression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

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

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C₁₀H₁₄N₅O₇P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			23	10	5	7	1	
3	B	1	Total	C	N	O	P	0
			23	10	5	7	1	
3	C	1	Total	C	N	O	P	0
			23	10	5	7	1	
3	D	1	Total	C	N	O	P	0
			23	10	5	7	1	

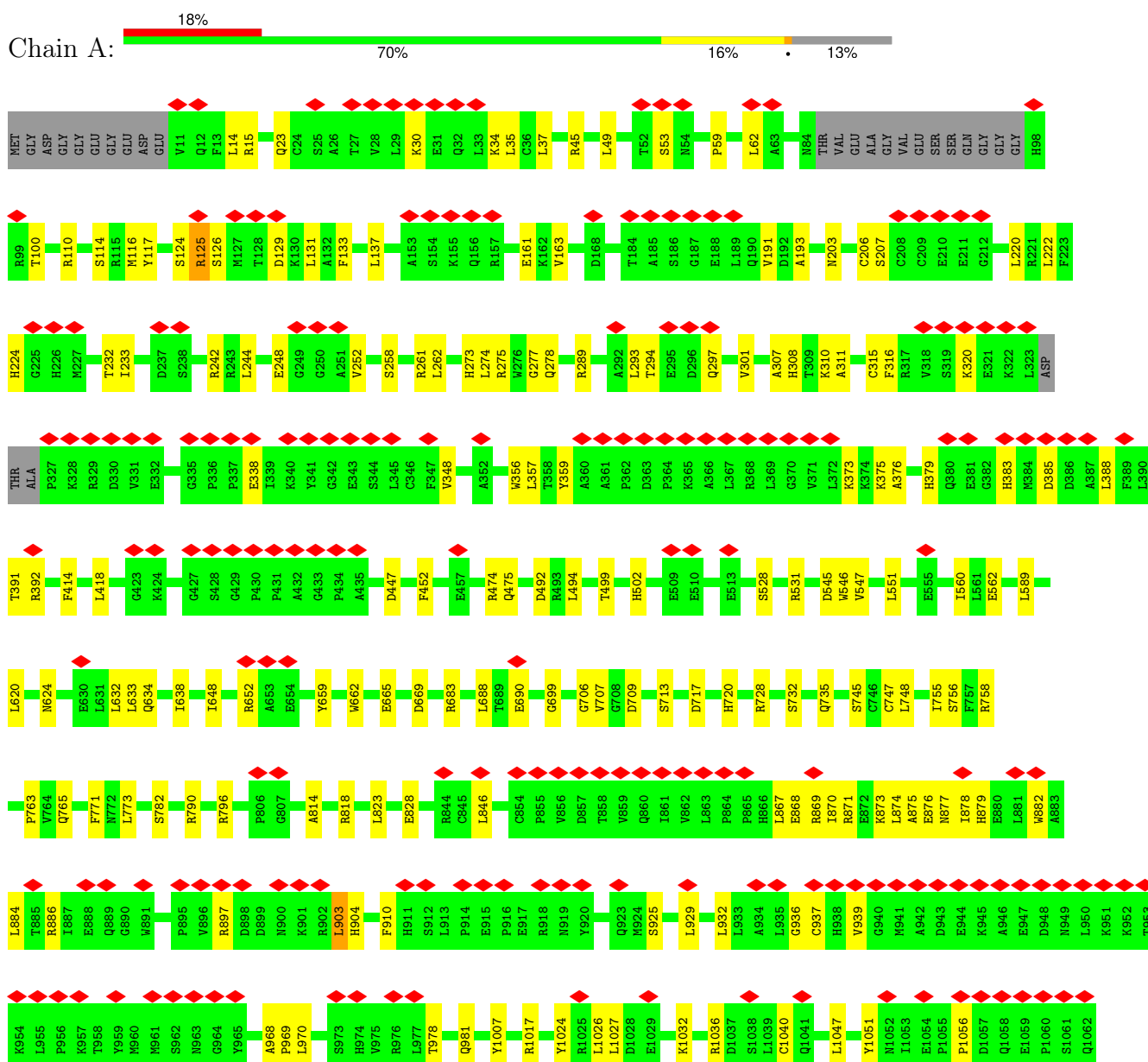
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

3 Residue-property plots

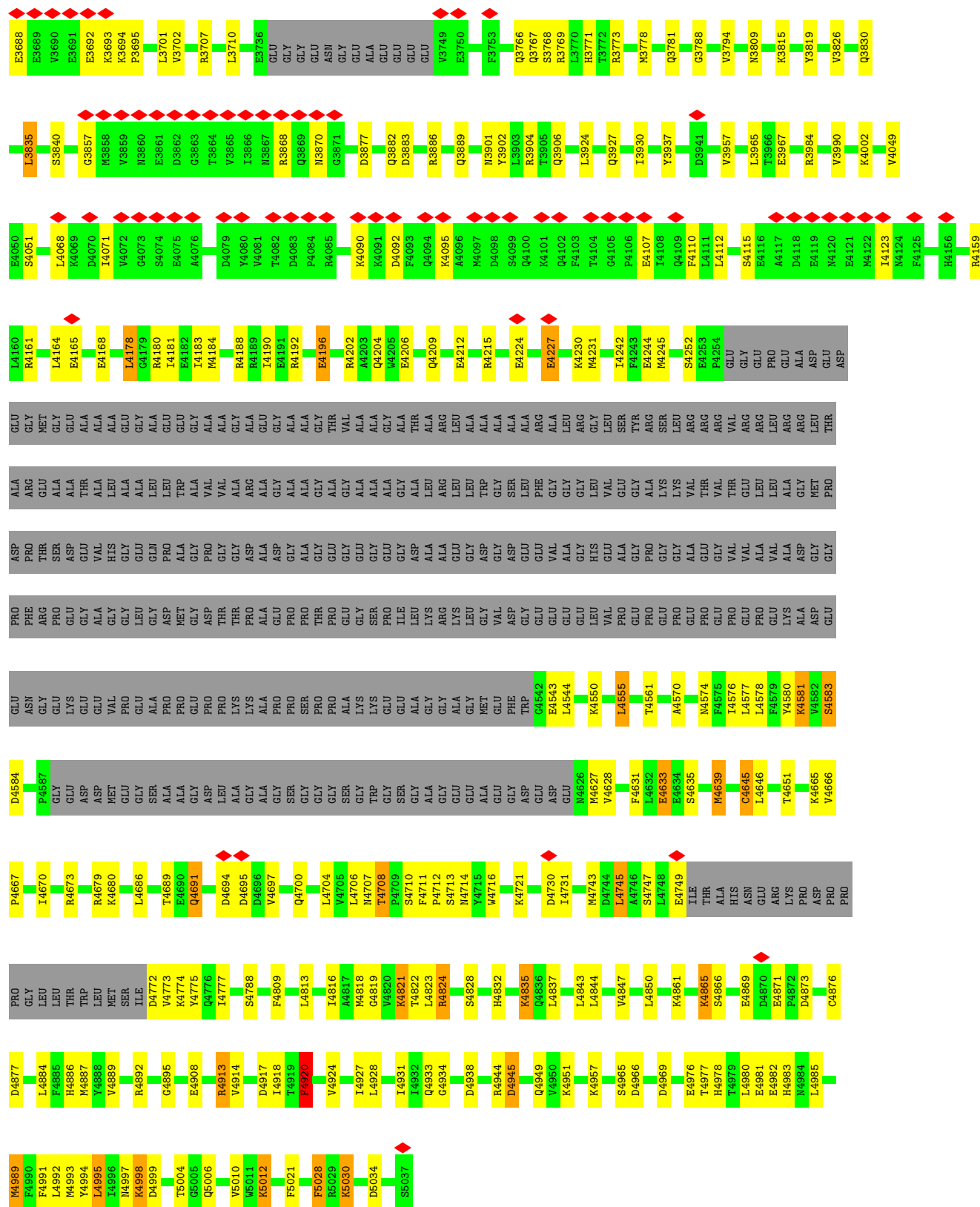
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Ryanodine receptor 1





V3593	N3523	V3459	G3363	E3290	Y3213	R3111	T3020	L2927	L2867	W2807	I2747	K2662
R3594	M3524	V3460	R3366	A3291	N3214	L3112	P3021	K2928	S2868	P2808	P2748	N2663
V3595	Q3530	Q3461	R3367	P3292	A3215	G3113	A3022	F2929	R2869	I2809	E2749	V2666
S3600	D3531	K3462	R3368	P3293	C3216	V3114	K3023	L2930	E2870	K2810	K2750	T2667
A3601		E3463		P3294	S3217	V3115	V3024	Q2931	L2871	E2811	L2751	S2668
V3602		T3464	V3373	A3295	V3218	S3116	L3025	M2932	Q2872	S2812	D2752	E2669
V3603		N3465	E3376	L3296	Y3219	GLN	G3026	N2933	A2873	L2813	L2753	E2670
H3605		N3466	E3377	P3297	T3220	ALA	G3027	Q2934	M2874	K2814	F2754	E2671
L3606		N3467	Q3378	A3298	T3221	ARG	S3028	G2935	A2875	A2815	I2755	L2672
L3607		S3468	L3379	G3299	K3222	THR	G3028	A2936	E2876	M2816	I2756	H2673
Q3608		F3469	R3380	A3300	S3223	VAL	G3029	V2937	Q2877	I2817	K2757	L2674
R3539		L3470	R3381	P3301	R3224	K3123		T2938	L2878	A2818	F2758	L2678
A3541		T3471	E3382	P3302	R3225	G3124		R2939	A2879	W2819	E2760	I2682
L3542		A3472	E3383	P3303	E3226	N3128	E3037	GLY	E2880	E2820	A2769	S2685
K3543		D3473	A3384	C3304	R3227		M3038	LEU	L2881	W2821	Y2761	L2686
D3544		K3474	A3385	T3305	A3228	V3134	L3042	LYS	Y2882	T2822	T2762	A2687
E3548		S3475	A3386	A3306	L3230	L3136	L3046	ASP	H2883	I2823	H2763	K2689
		S3476	E3387		G3231	H3146	A3047	MET	T2885	E2824	E2764	K2690
		K3477	E3388	S3309	L3232		A3048	D2947	V2886	K2825	K2765	K2690
		K3478	E3389	L3316	P3233	Q3149	R3051	GLU	G2887	A2826	A2767	Y2691
		A3479	G3390	G3317	N3234	H3150	H3052		K2888	E2827	F2768	Q2693
		LYS	E3391	T3319	S3235	Q3151	R3053	E2952	K2889	G2829	D2769	E2694
		ALA	L3392	L3320	V3236	D3154	G3058	G2958	K2890	E2830	K2770	L2695
		ALA	L3393	R3321	E3237	D3155	T3059	L2960	Q2891	GLU	I2771	V2715
		GLN	L3392	T3322	E3238	V3156		Q2961	THR	ARG	Q2772	S2718
		SER	R3395	T3323	M3239	I3157	P3062	Q2962	GLU	THR	N2773	L2719
		GLY	R3403	V3324	C3240	L3158	V3065	L2966	LYS	LYS	N2774	S2720
		GLY	D3404	N3325	P3241	D3159	L3075		LYS	LYS	W2775	S2721
		ASP	I3413	L3327	D3242	D3160			THR	THR	S2776	K2722
		GLN	R3414	G3328	I3243				ARG	ARG	Y2777	A2723
		ARG	D3417	L3329	P3244	S3171	R3078	L2974	G2778	ILE	N2780	K2725
		THR	N3418	D3330	D3247	L3175	T3079	L2977	G2898	THR	V2781	LYS
		LYS	N3419	E3331	R3248	V3080	V3081	A2979	G2899	GLN	D2782	ALA
		LYS	R3420	T3333	L3249	T3178	K3082	V2980	G2900	ALA	E2783	VAL
		LYS	A3421	V3334	M3250	K3179	S3083	V2981	L2904	GLN	E2784	ASP
		R3498	H3422	K3335	A3251	N3180	G3084	S2982	L2905	THR	L2785	ALA
		R3499	W3423	R3336	A3257	Y3182	P3085	S2983	V2906	TVR	K2786	GLY
		G3500	L3424	L3338	E3258	V3183	E3086	G2984	P2907	PRO	T2787	W2734
		D3501	L3424	L3338	E3258	E3184	I3087	R2985	ARG	ARG	H2788	F2735
		R3502	F3427	A3339	T3264	K3185	L3092	V2986	D2909	GLY	P2789	D2736
		R3503	N3430	V3340	E3265	L3197	R3093	E2987	T2910	GLY	M2790	P2737
		S3504	F3435	F3341	I3272	M3201	S3094	K2988	L2911	Y2855	L2791	R2738
		V3505		Q3343	P3275	P3202	A3099	S2989	T2912	N2856	R2792	P2739
		Q3506	F3442	P3344	M3276	V3203	D3102	P2990	L2913	Q2858	P2793	V2740
		T3507	I3443	I3345	L3277	S3207	K3106	H2991	K2914	P2859	Y2794	E2741
		S3508	Y3444	I3346	C3278	P3208	V3107	E2992	E2915	P2860	K2795	T2742
		T3509		S3347	S3279	Q3209	L3110	K2996	P2916	D2861	L2743	L2743
		T3510	H3449	R3348	Y3280	L3210		F2997	R2918	L2862	F2797	W2744
		V3511	N3450	R3351	P3282	N3211		P2998	A2917	S2863	E2798	V2745
		A3512		L3354	E3286	E3212		L3002	R2918	Q2864	S2799	I2746
		T3513	R3453	L3354	R3287			H3013	D2919	V2865	K2800	
		L3514	F3458	T3359	G3288				E2921	T2866	D2801	
		K3515		P3289	P3289				K2922		E2803	
									A2923		I2804	
									Q2924		Y2805	
									E2925			
									L2926			



- Molecule 1: Ryanodine receptor 1







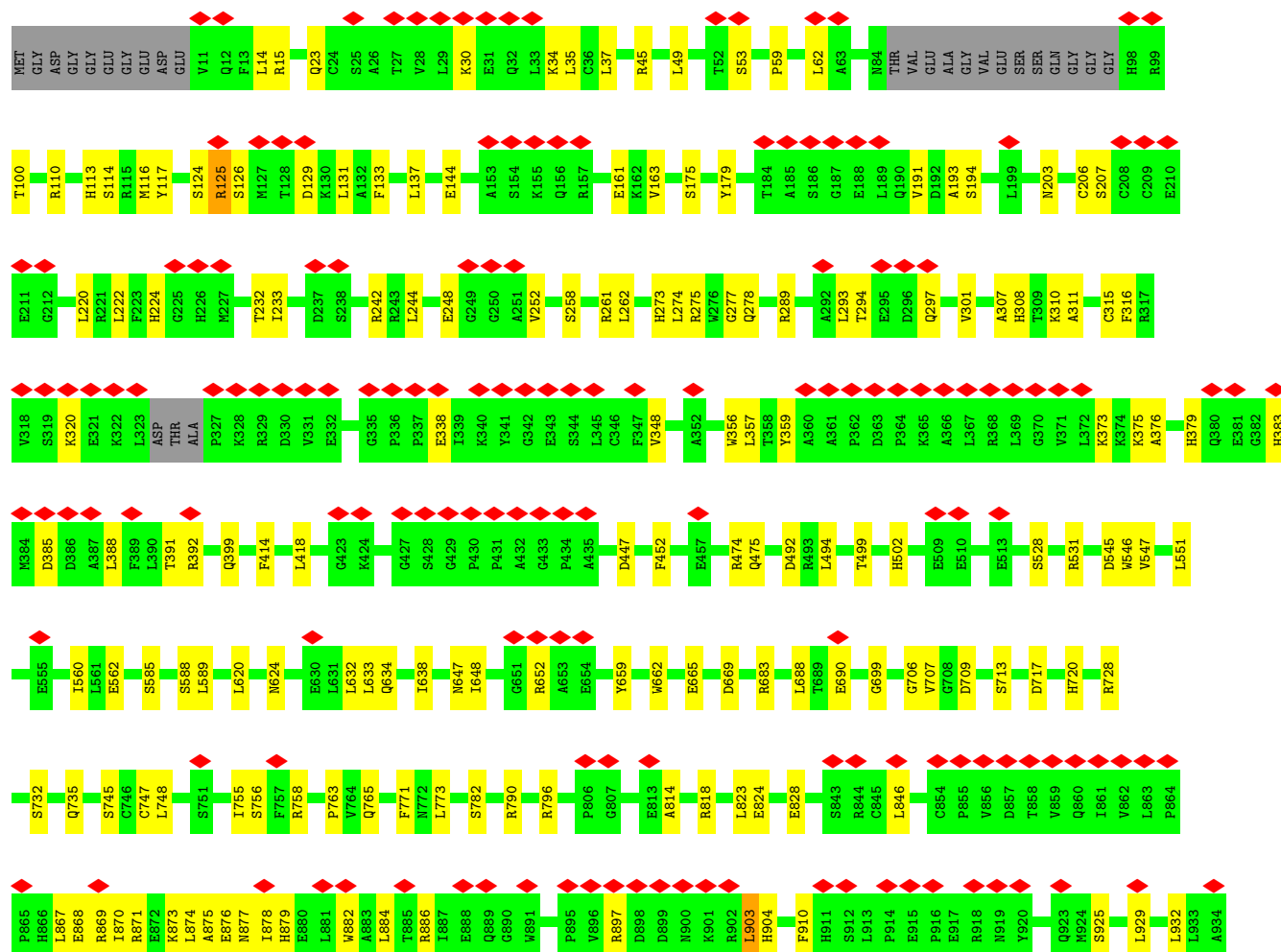












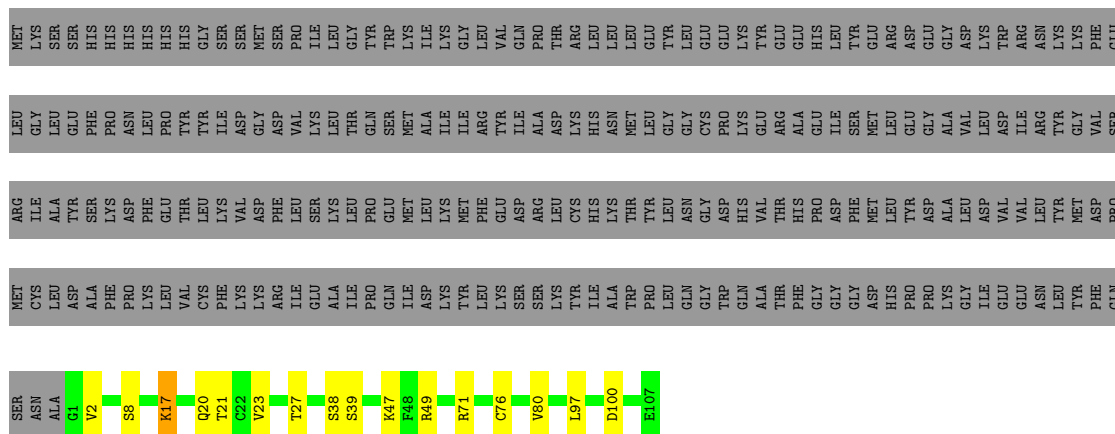






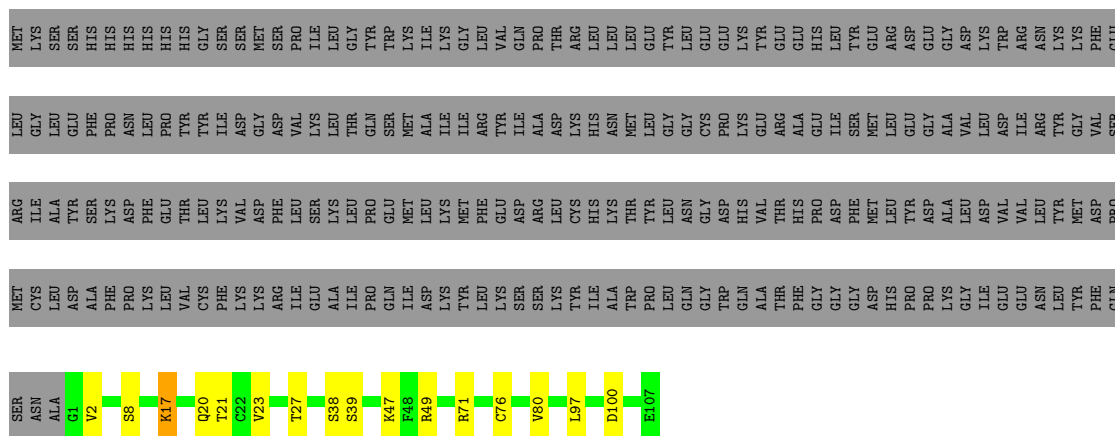
- Molecule 2: Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E: 26% 1% 69%



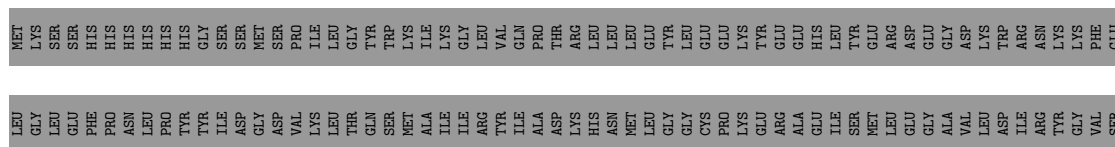
- Molecule 2: Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B

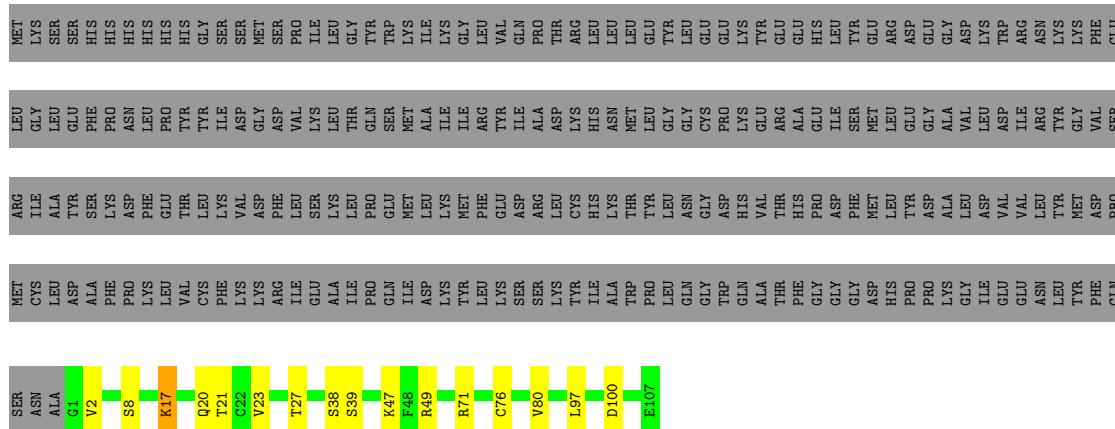
Chain F:  26% 69%



- Molecule 2: Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G: 26% . 69%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	133836	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	0.741	Depositor
Minimum map value	-0.326	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.132	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, AMP

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	0.34	0/35710	0.66	21/48359 (0.0%)
1	B	0.34	0/35710	0.66	21/48359 (0.0%)
1	C	0.34	0/35710	0.66	20/48359 (0.0%)
1	D	0.34	0/35710	0.66	20/48359 (0.0%)
2	E	0.31	0/834	0.64	0/1123
2	F	0.31	0/834	0.64	0/1123
2	G	0.31	0/834	0.64	0/1123
2	H	0.31	0/834	0.64	0/1123
All	All	0.34	0/146176	0.66	82/197928 (0.0%)

There are no bond length outliers.

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4945	ASP	CB-CG-OD1	10.69	127.92	118.30
1	C	4945	ASP	CB-CG-OD1	10.66	127.90	118.30
1	A	4945	ASP	CB-CG-OD1	10.58	127.82	118.30
1	D	4945	ASP	CB-CG-OD1	10.58	127.82	118.30
1	B	3417	ASP	CB-CG-OD1	8.19	125.67	118.30
1	A	3417	ASP	CB-CG-OD1	8.12	125.60	118.30
1	C	3417	ASP	CB-CG-OD1	8.12	125.60	118.30
1	D	3417	ASP	CB-CG-OD1	8.12	125.60	118.30
1	B	3835	LEU	CB-CG-CD2	-7.02	99.06	111.00
1	C	3835	LEU	CB-CG-CD2	-7.02	99.06	111.00
1	A	3835	LEU	CB-CG-CD2	-7.02	99.07	111.00
1	D	3835	LEU	CB-CG-CD2	-7.02	99.07	111.00
1	D	4920	PHE	CB-CG-CD1	6.94	125.66	120.80
1	C	4920	PHE	CB-CG-CD1	6.93	125.65	120.80
1	A	4920	PHE	CB-CG-CD1	6.93	125.65	120.80
1	C	5028	PHE	CB-CG-CD1	6.88	125.62	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4920	PHE	CB-CG-CD1	6.88	125.61	120.80
1	D	5028	PHE	CB-CG-CD1	6.87	125.61	120.80
1	A	5028	PHE	CB-CG-CD1	6.86	125.60	120.80
1	B	5028	PHE	CB-CG-CD1	6.81	125.57	120.80
1	B	4196	GLU	CA-CB-CG	6.61	127.95	113.40
1	C	4196	GLU	CA-CB-CG	6.61	127.95	113.40
1	D	4196	GLU	CA-CB-CG	6.61	127.95	113.40
1	A	4196	GLU	CA-CB-CG	6.60	127.92	113.40
1	A	903	LEU	CA-CB-CG	6.41	130.04	115.30
1	B	903	LEU	CA-CB-CG	6.40	130.02	115.30
1	C	903	LEU	CA-CB-CG	6.40	130.02	115.30
1	D	903	LEU	CA-CB-CG	6.40	130.02	115.30
1	A	3835	LEU	CA-CB-CG	6.28	129.74	115.30
1	B	3835	LEU	CA-CB-CG	6.27	129.72	115.30
1	D	3835	LEU	CA-CB-CG	6.26	129.71	115.30
1	C	3835	LEU	CA-CB-CG	6.25	129.69	115.30
1	B	3085	PRO	CA-N-CD	-5.91	103.23	111.50
1	C	3085	PRO	CA-N-CD	-5.91	103.23	111.50
1	D	3085	PRO	CA-N-CD	-5.91	103.23	111.50
1	A	3085	PRO	CA-N-CD	-5.89	103.26	111.50
1	B	3197	LEU	CA-CB-CG	5.88	128.83	115.30
1	C	3197	LEU	CA-CB-CG	5.87	128.80	115.30
1	D	3197	LEU	CA-CB-CG	5.86	128.78	115.30
1	A	3197	LEU	CA-CB-CG	5.85	128.76	115.30
1	D	131	LEU	CA-CB-CG	5.84	128.73	115.30
1	B	131	LEU	CA-CB-CG	5.84	128.72	115.30
1	C	131	LEU	CA-CB-CG	5.81	128.67	115.30
1	A	131	LEU	CA-CB-CG	5.81	128.66	115.30
1	A	3296	LEU	CA-CB-CG	5.54	128.05	115.30
1	C	3296	LEU	CA-CB-CG	5.54	128.04	115.30
1	D	3296	LEU	CA-CB-CG	5.54	128.04	115.30
1	B	3296	LEU	CA-CB-CG	5.51	127.98	115.30
1	D	3701	LEU	CA-CB-CG	5.48	127.90	115.30
1	A	3701	LEU	CA-CB-CG	5.47	127.88	115.30
1	B	3701	LEU	CA-CB-CG	5.47	127.88	115.30
1	C	3701	LEU	CA-CB-CG	5.47	127.88	115.30
1	A	2751	LEU	CA-CB-CG	5.34	127.58	115.30
1	C	2751	LEU	CA-CB-CG	5.34	127.58	115.30
1	D	2751	LEU	CA-CB-CG	5.33	127.55	115.30
1	B	2751	LEU	CA-CB-CG	5.32	127.54	115.30
1	C	5028	PHE	CB-CG-CD2	-5.29	117.10	120.80
1	D	5028	PHE	CB-CG-CD2	-5.28	117.11	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4196	GLU	CB-CA-C	-5.26	99.88	110.40
1	B	4196	GLU	CB-CA-C	-5.26	99.88	110.40
1	C	4196	GLU	CB-CA-C	-5.26	99.88	110.40
1	D	4196	GLU	CB-CA-C	-5.25	99.91	110.40
1	A	3531	ASP	CB-CG-OD1	5.24	123.01	118.30
1	A	5028	PHE	CB-CG-CD2	-5.24	117.14	120.80
1	D	4920	PHE	CB-CG-CD2	-5.22	117.15	120.80
1	B	3531	ASP	CB-CG-OD1	5.21	122.99	118.30
1	C	3531	ASP	CB-CG-OD1	5.21	122.99	118.30
1	D	3531	ASP	CB-CG-OD1	5.21	122.98	118.30
1	B	5028	PHE	CB-CG-CD2	-5.19	117.17	120.80
1	A	3085	PRO	N-CD-CG	-5.15	95.48	103.20
1	A	4920	PHE	CB-CG-CD2	-5.14	117.20	120.80
1	A	3835	LEU	CB-CG-CD1	5.14	119.74	111.00
1	D	3835	LEU	CB-CG-CD1	5.14	119.74	111.00
1	B	3085	PRO	N-CD-CG	-5.13	95.50	103.20
1	C	3085	PRO	N-CD-CG	-5.13	95.50	103.20
1	C	4920	PHE	CB-CG-CD2	-5.13	117.21	120.80
1	D	3085	PRO	N-CD-CG	-5.13	95.51	103.20
1	C	3835	LEU	CB-CG-CD1	5.11	119.69	111.00
1	B	3835	LEU	CB-CG-CD1	5.11	119.69	111.00
1	B	4920	PHE	CB-CG-CD2	-5.10	117.23	120.80
1	A	4178	LEU	CA-CB-CG	5.00	126.81	115.30
1	B	4178	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	34896	0	34522	451	0
1	B	34896	0	34522	440	0
1	C	34896	0	34522	448	0
1	D	34896	0	34522	451	0
2	E	818	0	824	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	818	0	824	8	0
2	G	818	0	824	8	0
2	H	818	0	824	8	0
3	A	23	0	12	1	0
3	B	23	0	12	1	0
3	C	23	0	12	1	0
3	D	23	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	142952	0	141432	1789	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 6.

All (1789) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4242:ILE:HG12	1:B:4993:MET:HG2	1.71	0.73
1:A:4242:ILE:HG12	1:A:4993:MET:HG2	1.71	0.72
1:D:4242:ILE:HG12	1:D:4993:MET:HG2	1.71	0.72
1:C:4242:ILE:HG12	1:C:4993:MET:HG2	1.71	0.71
1:D:233:ILE:HD12	1:D:242:ARG:HB3	1.73	0.71
1:C:1476:MET:HB3	1:C:1485:SER:HB3	1.73	0.71
1:A:233:ILE:HD12	1:A:242:ARG:HB3	1.73	0.71
1:B:1476:MET:HB3	1:B:1485:SER:HB3	1.73	0.70
1:C:233:ILE:HD12	1:C:242:ARG:HB3	1.73	0.70
1:C:3042:LEU:O	1:C:3046:LEU:HB2	1.91	0.70
1:A:1476:MET:HB3	1:A:1485:SER:HB3	1.73	0.70
1:B:3042:LEU:O	1:B:3046:LEU:HB2	1.91	0.70
1:D:3042:LEU:O	1:D:3046:LEU:HB2	1.91	0.69
1:B:233:ILE:HD12	1:B:242:ARG:HB3	1.73	0.69
1:D:1476:MET:HB3	1:D:1485:SER:HB3	1.73	0.69
1:A:3042:LEU:O	1:A:3046:LEU:HB2	1.91	0.69
1:B:745:SER:HB2	1:B:758:ARG:HB2	1.74	0.68
1:C:745:SER:HB2	1:C:758:ARG:HB2	1.74	0.68
1:D:745:SER:HB2	1:D:758:ARG:HB2	1.74	0.68
1:C:688:LEU:HD23	1:C:690:GLU:H	1.59	0.67
1:A:745:SER:HB2	1:A:758:ARG:HB2	1.74	0.67
1:D:688:LEU:HD23	1:D:690:GLU:H	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3346:VAL:HG11	1:D:3414:ARG:HB3	1.77	0.67
1:A:4978:HIS:HA	1:A:4982:GLU:HG3	1.77	0.66
1:A:3257:ALA:HB1	1:A:3321:ARG:HD2	1.76	0.66
1:C:3257:ALA:HB1	1:C:3321:ARG:HD2	1.76	0.66
1:A:688:LEU:HD23	1:A:690:GLU:H	1.59	0.66
1:A:3346:VAL:HG11	1:A:3414:ARG:HB3	1.77	0.66
1:B:688:LEU:HD23	1:B:690:GLU:H	1.59	0.66
1:B:3257:ALA:HB1	1:B:3321:ARG:HD2	1.76	0.66
1:D:3257:ALA:HB1	1:D:3321:ARG:HD2	1.76	0.66
1:B:4581:LYS:NZ	1:C:4877:ASP:O	2.28	0.66
1:C:4978:HIS:HA	1:C:4982:GLU:HG3	1.77	0.66
1:C:3346:VAL:HG11	1:C:3414:ARG:HB3	1.77	0.65
1:C:4581:LYS:NZ	1:D:4877:ASP:O	2.28	0.65
1:D:1116:GLY:HA3	1:D:1132:TRP:HB3	1.78	0.65
1:C:1116:GLY:HA3	1:C:1132:TRP:HB3	1.78	0.65
1:B:3346:VAL:HG11	1:B:3414:ARG:HB3	1.77	0.65
1:C:2007:ASN:O	1:C:2011:HIS:HB2	1.97	0.65
1:D:4978:HIS:HA	1:D:4982:GLU:HG3	1.77	0.65
1:A:4821:LYS:HG3	1:A:4824:ARG:HH21	1.62	0.65
1:B:1116:GLY:HA3	1:B:1132:TRP:HB3	1.78	0.65
1:B:4821:LYS:HG3	1:B:4824:ARG:HH21	1.62	0.65
1:B:4924:VAL:HA	1:B:4928:LEU:HD12	1.79	0.65
1:A:2961:GLN:NE2	1:A:3038:MET:SD	2.70	0.65
1:B:2007:ASN:O	1:B:2011:HIS:HB2	1.97	0.65
1:B:4978:HIS:HA	1:B:4982:GLU:HG3	1.77	0.64
1:A:4924:VAL:HA	1:A:4928:LEU:HD12	1.79	0.64
1:D:4821:LYS:HG3	1:D:4824:ARG:HH21	1.62	0.64
1:A:1116:GLY:HA3	1:A:1132:TRP:HB3	1.78	0.64
1:A:2007:ASN:O	1:A:2011:HIS:HB2	1.97	0.64
1:B:3332:ALA:HB3	1:B:3403:ARG:HD2	1.80	0.64
1:D:2007:ASN:O	1:D:2011:HIS:HB2	1.97	0.64
1:D:2961:GLN:NE2	1:D:3038:MET:SD	2.70	0.64
1:C:3332:ALA:HB3	1:C:3403:ARG:HD2	1.80	0.64
1:C:4924:VAL:HA	1:C:4928:LEU:HD12	1.79	0.64
1:A:3332:ALA:HB3	1:A:3403:ARG:HD2	1.80	0.64
1:A:1569:GLN:HB2	1:A:1572:ILE:HD12	1.80	0.64
1:B:2797:PHE:HE2	1:B:2802:LYS:HD3	1.63	0.64
1:D:4924:VAL:HA	1:D:4928:LEU:HD12	1.79	0.64
1:B:2958:GLY:O	1:B:2962:GLN:NE2	2.31	0.63
1:C:2797:PHE:HE2	1:C:2802:LYS:HD3	1.63	0.63
1:D:3332:ALA:HB3	1:D:3403:ARG:HD2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2958:GLY:O	1:D:2962:GLN:NE2	2.31	0.63
1:D:1569:GLN:HB2	1:D:1572:ILE:HD12	1.80	0.63
1:A:2958:GLY:O	1:A:2962:GLN:NE2	2.31	0.63
1:C:2958:GLY:O	1:C:2962:GLN:NE2	2.31	0.63
1:C:4821:LYS:HG3	1:C:4824:ARG:HH21	1.62	0.63
1:B:2961:GLN:NE2	1:B:3038:MET:SD	2.70	0.63
1:A:2797:PHE:HE2	1:A:2802:LYS:HD3	1.63	0.63
1:D:2797:PHE:HE2	1:D:2802:LYS:HD3	1.63	0.63
1:B:3075:LEU:O	1:B:3146:HIS:NE2	2.32	0.63
1:D:3075:LEU:O	1:D:3146:HIS:NE2	2.32	0.63
1:A:981:GLN:HG2	1:A:1047:LEU:HD11	1.81	0.62
1:B:659:TYR:O	1:B:662:TRP:NE1	2.33	0.62
1:B:1990:GLU:HB2	1:B:1993:ARG:HE	1.65	0.62
1:C:1024:TYR:O	1:C:1032:LYS:NZ	2.33	0.62
1:A:1990:GLU:HB2	1:A:1993:ARG:HE	1.64	0.62
1:A:3075:LEU:O	1:A:3146:HIS:NE2	2.32	0.62
1:C:1569:GLN:HB2	1:C:1572:ILE:HD12	1.80	0.62
1:C:659:TYR:O	1:C:662:TRP:NE1	2.32	0.62
1:D:659:TYR:O	1:D:662:TRP:NE1	2.32	0.62
1:A:659:TYR:O	1:A:662:TRP:NE1	2.32	0.62
1:A:3051:ARG:O	1:A:3053:ARG:NE	2.31	0.62
1:B:2978:GLU:OE2	1:B:3053:ARG:NH1	2.31	0.62
1:B:1569:GLN:HB2	1:B:1572:ILE:HD12	1.80	0.62
1:C:244:LEU:HD13	1:C:375:LYS:HD2	1.82	0.62
1:A:1024:TYR:O	1:A:1032:LYS:NZ	2.33	0.61
1:B:244:LEU:HD13	1:B:375:LYS:HD2	1.82	0.61
1:B:1024:TYR:O	1:B:1032:LYS:NZ	2.33	0.61
1:B:3051:ARG:O	1:B:3053:ARG:NE	2.31	0.61
1:C:1990:GLU:HB2	1:C:1993:ARG:HE	1.64	0.61
1:D:2978:GLU:OE2	1:D:3053:ARG:NH1	2.31	0.61
1:B:2630:VAL:HG12	1:B:2682:ILE:HD11	1.83	0.61
1:C:981:GLN:HG2	1:C:1047:LEU:HD11	1.81	0.61
1:D:981:GLN:HG2	1:D:1047:LEU:HD11	1.81	0.61
1:A:244:LEU:HD13	1:A:375:LYS:HD2	1.82	0.61
1:A:897:ARG:HB2	1:A:903:LEU:HD11	1.83	0.61
1:B:981:GLN:HG2	1:B:1047:LEU:HD11	1.81	0.61
1:C:3051:ARG:O	1:C:3053:ARG:NE	2.31	0.61
1:A:978:THR:OG1	1:A:981:GLN:OE1	2.19	0.61
1:A:3081:MET:HG3	1:A:3156:VAL:HA	1.83	0.61
1:D:1990:GLU:HB2	1:D:1993:ARG:HE	1.65	0.61
1:C:2630:VAL:HG12	1:C:2682:ILE:HD11	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3368:ARG:NH2	1:A:3404:ASP:OD2	2.34	0.61
1:B:3236:VAL:HA	1:B:3239:MET:HG3	1.83	0.61
1:D:244:LEU:HD13	1:D:375:LYS:HD2	1.82	0.61
1:D:1024:TYR:O	1:D:1032:LYS:NZ	2.33	0.61
1:A:3236:VAL:HA	1:A:3239:MET:HG3	1.83	0.61
1:D:897:ARG:HB2	1:D:903:LEU:HD11	1.83	0.61
1:D:3236:VAL:HA	1:D:3239:MET:HG3	1.83	0.60
1:D:3368:ARG:NH2	1:D:3404:ASP:OD2	2.34	0.60
1:A:2630:VAL:HG12	1:A:2682:ILE:HD11	1.83	0.60
1:B:897:ARG:HB2	1:B:903:LEU:HD11	1.83	0.60
1:C:897:ARG:HB2	1:C:903:LEU:HD11	1.83	0.60
1:D:3051:ARG:O	1:D:3053:ARG:NE	2.31	0.60
1:D:3081:MET:HG3	1:D:3156:VAL:HA	1.83	0.60
2:G:17:LYS:HG3	2:G:20:GLN:HE22	1.66	0.60
1:C:652:ARG:HB3	1:C:773:LEU:HD21	1.83	0.60
1:C:2961:GLN:NE2	1:C:3038:MET:SD	2.70	0.60
1:C:2978:GLU:OE2	1:C:3053:ARG:NH1	2.31	0.60
1:A:652:ARG:HB3	1:A:773:LEU:HD21	1.83	0.60
1:C:707:VAL:HG13	1:C:713:SER:HB2	1.83	0.60
1:A:2685:SER:O	1:A:2689:LYS:HB2	2.02	0.60
1:D:2630:VAL:HG12	1:D:2682:ILE:HD11	1.83	0.60
1:B:707:VAL:HG13	1:B:713:SER:HB2	1.83	0.60
1:B:2685:SER:O	1:B:2689:LYS:HB2	2.02	0.60
1:B:3081:MET:HG3	1:B:3156:VAL:HA	1.83	0.60
1:C:978:THR:OG1	1:C:981:GLN:OE1	2.19	0.60
1:C:3236:VAL:HA	1:C:3239:MET:HG3	1.83	0.60
1:B:978:THR:OG1	1:B:981:GLN:OE1	2.19	0.60
1:B:2992:GLU:OE2	1:B:2996:LYS:NZ	2.34	0.60
1:C:3075:LEU:O	1:C:3146:HIS:NE2	2.32	0.60
1:C:3368:ARG:NH2	1:C:3404:ASP:OD2	2.34	0.60
1:D:978:THR:OG1	1:D:981:GLN:OE1	2.19	0.60
1:A:707:VAL:HG13	1:A:713:SER:HB2	1.83	0.59
1:B:652:ARG:HB3	1:B:773:LEU:HD21	1.83	0.59
1:B:3368:ARG:NH2	1:B:3404:ASP:OD2	2.34	0.59
2:E:17:LYS:HG3	2:E:20:GLN:HE22	1.66	0.59
2:H:17:LYS:HG3	2:H:20:GLN:HE22	1.66	0.59
1:B:2619:LEU:HB3	1:B:2623:LEU:HD13	1.85	0.59
1:C:2992:GLU:OE2	1:C:2996:LYS:NZ	2.34	0.59
1:D:707:VAL:HG13	1:D:713:SER:HB2	1.84	0.59
2:F:17:LYS:HG3	2:F:20:GLN:HE22	1.66	0.59
1:A:475:GLN:NE2	1:A:528:SER:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1232:ARG:NH2	1:A:1828:ASP:O	2.35	0.59
1:A:2992:GLU:OE2	1:A:2996:LYS:NZ	2.34	0.59
1:C:2619:LEU:HB3	1:C:2623:LEU:HD13	1.85	0.59
1:D:652:ARG:HB3	1:D:773:LEU:HD21	1.83	0.59
1:D:1232:ARG:NH2	1:D:1828:ASP:O	2.35	0.59
1:D:2992:GLU:OE2	1:D:2996:LYS:NZ	2.34	0.59
1:A:551:LEU:HB3	1:A:589:LEU:HD11	1.85	0.59
1:C:1232:ARG:NH2	1:C:1828:ASP:O	2.35	0.59
1:C:3081:MET:HG3	1:C:3156:VAL:HA	1.83	0.59
1:D:551:LEU:HB3	1:D:589:LEU:HD11	1.85	0.59
1:D:2685:SER:O	1:D:2689:LYS:HB2	2.02	0.59
1:B:475:GLN:NE2	1:B:528:SER:O	2.36	0.58
1:C:551:LEU:HB3	1:C:589:LEU:HD11	1.85	0.58
1:D:2871:LEU:HG	1:D:2927:LEU:HD21	1.85	0.58
1:B:551:LEU:HB3	1:B:589:LEU:HD11	1.85	0.58
1:B:1252:HIS:O	1:B:1275:ARG:NH2	2.37	0.58
1:D:475:GLN:NE2	1:D:528:SER:O	2.36	0.58
1:D:1943:LEU:HD13	1:D:2098:VAL:HG22	1.86	0.58
1:B:1232:ARG:NH2	1:B:1828:ASP:O	2.35	0.58
1:C:475:GLN:NE2	1:C:528:SER:O	2.36	0.58
1:C:4994:TYR:OH	1:C:4998:LYS:NZ	2.35	0.58
1:A:882:TRP:O	1:A:886:ARG:NH1	2.37	0.58
1:A:2871:LEU:HG	1:A:2927:LEU:HD21	1.85	0.58
1:C:1252:HIS:O	1:C:1275:ARG:NH2	2.36	0.58
1:D:1252:HIS:O	1:D:1275:ARG:NH2	2.37	0.58
1:C:763:PRO:O	1:C:765:GLN:NE2	2.37	0.58
1:D:2619:LEU:HB3	1:D:2623:LEU:HD13	1.85	0.58
1:A:161:GLU:HB3	1:D:3984:ARG:HH22	1.68	0.58
1:A:1252:HIS:O	1:A:1275:ARG:NH2	2.36	0.58
1:A:4581:LYS:NZ	1:B:4877:ASP:O	2.35	0.58
1:C:1943:LEU:HD13	1:C:2098:VAL:HG22	1.86	0.58
1:C:2685:SER:O	1:C:2689:LYS:HB2	2.02	0.58
1:B:882:TRP:O	1:B:886:ARG:NH1	2.37	0.58
1:D:289:ARG:HB3	1:D:301:VAL:HB	1.85	0.58
1:B:62:LEU:HD23	1:B:261:ARG:HH12	1.69	0.58
1:B:3990:VAL:HG13	1:B:4051:SER:HB3	1.86	0.58
1:C:289:ARG:HB3	1:C:301:VAL:HB	1.86	0.58
1:C:882:TRP:O	1:C:886:ARG:NH1	2.37	0.58
1:C:2823:ILE:HD11	1:C:2935:TYR:HB3	1.86	0.58
1:C:3990:VAL:HG13	1:C:4051:SER:HB3	1.86	0.58
1:D:882:TRP:O	1:D:886:ARG:NH1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2619:LEU:HB3	1:A:2623:LEU:HD13	1.85	0.57
1:D:638:ILE:HD12	1:D:1638:ALA:HB3	1.86	0.57
1:C:2463:LEU:HA	1:C:2466:LEU:HD12	1.86	0.57
1:C:2871:LEU:HG	1:C:2927:LEU:HD21	1.85	0.57
1:C:3524:MET:HA	1:C:3582:ARG:HH22	1.70	0.57
1:C:3702:VAL:HG13	1:C:3778:MET:HG2	1.86	0.57
1:D:763:PRO:O	1:D:765:GLN:NE2	2.37	0.57
1:D:3702:VAL:HG13	1:D:3778:MET:HG2	1.86	0.57
1:A:763:PRO:O	1:A:765:GLN:NE2	2.37	0.57
1:A:62:LEU:HD23	1:A:261:ARG:HH12	1.69	0.57
1:B:289:ARG:HB3	1:B:301:VAL:HB	1.86	0.57
1:B:1943:LEU:HD13	1:B:2098:VAL:HG22	1.86	0.57
1:B:2309:SER:OG	1:B:2321:ILE:O	2.22	0.57
1:D:3524:MET:HA	1:D:3582:ARG:HH22	1.70	0.57
1:A:638:ILE:HD12	1:A:1638:ALA:HB3	1.86	0.57
1:A:2309:SER:OG	1:A:2321:ILE:O	2.22	0.57
1:B:3524:MET:HA	1:B:3582:ARG:HH22	1.70	0.57
1:A:1561:VAL:HG12	1:A:1562:ILE:HG13	1.87	0.57
1:A:3635:CYS:HA	1:A:3638:MET:HG3	1.86	0.57
1:C:2595:LEU:O	1:C:2600:ARG:NH1	2.38	0.57
1:C:3052:HIS:NE2	1:C:3128:ASN:OD1	2.35	0.57
1:D:2309:SER:OG	1:D:2321:ILE:O	2.22	0.57
1:B:2871:LEU:HG	1:B:2927:LEU:HD21	1.85	0.57
1:D:2823:ILE:HD11	1:D:2935:TYR:HB3	1.86	0.57
1:D:3990:VAL:HG13	1:D:4051:SER:HB3	1.86	0.57
1:A:1943:LEU:HD13	1:A:2098:VAL:HG22	1.86	0.57
1:A:2463:LEU:HA	1:A:2466:LEU:HD12	1.86	0.57
1:B:348:VAL:HB	1:B:357:LEU:HD22	1.87	0.57
1:C:62:LEU:HD23	1:C:261:ARG:HH12	1.69	0.57
1:C:2021:CYS:O	1:C:2028:ARG:NH2	2.38	0.57
1:D:2653:LYS:HB2	1:D:2661:TRP:HE3	1.70	0.57
1:D:3766:GLN:OE1	1:D:3769:ARG:NH2	2.38	0.57
1:B:747:CYS:HB2	1:B:756:SER:HB2	1.87	0.57
1:B:763:PRO:O	1:B:765:GLN:NE2	2.37	0.57
1:B:1653:LEU:O	1:B:1660:GLN:NE2	2.38	0.57
1:B:2595:LEU:O	1:B:2600:ARG:NH1	2.38	0.57
1:B:3635:CYS:HA	1:B:3638:MET:HG3	1.86	0.57
1:B:4994:TYR:OH	1:B:4998:LYS:NZ	2.35	0.57
1:C:728:ARG:NH2	1:C:1489:CYS:SG	2.78	0.57
1:A:1653:LEU:O	1:A:1660:GLN:NE2	2.38	0.57
1:A:2595:LEU:O	1:A:2600:ARG:NH1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2792:ARG:HB2	1:A:2797:PHE:HD1	1.70	0.57
1:A:3769:ARG:O	1:A:3773:ARG:NH1	2.38	0.57
1:A:3990:VAL:HG13	1:A:4051:SER:HB3	1.86	0.57
1:D:62:LEU:HD23	1:D:261:ARG:HH12	1.69	0.57
1:D:1561:VAL:HG12	1:D:1562:ILE:HG13	1.87	0.57
1:D:2018:GLU:OE1	1:D:2028:ARG:NH1	2.38	0.57
1:D:2792:ARG:HB2	1:D:2797:PHE:HD1	1.70	0.57
1:A:289:ARG:HB3	1:A:301:VAL:HB	1.86	0.56
1:C:3766:GLN:OE1	1:C:3769:ARG:NH2	2.38	0.56
1:D:133:PHE:O	1:D:193:ALA:N	2.38	0.56
1:D:728:ARG:NH2	1:D:1489:CYS:SG	2.78	0.56
1:A:2823:ILE:HD11	1:A:2935:TYR:HB3	1.86	0.56
1:B:638:ILE:HD12	1:B:1638:ALA:HB3	1.86	0.56
1:B:2000:SER:O	1:B:2005:GLN:NE2	2.33	0.56
1:C:1561:VAL:HG12	1:C:1562:ILE:HG13	1.87	0.56
1:D:2021:CYS:O	1:D:2028:ARG:NH2	2.38	0.56
1:A:348:VAL:HB	1:A:357:LEU:HD22	1.87	0.56
1:A:3766:GLN:OE1	1:A:3769:ARG:NH2	2.38	0.56
1:B:2653:LYS:HB2	1:B:2661:TRP:HE3	1.70	0.56
1:B:3766:GLN:OE1	1:B:3769:ARG:NH2	2.38	0.56
1:C:638:ILE:HD12	1:C:1638:ALA:HB3	1.86	0.56
1:C:3214:ASN:HB3	1:C:3217:SER:HB2	1.86	0.56
1:D:747:CYS:HB2	1:D:756:SER:HB2	1.87	0.56
1:A:728:ARG:NH2	1:A:1489:CYS:SG	2.78	0.56
1:A:2018:GLU:OE1	1:A:2028:ARG:NH1	2.38	0.56
1:B:2463:LEU:HA	1:B:2466:LEU:HD12	1.86	0.56
1:D:2463:LEU:HA	1:D:2466:LEU:HD12	1.86	0.56
1:D:2595:LEU:O	1:D:2600:ARG:NH1	2.38	0.56
1:A:2977:LEU:HA	1:A:2980:VAL:HG22	1.88	0.56
1:B:1454:THR:OG1	1:B:1456:ASP:OD1	2.23	0.56
1:B:1561:VAL:HG12	1:B:1562:ILE:HG13	1.87	0.56
1:B:2792:ARG:HB2	1:B:2797:PHE:HD1	1.70	0.56
1:B:3769:ARG:O	1:B:3773:ARG:NH1	2.38	0.56
1:C:2792:ARG:HB2	1:C:2797:PHE:HD1	1.70	0.56
1:D:3635:CYS:HA	1:D:3638:MET:HG3	1.86	0.56
1:D:4570:ALA:O	1:D:4574:ASN:ND2	2.39	0.56
1:A:3702:VAL:HG13	1:A:3778:MET:HG2	1.86	0.56
1:B:2021:CYS:O	1:B:2028:ARG:NH2	2.38	0.56
1:B:3702:VAL:HG13	1:B:3778:MET:HG2	1.86	0.56
1:D:348:VAL:HB	1:D:357:LEU:HD22	1.87	0.56
1:D:1694:LEU:HB3	1:D:1715:LEU:HD12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2977:LEU:HA	1:D:2980:VAL:HG22	1.87	0.56
1:A:34:LYS:HB3	1:A:53:SER:HB3	1.87	0.56
1:A:133:PHE:O	1:A:193:ALA:N	2.38	0.56
1:A:683:ARG:NH1	1:A:707:VAL:O	2.34	0.56
1:A:2021:CYS:O	1:A:2028:ARG:NH2	2.38	0.56
1:B:3052:HIS:NE2	1:B:3128:ASN:OD1	2.35	0.56
1:D:3769:ARG:O	1:D:3773:ARG:NH1	2.38	0.56
1:A:4938:ASP:OD1	1:D:4944:ARG:NH2	2.36	0.56
1:B:728:ARG:NH2	1:B:1489:CYS:SG	2.78	0.56
1:B:2823:ILE:HD11	1:B:2935:TYR:HB3	1.86	0.56
1:B:3214:ASN:HB3	1:B:3217:SER:HB2	1.86	0.56
1:B:4570:ALA:O	1:B:4574:ASN:ND2	2.39	0.56
1:A:2653:LYS:HB2	1:A:2661:TRP:HE3	1.70	0.56
1:B:3048:ALA:O	1:B:3053:ARG:NH2	2.39	0.56
1:C:1694:LEU:HB3	1:C:1715:LEU:HD12	1.88	0.56
1:C:2018:GLU:OE1	1:C:2028:ARG:NH1	2.38	0.56
1:D:1653:LEU:O	1:D:1660:GLN:NE2	2.38	0.56
1:D:4994:TYR:OH	1:D:4998:LYS:NZ	2.35	0.56
1:C:2512:ILE:HG21	1:C:2518:LEU:HD13	1.88	0.56
1:D:3048:ALA:O	1:D:3053:ARG:NH2	2.39	0.56
1:A:747:CYS:HB2	1:A:756:SER:HB2	1.87	0.55
1:A:2000:SER:O	1:A:2005:GLN:NE2	2.32	0.55
1:A:3524:MET:HA	1:A:3582:ARG:HH22	1.70	0.55
1:B:1694:LEU:HB3	1:B:1715:LEU:HD12	1.88	0.55
1:B:2018:GLU:OE1	1:B:2028:ARG:NH1	2.38	0.55
1:B:2977:LEU:HA	1:B:2980:VAL:HG22	1.87	0.55
1:C:683:ARG:NH1	1:C:707:VAL:O	2.34	0.55
1:C:3459:VAL:HG13	1:C:3464:ILE:HB	1.89	0.55
1:A:707:VAL:HG23	1:A:782:SER:HB3	1.88	0.55
1:A:3459:VAL:HG13	1:A:3464:ILE:HB	1.89	0.55
1:B:707:VAL:HG23	1:B:782:SER:HB3	1.88	0.55
1:C:348:VAL:HB	1:C:357:LEU:HD22	1.87	0.55
1:C:2927:LEU:HD12	1:C:2930:LEU:HD12	1.88	0.55
1:C:4570:ALA:O	1:C:4574:ASN:ND2	2.39	0.55
1:D:3214:ASN:HB3	1:D:3217:SER:HB2	1.87	0.55
1:D:4583:SER:HB2	1:D:4631:PHE:HE1	1.72	0.55
1:A:277:GLY:HA2	1:A:315:CYS:HB3	1.89	0.55
1:A:1454:THR:OG1	1:A:1456:ASP:OD1	2.23	0.55
1:B:34:LYS:HB3	1:B:53:SER:HB3	1.87	0.55
1:C:2653:LYS:HB2	1:C:2661:TRP:HE3	1.70	0.55
1:D:277:GLY:HA2	1:D:315:CYS:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2114:PRO:HB3	1:D:3707:ARG:HH12	1.72	0.55
1:D:3099:ALA:HA	1:D:3136:LEU:HD21	1.89	0.55
1:A:1694:LEU:HB3	1:A:1715:LEU:HD12	1.88	0.55
1:A:2512:ILE:HG21	1:A:2518:LEU:HD13	1.88	0.55
1:A:4583:SER:HB2	1:A:4631:PHE:HE1	1.72	0.55
1:C:3635:CYS:HA	1:C:3638:MET:HG3	1.86	0.55
1:A:3214:ASN:HB3	1:A:3217:SER:HB2	1.87	0.55
1:B:133:PHE:O	1:B:193:ALA:N	2.38	0.55
1:B:2512:ILE:HG21	1:B:2518:LEU:HD13	1.88	0.55
1:B:3459:VAL:HG13	1:B:3464:ILE:HB	1.89	0.55
1:C:633:LEU:HD13	1:C:1639:LEU:HD21	1.89	0.55
1:C:3769:ARG:O	1:C:3773:ARG:NH1	2.38	0.55
1:A:3048:ALA:O	1:A:3053:ARG:NH2	2.39	0.55
1:A:4570:ALA:O	1:A:4574:ASN:ND2	2.39	0.55
1:B:2265:LEU:O	1:B:2330:ARG:NH1	2.39	0.55
1:C:1653:LEU:O	1:C:1660:GLN:NE2	2.38	0.55
1:C:3048:ALA:O	1:C:3053:ARG:NH2	2.39	0.55
1:C:3419:ASN:OD1	1:C:3423:TRP:NE1	2.40	0.55
1:D:3459:VAL:HG13	1:D:3464:ILE:HB	1.89	0.55
1:D:23:GLN:NE2	1:D:203:ASN:OD1	2.40	0.55
1:A:1730:MET:O	1:A:1772:ARG:NH1	2.40	0.55
1:C:747:CYS:HB2	1:C:756:SER:HB2	1.87	0.55
1:C:2265:LEU:O	1:C:2330:ARG:NH1	2.39	0.55
1:C:2977:LEU:HA	1:C:2980:VAL:HG22	1.87	0.55
1:C:4583:SER:HB2	1:C:4631:PHE:HE1	1.72	0.55
1:D:1730:MET:O	1:D:1772:ARG:NH1	2.40	0.55
1:D:2000:SER:O	1:D:2005:GLN:NE2	2.33	0.55
1:A:2114:PRO:HB3	1:A:3707:ARG:HH12	1.72	0.55
1:B:633:LEU:HD13	1:B:1639:LEU:HD21	1.89	0.55
1:B:3419:ASN:OD1	1:B:3423:TRP:NE1	2.40	0.55
1:C:23:GLN:NE2	1:C:203:ASN:OD1	2.40	0.55
1:C:796:ARG:O	1:C:1619:ARG:NH2	2.40	0.55
1:B:796:ARG:O	1:B:1619:ARG:NH2	2.40	0.54
1:A:796:ARG:O	1:A:1619:ARG:NH2	2.40	0.54
1:A:2978:GLU:OE2	1:A:3053:ARG:NH1	2.31	0.54
1:A:3419:ASN:OD1	1:A:3423:TRP:NE1	2.40	0.54
1:B:1730:MET:O	1:B:1772:ARG:NH1	2.40	0.54
1:B:2114:PRO:HB3	1:B:3707:ARG:HH12	1.72	0.54
1:B:3840:SER:OG	1:B:3877:ASP:OD1	2.24	0.54
1:B:4583:SER:HB2	1:B:4631:PHE:HE1	1.72	0.54
1:C:2114:PRO:HB3	1:C:3707:ARG:HH12	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:LYS:HB3	1:D:53:SER:HB3	1.87	0.54
1:A:2265:LEU:O	1:A:2330:ARG:NH1	2.40	0.54
1:B:23:GLN:NE2	1:B:203:ASN:OD1	2.40	0.54
1:C:3099:ALA:HA	1:C:3136:LEU:HD21	1.89	0.54
1:A:23:GLN:NE2	1:A:203:ASN:OD1	2.40	0.54
1:A:2927:LEU:HD12	1:A:2930:LEU:HD12	1.88	0.54
1:D:2265:LEU:O	1:D:2330:ARG:NH1	2.39	0.54
1:C:707:VAL:HG23	1:C:782:SER:HB3	1.88	0.54
1:D:707:VAL:HG23	1:D:782:SER:HB3	1.88	0.54
1:D:4886:HIS:HD2	1:D:4920:PHE:HE2	1.56	0.54
1:A:1944:GLU:HB3	1:A:2123:LEU:HD21	1.90	0.54
1:A:2131:LEU:HD12	1:A:3662:ILE:HG23	1.90	0.54
1:C:34:LYS:HB3	1:C:53:SER:HB3	1.87	0.54
1:A:867:LEU:HD13	1:A:929:LEU:HB3	1.90	0.54
1:B:3099:ALA:HA	1:B:3136:LEU:HD21	1.89	0.54
1:B:4886:HIS:HD2	1:B:4920:PHE:HE2	1.56	0.54
1:C:1730:MET:O	1:C:1772:ARG:NH1	2.40	0.54
1:C:1944:GLU:HB3	1:C:2123:LEU:HD21	1.90	0.54
1:C:2309:SER:OG	1:C:2321:ILE:O	2.22	0.54
1:D:669:ASP:OD1	1:D:790:ARG:NH1	2.40	0.54
1:A:2247:GLN:NE2	1:A:2281:ILE:O	2.41	0.54
1:A:3099:ALA:HA	1:A:3136:LEU:HD21	1.88	0.54
1:A:4886:HIS:HD2	1:A:4920:PHE:HE2	1.56	0.54
1:B:632:LEU:O	1:B:634:GLN:NE2	2.40	0.54
1:B:669:ASP:OD1	1:B:790:ARG:NH1	2.40	0.54
1:B:1944:GLU:HB3	1:B:2123:LEU:HD21	1.90	0.54
1:B:2247:GLN:NE2	1:B:2281:ILE:O	2.41	0.54
1:C:669:ASP:OD1	1:C:790:ARG:NH1	2.40	0.54
1:C:867:LEU:HD13	1:C:929:LEU:HB3	1.90	0.54
1:C:4112:LEU:O	1:C:4115:SER:OG	2.25	0.54
1:D:633:LEU:HD13	1:D:1639:LEU:HD21	1.89	0.54
1:D:2512:ILE:HG21	1:D:2518:LEU:HD13	1.88	0.54
1:D:3380:ARG:NH2	1:D:3450:ASN:OD1	2.41	0.54
1:A:4112:LEU:O	1:A:4115:SER:OG	2.25	0.54
1:B:2927:LEU:HD12	1:B:2930:LEU:HD12	1.89	0.54
1:C:277:GLY:HA2	1:C:315:CYS:HB3	1.89	0.54
1:C:1277:TRP:O	1:C:1559:GLN:NE2	2.41	0.54
1:C:3380:ARG:NH2	1:C:3450:ASN:OD1	2.40	0.54
1:D:632:LEU:O	1:D:634:GLN:NE2	2.40	0.54
1:D:1277:TRP:O	1:D:1559:GLN:NE2	2.41	0.54
1:B:3380:ARG:NH2	1:B:3450:ASN:OD1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:LEU:O	1:A:634:GLN:NE2	2.40	0.53
1:A:669:ASP:OD1	1:A:790:ARG:NH1	2.40	0.53
1:B:277:GLY:HA2	1:B:315:CYS:HB3	1.89	0.53
1:B:867:LEU:HD13	1:B:929:LEU:HB3	1.90	0.53
1:B:2131:LEU:HD12	1:B:3662:ILE:HG23	1.90	0.53
1:D:1454:THR:OG1	1:D:1456:ASP:OD1	2.23	0.53
1:D:4112:LEU:O	1:D:4115:SER:OG	2.25	0.53
1:A:633:LEU:HD13	1:A:1639:LEU:HD21	1.89	0.53
1:A:4994:TYR:OH	1:A:4998:LYS:NZ	2.35	0.53
1:B:3322:ILE:O	1:B:3326:ASN:ND2	2.41	0.53
1:D:796:ARG:O	1:D:1619:ARG:NH2	2.40	0.53
1:D:1944:GLU:HB3	1:D:2123:LEU:HD21	1.90	0.53
1:D:2927:LEU:HD12	1:D:2930:LEU:HD12	1.88	0.53
1:D:3322:ILE:O	1:D:3326:ASN:ND2	2.41	0.53
1:D:3419:ASN:OD1	1:D:3423:TRP:NE1	2.40	0.53
1:C:3882:GLN:HG3	1:C:3957:VAL:HG22	1.91	0.53
1:D:867:LEU:HD13	1:D:929:LEU:HB3	1.90	0.53
1:A:1277:TRP:O	1:A:1559:GLN:NE2	2.41	0.53
1:A:3380:ARG:NH2	1:A:3450:ASN:OD1	2.41	0.53
1:B:1277:TRP:O	1:B:1559:GLN:NE2	2.41	0.53
1:C:2000:SER:O	1:C:2005:GLN:NE2	2.33	0.53
1:D:3107:VAL:HG11	1:D:3171:SER:HB2	1.91	0.53
1:A:3322:ILE:O	1:A:3326:ASN:ND2	2.41	0.53
1:A:3924:LEU:HD21	1:A:3984:ARG:HH21	1.73	0.53
1:C:632:LEU:O	1:C:634:GLN:NE2	2.40	0.53
1:D:3524:MET:O	1:D:3595:ARG:NH1	2.42	0.53
1:D:3882:GLN:HG3	1:D:3957:VAL:HG22	1.91	0.53
1:A:2960:LEU:HD23	1:A:2963:LEU:HD12	1.91	0.53
1:A:3882:GLN:HG3	1:A:3957:VAL:HG22	1.91	0.53
1:B:2960:LEU:HD23	1:B:2963:LEU:HD12	1.91	0.53
1:D:125:ARG:NH1	1:D:126:SER:OG	2.42	0.53
1:D:1066:GLN:NE2	1:D:1461:ASP:OD1	2.39	0.53
1:B:3767:GLN:OE1	1:B:3809:ASN:ND2	2.38	0.53
1:C:4886:HIS:HD2	1:C:4920:PHE:HE2	1.56	0.53
1:D:3208:PRO:HA	1:D:3211:ASN:HB2	1.91	0.53
1:B:3020:THR:HG23	1:B:3023:LYS:H	1.74	0.53
1:B:3524:MET:O	1:B:3595:ARG:NH1	2.42	0.53
1:C:3524:MET:O	1:C:3595:ARG:NH1	2.42	0.53
1:D:683:ARG:NH1	1:D:707:VAL:O	2.34	0.53
1:D:1099:GLU:OE2	1:D:1125:ASN:ND2	2.40	0.53
1:D:2131:LEU:HD12	1:D:3662:ILE:HG23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3984:ARG:HH22	1:B:161:GLU:HB3	1.74	0.53
1:B:3984:ARG:HH22	1:C:161:GLU:HB3	1.74	0.53
1:C:3573:MET:HB3	1:C:3577:ARG:HH21	1.73	0.53
1:D:3573:MET:HB3	1:D:3577:ARG:HH21	1.73	0.53
1:A:818:ARG:NH2	1:A:1027:LEU:O	2.42	0.53
1:A:4161:ARG:HA	1:A:4164:LEU:HD13	1.91	0.53
1:C:133:PHE:O	1:C:193:ALA:N	2.38	0.53
1:C:3020:THR:HG23	1:C:3023:LYS:H	1.74	0.53
1:B:3573:MET:HB3	1:B:3577:ARG:HH21	1.73	0.52
1:C:1066:GLN:NE2	1:C:1461:ASP:OD1	2.39	0.52
1:C:3984:ARG:HH22	1:D:161:GLU:HB3	1.74	0.52
1:D:1674:CYS:HG	1:D:1717:SER:HG	1.56	0.52
1:B:224:HIS:NE2	1:B:385:ASP:O	2.42	0.52
1:C:3107:VAL:HG11	1:C:3171:SER:HB2	1.91	0.52
1:C:3924:LEU:HD21	1:C:3984:ARG:HH21	1.74	0.52
1:A:1739:THR:OG1	1:A:1742:THR:OG1	2.25	0.52
1:B:818:ARG:NH2	1:B:1027:LEU:O	2.42	0.52
1:B:3208:PRO:HA	1:B:3211:ASN:HB2	1.91	0.52
1:B:4866:SER:HB3	1:B:4873:ASP:HB2	1.92	0.52
1:C:222:LEU:HD23	1:C:388:LEU:HD13	1.92	0.52
1:C:224:HIS:NE2	1:C:385:ASP:O	2.42	0.52
1:C:1443:GLN:NE2	1:C:1555:LEU:O	2.40	0.52
1:C:2131:LEU:HD12	1:C:3662:ILE:HG23	1.90	0.52
1:D:222:LEU:HD23	1:D:388:LEU:HD13	1.92	0.52
1:A:1443:GLN:NE2	1:A:1555:LEU:O	2.41	0.52
1:A:2268[A]:GLN:OE1	1:A:2414:ASN:ND2	2.43	0.52
1:A:2268[B]:GLN:OE1	1:A:2414:ASN:ND2	2.43	0.52
1:A:3524:MET:O	1:A:3595:ARG:NH1	2.42	0.52
1:A:3573:MET:HB3	1:A:3577:ARG:HH21	1.73	0.52
1:A:4107:GLU:HA	1:A:4110:PHE:HB3	1.92	0.52
1:B:3107:VAL:HG11	1:B:3171:SER:HB2	1.91	0.52
1:C:818:ARG:NH2	1:C:1027:LEU:O	2.42	0.52
1:D:2268[A]:GLN:OE1	1:D:2414:ASN:ND2	2.43	0.52
1:D:3052:HIS:NE2	1:D:3128:ASN:OD1	2.35	0.52
1:D:3924:LEU:HD21	1:D:3984:ARG:HH21	1.74	0.52
1:D:4161:ARG:HA	1:D:4164:LEU:HD13	1.91	0.52
1:B:125:ARG:NH1	1:B:126:SER:OG	2.42	0.52
1:B:3882:GLN:HG3	1:B:3957:VAL:HG22	1.90	0.52
1:C:125:ARG:NH1	1:C:126:SER:OG	2.42	0.52
1:C:4866:SER:HB3	1:C:4873:ASP:HB2	1.92	0.52
1:D:3767:GLN:OE1	1:D:3809:ASN:ND2	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3208:PRO:HA	1:A:3211:ASN:HB2	1.91	0.52
1:A:3556:ASN:HA	1:A:3559:LEU:HD23	1.92	0.52
1:B:222:LEU:HD23	1:B:388:LEU:HD13	1.92	0.52
1:C:2247:GLN:NE2	1:C:2281:ILE:O	2.41	0.52
1:A:125:ARG:NH1	1:A:126:SER:OG	2.42	0.52
1:B:2365:GLY:O	1:B:2369[B]:ARG:NE	2.39	0.52
1:B:3924:LEU:HD21	1:B:3984:ARG:HH21	1.73	0.52
1:D:818:ARG:NH2	1:D:1027:LEU:O	2.42	0.52
1:D:4107:GLU:HA	1:D:4110:PHE:HB3	1.92	0.52
1:A:3318:ASN:OD1	1:A:3321:ARG:NH1	2.43	0.52
1:A:4866:SER:HB3	1:A:4873:ASP:HB2	1.92	0.52
1:A:4877:ASP:O	1:D:4581:LYS:NZ	2.42	0.52
1:B:3318:ASN:OD1	1:B:3321:ARG:NH1	2.43	0.52
1:C:2879:ALA:HB1	1:C:2919:ASP:HB3	1.92	0.52
1:C:3318:ASN:OD1	1:C:3321:ARG:NH1	2.43	0.52
1:D:3020:THR:HG23	1:D:3023:LYS:H	1.74	0.52
1:D:3556:ASN:HA	1:D:3559:LEU:HD23	1.92	0.52
1:D:4866:SER:HB3	1:D:4873:ASP:HB2	1.92	0.52
1:A:2879:ALA:HB1	1:A:2919:ASP:HB3	1.92	0.52
1:B:1443:GLN:NE2	1:B:1555:LEU:O	2.41	0.52
1:D:2247:GLN:NE2	1:D:2281:ILE:O	2.41	0.52
1:D:2960:LEU:HD23	1:D:2963:LEU:HD12	1.91	0.52
1:A:3020:THR:HG23	1:A:3023:LYS:H	1.74	0.52
1:B:2268[A]:GLN:OE1	1:B:2414:ASN:ND2	2.43	0.52
1:B:2879:ALA:HB1	1:B:2919:ASP:HB3	1.92	0.52
1:C:2268[A]:GLN:OE1	1:C:2414:ASN:ND2	2.43	0.52
1:D:2268[B]:GLN:OE1	1:D:2414:ASN:ND2	2.43	0.52
1:A:4914:VAL:HG11	1:D:4884:LEU:HD11	1.92	0.51
1:B:2268[B]:GLN:OE1	1:B:2414:ASN:ND2	2.43	0.51
1:B:4068:LEU:HA	1:B:4071:ILE:HB	1.92	0.51
1:B:4161:ARG:HA	1:B:4164:LEU:HD13	1.91	0.51
1:B:4823:LEU:HD22	1:C:4843:LEU:HD22	1.91	0.51
1:C:3322:ILE:O	1:C:3326:ASN:ND2	2.41	0.51
1:C:4708:THR:HG21	1:C:4775:TYR:HB2	1.93	0.51
1:D:224:HIS:NE2	1:D:385:ASP:O	2.42	0.51
1:D:1443:GLN:NE2	1:D:1555:LEU:O	2.40	0.51
1:A:4068:LEU:HA	1:A:4071:ILE:HB	1.92	0.51
1:B:1084:GLN:NE2	1:B:1186:ASP:O	2.43	0.51
1:C:2749:GLU:HG3	1:C:2752:ASP:HB2	1.93	0.51
1:D:3458:PHE:O	1:D:3462:ASN:ND2	2.36	0.51
1:D:3596:VAL:O	1:D:3600:SER:OG	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:HIS:NE2	1:A:385:ASP:O	2.42	0.51
1:B:45:ARG:NH2	1:B:447:ASP:OD1	2.42	0.51
1:D:2437:ALA:O	1:D:2508:ARG:NH2	2.44	0.51
1:D:2749:GLU:HG3	1:D:2752:ASP:HB2	1.93	0.51
1:D:4708:THR:HG21	1:D:4775:TYR:HB2	1.93	0.51
1:A:222:LEU:HD23	1:A:388:LEU:HD13	1.92	0.51
1:A:796:ARG:HG3	1:A:1619:ARG:HH22	1.74	0.51
1:A:1099:GLU:OE2	1:A:1125:ASN:ND2	2.40	0.51
1:C:2960:LEU:HD23	1:C:2963:LEU:HD12	1.91	0.51
1:D:3318:ASN:OD1	1:D:3321:ARG:NH1	2.43	0.51
1:B:356:TRP:O	1:B:379:HIS:N	2.43	0.51
1:B:2749:GLU:HG3	1:B:2752:ASP:HB2	1.93	0.51
1:C:3556:ASN:HA	1:C:3559:LEU:HD23	1.92	0.51
1:B:3781:GLN:NE2	1:B:3819:TYR:OH	2.40	0.51
1:C:4161:ARG:HA	1:C:4164:LEU:HD13	1.91	0.51
1:C:4823:LEU:HD22	1:D:4843:LEU:HD22	1.91	0.51
1:D:1947:CYS:SG	1:D:2127:GLN:NE2	2.79	0.51
1:D:2365:GLY:O	1:D:2369[B]:ARG:NE	2.39	0.51
1:D:2879:ALA:HB1	1:D:2919:ASP:HB3	1.92	0.51
1:A:818:ARG:HH12	1:A:1026:LEU:HA	1.76	0.51
1:A:3052:HIS:NE2	1:A:3128:ASN:OD1	2.35	0.51
1:B:1947:CYS:SG	1:B:2127:GLN:NE2	2.79	0.51
1:B:2437:ALA:O	1:B:2508:ARG:NH2	2.44	0.51
1:C:356:TRP:O	1:C:379:HIS:N	2.43	0.51
1:C:2268[B]:GLN:OE1	1:C:2414:ASN:ND2	2.43	0.51
1:D:45:ARG:NH2	1:D:447:ASP:OD1	2.42	0.51
1:D:4068:LEU:HA	1:D:4071:ILE:HB	1.93	0.51
1:B:818:ARG:HH12	1:B:1026:LEU:HA	1.76	0.51
1:B:1225:PRO:HG2	1:B:1228:ILE:HD13	1.93	0.51
1:B:1618:ARG:NH2	1:B:1619:ARG:O	2.44	0.51
1:B:3107:VAL:O	1:B:3111:ARG:HB2	2.11	0.51
1:B:4107:GLU:HA	1:B:4110:PHE:HB3	1.92	0.51
1:C:320:LYS:NZ	1:C:383:HIS:O	2.44	0.51
1:C:4107:GLU:HA	1:C:4110:PHE:HB3	1.92	0.51
1:A:2437:ALA:O	1:A:2508:ARG:NH2	2.44	0.51
1:A:2749:GLU:HG3	1:A:2752:ASP:HB2	1.93	0.51
1:B:796:ARG:HG3	1:B:1619:ARG:HH22	1.74	0.51
1:B:2806:ARG:HD2	1:B:2810:LYS:HZ3	1.75	0.51
1:B:3556:ASN:HA	1:B:3559:LEU:HD23	1.92	0.51
1:A:356:TRP:O	1:A:379:HIS:N	2.43	0.51
1:A:1225:PRO:HG2	1:A:1228:ILE:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4708:THR:HG21	1:B:4775:TYR:HB2	1.93	0.51
1:C:796:ARG:HG3	1:C:1619:ARG:HH22	1.74	0.51
1:C:1084:GLN:NE2	1:C:1186:ASP:O	2.43	0.51
1:C:3771:HIS:O	1:C:3815:LYS:NZ	2.44	0.51
1:A:45:ARG:NH2	1:A:447:ASP:OD1	2.42	0.50
1:A:320:LYS:NZ	1:A:383:HIS:O	2.44	0.50
1:A:3107:VAL:HG11	1:A:3171:SER:HB2	1.91	0.50
1:C:1454:THR:OG1	1:C:1456:ASP:OD1	2.23	0.50
1:C:1739:THR:OG1	1:C:1742:THR:OG1	2.25	0.50
1:C:3458:PHE:O	1:C:3462:ASN:ND2	2.36	0.50
1:D:1739:THR:OG1	1:D:1742:THR:OG1	2.25	0.50
1:A:2788:HIS:HB3	1:A:2791:LEU:HD23	1.93	0.50
1:B:273:HIS:CE1	1:B:338:GLU:H	2.30	0.50
1:C:1618:ARG:NH2	1:C:1619:ARG:O	2.44	0.50
1:C:3208:PRO:HA	1:C:3211:ASN:HB2	1.91	0.50
1:A:545:ASP:N	1:A:545:ASP:OD1	2.44	0.50
1:A:2754:PHE:HE2	1:A:2813:LEU:HD11	1.76	0.50
1:B:1676:LEU:HD22	1:B:2167:ILE:HD12	1.93	0.50
1:B:2745:VAL:HG13	1:B:2814:LYS:HD2	1.94	0.50
1:C:273:HIS:CE1	1:C:338:GLU:H	2.29	0.50
1:C:1225:PRO:HG2	1:C:1228:ILE:HD13	1.93	0.50
1:D:273:HIS:CE1	1:D:338:GLU:H	2.29	0.50
1:A:706:GLY:N	1:A:709:ASP:OD2	2.39	0.50
1:A:1066:GLN:NE2	1:A:1461:ASP:OD1	2.39	0.50
1:B:2754:PHE:HE2	1:B:2813:LEU:HD11	1.76	0.50
1:B:2788:HIS:HB3	1:B:2791:LEU:HD23	1.93	0.50
1:C:1751:GLY:HA3	1:C:1758:ARG:HE	1.77	0.50
1:C:2745:VAL:HG13	1:C:2814:LYS:HD2	1.94	0.50
1:C:3107:VAL:O	1:C:3111:ARG:HB2	2.11	0.50
1:C:4068:LEU:HA	1:C:4071:ILE:HB	1.93	0.50
1:D:3107:VAL:O	1:D:3111:ARG:HB2	2.11	0.50
1:D:3771:HIS:O	1:D:3815:LYS:NZ	2.44	0.50
1:A:273:HIS:CE1	1:A:338:GLU:H	2.29	0.50
1:A:1084:GLN:NE2	1:A:1186:ASP:O	2.43	0.50
1:A:1679:ASN:HA	1:A:1682:ALA:HB3	1.93	0.50
1:A:1947:CYS:SG	1:A:2127:GLN:NE2	2.79	0.50
1:A:2299:VAL:HG11	1:A:2356:LEU:HB3	1.93	0.50
1:C:3781:GLN:NE2	1:C:3819:TYR:OH	2.40	0.50
1:C:3868:ARG:HH11	1:C:3870:ASN:HB3	1.76	0.50
1:D:3840:SER:OG	1:D:3877:ASP:OD1	2.24	0.50
1:A:932:LEU:HB3	1:A:937:CYS:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1618:ARG:NH2	1:A:1619:ARG:O	2.44	0.50
1:A:3840:SER:OG	1:A:3877:ASP:OD1	2.24	0.50
1:A:3868:ARG:HH11	1:A:3870:ASN:HB3	1.76	0.50
1:A:4204:GLN:HG2	1:A:4245:MET:HG2	1.94	0.50
1:B:2764:GLU:HG3	1:B:2857:PRO:HB3	1.94	0.50
1:C:2437:ALA:O	1:C:2508:ARG:NH2	2.44	0.50
1:D:2745:VAL:HG13	1:D:2814:LYS:HD2	1.94	0.50
1:A:3107:VAL:O	1:A:3111:ARG:HB2	2.11	0.50
1:A:3458:PHE:O	1:A:3462:ASN:ND2	2.36	0.50
1:A:3767:GLN:OE1	1:A:3809:ASN:ND2	2.38	0.50
1:A:4708:THR:HG21	1:A:4775:TYR:HB2	1.93	0.50
1:A:4892:ARG:NH1	1:B:4895:GLY:O	2.37	0.50
1:B:932:LEU:HB3	1:B:937:CYS:HB3	1.94	0.50
1:B:2310:CYS:HB3	1:B:2313:LEU:HB2	1.94	0.50
1:C:648:ILE:HG23	1:C:814:ALA:HB3	1.94	0.50
1:C:2299:VAL:HG11	1:C:2356:LEU:HB3	1.93	0.50
1:C:2764:GLU:HG3	1:C:2857:PRO:HB3	1.94	0.50
1:D:545:ASP:N	1:D:545:ASP:OD1	2.44	0.50
1:B:1739:THR:OG1	1:B:1742:THR:OG1	2.25	0.50
1:B:4204:GLN:HG2	1:B:4245:MET:HG2	1.94	0.50
1:D:796:ARG:HG3	1:D:1619:ARG:HH22	1.74	0.50
1:A:1676:LEU:HD22	1:A:2167:ILE:HD12	1.93	0.50
1:A:4917:ASP:HB2	1:D:4888:TYR:HE1	1.76	0.50
1:B:1679:ASN:HA	1:B:1682:ALA:HB3	1.93	0.50
1:B:2882:TYR:O	1:B:2885:THR:OG1	2.28	0.50
1:C:2882:TYR:O	1:C:2885:THR:OG1	2.28	0.50
1:C:3227:ARG:NH1	1:C:3234:ASN:OD1	2.37	0.50
1:C:3767:GLN:OE1	1:C:3809:ASN:ND2	2.38	0.50
1:D:356:TRP:O	1:D:379:HIS:N	2.43	0.50
1:D:2764:GLU:HG3	1:D:2857:PRO:HB3	1.94	0.50
1:A:2764:GLU:HG3	1:A:2857:PRO:HB3	1.94	0.49
1:C:758:ARG:HA	1:C:763:PRO:HA	1.94	0.49
1:C:4204:GLN:HG2	1:C:4245:MET:HG2	1.94	0.49
1:D:758:ARG:HA	1:D:763:PRO:HA	1.94	0.49
1:D:1618:ARG:NH2	1:D:1619:ARG:O	2.44	0.49
1:D:1676:LEU:HD22	1:D:2167:ILE:HD12	1.93	0.49
1:D:3244:PRO:HA	1:D:3248:ARG:HH21	1.76	0.49
1:D:3868:ARG:HH11	1:D:3870:ASN:HB3	1.76	0.49
1:B:320:LYS:NZ	1:B:383:HIS:O	2.44	0.49
1:B:3244:PRO:HA	1:B:3248:ARG:HH21	1.76	0.49
1:C:45:ARG:NH2	1:C:447:ASP:OD1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2310:CYS:HB3	1:C:2313:LEU:HB2	1.94	0.49
1:D:932:LEU:HB3	1:D:937:CYS:HB3	1.94	0.49
1:D:1225:PRO:HG2	1:D:1228:ILE:HD13	1.93	0.49
1:D:1423:ASP:N	1:D:1571:ASN:OD1	2.45	0.49
1:D:2648:TYR:O	1:D:2652:TRP:HB3	2.12	0.49
1:D:3781:GLN:NE2	1:D:3819:TYR:OH	2.40	0.49
2:E:21:THR:HA	2:E:49:ARG:HA	1.94	0.49
1:B:545:ASP:N	1:B:545:ASP:OD1	2.44	0.49
1:B:4112:LEU:O	1:B:4115:SER:OG	2.25	0.49
1:C:818:ARG:HH12	1:C:1026:LEU:HA	1.76	0.49
1:C:932:LEU:HB3	1:C:937:CYS:HB3	1.94	0.49
1:D:2788:HIS:HB3	1:D:2791:LEU:HD23	1.93	0.49
1:A:2648:TYR:O	1:A:2652:TRP:HB3	2.12	0.49
1:A:3244:PRO:HA	1:A:3248:ARG:HH21	1.76	0.49
1:B:683:ARG:NH1	1:B:707:VAL:O	2.34	0.49
1:B:1131:ARG:NH1	1:B:1178:ALA:O	2.46	0.49
1:B:2299:VAL:HG11	1:B:2356:LEU:HB3	1.93	0.49
1:C:1676:LEU:HD22	1:C:2167:ILE:HD12	1.93	0.49
1:C:2648:TYR:O	1:C:2652:TRP:HB3	2.13	0.49
1:C:3244:PRO:HA	1:C:3248:ARG:HH21	1.76	0.49
1:D:648:ILE:HG23	1:D:814:ALA:HB3	1.94	0.49
1:D:818:ARG:HH12	1:D:1026:LEU:HA	1.76	0.49
1:D:4204:GLN:HG2	1:D:4245:MET:HG2	1.94	0.49
1:A:2768:PHE:HD1	1:A:2857:PRO:HG2	1.78	0.49
1:A:4090:LYS:HG2	1:A:4123:ILE:HD11	1.95	0.49
1:A:4828:SER:O	1:A:4832:HIS:HB2	2.12	0.49
1:B:1066:GLN:NE2	1:B:1461:ASP:OD1	2.39	0.49
1:B:3391:GLU:HA	1:B:3394:VAL:HG22	1.95	0.49
1:B:3868:ARG:HH11	1:B:3870:ASN:HB3	1.76	0.49
1:B:4828:SER:O	1:B:4832:HIS:HB2	2.13	0.49
1:D:320:LYS:NZ	1:D:383:HIS:O	2.44	0.49
1:D:1256:GLU:HB3	1:D:1275:ARG:HE	1.77	0.49
1:D:2754:PHE:HE2	1:D:2813:LEU:HD11	1.76	0.49
1:A:2745:VAL:HG13	1:A:2814:LYS:HD2	1.94	0.49
1:A:3202:PRO:O	1:A:3214:ASN:ND2	2.45	0.49
1:B:1256:GLU:HB3	1:B:1275:ARG:HE	1.77	0.49
1:B:1751:GLY:HA3	1:B:1758:ARG:HE	1.77	0.49
1:B:4090:LYS:HG2	1:B:4123:ILE:HD11	1.95	0.49
1:C:262:LEU:HD13	1:C:274:LEU:HD11	1.94	0.49
1:C:1099:GLU:OE2	1:C:1125:ASN:ND2	2.40	0.49
1:C:1679:ASN:HA	1:C:1682:ALA:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2299:VAL:HG11	1:D:2356:LEU:HB3	1.93	0.49
1:D:2470:ILE:O	1:D:2499:LYS:NZ	2.39	0.49
1:D:2742:THR:O	1:D:2814:LYS:NZ	2.46	0.49
1:D:4999:ASP:OD1	1:D:4999:ASP:N	2.46	0.49
1:A:939:VAL:HB	1:A:1051:TYR:HB3	1.95	0.49
1:A:1131:ARG:NH1	1:A:1178:ALA:O	2.46	0.49
1:A:3180:ASN:HB2	1:A:3183:VAL:HG23	1.95	0.49
1:A:3391:GLU:HA	1:A:3394:VAL:HG22	1.95	0.49
1:A:4928:LEU:HD23	1:A:4931:ILE:HD12	1.95	0.49
1:B:3180:ASN:HB2	1:B:3183:VAL:HG23	1.95	0.49
1:C:936:GLY:HA3	1:C:1056:PRO:HB3	1.95	0.49
1:C:2998:PHE:HA	1:C:3002:LEU:HD13	1.95	0.49
1:C:3575:LEU:HD23	1:D:1219:LEU:HD22	1.95	0.49
1:C:4828:SER:O	1:C:4832:HIS:HB2	2.13	0.49
1:D:1679:ASN:HA	1:D:1682:ALA:HB3	1.93	0.49
1:D:1751:GLY:HA3	1:D:1758:ARG:HE	1.77	0.49
2:F:21:THR:HA	2:F:49:ARG:HA	1.94	0.49
2:H:21:THR:HA	2:H:49:ARG:HA	1.94	0.49
1:A:1423:ASP:N	1:A:1571:ASN:OD1	2.45	0.49
1:A:3051:ARG:NH2	1:A:3102:ASP:OD1	2.46	0.49
1:B:3771:HIS:O	1:B:3815:LYS:NZ	2.44	0.49
1:C:2788:HIS:HB3	1:C:2791:LEU:HD23	1.93	0.49
1:C:3051:ARG:NH2	1:C:3102:ASP:OD1	2.46	0.49
1:C:3523:ASN:O	1:C:3582:ARG:NH2	2.46	0.49
1:D:717:ASP:OD1	1:D:720:HIS:N	2.41	0.49
1:D:3227:ARG:NH1	1:D:3234:ASN:OD1	2.37	0.49
2:G:21:THR:HA	2:G:49:ARG:HA	1.94	0.49
1:A:870:ILE:HG13	1:A:874:LEU:HD23	1.95	0.49
1:A:2093:SER:OG	1:A:2096:GLU:OE1	2.31	0.49
1:B:2768:PHE:HD1	1:B:2857:PRO:HG2	1.78	0.49
1:C:2093:SER:OG	1:C:2096:GLU:OE1	2.31	0.49
1:D:939:VAL:HB	1:D:1051:TYR:HB3	1.95	0.49
1:D:2310:CYS:HB3	1:D:2313:LEU:HB2	1.94	0.49
1:A:262:LEU:HD13	1:A:274:LEU:HD11	1.95	0.49
1:B:5012:LYS:HD3	1:B:5012:LYS:HA	1.64	0.49
1:C:870:ILE:HG13	1:C:874:LEU:HD23	1.95	0.49
1:D:1131:ARG:NH1	1:D:1178:ALA:O	2.46	0.49
1:D:3391:GLU:HA	1:D:3394:VAL:HG22	1.95	0.49
1:A:648:ILE:HG23	1:A:814:ALA:HB3	1.94	0.48
1:A:758:ARG:HA	1:A:763:PRO:HA	1.94	0.48
1:A:2365:GLY:O	1:A:2369[B]:ARG:NE	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3902:TYR:O	1:A:3906:GLN:NE2	2.45	0.48
1:B:717:ASP:OD1	1:B:720:HIS:N	2.41	0.48
1:B:870:ILE:HG13	1:B:874:LEU:HD23	1.95	0.48
1:C:4944:ARG:NH2	1:D:4938:ASP:OD1	2.43	0.48
1:D:2093:SER:OG	1:D:2096:GLU:OE1	2.31	0.48
1:D:2386:ILE:HG23	1:D:2392:ARG:HG3	1.95	0.48
1:B:939:VAL:HB	1:B:1051:TYR:HB3	1.95	0.48
1:C:2754:PHE:HE2	1:C:2813:LEU:HD11	1.76	0.48
1:C:3391:GLU:HA	1:C:3394:VAL:HG22	1.95	0.48
1:C:3442:PHE:HE1	1:C:3511:VAL:HG12	1.78	0.48
1:D:4821:LYS:HE2	1:D:4821:LYS:HB2	1.54	0.48
1:D:4828:SER:O	1:D:4832:HIS:HB2	2.12	0.48
1:A:1256:GLU:HB3	1:A:1275:ARG:HE	1.77	0.48
1:A:4227:GLU:H	1:A:4227:GLU:HG3	1.43	0.48
1:B:758:ARG:HA	1:B:763:PRO:HA	1.94	0.48
1:B:2093:SER:OG	1:B:2096:GLU:OE1	2.31	0.48
1:B:2736:ASP:OD1	1:B:2736:ASP:N	2.47	0.48
1:C:1256:GLU:HB3	1:C:1275:ARG:HE	1.77	0.48
1:C:1423:ASP:N	1:C:1571:ASN:OD1	2.45	0.48
1:C:2512:ILE:HD13	1:C:2561:LEU:HD11	1.95	0.48
1:A:1751:GLY:HA3	1:A:1758:ARG:HE	1.77	0.48
1:A:3781:GLN:NE2	1:A:3819:TYR:OH	2.40	0.48
1:B:648:ILE:HG23	1:B:814:ALA:HB3	1.94	0.48
1:C:1131:ARG:NH1	1:C:1178:ALA:O	2.46	0.48
1:C:2742:THR:O	1:C:2814:LYS:NZ	2.46	0.48
1:D:3180:ASN:HB2	1:D:3183:VAL:HG23	1.95	0.48
1:D:4928:LEU:HD23	1:D:4931:ILE:HD12	1.95	0.48
1:A:936:GLY:HA3	1:A:1056:PRO:HB3	1.95	0.48
1:B:1099:GLU:OE2	1:B:1125:ASN:ND2	2.40	0.48
1:B:2512:ILE:HD13	1:B:2561:LEU:HD11	1.95	0.48
1:B:4928:LEU:HD23	1:B:4931:ILE:HD12	1.95	0.48
1:B:4999:ASP:OD1	1:B:4999:ASP:N	2.46	0.48
1:D:3442:PHE:HE1	1:D:3511:VAL:HG12	1.78	0.48
1:D:4090:LYS:HG2	1:D:4123:ILE:HD11	1.95	0.48
1:A:356:TRP:N	1:A:379:HIS:O	2.38	0.48
1:A:359:TYR:HA	1:A:376:ALA:HA	1.96	0.48
1:A:3442:PHE:HE1	1:A:3511:VAL:HG12	1.78	0.48
1:A:3523:ASN:O	1:A:3582:ARG:NH2	2.46	0.48
1:A:3788:GLY:HA2	1:A:3835:LEU:HD12	1.96	0.48
1:B:2648:TYR:O	1:B:2652:TRP:HB3	2.13	0.48
1:C:886:ARG:HE	1:C:904:HIS:HB2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2377:LEU:HA	1:C:2380:ILE:HG22	1.96	0.48
1:C:3794:VAL:HG11	1:C:3835:LEU:HD21	1.96	0.48
1:D:870:ILE:HG13	1:D:874:LEU:HD23	1.95	0.48
1:D:886:ARG:HE	1:D:904:HIS:HB2	1.79	0.48
1:D:936:GLY:HA3	1:D:1056:PRO:HB3	1.95	0.48
1:D:2768:PHE:HD1	1:D:2857:PRO:HG2	1.78	0.48
1:A:1253:PRO:O	1:A:1275:ARG:NH1	2.46	0.48
1:A:4165:GLU:HA	1:A:4168:GLU:HG2	1.95	0.48
1:B:359:TYR:HA	1:B:376:ALA:HA	1.96	0.48
1:B:936:GLY:HA3	1:B:1056:PRO:HB3	1.95	0.48
1:B:1698:LEU:HD21	1:B:1715:LEU:HD13	1.95	0.48
1:B:2165:LEU:HD12	1:B:2178:MET:HB3	1.95	0.48
1:B:3051:ARG:NH2	1:B:3102:ASP:OD1	2.46	0.48
1:B:3363:GLY:HA2	1:B:3366:ARG:HG2	1.96	0.48
1:B:4835:LYS:HB3	1:B:4835:LYS:HE2	1.56	0.48
1:C:3180:ASN:HB2	1:C:3183:VAL:HG23	1.95	0.48
1:C:4165:GLU:HA	1:C:4168:GLU:HG2	1.95	0.48
1:C:4928:LEU:HD23	1:C:4931:ILE:HD12	1.95	0.48
1:D:2165:LEU:HD12	1:D:2178:MET:HB3	1.95	0.48
1:B:3575:LEU:HD23	1:C:1219:LEU:HD22	1.95	0.48
1:B:3794:VAL:HG11	1:B:3835:LEU:HD21	1.96	0.48
1:C:875:ALA:O	1:C:879:HIS:ND1	2.47	0.48
1:C:2165:LEU:HD12	1:C:2178:MET:HB3	1.95	0.48
1:C:4090:LYS:HG2	1:C:4123:ILE:HD11	1.95	0.48
1:D:748:LEU:HD13	1:D:755:ILE:HG12	1.96	0.48
1:A:886:ARG:HE	1:A:904:HIS:HB2	1.79	0.48
1:A:2998:PHE:HA	1:A:3002:LEU:HD13	1.95	0.48
1:B:706:GLY:N	1:B:709:ASP:OD2	2.39	0.48
1:B:875:ALA:O	1:B:879:HIS:ND1	2.47	0.48
1:B:1253:PRO:O	1:B:1275:ARG:NH1	2.46	0.48
1:C:939:VAL:HB	1:C:1051:TYR:HB3	1.95	0.48
1:C:1253:PRO:O	1:C:1275:ARG:NH1	2.46	0.48
1:C:2768:PHE:HD1	1:C:2857:PRO:HG2	1.78	0.48
1:D:262:LEU:HD13	1:D:274:LEU:HD11	1.94	0.48
1:D:1448:VAL:HG22	1:D:1554:VAL:HG23	1.96	0.48
1:D:2512:ILE:HD13	1:D:2561:LEU:HD11	1.95	0.48
1:A:110:ARG:NH2	1:A:117:TYR:OH	2.47	0.48
1:A:1448:VAL:HG22	1:A:1554:VAL:HG23	1.96	0.48
1:A:2310:CYS:HB3	1:A:2313:LEU:HB2	1.94	0.48
1:A:2386:ILE:HG23	1:A:2392:ARG:HG3	1.95	0.48
1:A:2863:SER:HA	1:A:2928:LYS:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:LEU:HD13	1:B:274:LEU:HD11	1.94	0.48
1:B:2742:THR:O	1:B:2814:LYS:NZ	2.46	0.48
1:B:3537:LYS:NZ	1:B:3600:SER:O	2.44	0.48
1:C:110:ARG:NH2	1:C:117:TYR:OH	2.47	0.48
1:C:248:GLU:HG2	1:C:252:VAL:HG21	1.96	0.48
1:C:359:TYR:HA	1:C:376:ALA:HA	1.96	0.48
1:C:1100:MET:HB2	1:C:1143:TRP:HZ2	1.79	0.48
1:C:2736:ASP:OD1	1:C:2736:ASP:N	2.47	0.48
1:A:877:ASN:HA	1:A:970:LEU:H	1.79	0.47
1:B:886:ARG:HE	1:B:904:HIS:HB2	1.79	0.47
1:C:748:LEU:HD13	1:C:755:ILE:HG12	1.96	0.47
1:C:2365:GLY:O	1:C:2369[B]:ARG:NE	2.39	0.47
1:C:2870[A]:GLU:OE1	1:C:2939:ARG:NH2	2.47	0.47
1:C:3902:TYR:O	1:C:3906:GLN:NE2	2.45	0.47
1:D:875:ALA:O	1:D:879:HIS:ND1	2.47	0.47
1:D:1100:MET:HB2	1:D:1143:TRP:HZ2	1.79	0.47
1:D:2863:SER:HA	1:D:2928:LYS:HG3	1.96	0.47
1:D:2998:PHE:HA	1:D:3002:LEU:HD13	1.95	0.47
1:D:3523:ASN:O	1:D:3582:ARG:NH2	2.46	0.47
1:A:1292:SER:OG	1:A:1596:GLU:N	2.44	0.47
1:A:2165:LEU:HD12	1:A:2178:MET:HB3	1.95	0.47
1:A:3159:ASP:OD1	1:A:3159:ASP:N	2.46	0.47
1:A:3227:ARG:NH1	1:A:3234:ASN:OD1	2.37	0.47
1:A:3363:GLY:HA2	1:A:3366:ARG:HG2	1.96	0.47
1:B:2377:LEU:HA	1:B:2380:ILE:HG22	1.96	0.47
1:B:2998:PHE:HA	1:B:3002:LEU:HD13	1.95	0.47
1:C:877:ASN:HA	1:C:970:LEU:H	1.79	0.47
1:D:110:ARG:NH2	1:D:117:TYR:OH	2.47	0.47
1:D:359:TYR:HA	1:D:376:ALA:HA	1.96	0.47
1:D:1253:PRO:O	1:D:1275:ARG:NH1	2.46	0.47
1:D:2377:LEU:HA	1:D:2380:ILE:HG22	1.96	0.47
1:D:3233:PRO:HG2	1:D:3239:MET:HA	1.96	0.47
1:D:4835:LYS:HB3	1:D:4835:LYS:HE2	1.56	0.47
1:A:875:ALA:O	1:A:879:HIS:ND1	2.47	0.47
1:A:2736:ASP:OD1	1:A:2736:ASP:N	2.47	0.47
1:B:3442:PHE:HE1	1:B:3511:VAL:HG12	1.78	0.47
1:C:1653:LEU:HD23	1:C:1660:GLN:HA	1.96	0.47
1:C:2477:PRO:HB3	1:C:2487:GLN:HG2	1.97	0.47
1:D:15:ARG:HG3	1:D:100:THR:HA	1.96	0.47
1:D:1712:TYR:OH	1:D:1814:MET:SD	2.72	0.47
1:B:14:LEU:HB2	1:B:163:VAL:HG13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:ARG:HG3	1:B:100:THR:HA	1.96	0.47
1:B:3523:ASN:O	1:B:3582:ARG:NH2	2.46	0.47
1:B:4049:VAL:HG11	1:B:4159:ARG:HH11	1.80	0.47
1:C:545:ASP:OD1	1:C:545:ASP:N	2.44	0.47
1:C:3840:SER:OG	1:C:3877:ASP:OD1	2.24	0.47
1:D:2736:ASP:N	1:D:2736:ASP:OD1	2.47	0.47
1:D:4165:GLU:HA	1:D:4168:GLU:HG2	1.95	0.47
1:A:868:GLU:HA	1:A:871:ARG:HB2	1.97	0.47
1:A:2748:PRO:HG2	1:A:2817:ILE:HD13	1.97	0.47
1:B:3233:PRO:HG2	1:B:3239:MET:HA	1.96	0.47
1:C:356:TRP:N	1:C:379:HIS:O	2.38	0.47
1:D:868:GLU:HA	1:D:871:ARG:HB2	1.97	0.47
1:D:1469:VAL:HG13	1:D:1492:CYS:HB3	1.96	0.47
1:D:2875:ALA:HB2	1:D:2927:LEU:HD22	1.97	0.47
1:A:1698:LEU:HD21	1:A:1715:LEU:HD13	1.95	0.47
1:C:15:ARG:HG3	1:C:100:THR:HA	1.96	0.47
1:D:37:LEU:HD21	1:D:191:VAL:HG21	1.97	0.47
1:D:2870[A]:GLU:OE1	1:D:2939:ARG:NH2	2.47	0.47
1:D:3567:PRO:HA	1:D:3570:ARG:HD3	1.96	0.47
1:D:3902:TYR:O	1:D:3906:GLN:NE2	2.45	0.47
1:A:15:ARG:HG3	1:A:100:THR:HA	1.96	0.47
1:A:1469:VAL:HG13	1:A:1492:CYS:HB3	1.96	0.47
1:A:1653:LEU:HD23	1:A:1660:GLN:HA	1.96	0.47
1:A:2870[A]:GLU:OE1	1:A:2939:ARG:NH2	2.47	0.47
1:A:3233:PRO:HG2	1:A:3239:MET:HA	1.96	0.47
1:A:3537:LYS:NZ	1:A:3600:SER:O	2.44	0.47
1:A:4895:GLY:O	1:D:4892:ARG:NH1	2.45	0.47
1:A:4999:ASP:N	1:A:4999:ASP:OD1	2.46	0.47
1:B:35:LEU:HD13	1:B:49:LEU:HD13	1.97	0.47
1:B:877:ASN:HA	1:B:970:LEU:H	1.79	0.47
1:B:1100:MET:HB2	1:B:1143:TRP:HZ2	1.79	0.47
1:B:1469:VAL:HG13	1:B:1492:CYS:HB3	1.96	0.47
1:B:2386:ILE:HG23	1:B:2392:ARG:HG3	1.95	0.47
1:B:2748:PRO:HG2	1:B:2817:ILE:HD13	1.97	0.47
1:B:2867:LEU:HD12	1:B:2928:LYS:HZ3	1.79	0.47
1:B:3567:PRO:HA	1:B:3570:ARG:HD3	1.96	0.47
1:B:4944:ARG:NH2	1:C:4938:ASP:OD1	2.43	0.47
1:C:37:LEU:HD21	1:C:191:VAL:HG21	1.97	0.47
1:C:1698:LEU:HD21	1:C:1715:LEU:HD13	1.95	0.47
1:C:2875:ALA:HB2	1:C:2927:LEU:HD22	1.97	0.47
1:C:3363:GLY:HA2	1:C:3366:ARG:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4227:GLU:H	1:C:4227:GLU:HG3	1.43	0.47
1:D:35:LEU:HD13	1:D:49:LEU:HD13	1.97	0.47
1:D:877:ASN:HA	1:D:970:LEU:H	1.79	0.47
1:D:1698:LEU:HD21	1:D:1715:LEU:HD13	1.95	0.47
1:D:1753:LYS:HB3	1:D:1758:ARG:HD2	1.96	0.47
1:D:2477:PRO:HB3	1:D:2487:GLN:HG2	1.97	0.47
1:D:2692:ASP:HB3	1:D:2695:LEU:HB3	1.96	0.47
1:D:2748:PRO:HG2	1:D:2817:ILE:HD13	1.97	0.47
1:D:2882:TYR:O	1:D:2885:THR:OG1	2.28	0.47
1:A:37:LEU:HD21	1:A:191:VAL:HG21	1.97	0.47
1:A:1100:MET:HB2	1:A:1143:TRP:HZ2	1.79	0.47
1:A:2512:ILE:HD13	1:A:2561:LEU:HD11	1.95	0.47
1:A:2692:ASP:HB3	1:A:2695:LEU:HB3	1.96	0.47
1:A:2742:THR:O	1:A:2814:LYS:NZ	2.46	0.47
1:B:356:TRP:N	1:B:379:HIS:O	2.38	0.47
1:B:1292:SER:OG	1:B:1596:GLU:N	2.44	0.47
1:B:1653:LEU:HD23	1:B:1660:GLN:HA	1.96	0.47
1:B:1712:TYR:OH	1:B:1814:MET:SD	2.72	0.47
1:C:35:LEU:HD13	1:C:49:LEU:HD13	1.97	0.47
1:C:1469:VAL:HG13	1:C:1492:CYS:HB3	1.96	0.47
1:C:2863:SER:HA	1:C:2928:LYS:HG3	1.96	0.47
1:D:1292:SER:OG	1:D:1596:GLU:N	2.44	0.47
1:D:2614:ILE:O	1:D:2650:ARG:NH2	2.43	0.47
1:D:2806:ARG:HD2	1:D:2810:LYS:HZ3	1.79	0.47
1:A:248:GLU:HG2	1:A:252:VAL:HG21	1.96	0.47
1:B:248:GLU:HG2	1:B:252:VAL:HG21	1.96	0.47
1:B:2870[A]:GLU:OE1	1:B:2939:ARG:NH2	2.47	0.47
1:B:3788:GLY:HA2	1:B:3835:LEU:HD12	1.96	0.47
1:C:3316:LEU:HD11	1:C:3346:VAL:HA	1.97	0.47
1:C:4694:ASP:HA	1:C:4700:GLN:HE21	1.80	0.47
1:D:706:GLY:N	1:D:709:ASP:OD2	2.39	0.47
1:D:3051:ARG:NH2	1:D:3102:ASP:OD1	2.46	0.47
2:F:23:VAL:HG22	2:F:47:LYS:HG2	1.97	0.47
1:A:14:LEU:HB2	1:A:163:VAL:HG13	1.97	0.47
1:B:748:LEU:HD13	1:B:755:ILE:HG12	1.96	0.47
1:B:1753:LYS:HB3	1:B:1758:ARG:HD2	1.96	0.47
1:C:3567:PRO:HA	1:C:3570:ARG:HD3	1.96	0.47
1:C:4999:ASP:N	1:C:4999:ASP:OD1	2.46	0.47
1:D:3333:THR:O	1:D:3337:ARG:NH1	2.48	0.47
1:D:3788:GLY:HA2	1:D:3835:LEU:HD12	1.96	0.47
1:D:4694:ASP:HA	1:D:4700:GLN:HE21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:27:THR:HB	2:F:100:ASP:HB3	1.97	0.47
2:G:27:THR:HB	2:G:100:ASP:HB3	1.97	0.47
1:A:2377:LEU:HA	1:A:2380:ILE:HG22	1.96	0.46
1:A:3536:ALA:HA	1:A:3539:ARG:HG2	1.97	0.46
1:A:3567:PRO:HA	1:A:3570:ARG:HD3	1.97	0.46
1:A:3794:VAL:HG11	1:A:3835:LEU:HD21	1.96	0.46
1:B:2863:SER:HA	1:B:2928:LYS:HG3	1.96	0.46
1:B:3333:THR:O	1:B:3337:ARG:NH1	2.48	0.46
1:C:1292:SER:OG	1:C:1596:GLU:N	2.44	0.46
1:D:248:GLU:HG2	1:D:252:VAL:HG21	1.96	0.46
1:D:1653:LEU:HD23	1:D:1660:GLN:HA	1.96	0.46
1:D:3794:VAL:HG11	1:D:3835:LEU:HD21	1.96	0.46
2:E:23:VAL:HG22	2:E:47:LYS:HG2	1.97	0.46
2:F:8:SER:HB2	2:F:71:ARG:HB2	1.97	0.46
2:G:23:VAL:HG22	2:G:47:LYS:HG2	1.97	0.46
1:A:1712:TYR:OH	1:A:1814:MET:SD	2.72	0.46
1:A:1753:LYS:HB3	1:A:1758:ARG:HD2	1.97	0.46
1:B:37:LEU:HD21	1:B:191:VAL:HG21	1.97	0.46
1:C:14:LEU:HB2	1:C:163:VAL:HG13	1.97	0.46
1:C:3788:GLY:HA2	1:C:3835:LEU:HD12	1.96	0.46
1:D:294:THR:HG23	1:D:297:GLN:H	1.81	0.46
1:D:3202:PRO:O	1:D:3214:ASN:ND2	2.45	0.46
2:E:8:SER:HB2	2:E:71:ARG:HB2	1.97	0.46
2:H:23:VAL:HG22	2:H:47:LYS:HG2	1.97	0.46
1:A:717:ASP:OD1	1:A:720:HIS:N	2.41	0.46
1:A:4835:LYS:HB3	1:A:4835:LYS:HE2	1.56	0.46
1:B:110:ARG:NH2	1:B:117:TYR:OH	2.47	0.46
1:B:2109:ASP:OD1	1:B:2109:ASP:N	2.49	0.46
1:C:1947:CYS:SG	1:C:2127:GLN:NE2	2.79	0.46
1:C:2386:ILE:HG23	1:C:2392:ARG:HG3	1.95	0.46
1:C:2623:LEU:HD12	1:C:2626:LEU:HD12	1.97	0.46
1:A:294:THR:HG23	1:A:297:GLN:H	1.81	0.46
1:A:2466:LEU:HB3	1:A:2502:MET:HE1	1.97	0.46
1:A:3316:LEU:HD11	1:A:3346:VAL:HA	1.97	0.46
1:A:3333:THR:O	1:A:3337:ARG:NH1	2.48	0.46
1:B:3316:LEU:HD11	1:B:3346:VAL:HA	1.97	0.46
1:C:1753:LYS:HB3	1:C:1758:ARG:HD2	1.96	0.46
1:C:2109:ASP:N	1:C:2109:ASP:OD1	2.49	0.46
1:C:4049:VAL:HG11	1:C:4159:ARG:HH11	1.80	0.46
1:D:492:ASP:OD1	1:D:546:TRP:NE1	2.42	0.46
1:A:748:LEU:HD13	1:A:755:ILE:HG12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2882:TYR:O	1:A:2885:THR:OG1	2.28	0.46
1:B:277:GLY:N	1:B:316:PHE:O	2.48	0.46
1:B:884:LEU:HB2	1:B:969:PRO:HD3	1.98	0.46
1:B:3902:TYR:O	1:B:3906:GLN:NE2	2.45	0.46
1:C:868:GLU:HA	1:C:871:ARG:HB2	1.97	0.46
1:C:1448:VAL:HG22	1:C:1554:VAL:HG23	1.96	0.46
1:C:2748:PRO:HG2	1:C:2817:ILE:HD13	1.97	0.46
1:C:3233:PRO:HG2	1:C:3239:MET:HA	1.96	0.46
1:C:3537:LYS:NZ	1:C:3600:SER:O	2.44	0.46
1:D:1243:PRO:O	1:D:1458:HIS:ND1	2.34	0.46
1:D:3363:GLY:HA2	1:D:3366:ARG:HG2	1.96	0.46
1:A:161:GLU:OE1	1:D:3984:ARG:NH1	2.49	0.46
1:A:4049:VAL:HG11	1:A:4159:ARG:HH11	1.80	0.46
1:A:4694:ASP:HA	1:A:4700:GLN:HE21	1.80	0.46
1:B:232:THR:HG22	1:B:258:SER:HB3	1.98	0.46
1:B:1448:VAL:HG22	1:B:1554:VAL:HG23	1.96	0.46
1:B:2477:PRO:HB3	1:B:2487:GLN:HG2	1.97	0.46
1:B:2623:LEU:HD12	1:B:2626:LEU:HD12	1.97	0.46
1:B:4165:GLU:HA	1:B:4168:GLU:HG2	1.95	0.46
1:B:4865:LYS:HA	1:B:4865:LYS:HD2	1.49	0.46
1:C:5012:LYS:HD3	1:C:5012:LYS:HA	1.64	0.46
1:D:14:LEU:HB2	1:D:163:VAL:HG13	1.97	0.46
1:D:2623:LEU:HD12	1:D:2626:LEU:HD12	1.97	0.46
2:H:8:SER:HB2	2:H:71:ARG:HB2	1.97	0.46
1:B:275:ARG:NH1	1:B:278:GLN:OE1	2.49	0.46
1:B:492:ASP:OD1	1:B:546:TRP:NE1	2.42	0.46
1:B:868:GLU:HA	1:B:871:ARG:HB2	1.97	0.46
1:B:2410:PRO:HB3	1:B:2415:ARG:HB3	1.97	0.46
1:B:2692:ASP:HB3	1:B:2695:LEU:HB3	1.96	0.46
1:D:3275:PRO:HA	1:D:3278:CYS:HB2	1.98	0.46
1:D:4049:VAL:HG11	1:D:4159:ARG:HH11	1.80	0.46
1:A:2109:ASP:N	1:A:2109:ASP:OD1	2.49	0.46
1:A:2627:VAL:HG22	1:A:2678:LEU:HG	1.98	0.46
1:A:3771:HIS:O	1:A:3815:LYS:NZ	2.44	0.46
1:B:620:LEU:O	1:B:624:ASN:ND2	2.49	0.46
1:B:2742:THR:HB	1:B:2814:LYS:HG2	1.98	0.46
1:B:2875:ALA:HB2	1:B:2927:LEU:HD22	1.97	0.46
1:B:3536:ALA:HA	1:B:3539:ARG:HG2	1.97	0.46
1:B:4694:ASP:HA	1:B:4700:GLN:HE21	1.80	0.46
1:C:294:THR:HG23	1:C:297:GLN:H	1.81	0.46
1:C:3175:LEU:O	1:C:3178:THR:OG1	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3202:PRO:O	1:C:3214:ASN:ND2	2.45	0.46
1:C:3536:ALA:HA	1:C:3539:ARG:HG2	1.97	0.46
1:D:277:GLY:N	1:D:316:PHE:O	2.48	0.46
1:D:1084:GLN:NE2	1:D:1186:ASP:O	2.43	0.46
2:H:27:THR:HB	2:H:100:ASP:HB3	1.97	0.46
1:A:35:LEU:HD13	1:A:49:LEU:HD13	1.97	0.46
1:A:1473:THR:HA	1:A:1487:LEU:O	2.16	0.46
1:A:2470:ILE:HG22	1:A:2525:GLY:HA3	1.98	0.46
1:A:2477:PRO:HB3	1:A:2487:GLN:HG2	1.97	0.46
1:B:1423:ASP:N	1:B:1571:ASN:OD1	2.45	0.46
1:C:732:SER:HB2	1:C:735:GLN:HB3	1.98	0.46
1:C:2410:PRO:HB3	1:C:2415:ARG:HB3	1.97	0.46
1:C:2500:ALA:HB2	1:C:2553:TYR:HD1	1.81	0.46
1:C:3275:PRO:HA	1:C:3278:CYS:HB2	1.98	0.46
1:D:732:SER:HB2	1:D:735:GLN:HB3	1.98	0.46
1:D:2410:PRO:HB3	1:D:2415:ARG:HB3	1.97	0.46
1:D:3316:LEU:HD11	1:D:3346:VAL:HA	1.97	0.46
1:D:4631:PHE:HE2	1:D:4633:GLU:HG2	1.81	0.46
1:A:531:ARG:NH2	1:A:562:GLU:OE2	2.37	0.46
1:A:620:LEU:O	1:A:624:ASN:ND2	2.49	0.46
1:A:4989:MET:HE3	1:A:4989:MET:HB3	1.82	0.46
1:B:3159:ASP:OD1	1:B:3159:ASP:N	2.46	0.46
1:B:3275:PRO:HA	1:B:3278:CYS:HB2	1.98	0.46
1:C:2692:ASP:HB3	1:C:2695:LEU:HB3	1.96	0.46
1:C:3333:THR:O	1:C:3337:ARG:NH1	2.48	0.46
1:D:2109:ASP:OD1	1:D:2109:ASP:N	2.49	0.46
2:G:8:SER:HB2	2:G:71:ARG:HB2	1.97	0.46
1:A:3275:PRO:HA	1:A:3278:CYS:HB2	1.98	0.45
1:C:277:GLY:N	1:C:316:PHE:O	2.48	0.45
1:D:275:ARG:NH1	1:D:278:GLN:OE1	2.49	0.45
1:D:665:GLU:HG2	1:D:745:SER:HA	1.98	0.45
1:A:232:THR:HG22	1:A:258:SER:HB3	1.98	0.45
1:A:277:GLY:N	1:A:316:PHE:O	2.48	0.45
1:C:275:ARG:NH1	1:C:278:GLN:OE1	2.49	0.45
1:D:1473:THR:HA	1:D:1487:LEU:O	2.16	0.45
1:D:2500:ALA:HB2	1:D:2553:TYR:HD1	1.81	0.45
1:D:3536:ALA:HA	1:D:3539:ARG:HG2	1.97	0.45
1:A:2500:ALA:HB2	1:A:2553:TYR:HD1	1.81	0.45
1:B:2559:LEU:HA	1:B:2562:ILE:HD12	1.99	0.45
1:A:884:LEU:HB2	1:A:969:PRO:HD3	1.98	0.45
1:A:2623:LEU:HD12	1:A:2626:LEU:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1473:THR:HA	1:B:1487:LEU:O	2.16	0.45
1:C:620:LEU:O	1:C:624:ASN:ND2	2.49	0.45
1:C:4631:PHE:HE2	1:C:4633:GLU:HG2	1.81	0.45
1:D:2627:VAL:HG22	1:D:2678:LEU:HG	1.98	0.45
1:A:665:GLU:HG2	1:A:745:SER:HA	1.98	0.45
1:A:2875:ALA:HB2	1:A:2927:LEU:HD22	1.97	0.45
1:A:3175:LEU:O	1:A:3178:THR:OG1	2.33	0.45
1:A:4576:ILE:HG23	1:A:4639:MET:HG2	1.99	0.45
1:B:4631:PHE:HE2	1:B:4633:GLU:HG2	1.81	0.45
1:B:4821:LYS:HE2	1:B:4821:LYS:HB2	1.54	0.45
1:C:2466:LEU:HB3	1:C:2502:MET:HE1	1.99	0.45
1:C:2559:LEU:HA	1:C:2562:ILE:HD12	1.99	0.45
1:D:620:LEU:O	1:D:624:ASN:ND2	2.49	0.45
1:D:5030:LYS:HE2	1:D:5030:LYS:HB2	1.76	0.45
1:A:232:THR:HG21	1:A:252:VAL:HG12	1.99	0.45
1:A:699:GLY:N	1:A:1647:CYS:O	2.50	0.45
1:A:2742:THR:HB	1:A:2814:LYS:HG2	1.98	0.45
1:A:4049:VAL:HG21	1:A:4159:ARG:HG2	1.99	0.45
1:C:699:GLY:N	1:C:1647:CYS:O	2.50	0.45
1:C:876:GLU:HG2	1:C:910:PHE:CE2	2.52	0.45
1:C:2667:THR:HG21	1:C:2672:LEU:HD21	1.99	0.45
1:C:4581:LYS:HE3	1:C:4581:LYS:HB3	1.82	0.45
1:D:771:PHE:HB3	1:D:1472:VAL:HG23	1.99	0.45
1:D:884:LEU:HB2	1:D:969:PRO:HD3	1.98	0.45
1:D:1671:ARG:O	1:D:1675:ALA:HB2	2.17	0.45
1:D:2742:THR:HB	1:D:2814:LYS:HG2	1.98	0.45
1:A:275:ARG:NH1	1:A:278:GLN:OE1	2.49	0.45
1:B:732:SER:HB2	1:B:735:GLN:HB3	1.98	0.45
1:B:2500:ALA:HB2	1:B:2553:TYR:HD1	1.81	0.45
1:C:884:LEU:HB2	1:C:969:PRO:HD3	1.98	0.45
1:C:1519:LEU:HD21	1:C:1572:ILE:HD13	1.99	0.45
1:D:232:THR:HG21	1:D:252:VAL:HG12	1.99	0.45
1:D:2466:LEU:HB3	1:D:2502:MET:HE1	1.98	0.45
2:E:27:THR:HB	2:E:100:ASP:HB3	1.97	0.45
1:A:1116:GLY:O	1:A:1134:LEU:N	2.50	0.45
1:A:2986:VAL:HG22	1:A:2988:LYS:H	1.82	0.45
1:A:3519:PRO:HB3	1:B:1220:GLN:HB2	1.99	0.45
1:A:4184:MET:N	1:A:5021:PHE:O	2.50	0.45
1:B:294:THR:HG23	1:B:297:GLN:H	1.81	0.45
1:B:665:GLU:HG2	1:B:745:SER:HA	1.98	0.45
1:B:2039:LEU:HB3	1:B:2044:ILE:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:LYS:HA	1:C:30:LYS:HD2	1.79	0.45
1:C:206:CYS:SG	1:C:207:SER:N	2.90	0.45
1:C:1000:ARG:HD3	1:C:1000:ARG:HA	1.82	0.45
1:C:1473:THR:HA	1:C:1487:LEU:O	2.16	0.45
1:D:585:SER:O	1:D:588:SER:OG	2.28	0.45
2:G:38:SER:OG	2:G:39:SER:N	2.50	0.45
1:A:2410:PRO:HB3	1:A:2415:ARG:HB3	1.97	0.45
1:B:2470:ILE:HG22	1:B:2525:GLY:HA3	1.98	0.45
1:B:2614:ILE:O	1:B:2650:ARG:NH2	2.43	0.45
1:B:2667:THR:HG21	1:B:2672:LEU:HD21	1.99	0.45
1:B:4576:ILE:HG23	1:B:4639:MET:HG2	1.99	0.45
1:C:2470:ILE:HG22	1:C:2525:GLY:HA3	1.98	0.45
1:C:2742:THR:HB	1:C:2814:LYS:HG2	1.98	0.45
1:C:2806:ARG:HD2	1:C:2810:LYS:HZ3	1.82	0.45
1:D:232:THR:HG22	1:D:258:SER:HB3	1.98	0.45
1:D:876:GLU:HG2	1:D:910:PHE:CE2	2.52	0.45
1:D:1658:ASP:N	1:D:1658:ASP:OD1	2.50	0.45
1:D:1690:ASP:HB2	1:D:1693:GLN:HG3	1.99	0.45
1:A:1671:ARG:O	1:A:1675:ALA:HB2	2.17	0.45
1:A:3693:LYS:HD2	1:A:3693:LYS:HA	1.78	0.45
1:A:4202:ARG:O	1:A:4206:GLU:HG2	2.17	0.45
1:A:4631:PHE:HE2	1:A:4633:GLU:HG2	1.81	0.45
1:B:1671:ARG:O	1:B:1675:ALA:HB2	2.17	0.45
1:C:1419:ASP:OD1	1:C:1421:ARG:NH1	2.50	0.45
1:D:4202:ARG:O	1:D:4206:GLU:HG2	2.17	0.45
1:D:4745:LEU:H	1:D:4745:LEU:HG	1.55	0.45
2:H:38:SER:OG	2:H:39:SER:N	2.50	0.45
1:A:732:SER:HB2	1:A:735:GLN:HB3	1.98	0.44
1:B:876:GLU:HG2	1:B:910:PHE:CE2	2.52	0.44
1:B:1658:ASP:OD1	1:B:1658:ASP:N	2.50	0.44
1:C:771:PHE:HB3	1:C:1472:VAL:HG23	1.99	0.44
1:C:1690:ASP:HB2	1:C:1693:GLN:HG3	1.99	0.44
1:C:2627:VAL:HG22	1:C:2678:LEU:HG	1.98	0.44
1:C:4049:VAL:HG21	1:C:4159:ARG:HG2	1.99	0.44
1:D:356:TRP:N	1:D:379:HIS:O	2.38	0.44
1:D:2296:GLU:HA	1:D:2299:VAL:HG12	1.99	0.44
1:D:3420:ARG:HH22	1:D:3519:PRO:HG2	1.82	0.44
1:A:206:CYS:SG	1:A:207:SER:N	2.90	0.44
1:A:876:GLU:HG2	1:A:910:PHE:CE2	2.52	0.44
1:A:1156:THR:OG1	1:A:1157:GLU:OE1	2.36	0.44
1:A:4821:LYS:HE2	1:A:4821:LYS:HB2	1.54	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:CYS:SG	1:B:207:SER:N	2.90	0.44
1:B:531:ARG:NH2	1:B:562:GLU:OE2	2.37	0.44
1:B:1116:GLY:O	1:B:1134:LEU:N	2.50	0.44
1:B:1147:ASP:HB3	1:B:1164:LEU:HD11	2.00	0.44
1:B:3202:PRO:O	1:B:3214:ASN:ND2	2.45	0.44
1:C:232:THR:HG22	1:C:258:SER:HB3	1.98	0.44
1:C:823:LEU:HD12	1:C:823:LEU:HA	1.89	0.44
1:D:206:CYS:SG	1:D:207:SER:N	2.90	0.44
1:D:1116:GLY:O	1:D:1134:LEU:N	2.50	0.44
1:D:2470:ILE:HG22	1:D:2525:GLY:HA3	1.98	0.44
1:D:2559:LEU:HA	1:D:2562:ILE:HD12	1.99	0.44
1:D:2770:LYS:HD2	1:D:2788:HIS:H	1.82	0.44
1:A:2559:LEU:HA	1:A:2562:ILE:HD12	1.99	0.44
1:A:4938:ASP:CG	1:D:4944:ARG:HH21	2.20	0.44
1:B:2466:LEU:HB3	1:B:2502:MET:HE1	2.00	0.44
1:C:499:THR:HG23	1:C:502:HIS:H	1.83	0.44
1:C:1147:ASP:HB3	1:C:1164:LEU:HD11	2.00	0.44
1:A:499:THR:HG23	1:A:502:HIS:H	1.83	0.44
1:A:1658:ASP:N	1:A:1658:ASP:OD1	2.50	0.44
1:A:2039:LEU:HB3	1:A:2044:ILE:HB	1.99	0.44
1:B:499:THR:HG23	1:B:502:HIS:H	1.83	0.44
1:B:2986:VAL:HG22	1:B:2988:LYS:H	1.82	0.44
1:C:4913:ARG:NH2	1:C:4917:ASP:OD2	2.51	0.44
1:D:30:LYS:HA	1:D:30:LYS:HD2	1.79	0.44
1:D:3159:ASP:OD1	1:D:3159:ASP:N	2.46	0.44
1:A:1147:ASP:HB3	1:A:1164:LEU:HD11	2.00	0.44
1:A:1220:GLN:HB2	1:D:3519:PRO:HB3	1.99	0.44
1:A:1243:PRO:O	1:A:1458:HIS:ND1	2.33	0.44
1:A:2355:ARG:HA	1:A:2358:ILE:HG12	1.99	0.44
1:A:2654:TYR:HA	1:A:2661:TRP:H	1.83	0.44
1:A:2770:LYS:HD2	1:A:2788:HIS:H	1.83	0.44
1:A:4865:LYS:HA	1:A:4865:LYS:HD2	1.49	0.44
1:B:863:LEU:HA	1:B:864:PRO:HD3	1.85	0.44
1:C:717:ASP:OD1	1:C:720:HIS:N	2.41	0.44
1:C:4865:LYS:HD2	1:C:4865:LYS:HA	1.49	0.44
1:D:4576:ILE:HG23	1:D:4639:MET:HG2	1.99	0.44
1:A:161:GLU:HB3	1:D:3984:ARG:NH2	2.32	0.44
1:A:1690:ASP:HB2	1:A:1693:GLN:HG3	1.99	0.44
1:A:5012:LYS:HD3	1:A:5012:LYS:HA	1.64	0.44
1:B:2355:ARG:HA	1:B:2358:ILE:HG12	1.99	0.44
1:B:4202:ARG:O	1:B:4206:GLU:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:THR:HG21	1:C:252:VAL:HG12	1.99	0.44
1:C:665:GLU:HG2	1:C:745:SER:HA	1.98	0.44
1:C:2355:ARG:HA	1:C:2358:ILE:HG12	1.99	0.44
1:C:2614:ILE:O	1:C:2650:ARG:NH2	2.43	0.44
1:C:2770:LYS:HD2	1:C:2788:HIS:H	1.83	0.44
1:D:1519:LEU:HD21	1:D:1572:ILE:HD13	1.99	0.44
1:D:2251:PHE:HB2	1:D:2286:LEU:HD13	2.00	0.44
1:D:2560:PRO:O	1:D:2564:LYS:HD2	2.18	0.44
1:D:2654:TYR:HA	1:D:2661:TRP:H	1.83	0.44
1:D:2667:THR:HG21	1:D:2672:LEU:HD21	1.99	0.44
1:D:2986:VAL:HG22	1:D:2988:LYS:H	1.82	0.44
2:E:38:SER:OG	2:E:39:SER:N	2.50	0.44
1:A:308:HIS:HD2	1:A:310:LYS:HB3	1.83	0.44
1:A:771:PHE:HB3	1:A:1472:VAL:HG23	1.99	0.44
1:A:2671:GLU:HA	1:A:2674:LEU:HB2	2.00	0.44
1:A:3420:ARG:HH22	1:A:3519:PRO:HG2	1.82	0.44
1:A:4983:HIS:O	3:A:5101:AMP:N6	2.51	0.44
1:B:771:PHE:HB3	1:B:1472:VAL:HG23	1.99	0.44
1:B:1519:LEU:HD21	1:B:1572:ILE:HD13	1.99	0.44
1:B:2560:PRO:O	1:B:2564:LYS:HD2	2.18	0.44
1:B:2806:ARG:HA	1:B:2809:ILE:HD13	2.00	0.44
1:B:3321:ARG:HA	1:B:3324:VAL:HG12	2.00	0.44
1:C:414:PHE:O	1:C:418:LEU:HB2	2.18	0.44
1:C:2039:LEU:HB3	1:C:2044:ILE:HB	1.99	0.44
1:C:2251:PHE:HB2	1:C:2286:LEU:HD13	2.00	0.44
1:D:1147:ASP:HB3	1:D:1164:LEU:HD11	2.00	0.44
1:D:3092:LEU:HD12	1:D:3093:ARG:HG3	2.00	0.44
1:A:414:PHE:O	1:A:418:LEU:HB2	2.18	0.44
1:A:2806:ARG:HA	1:A:2809:ILE:HD13	2.00	0.44
1:B:1156:THR:OG1	1:B:1157:GLU:OE1	2.35	0.44
1:B:2770:LYS:HD2	1:B:2788:HIS:H	1.83	0.44
1:C:308:HIS:HD2	1:C:310:LYS:HB3	1.83	0.44
1:C:1671:ARG:O	1:C:1675:ALA:HB2	2.17	0.44
1:C:1712:TYR:OH	1:C:1814:MET:SD	2.72	0.44
1:D:2633:LEU:HG	1:D:2695:LEU:HD21	2.00	0.44
1:D:4913:ARG:NH2	1:D:4917:ASP:OD2	2.51	0.44
2:F:38:SER:OG	2:F:39:SER:N	2.50	0.44
1:A:452:PHE:HE1	1:A:474:ARG:HB3	1.83	0.44
1:A:492:ASP:OD1	1:A:546:TRP:NE1	2.42	0.44
1:A:2621:HIS:HB3	1:A:2624:ARG:HH21	1.83	0.44
1:A:3321:ARG:HA	1:A:3324:VAL:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:699:GLY:N	1:B:1647:CYS:O	2.50	0.44
1:B:3218:VAL:O	1:B:3222:LYS:HB2	2.18	0.44
1:C:1156:THR:OG1	1:C:1157:GLU:OE1	2.36	0.44
1:C:1652:GLU:OE1	1:C:1656:ARG:NH2	2.46	0.44
1:C:2296:GLU:HA	1:C:2299:VAL:HG12	1.99	0.44
1:C:4202:ARG:O	1:C:4206:GLU:HG2	2.17	0.44
1:D:3218:VAL:O	1:D:3222:LYS:HB2	2.18	0.44
1:D:3694:LYS:HA	1:D:3695:PRO:HD3	1.90	0.44
1:D:4049:VAL:HG21	1:D:4159:ARG:HG2	1.99	0.44
1:A:683:ARG:HG2	1:A:717:ASP:HB3	2.00	0.43
1:B:3264:THR:OG1	1:B:3265:GLU:OE1	2.36	0.43
1:C:2472:LEU:HD23	1:C:2472:LEU:HA	1.87	0.43
1:C:2560:PRO:O	1:C:2564:LYS:HD2	2.18	0.43
1:C:2633:LEU:HG	1:C:2695:LEU:HD21	2.00	0.43
1:C:2825:LYS:NZ	1:C:2935:TYR:OH	2.45	0.43
1:C:3420:ARG:HH22	1:C:3519:PRO:HG2	1.82	0.43
1:C:4576:ILE:HG23	1:C:4639:MET:HG2	1.99	0.43
1:C:4983:HIS:O	3:C:5101:AMP:N6	2.51	0.43
1:D:1419:ASP:OD1	1:D:1421:ARG:NH1	2.50	0.43
1:D:4184:MET:N	1:D:5021:PHE:O	2.50	0.43
2:E:76:CYS:HB3	2:E:97:LEU:HB2	2.00	0.43
2:H:76:CYS:HB3	2:H:97:LEU:HB2	2.00	0.43
1:A:2357:LEU:HB3	1:A:2364:PHE:HE1	1.83	0.43
1:A:2667:THR:HG21	1:A:2672:LEU:HD21	1.99	0.43
1:A:4823:LEU:HD23	1:A:4823:LEU:HA	1.79	0.43
1:A:4965:SER:O	1:A:4969:ASP:HB2	2.18	0.43
1:B:232:THR:HG21	1:B:252:VAL:HG12	1.99	0.43
1:B:452:PHE:HE1	1:B:474:ARG:HB3	1.83	0.43
1:B:683:ARG:HG2	1:B:717:ASP:HB3	2.00	0.43
1:B:1036:ARG:O	1:B:1040:CYS:HB2	2.18	0.43
1:B:2686:LEU:HB3	1:B:2997:PHE:HE1	1.83	0.43
1:B:3592:ILE:HG22	1:B:3595:ARG:HH21	1.83	0.43
1:B:4049:VAL:HG21	1:B:4159:ARG:HG2	1.99	0.43
1:B:4823:LEU:HA	1:B:4823:LEU:HD23	1.79	0.43
1:C:2357:LEU:HB3	1:C:2364:PHE:HE1	1.83	0.43
1:C:3798:LEU:HD23	1:C:3798:LEU:HA	1.89	0.43
1:D:2621:HIS:HB3	1:D:2624:ARG:HH21	1.83	0.43
1:D:2806:ARG:HA	1:D:2809:ILE:HD13	2.00	0.43
1:A:2175:GLU:HG3	1:A:2228:MET:HB2	2.00	0.43
1:A:2633:LEU:HG	1:A:2695:LEU:HD21	2.00	0.43
1:A:2766:TRP:HE1	1:A:2788:HIS:HB2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3092:LEU:HD12	1:A:3093:ARG:HG3	1.99	0.43
1:A:4823:LEU:HD22	1:B:4843:LEU:HD22	1.99	0.43
1:B:1690:ASP:HB2	1:B:1693:GLN:HG3	1.99	0.43
1:B:2782:ASP:N	1:B:2782:ASP:OD1	2.52	0.43
1:B:4184:MET:N	1:B:5021:PHE:O	2.50	0.43
1:B:4913:ARG:NH2	1:B:4917:ASP:OD2	2.51	0.43
1:C:1116:GLY:O	1:C:1134:LEU:N	2.50	0.43
1:C:1658:ASP:N	1:C:1658:ASP:OD1	2.50	0.43
1:C:2591:ARG:HG2	1:C:2636:PHE:HB3	2.01	0.43
1:C:2986:VAL:HG22	1:C:2988:LYS:H	1.82	0.43
1:C:4965:SER:O	1:C:4969:ASP:HB2	2.18	0.43
1:D:452:PHE:HE1	1:D:474:ARG:HB3	1.83	0.43
1:D:1036:ARG:O	1:D:1040:CYS:HB2	2.18	0.43
1:D:3227:ARG:HA	1:D:3232:LEU:HD12	2.01	0.43
1:D:3264:THR:OG1	1:D:3265:GLU:OE1	2.36	0.43
1:D:4227:GLU:H	1:D:4227:GLU:HG3	1.43	0.43
1:D:4823:LEU:HD23	1:D:4823:LEU:HA	1.79	0.43
2:E:2:VAL:HG23	2:E:80:VAL:HG21	2.01	0.43
1:A:2782:ASP:N	1:A:2782:ASP:OD1	2.52	0.43
1:A:4934:GLY:HA2	1:D:4937:ILE:HG12	2.00	0.43
1:B:124:SER:HB2	1:B:133:PHE:HA	2.01	0.43
1:B:414:PHE:O	1:B:418:LEU:HB2	2.18	0.43
1:B:2159:LEU:HG	1:B:2163:ARG:HE	1.84	0.43
1:B:2627:VAL:HG22	1:B:2678:LEU:HG	1.98	0.43
1:B:2654:TYR:HA	1:B:2661:TRP:H	1.83	0.43
1:B:3092:LEU:HD12	1:B:3093:ARG:HG3	2.00	0.43
1:C:1036:ARG:O	1:C:1040:CYS:HB2	2.18	0.43
1:C:2930:LEU:O	1:C:2935:TYR:N	2.49	0.43
1:C:3694:LYS:HA	1:C:3695:PRO:HD3	1.90	0.43
1:D:414:PHE:O	1:D:418:LEU:HB2	2.18	0.43
1:A:2560:PRO:O	1:A:2564:LYS:HD2	2.18	0.43
1:A:2686:LEU:HB3	1:A:2997:PHE:HE1	1.83	0.43
1:B:308:HIS:HD2	1:B:310:LYS:HB3	1.83	0.43
1:B:2591:ARG:HG2	1:B:2636:PHE:HB3	2.01	0.43
1:B:3458:PHE:O	1:B:3462:ASN:ND2	2.36	0.43
1:B:4965:SER:O	1:B:4969:ASP:HB2	2.18	0.43
1:B:4983:HIS:O	3:B:5101:AMP:N6	2.51	0.43
1:C:2621:HIS:HB3	1:C:2624:ARG:HH21	1.83	0.43
1:C:2806:ARG:HA	1:C:2809:ILE:HD13	2.00	0.43
1:C:3092:LEU:HD12	1:C:3093:ARG:HG3	2.00	0.43
1:C:3227:ARG:HA	1:C:3232:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3535:LEU:O	1:C:3538:THR:OG1	2.32	0.43
1:D:2039:LEU:HB3	1:D:2044:ILE:HB	1.99	0.43
1:D:3157:ILE:HB	1:D:3202:PRO:HG3	2.01	0.43
1:D:4965:SER:O	1:D:4969:ASP:HB2	2.18	0.43
1:A:1519:LEU:HD21	1:A:1572:ILE:HD13	1.99	0.43
1:A:2158:CYS:O	1:A:2162:ILE:HG12	2.19	0.43
1:A:2251:PHE:HB2	1:A:2286:LEU:HD13	2.00	0.43
1:A:4670:ILE:HB	1:A:4714:ASN:HD22	1.84	0.43
1:B:2621:HIS:HB3	1:B:2624:ARG:HH21	1.83	0.43
1:B:2633:LEU:HG	1:B:2695:LEU:HD21	2.00	0.43
1:C:492:ASP:OD1	1:C:546:TRP:NE1	2.42	0.43
1:C:2654:TYR:HA	1:C:2661:TRP:H	1.83	0.43
1:C:3592:ILE:HG22	1:C:3595:ARG:HH21	1.83	0.43
1:C:3693:LYS:HD2	1:C:3693:LYS:HA	1.78	0.43
1:D:308:HIS:HD2	1:D:310:LYS:HB3	1.83	0.43
1:D:499:THR:HG23	1:D:502:HIS:H	1.83	0.43
1:D:3592:ILE:HG22	1:D:3595:ARG:HH21	1.83	0.43
1:D:4983:HIS:O	3:D:5101:AMP:N6	2.51	0.43
1:A:1036:ARG:O	1:A:1040:CYS:HB2	2.18	0.43
1:A:2296:GLU:HA	1:A:2299:VAL:HG12	1.99	0.43
1:A:4913:ARG:NH2	1:A:4917:ASP:OD2	2.51	0.43
1:A:5030:LYS:HB2	1:A:5030:LYS:HE2	1.76	0.43
1:B:823:LEU:HD23	1:B:1617:THR:HB	2.01	0.43
1:B:1419:ASP:OD1	1:B:1421:ARG:NH1	2.50	0.43
1:B:2205:GLU:O	1:B:2208:MET:N	2.52	0.43
1:C:2009:LEU:HD23	1:C:2022:PRO:HD2	2.01	0.43
1:C:2686:LEU:HB3	1:C:2997:PHE:HE1	1.83	0.43
1:C:3218:VAL:O	1:C:3222:LYS:HB2	2.18	0.43
1:C:3321:ARG:HA	1:C:3324:VAL:HG12	2.00	0.43
1:C:4670:ILE:HB	1:C:4714:ASN:HD22	1.84	0.43
1:D:2671:GLU:HA	1:D:2674:LEU:HB2	2.00	0.43
1:D:4670:ILE:HB	1:D:4714:ASN:HD22	1.84	0.43
1:A:1007:TYR:O	1:A:1017:ARG:NH2	2.51	0.43
1:A:3227:ARG:HA	1:A:3232:LEU:HD12	2.01	0.43
1:A:4884:LEU:HD11	1:B:4914:VAL:HG11	2.01	0.43
1:B:2296:GLU:HA	1:B:2299:VAL:HG12	1.99	0.43
1:B:2476:ILE:HG23	1:B:2536:LEU:HD21	2.01	0.43
1:B:2575:ARG:HA	1:B:2575:ARG:HD2	1.79	0.43
1:B:2766:TRP:HE1	1:B:2788:HIS:HB2	1.84	0.43
1:B:2911:LEU:HD13	1:B:2915:GLU:HG3	2.00	0.43
1:B:3420:ARG:HH22	1:B:3519:PRO:HG2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:823:LEU:HD23	1:C:1617:THR:HB	2.01	0.43
1:D:1156:THR:OG1	1:D:1157:GLU:OE1	2.36	0.43
1:D:2205:GLU:O	1:D:2208:MET:N	2.52	0.43
1:D:2357:LEU:HB3	1:D:2364:PHE:HE1	1.83	0.43
1:D:2782:ASP:OD1	1:D:2782:ASP:N	2.52	0.43
1:A:2301:TYR:HB3	1:A:2331:TYR:CE2	2.54	0.43
1:A:3575:LEU:HD23	1:B:1219:LEU:HD22	2.00	0.43
1:A:4745:LEU:H	1:A:4745:LEU:HG	1.55	0.43
1:B:113:HIS:NE2	1:B:399:GLN:O	2.51	0.43
1:B:2177:LEU:O	1:B:2181:SER:OG	2.36	0.43
1:C:1444:GLU:HG2	1:C:1446:SER:H	1.84	0.43
1:C:2766:TRP:HE1	1:C:2788:HIS:HB2	1.84	0.43
1:C:3264:THR:OG1	1:C:3265:GLU:OE1	2.36	0.43
1:C:4892:ARG:NH1	1:D:4895:GLY:O	2.48	0.43
1:D:113:HIS:NE2	1:D:399:GLN:O	2.51	0.43
1:D:683:ARG:HG2	1:D:717:ASP:HB3	2.00	0.43
1:D:2765:LYS:HA	1:D:2765:LYS:HD3	1.87	0.43
2:G:76:CYS:HB3	2:G:97:LEU:HB2	2.00	0.43
2:H:2:VAL:HG23	2:H:80:VAL:HG21	2.01	0.43
1:A:293:LEU:H	1:A:311:ALA:HB1	1.84	0.43
1:A:2591:ARG:HG2	1:A:2636:PHE:HB3	2.01	0.43
1:A:4977:THR:O	1:A:4981:GLU:HB2	2.19	0.43
1:B:765:GLN:NE2	1:B:1479:GLU:OE1	2.52	0.43
1:B:1000:ARG:HA	1:B:1000:ARG:HD3	1.82	0.43
1:B:1444:GLU:HG2	1:B:1446:SER:H	1.84	0.43
1:B:2009:LEU:HD23	1:B:2022:PRO:HD2	2.01	0.43
1:B:2301:TYR:HB3	1:B:2331:TYR:CE2	2.54	0.43
1:B:4686:LEU:O	1:B:4691:GLN:N	2.49	0.43
1:C:706:GLY:N	1:C:709:ASP:OD2	2.39	0.43
1:C:1007:TYR:O	1:C:1017:ARG:NH2	2.51	0.43
1:C:2911:LEU:HD13	1:C:2915:GLU:HG3	2.00	0.43
1:C:3901:ASN:OD1	1:C:3904:ARG:NH1	2.34	0.43
1:D:765:GLN:NE2	1:D:1479:GLU:OE1	2.52	0.43
1:D:3537:LYS:HZ1	1:D:3603:LEU:HB2	1.84	0.43
1:D:4991:PHE:HE2	1:D:5010:VAL:HG11	1.84	0.43
1:A:2948:THR:HG23	1:A:2952:GLU:HB2	2.01	0.42
1:A:3218:VAL:O	1:A:3222:LYS:HB2	2.18	0.42
1:A:3424:LEU:HD23	1:A:3424:LEU:HA	1.88	0.42
1:B:2251:PHE:HB2	1:B:2286:LEU:HD13	2.00	0.42
1:B:3106:MET:HG3	1:B:3110:LEU:HD13	2.01	0.42
1:B:3889:GLN:HG3	1:B:3967:GLU:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:452:PHE:HE1	1:C:474:ARG:HB3	1.83	0.42
1:C:1231[B]:GLN:H	1:C:1231[B]:GLN:HG3	1.61	0.42
1:C:2671:GLU:HA	1:C:2674:LEU:HB2	2.00	0.42
1:C:3218:VAL:HG22	1:C:3227:ARG:HD3	2.00	0.42
1:D:3218:VAL:HG22	1:D:3227:ARG:HD3	2.00	0.42
1:D:3927:GLN:HA	1:D:3930:ILE:HG22	2.01	0.42
1:D:4977:THR:O	1:D:4981:GLU:HB2	2.19	0.42
1:A:1219:LEU:HD22	1:D:3575:LEU:HD23	2.01	0.42
1:A:1444:GLU:HG2	1:A:1446:SER:H	1.84	0.42
1:A:2205:GLU:O	1:A:2208:MET:N	2.52	0.42
1:A:3106:MET:HG3	1:A:3110:LEU:HD13	2.01	0.42
1:B:1076:ARG:HB3	1:B:1191:VAL:HG23	2.01	0.42
1:B:1291:LEU:HD23	1:B:1291:LEU:HA	1.91	0.42
1:B:2671:GLU:HA	1:B:2674:LEU:HB2	2.00	0.42
1:B:2974:ILE:HD12	1:B:3053:ARG:HH12	1.84	0.42
1:B:4581:LYS:HE3	1:B:4581:LYS:HB3	1.82	0.42
1:B:4977:THR:O	1:B:4981:GLU:HB2	2.20	0.42
1:C:1066:GLN:HG3	1:C:1462:MET:HG2	2.01	0.42
1:C:2205:GLU:O	1:C:2208:MET:N	2.52	0.42
1:C:2301:TYR:HB3	1:C:2331:TYR:CE2	2.54	0.42
1:C:2476:ILE:HG23	1:C:2536:LEU:HD21	2.01	0.42
1:C:2519:LEU:HD12	1:C:2578:MET:HE1	2.01	0.42
1:C:4821:LYS:HB2	1:C:4821:LYS:HE2	1.54	0.42
1:C:4977:THR:O	1:C:4981:GLU:HB2	2.20	0.42
1:D:114:SER:HB2	1:D:116:MET:HG3	2.02	0.42
1:D:2355:ARG:HA	1:D:2358:ILE:HG12	1.99	0.42
1:D:3768:SER:HA	1:D:3771:HIS:CD2	2.54	0.42
1:A:823:LEU:HD22	1:A:1626:TRP:HB3	2.01	0.42
1:A:823:LEU:HD23	1:A:1617:THR:HB	2.01	0.42
1:A:1419:ASP:OD1	1:A:1421:ARG:NH1	2.50	0.42
1:A:2302:LEU:HD23	1:A:2363:CYS:HB3	2.02	0.42
1:A:2974:ILE:HD12	1:A:3053:ARG:HH12	1.84	0.42
1:A:3207:GLU:OE1	1:A:3280:TYR:OH	2.33	0.42
1:A:3335:MET:HE3	1:A:3338:LEU:HD23	2.00	0.42
1:A:3554:GLN:HA	1:A:3557:LEU:HG	2.02	0.42
1:A:3768:SER:HA	1:A:3771:HIS:CD2	2.54	0.42
1:B:1007:TYR:O	1:B:1017:ARG:NH2	2.51	0.42
1:B:2519:LEU:HD12	1:B:2578:MET:HE1	2.01	0.42
1:B:3157:ILE:HB	1:B:3202:PRO:HG3	2.00	0.42
1:B:3218:VAL:HG22	1:B:3227:ARG:HD3	2.01	0.42
1:B:3335:MET:HE3	1:B:3338:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4016:LEU:HD12	1:B:4016:LEU:HA	1.84	0.42
1:C:114:SER:HB2	1:C:116:MET:HG3	2.02	0.42
1:C:683:ARG:HG2	1:C:717:ASP:HB3	2.00	0.42
1:C:2159:LEU:HG	1:C:2163:ARG:HE	1.84	0.42
1:C:2175:GLU:HG3	1:C:2228:MET:HB2	2.00	0.42
1:C:3159:ASP:OD1	1:C:3159:ASP:N	2.46	0.42
1:C:3768:SER:HA	1:C:3771:HIS:CD2	2.54	0.42
1:C:4092:ASP:HA	1:C:4095:LYS:HG2	2.02	0.42
1:D:823:LEU:HD23	1:D:1617:THR:HB	2.01	0.42
1:D:1444:GLU:HG2	1:D:1446:SER:H	1.84	0.42
1:D:2009:LEU:HD23	1:D:2022:PRO:HD2	2.01	0.42
1:D:2302:LEU:HD23	1:D:2363:CYS:HB3	2.02	0.42
1:D:2591:ARG:HG2	1:D:2636:PHE:HB3	2.00	0.42
1:D:2948:THR:HG23	1:D:2952:GLU:HB2	2.01	0.42
1:D:3321:ARG:HA	1:D:3324:VAL:HG12	2.00	0.42
2:F:2:VAL:HG23	2:F:80:VAL:HG21	2.01	0.42
1:A:2624:ARG:HD2	1:A:2906:VAL:HG11	2.02	0.42
1:A:2867:LEU:HD12	1:A:2928:LYS:HZ3	1.84	0.42
1:A:3592:ILE:HG22	1:A:3595:ARG:HH21	1.83	0.42
1:B:293:LEU:H	1:B:311:ALA:HB1	1.84	0.42
1:B:869:ARG:CZ	1:B:870:ILE:HB	2.50	0.42
1:B:884:LEU:HD13	1:B:968:ALA:H	1.84	0.42
1:C:765:GLN:NE2	1:C:1479:GLU:OE1	2.52	0.42
1:C:884:LEU:HD13	1:C:968:ALA:H	1.84	0.42
1:C:2974:ILE:HD12	1:C:3053:ARG:HH12	1.84	0.42
1:C:3889:GLN:HG3	1:C:3967:GLU:HG3	2.01	0.42
1:C:4814:LEU:HD23	1:C:4814:LEU:HA	1.89	0.42
1:C:4991:PHE:HE2	1:C:5010:VAL:HG11	1.84	0.42
1:D:2159:LEU:HG	1:D:2163:ARG:HE	1.84	0.42
1:D:2175:GLU:HG3	1:D:2228:MET:HB2	2.00	0.42
2:F:76:CYS:HB3	2:F:97:LEU:HB2	2.00	0.42
1:A:1076:ARG:HB3	1:A:1191:VAL:HG23	2.01	0.42
1:A:3264:THR:OG1	1:A:3265:GLU:OE1	2.36	0.42
1:B:30:LYS:HA	1:B:30:LYS:HD2	1.80	0.42
1:B:1066:GLN:HG3	1:B:1462:MET:HG2	2.01	0.42
1:B:2158:CYS:O	1:B:2162:ILE:HG12	2.19	0.42
1:B:2302:LEU:HD23	1:B:2363:CYS:HB3	2.02	0.42
1:B:3227:ARG:HA	1:B:3232:LEU:HD12	2.01	0.42
1:C:2302:LEU:HD23	1:C:2363:CYS:HB3	2.02	0.42
1:C:4184:MET:N	1:C:5021:PHE:O	2.50	0.42
1:C:5030:LYS:HE2	1:C:5030:LYS:HB2	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:828:GLU:O	1:D:1073:ARG:NH1	2.53	0.42
1:D:878:ILE:HD11	1:D:925:SER:HB2	2.02	0.42
1:A:30:LYS:HD2	1:A:30:LYS:HA	1.79	0.42
1:A:878:ILE:HD11	1:A:925:SER:HB2	2.02	0.42
1:A:884:LEU:HD13	1:A:968:ALA:H	1.84	0.42
1:A:3927:GLN:HA	1:A:3930:ILE:HG22	2.01	0.42
1:A:4991:PHE:HE2	1:A:5010:VAL:HG11	1.84	0.42
1:B:199:LEU:HD12	1:B:199:LEU:HA	1.90	0.42
1:C:863:LEU:HA	1:C:864:PRO:HD3	1.85	0.42
1:C:3157:ILE:HB	1:C:3202:PRO:HG3	2.00	0.42
1:C:3288:GLY:HA2	1:C:3303:PRO:HB3	2.01	0.42
1:D:1007:TYR:O	1:D:1017:ARG:NH2	2.51	0.42
1:D:2686:LEU:HB3	1:D:2997:PHE:HE1	1.83	0.42
1:A:1066:GLN:HG3	1:A:1462:MET:HG2	2.01	0.42
1:A:2009:LEU:HD23	1:A:2022:PRO:HD2	2.01	0.42
1:A:2911:LEU:HD13	1:A:2915:GLU:HG3	2.00	0.42
1:A:2930:LEU:O	1:A:2935:TYR:N	2.49	0.42
1:A:3218:VAL:HG22	1:A:3227:ARG:HD3	2.00	0.42
1:A:3288:GLY:HA2	1:A:3303:PRO:HB3	2.01	0.42
1:A:3582:ARG:HD3	1:A:3582:ARG:HA	1.88	0.42
1:B:114:SER:HB2	1:B:116:MET:HG3	2.02	0.42
1:B:2039:LEU:HD22	1:B:2044:ILE:HG13	2.02	0.42
1:B:2175:GLU:HG3	1:B:2228:MET:HB2	2.00	0.42
1:B:2472:LEU:HA	1:B:2472:LEU:HD23	1.87	0.42
1:C:2867:LEU:HD12	1:C:2928:LYS:HZ3	1.85	0.42
1:C:3207:GLU:OE1	1:C:3280:TYR:OH	2.33	0.42
1:C:3927:GLN:HA	1:C:3930:ILE:HG22	2.01	0.42
1:C:4827:LEU:HD23	1:C:4827:LEU:HA	1.89	0.42
1:C:4976:GLU:H	1:C:4976:GLU:HG2	1.59	0.42
1:D:124:SER:HB2	1:D:133:PHE:HA	2.01	0.42
1:D:1434:TYR:HA	1:D:1518:CYS:O	2.20	0.42
1:D:2158:CYS:O	1:D:2162:ILE:HG12	2.19	0.42
1:D:2301:TYR:HB3	1:D:2331:TYR:CE2	2.54	0.42
1:D:2624:ARG:HD2	1:D:2906:VAL:HG11	2.02	0.42
1:D:2867:LEU:HD12	1:D:2928:LYS:HZ3	1.85	0.42
1:D:3175:LEU:O	1:D:3178:THR:OG1	2.33	0.42
1:D:3335:MET:HE3	1:D:3338:LEU:HD23	2.02	0.42
1:D:4092:ASP:HA	1:D:4095:LYS:HG2	2.02	0.42
2:G:2:VAL:HG23	2:G:80:VAL:HG21	2.01	0.42
1:A:765:GLN:NE2	1:A:1479:GLU:OE1	2.52	0.42
1:A:2039:LEU:HD22	1:A:2044:ILE:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2159:LEU:HG	1:A:2163:ARG:HE	1.84	0.42
1:A:2580:ASP:HB2	1:A:2618:MET:HE1	2.02	0.42
1:A:3157:ILE:HB	1:A:3202:PRO:HG3	2.00	0.42
1:A:3889:GLN:HG3	1:A:3967:GLU:HG3	2.01	0.42
1:B:2357:LEU:HB3	1:B:2364:PHE:HE1	1.83	0.42
1:B:2825:LYS:NZ	1:B:2935:TYR:OH	2.45	0.42
1:B:2902:HIS:HB3	1:B:2905:LEU:HG	2.02	0.42
1:B:3554:GLN:HA	1:B:3557:LEU:HG	2.01	0.42
1:B:3710:LEU:HD21	1:B:3781:GLN:HG2	2.02	0.42
1:B:4092:ASP:HA	1:B:4095:LYS:HG2	2.02	0.42
1:C:124:SER:HB2	1:C:133:PHE:HA	2.01	0.42
1:C:293:LEU:H	1:C:311:ALA:HB1	1.84	0.42
1:D:699:GLY:N	1:D:1647:CYS:O	2.50	0.42
1:D:2766:TRP:HE1	1:D:2788:HIS:HB2	1.84	0.42
1:A:1773:PRO:HA	1:A:1774:PRO:HD3	1.94	0.42
1:C:1253:PRO:HG2	1:C:1254:HIS:CD2	2.55	0.42
1:C:3648:ARG:O	1:C:3652:MET:HG2	2.20	0.42
1:D:59:PRO:HD3	1:D:307:ALA:HB3	2.02	0.42
1:D:823:LEU:HD22	1:D:1626:TRP:HB3	2.01	0.42
1:D:1066:GLN:HG3	1:D:1462:MET:HG2	2.01	0.42
1:D:1253:PRO:HG2	1:D:1254:HIS:CD2	2.55	0.42
1:D:1773:PRO:HA	1:D:1774:PRO:HD3	1.94	0.42
1:D:2911:LEU:HD13	1:D:2915:GLU:HG3	2.00	0.42
1:D:4865:LYS:HA	1:D:4865:LYS:HD2	1.49	0.42
1:A:3575:LEU:HD12	1:A:3575:LEU:HA	1.93	0.42
1:A:4645:CYS:SG	1:A:4646:LEU:N	2.93	0.42
1:B:418:LEU:HD11	1:B:494:LEU:HD22	2.02	0.42
1:B:2948:THR:HG23	1:B:2952:GLU:HB2	2.01	0.42
1:B:3376:GLU:O	1:B:3380:ARG:HG2	2.20	0.42
1:B:3539:ARG:NH1	1:B:3553:LEU:HG	2.35	0.42
1:B:3648:ARG:O	1:B:3652:MET:HG2	2.20	0.42
1:B:4645:CYS:SG	1:B:4646:LEU:N	2.93	0.42
1:B:4670:ILE:HB	1:B:4714:ASN:HD22	1.84	0.42
1:B:4991:PHE:HE2	1:B:5010:VAL:HG11	1.84	0.42
1:C:869:ARG:CZ	1:C:870:ILE:HB	2.50	0.42
1:C:878:ILE:HD11	1:C:925:SER:HB2	2.02	0.42
1:C:1773:PRO:HA	1:C:1774:PRO:HD3	1.94	0.42
1:C:2782:ASP:OD1	1:C:2782:ASP:N	2.52	0.42
1:C:3965:LEU:HD23	1:C:3965:LEU:HA	1.94	0.42
1:D:3106:MET:HG3	1:D:3110:LEU:HD13	2.01	0.42
1:A:114:SER:HB2	1:A:116:MET:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1253:PRO:HG2	1:A:1254:HIS:CD2	2.55	0.41
1:B:1290:ARG:HH12	1:B:1455:PRO:HA	1.85	0.41
1:B:1434:TYR:HA	1:B:1518:CYS:O	2.20	0.41
1:B:3033:ASN:O	1:B:3037:GLU:HG2	2.21	0.41
1:B:3823:LYS:HA	1:B:3823:LYS:HD3	1.83	0.41
1:C:1434:TYR:HA	1:C:1518:CYS:O	2.20	0.41
1:C:3106:MET:HG3	1:C:3110:LEU:HD13	2.01	0.41
1:C:3335:MET:HE3	1:C:3338:LEU:HD23	2.02	0.41
1:D:293:LEU:H	1:D:311:ALA:HB1	1.84	0.41
1:D:869:ARG:CZ	1:D:870:ILE:HB	2.50	0.41
1:D:3889:GLN:HG3	1:D:3967:GLU:HG3	2.02	0.41
1:A:828:GLU:O	1:A:1073:ARG:NH1	2.53	0.41
1:A:1568:LYS:O	1:A:1569:GLN:NE2	2.53	0.41
1:A:2614:ILE:O	1:A:2650:ARG:NH2	2.43	0.41
1:B:878:ILE:HD11	1:B:925:SER:HB2	2.02	0.41
1:B:2624:ARG:HD2	1:B:2906:VAL:HG11	2.02	0.41
1:B:3227:ARG:NH1	1:B:3234:ASN:OD1	2.37	0.41
1:B:3768:SER:HA	1:B:3771:HIS:CD2	2.54	0.41
1:C:418:LEU:HD11	1:C:494:LEU:HD22	2.02	0.41
1:C:2624:ARG:HD2	1:C:2906:VAL:HG11	2.02	0.41
1:C:2948:THR:HG23	1:C:2952:GLU:HB2	2.01	0.41
1:C:3033:ASN:O	1:C:3037:GLU:HG2	2.21	0.41
1:C:4835:LYS:HE2	1:C:4835:LYS:HB3	1.56	0.41
1:D:1568:LYS:O	1:D:1569:GLN:NE2	2.53	0.41
1:D:1749:PRO:HA	1:D:1750:PRO:HD3	1.95	0.41
1:A:124:SER:HB2	1:A:133:PHE:HA	2.01	0.41
1:A:2454:ARG:CZ	1:A:2458:ARG:HH21	2.34	0.41
1:A:4686:LEU:O	1:A:4691:GLN:N	2.49	0.41
1:A:4995:LEU:HD23	1:A:4995:LEU:HA	1.93	0.41
1:B:2682:ILE:HD13	1:B:2682:ILE:HA	1.93	0.41
1:B:3160:ASP:OD1	1:B:3160:ASP:N	2.53	0.41
1:B:3288:GLY:HA2	1:B:3303:PRO:HB3	2.01	0.41
1:B:3467:MET:O	1:B:3471:THR:OG1	2.37	0.41
1:C:1849:LEU:HD23	1:C:1849:LEU:HA	1.87	0.41
1:C:2454:ARG:CZ	1:C:2458:ARG:HH21	2.34	0.41
1:C:3823:LYS:HD3	1:C:3823:LYS:HA	1.83	0.41
1:D:1076:ARG:HB3	1:D:1191:VAL:HG23	2.01	0.41
1:D:3288:GLY:HA2	1:D:3303:PRO:HB3	2.01	0.41
1:D:3554:GLN:HA	1:D:3557:LEU:HG	2.02	0.41
1:B:823:LEU:HD22	1:B:1626:TRP:HB3	2.01	0.41
1:B:2454:ARG:CZ	1:B:2458:ARG:HH21	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3628:ARG:NH2	1:B:3857:GLY:O	2.54	0.41
1:B:3693:LYS:HA	1:B:3693:LYS:HD2	1.78	0.41
1:C:59:PRO:HD3	1:C:307:ALA:HB3	2.02	0.41
1:C:129:ASP:N	1:C:129:ASP:OD1	2.54	0.41
1:C:823:LEU:HD22	1:C:1626:TRP:HB3	2.01	0.41
1:C:1076:ARG:HB3	1:C:1191:VAL:HG23	2.01	0.41
1:C:1290:ARG:HH12	1:C:1455:PRO:HA	1.85	0.41
1:C:2902:HIS:HB3	1:C:2905:LEU:HG	2.02	0.41
1:C:3272:ILE:O	1:C:3276:MET:HG2	2.20	0.41
1:D:531:ARG:NH2	1:D:562:GLU:OE2	2.37	0.41
1:D:2476:ILE:HG23	1:D:2536:LEU:HD21	2.01	0.41
1:D:2974:ILE:HD12	1:D:3053:ARG:HH12	1.84	0.41
1:D:4995:LEU:HD23	1:D:4995:LEU:HA	1.94	0.41
1:A:59:PRO:HD3	1:A:307:ALA:HB3	2.02	0.41
1:A:1863:LEU:HB3	1:A:1871:PHE:HD2	1.86	0.41
1:A:4944:ARG:NH2	1:B:4938:ASP:O	2.54	0.41
1:B:220:LEU:HB2	1:B:391:THR:O	2.20	0.41
1:B:3175:LEU:O	1:B:3178:THR:OG1	2.33	0.41
1:C:137:LEU:HD23	1:C:137:LEU:HA	1.87	0.41
1:C:531:ARG:NH2	1:C:562:GLU:OE2	2.37	0.41
1:C:3376:GLU:O	1:C:3380:ARG:HG2	2.20	0.41
1:D:3272:ILE:O	1:D:3276:MET:HG2	2.20	0.41
1:D:3376:GLU:O	1:D:3380:ARG:HG2	2.20	0.41
1:D:3823:LYS:HD3	1:D:3823:LYS:HA	1.83	0.41
1:D:4843:LEU:O	1:D:4847:VAL:HG13	2.21	0.41
1:A:418:LEU:HD11	1:A:494:LEU:HD22	2.02	0.41
1:A:823:LEU:HD12	1:A:823:LEU:HA	1.89	0.41
1:A:3033:ASN:O	1:A:3037:GLU:HG2	2.20	0.41
1:A:3539:ARG:NH1	1:A:3553:LEU:HG	2.35	0.41
1:A:4092:ASP:HA	1:A:4095:LYS:HG2	2.02	0.41
1:A:4843:LEU:O	1:A:4847:VAL:HG13	2.21	0.41
1:B:828:GLU:O	1:B:1073:ARG:NH1	2.53	0.41
1:B:1229:ASN:HB2	1:B:1827:ARG:HG3	2.03	0.41
1:B:3927:GLN:HA	1:B:3930:ILE:HG22	2.01	0.41
1:C:1863:LEU:HB3	1:C:1871:PHE:HD2	1.86	0.41
1:D:137:LEU:HA	1:D:137:LEU:HD23	1.88	0.41
1:D:418:LEU:HD11	1:D:494:LEU:HD22	2.02	0.41
1:D:873:LYS:HG2	1:D:970:LEU:HD13	2.02	0.41
1:D:884:LEU:HD13	1:D:968:ALA:H	1.84	0.41
1:D:1088:TRP:HB2	1:D:1153:ILE:HG22	2.01	0.41
1:D:2825:LYS:NZ	1:D:2935:TYR:OH	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:LEU:HB2	1:A:391:THR:O	2.20	0.41
1:A:2806:ARG:HD2	1:A:2810:LYS:HZ3	1.86	0.41
1:A:3062:PRO:HA	1:A:3065:VAL:HG22	2.03	0.41
1:A:3373:VAL:HG11	1:A:3444:TYR:HB3	2.03	0.41
1:B:129:ASP:N	1:B:129:ASP:OD1	2.54	0.41
1:B:932:LEU:HD22	1:B:984:LEU:HD21	2.03	0.41
1:C:49:LEU:HD23	1:C:49:LEU:HA	1.93	0.41
1:C:1243:PRO:O	1:C:1458:HIS:ND1	2.33	0.41
1:C:2158:CYS:O	1:C:2162:ILE:HG12	2.19	0.41
1:C:2866:THR:OG1	1:C:2867:LEU:N	2.54	0.41
1:C:3883:ASP:HA	1:C:3886:ARG:HB3	2.03	0.41
1:D:2454:ARG:CZ	1:D:2458:ARG:HH21	2.34	0.41
1:D:3648:ARG:O	1:D:3652:MET:HG2	2.20	0.41
1:A:869:ARG:CZ	1:A:870:ILE:HB	2.50	0.41
1:A:1259:ARG:HH12	1:A:1596:GLU:HA	1.85	0.41
1:A:1434:TYR:HA	1:A:1518:CYS:O	2.20	0.41
1:A:2866:THR:OG1	1:A:2867:LEU:N	2.54	0.41
1:A:3659:ALA:HA	1:A:3663:LEU:HD12	2.03	0.41
1:A:3694:LYS:HA	1:A:3695:PRO:HD3	1.90	0.41
1:A:3937:TYR:O	1:A:4002:LYS:NZ	2.44	0.41
1:B:2930:LEU:O	1:B:2935:TYR:N	2.49	0.41
1:C:113:HIS:NE2	1:C:399:GLN:O	2.51	0.41
1:C:2039:LEU:HD22	1:C:2044:ILE:HG13	2.02	0.41
1:C:3582:ARG:HD3	1:C:3582:ARG:HA	1.87	0.41
1:D:129:ASP:OD1	1:D:129:ASP:N	2.54	0.41
1:D:2039:LEU:HD22	1:D:2044:ILE:HG13	2.02	0.41
1:D:2656:CYS:SG	1:D:3013:HIS:NE2	2.93	0.41
1:D:3033:ASN:O	1:D:3037:GLU:HG2	2.21	0.41
1:D:3659:ALA:HA	1:D:3663:LEU:HD12	2.03	0.41
1:A:137:LEU:HD23	1:A:137:LEU:HA	1.87	0.41
1:A:873:LYS:HG2	1:A:970:LEU:HD13	2.02	0.41
1:A:1088:TRP:HB2	1:A:1153:ILE:HG22	2.01	0.41
1:A:2017:ASP:OD1	1:A:2017:ASP:N	2.54	0.41
1:A:2476:ILE:HG23	1:A:2536:LEU:HD21	2.01	0.41
1:A:2765:LYS:HA	1:A:2765:LYS:HD3	1.87	0.41
1:A:3272:ILE:O	1:A:3276:MET:HG2	2.20	0.41
1:A:3376:GLU:O	1:A:3380:ARG:HG2	2.20	0.41
1:A:3628:ARG:NH2	1:A:3857:GLY:O	2.54	0.41
1:A:3710:LEU:HD21	1:A:3781:GLN:HG2	2.02	0.41
1:A:3883:ASP:HA	1:A:3886:ARG:HB3	2.03	0.41
1:A:3965:LEU:HD23	1:A:3965:LEU:HA	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4850:LEU:HD23	1:A:4850:LEU:HA	1.93	0.41
1:B:1253:PRO:HG2	1:B:1254:HIS:CD2	2.55	0.41
1:B:1568:LYS:O	1:B:1569:GLN:NE2	2.53	0.41
1:B:3062:PRO:HA	1:B:3065:VAL:HG22	2.03	0.41
1:B:3703:LEU:HD23	1:B:3703:LEU:HA	1.93	0.41
1:B:3901:ASN:OD1	1:B:3904:ARG:NH1	2.34	0.41
1:C:547:VAL:HB	1:C:560:ILE:HD11	2.03	0.41
1:C:829:TYR:HB3	1:C:1073:ARG:HH11	1.86	0.41
1:C:1088:TRP:HB2	1:C:1153:ILE:HG22	2.02	0.41
1:C:1433:TYR:HB3	1:C:1575:LEU:HD23	2.03	0.41
1:C:1446:SER:O	1:C:1496:TRP:NE1	2.43	0.41
1:C:1842:LEU:HD23	1:C:1842:LEU:HA	1.95	0.41
1:C:2580:ASP:HB2	1:C:2618:MET:HE1	2.03	0.41
1:C:2971:GLN:HG2	1:C:3045:LYS:NZ	2.36	0.41
1:C:3539:ARG:NH1	1:C:3553:LEU:HG	2.35	0.41
1:C:3554:GLN:HA	1:C:3557:LEU:HG	2.02	0.41
1:D:49:LEU:HD23	1:D:49:LEU:HA	1.93	0.41
1:D:2472:LEU:HD23	1:D:2472:LEU:HA	1.87	0.41
1:D:2902:HIS:HB3	1:D:2905:LEU:HG	2.02	0.41
1:D:4645:CYS:SG	1:D:4646:LEU:N	2.93	0.41
1:A:2902:HIS:HB3	1:A:2905:LEU:HG	2.02	0.41
1:A:3562:LYS:HE2	1:A:3562:LYS:HB2	1.92	0.41
1:B:865:PRO:HA	1:B:868:GLU:HG2	2.03	0.41
1:B:1433:TYR:HB3	1:B:1575:LEU:HD23	2.03	0.41
1:B:2531:ARG:HH22	1:B:2581:SER:HB2	1.85	0.41
1:B:2640:PRO:HA	1:B:2643:LEU:HB3	2.03	0.41
1:B:4813:LEU:O	1:B:4816:ILE:HG12	2.20	0.41
1:C:865:PRO:HA	1:C:868:GLU:HG2	2.03	0.41
1:C:1229:ASN:HB2	1:C:1827:ARG:HG3	2.03	0.41
1:C:1259:ARG:HH12	1:C:1596:GLU:HA	1.85	0.41
1:C:3826:VAL:HG12	1:C:3830:GLN:HG3	2.03	0.41
1:C:4813:LEU:O	1:C:4816:ILE:HG12	2.20	0.41
1:D:547:VAL:HB	1:D:560:ILE:HD11	2.03	0.41
1:D:1126:GLY:HA3	1:D:1143:TRP:CZ3	2.56	0.41
1:D:2710:LEU:HA	1:D:2711:PRO:HD3	1.98	0.41
1:D:3201:MET:HG2	1:D:3203:VAL:H	1.86	0.41
1:D:3628:ARG:NH2	1:D:3857:GLY:O	2.54	0.41
1:D:3852:LYS:HE3	1:D:3852:LYS:HB3	1.94	0.41
1:A:1433:TYR:HB3	1:A:1575:LEU:HD23	2.03	0.40
1:A:2656:CYS:SG	1:A:3013:HIS:NE2	2.93	0.40
1:A:3201:MET:HG2	1:A:3203:VAL:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3537:LYS:HZ1	1:A:3603:LEU:HB2	1.86	0.40
1:A:3648:ARG:O	1:A:3652:MET:HG2	2.20	0.40
1:A:3826:VAL:HG12	1:A:3830:GLN:HG3	2.03	0.40
1:A:4581:LYS:HE3	1:A:4581:LYS:HB3	1.82	0.40
1:A:4918:ILE:HD11	1:D:4888:TYR:HA	2.03	0.40
1:B:1863:LEU:HB3	1:B:1871:PHE:HD2	1.86	0.40
1:B:2159:LEU:HD21	1:B:2163:ARG:HH21	1.86	0.40
1:B:2710:LEU:HA	1:B:2711:PRO:HD3	1.98	0.40
1:B:3965:LEU:HD23	1:B:3965:LEU:HA	1.94	0.40
1:C:220:LEU:HB2	1:C:391:THR:O	2.20	0.40
1:C:2531:ARG:HH22	1:C:2581:SER:HB2	1.85	0.40
1:C:3062:PRO:HA	1:C:3065:VAL:HG22	2.03	0.40
1:C:3628:ARG:NH2	1:C:3857:GLY:O	2.54	0.40
1:C:4577:LEU:HD12	1:C:4577:LEU:HA	1.94	0.40
1:D:220:LEU:HB2	1:D:391:THR:O	2.20	0.40
1:D:1259:ARG:HH12	1:D:1596:GLU:HA	1.85	0.40
1:D:1488:LYS:HB2	1:D:1488:LYS:HE3	1.86	0.40
1:D:2531:ARG:HH22	1:D:2581:SER:HB2	1.85	0.40
1:D:3710:LEU:HD21	1:D:3781:GLN:HG2	2.02	0.40
1:A:1290:ARG:HH12	1:A:1455:PRO:HA	1.85	0.40
1:A:3390:GLY:HA2	1:A:3393:LEU:HD13	2.04	0.40
1:A:3601:ALA:O	1:A:3605:HIS:ND1	2.40	0.40
1:A:4555:LEU:HD12	1:A:4555:LEU:HA	1.94	0.40
1:A:4666:VAL:O	1:A:4670:ILE:HG12	2.21	0.40
1:A:4813:LEU:O	1:A:4816:ILE:HG12	2.20	0.40
1:B:1088:TRP:HB2	1:B:1153:ILE:HG22	2.02	0.40
1:B:1259:ARG:HH12	1:B:1596:GLU:HA	1.85	0.40
1:B:2866:THR:OG1	1:B:2867:LEU:N	2.54	0.40
1:B:3201:MET:HG2	1:B:3203:VAL:H	1.86	0.40
1:B:3272:ILE:O	1:B:3276:MET:HG2	2.20	0.40
1:B:4745:LEU:H	1:B:4745:LEU:HG	1.55	0.40
1:C:1568:LYS:O	1:C:1569:GLN:NE2	2.53	0.40
1:C:1776:HIS:HB3	1:C:1798:LEU:HD13	2.04	0.40
1:C:3573:MET:HB3	1:C:3577:ARG:NH2	2.36	0.40
1:C:4686:LEU:O	1:C:4691:GLN:N	2.49	0.40
1:D:2159:LEU:HD21	1:D:2163:ARG:HH21	1.86	0.40
1:D:2640:PRO:HA	1:D:2643:LEU:HB3	2.03	0.40
1:D:4152:GLU:OE1	1:D:4192:ARG:NH1	2.51	0.40
1:D:4976:GLU:H	1:D:4976:GLU:HG2	1.59	0.40
1:A:3160:ASP:OD1	1:A:3160:ASP:N	2.53	0.40
1:A:4843:LEU:HD22	1:D:4823:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:PRO:HD3	1:B:307:ALA:HB3	2.02	0.40
1:B:873:LYS:HG2	1:B:970:LEU:HD13	2.02	0.40
1:B:2765:LYS:HA	1:B:2765:LYS:HD3	1.87	0.40
1:B:4000:MET:HG2	1:B:4016:LEU:HD23	2.04	0.40
1:C:2640:PRO:HA	1:C:2643:LEU:HB3	2.04	0.40
1:C:3201:MET:HG2	1:C:3203:VAL:H	1.86	0.40
1:C:4016:LEU:HD12	1:C:4016:LEU:HA	1.84	0.40
1:D:179:TYR:N	1:D:194:SER:O	2.54	0.40
1:D:1776:HIS:HB3	1:D:1798:LEU:HD13	2.04	0.40
1:D:1849:LEU:HD23	1:D:1849:LEU:HA	1.87	0.40
1:D:3573:MET:HB3	1:D:3577:ARG:NH2	2.36	0.40
1:D:3826:VAL:HG12	1:D:3830:GLN:HG3	2.04	0.40
1:D:4993:MET:HE2	1:D:4993:MET:HB3	2.00	0.40
1:A:129:ASP:OD1	1:A:129:ASP:N	2.54	0.40
1:A:2825:LYS:NZ	1:A:2935:TYR:OH	2.45	0.40
1:A:3901:ASN:OD1	1:A:3904:ARG:NH1	2.34	0.40
1:B:647:ASN:ND2	1:B:824:GLU:OE2	2.54	0.40
1:B:1776:HIS:HB3	1:B:1798:LEU:HD13	2.04	0.40
1:B:2325:PRO:HB2	1:B:2421:ALA:HB1	2.04	0.40
1:C:484:LEU:HD21	1:C:540:PHE:HE1	1.87	0.40
1:C:873:LYS:HG2	1:C:970:LEU:HD13	2.02	0.40
1:C:932:LEU:HD22	1:C:984:LEU:HD21	2.03	0.40
1:D:144:GLU:HG3	1:D:175:SER:HB3	2.04	0.40
1:D:647:ASN:ND2	1:D:824:GLU:OE2	2.54	0.40
1:D:1229:ASN:HB2	1:D:1827:ARG:HG3	2.03	0.40
1:D:1863:LEU:HB3	1:D:1871:PHE:HD2	1.86	0.40
1:D:3390:GLY:HA2	1:D:3393:LEU:HD13	2.04	0.40
1:D:3539:ARG:NH1	1:D:3553:LEU:HG	2.35	0.40
1:D:4000:MET:HG2	1:D:4016:LEU:HD23	2.04	0.40
1:D:4813:LEU:O	1:D:4816:ILE:HG12	2.20	0.40
1:D:4869:GLU:H	1:D:4869:GLU:HG2	1.74	0.40
1:D:5012:LYS:HD3	1:D:5012:LYS:HA	1.64	0.40
1:A:547:VAL:HB	1:A:560:ILE:HD11	2.03	0.40
1:A:2159:LEU:HD21	1:A:2163:ARG:HH21	1.86	0.40
1:B:317:ARG:HH12	1:B:349:GLN:N	2.20	0.40
1:B:880:GLU:HB3	1:B:883:ALA:HB3	2.03	0.40
1:B:2017:ASP:OD1	1:B:2017:ASP:N	2.54	0.40
1:B:3717:ASP:N	1:B:3717:ASP:OD1	2.54	0.40
1:C:266:ARG:NH2	1:C:331:VAL:O	2.51	0.40
1:C:2325:PRO:HB2	1:C:2421:ALA:HB1	2.04	0.40
1:C:3710:LEU:HD21	1:C:3781:GLN:HG2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4801:LEU:HD23	1:C:4801:LEU:HA	1.87	0.40
1:D:1290:ARG:HH12	1:D:1455:PRO:HA	1.85	0.40
1:D:1445:PRO:HG2	1:D:1501:VAL:HG11	2.04	0.40
1:D:3062:PRO:HA	1:D:3065:VAL:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4353/5037 (86%)	4199 (96%)	149 (3%)	5 (0%)	48	78
1	B	4353/5037 (86%)	4199 (96%)	149 (3%)	5 (0%)	48	78
1	C	4353/5037 (86%)	4200 (96%)	148 (3%)	5 (0%)	48	78
1	D	4353/5037 (86%)	4199 (96%)	149 (3%)	5 (0%)	48	78
2	E	105/350 (30%)	102 (97%)	3 (3%)	0	100	100
2	F	105/350 (30%)	102 (97%)	3 (3%)	0	100	100
2	G	105/350 (30%)	102 (97%)	3 (3%)	0	100	100
2	H	105/350 (30%)	102 (97%)	3 (3%)	0	100	100
All	All	17832/21548 (83%)	17205 (96%)	607 (3%)	20 (0%)	50	78

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3692	GLU
1	A	4691	GLN
1	B	3692	GLU
1	B	4691	GLN
1	C	3692	GLU
1	C	4691	GLN

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Mol	Chain	Res	Type
1	D	3692	GLU
1	D	4691	GLN
1	A	4712	PRO
1	B	4712	PRO
1	C	4712	PRO
1	D	4712	PRO
1	A	4819	GLY
1	B	4819	GLY
1	C	4819	GLY
1	D	4819	GLY
1	A	3292	PRO
1	B	3292	PRO
1	C	3292	PRO
1	D	3292	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%)	3675 (97%)	130 (3%)	32	57
1	B	3805/4276 (89%)	3675 (97%)	130 (3%)	32	57
1	C	3805/4276 (89%)	3674 (97%)	131 (3%)	32	57
1	D	3805/4276 (89%)	3674 (97%)	131 (3%)	32	57
2	E	88/304 (29%)	87 (99%)	1 (1%)	70	81
2	F	88/304 (29%)	87 (99%)	1 (1%)	70	81
2	G	88/304 (29%)	87 (99%)	1 (1%)	70	81
2	H	88/304 (29%)	87 (99%)	1 (1%)	70	81
All	All	15572/18320 (85%)	15046 (97%)	526 (3%)	35	57

All (526) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	ARG

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Mol	Chain	Res	Type
1	A	373	LYS
1	A	392	ARG
1	A	846	LEU
1	A	1534	LYS
1	A	1743[A]	ARG
1	A	1743[B]	ARG
1	A	1752	ARG
1	A	2100[A]	HIS
1	A	2100[B]	HIS
1	A	2336	ARG
1	A	2369[A]	ARG
1	A	2369[B]	ARG
1	A	2690	LYS
1	A	2786	LYS
1	A	2827	ARG
1	A	2870[A]	GLU
1	A	2870[B]	GLU
1	A	2914	LYS
1	A	2985	ARG
1	A	3053	ARG
1	A	3185	LYS
1	A	3325	ASN
1	A	3453	ARG
1	A	3577	ARG
1	A	3614	LYS
1	A	3622	LYS
1	A	3688	GLU
1	A	4178	LEU
1	A	4180	ARG
1	A	4181	ILE
1	A	4183	ILE
1	A	4188	ARG
1	A	4190	ILE
1	A	4192	ARG
1	A	4196	GLU
1	A	4209	GLN
1	A	4212	GLU
1	A	4215	ARG
1	A	4224	GLU
1	A	4227	GLU
1	A	4230	LYS
1	A	4231	MET

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Mol	Chain	Res	Type
1	A	4244	GLU
1	A	4252	SER
1	A	4543	GLU
1	A	4544	LEU
1	A	4550	LYS
1	A	4555	LEU
1	A	4561	THR
1	A	4577	LEU
1	A	4578	LEU
1	A	4580	TYR
1	A	4581	LYS
1	A	4583	SER
1	A	4584	ASP
1	A	4627	MET
1	A	4628	VAL
1	A	4633	GLU
1	A	4635	SER
1	A	4639	MET
1	A	4645	CYS
1	A	4651	THR
1	A	4665	LYS
1	A	4667	PRO
1	A	4673	ARG
1	A	4679	ARG
1	A	4680	LYS
1	A	4689	THR
1	A	4695	ASP
1	A	4697	VAL
1	A	4704	LEU
1	A	4706	LEU
1	A	4707	ASN
1	A	4708	THR
1	A	4710	SER
1	A	4711	PHE
1	A	4713	SER
1	A	4716	TRP
1	A	4721	LYS
1	A	4730	ASP
1	A	4731	ILE
1	A	4743	MET
1	A	4745	LEU
1	A	4747	SER

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Mol	Chain	Res	Type
1	A	4749	GLU
1	A	4772	ASP
1	A	4773	VAL
1	A	4774	LYS
1	A	4777	ILE
1	A	4788	SER
1	A	4809	PHE
1	A	4818	MET
1	A	4821	LYS
1	A	4822	THR
1	A	4824	ARG
1	A	4835	LYS
1	A	4837	LEU
1	A	4844	LEU
1	A	4861	LYS
1	A	4865	LYS
1	A	4869	GLU
1	A	4871	GLU
1	A	4876	CYS
1	A	4887	MET
1	A	4889	VAL
1	A	4908	GLU
1	A	4913	ARG
1	A	4920	PHE
1	A	4927	ILE
1	A	4933	GLN
1	A	4945	ASP
1	A	4949	GLN
1	A	4951	LYS
1	A	4957	LYS
1	A	4966	ASP
1	A	4976	GLU
1	A	4980	LEU
1	A	4985	LEU
1	A	4989	MET
1	A	4992	LEU
1	A	4995	LEU
1	A	4997	ASN
1	A	4998	LYS
1	A	5004	THR
1	A	5006	GLN
1	A	5012	LYS

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Mol	Chain	Res	Type
1	A	5028	PHE
1	A	5030	LYS
1	A	5034	ASP
1	B	125	ARG
1	B	373	LYS
1	B	392	ARG
1	B	846	LEU
1	B	1534	LYS
1	B	1743[A]	ARG
1	B	1743[B]	ARG
1	B	1752	ARG
1	B	2100[A]	HIS
1	B	2100[B]	HIS
1	B	2336	ARG
1	B	2369[A]	ARG
1	B	2369[B]	ARG
1	B	2690	LYS
1	B	2786	LYS
1	B	2827	ARG
1	B	2870[A]	GLU
1	B	2870[B]	GLU
1	B	2914	LYS
1	B	2985	ARG
1	B	3053	ARG
1	B	3185	LYS
1	B	3325	ASN
1	B	3453	ARG
1	B	3577	ARG
1	B	3614	LYS
1	B	3622	LYS
1	B	3688	GLU
1	B	4178	LEU
1	B	4180	ARG
1	B	4181	ILE
1	B	4183	ILE
1	B	4188	ARG
1	B	4190	ILE
1	B	4192	ARG
1	B	4196	GLU
1	B	4209	GLN
1	B	4212	GLU
1	B	4215	ARG

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Mol	Chain	Res	Type
1	B	4224	GLU
1	B	4227	GLU
1	B	4230	LYS
1	B	4231	MET
1	B	4244	GLU
1	B	4252	SER
1	B	4543	GLU
1	B	4544	LEU
1	B	4550	LYS
1	B	4555	LEU
1	B	4561	THR
1	B	4577	LEU
1	B	4578	LEU
1	B	4580	TYR
1	B	4581	LYS
1	B	4583	SER
1	B	4584	ASP
1	B	4627	MET
1	B	4628	VAL
1	B	4633	GLU
1	B	4635	SER
1	B	4639	MET
1	B	4645	CYS
1	B	4651	THR
1	B	4665	LYS
1	B	4667	PRO
1	B	4673	ARG
1	B	4679	ARG
1	B	4680	LYS
1	B	4689	THR
1	B	4695	ASP
1	B	4697	VAL
1	B	4704	LEU
1	B	4706	LEU
1	B	4707	ASN
1	B	4708	THR
1	B	4710	SER
1	B	4711	PHE
1	B	4713	SER
1	B	4716	TRP
1	B	4721	LYS
1	B	4730	ASP

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Mol	Chain	Res	Type
1	B	4731	ILE
1	B	4743	MET
1	B	4745	LEU
1	B	4747	SER
1	B	4749	GLU
1	B	4772	ASP
1	B	4773	VAL
1	B	4774	LYS
1	B	4777	ILE
1	B	4788	SER
1	B	4809	PHE
1	B	4818	MET
1	B	4821	LYS
1	B	4822	THR
1	B	4824	ARG
1	B	4835	LYS
1	B	4837	LEU
1	B	4844	LEU
1	B	4861	LYS
1	B	4865	LYS
1	B	4869	GLU
1	B	4871	GLU
1	B	4876	CYS
1	B	4887	MET
1	B	4889	VAL
1	B	4908	GLU
1	B	4913	ARG
1	B	4920	PHE
1	B	4927	ILE
1	B	4933	GLN
1	B	4945	ASP
1	B	4949	GLN
1	B	4951	LYS
1	B	4957	LYS
1	B	4966	ASP
1	B	4976	GLU
1	B	4980	LEU
1	B	4985	LEU
1	B	4989	MET
1	B	4992	LEU
1	B	4995	LEU
1	B	4997	ASN

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Mol	Chain	Res	Type
1	B	4998	LYS
1	B	5004	THR
1	B	5006	GLN
1	B	5012	LYS
1	B	5028	PHE
1	B	5030	LYS
1	B	5034	ASP
1	C	125	ARG
1	C	373	LYS
1	C	392	ARG
1	C	846	LEU
1	C	1534	LYS
1	C	1743[A]	ARG
1	C	1743[B]	ARG
1	C	1752	ARG
1	C	2100[A]	HIS
1	C	2100[B]	HIS
1	C	2336	ARG
1	C	2369[A]	ARG
1	C	2369[B]	ARG
1	C	2690	LYS
1	C	2786	LYS
1	C	2827	ARG
1	C	2870[A]	GLU
1	C	2870[B]	GLU
1	C	2914	LYS
1	C	2985	ARG
1	C	3053	ARG
1	C	3185	LYS
1	C	3325	ASN
1	C	3453	ARG
1	C	3577	ARG
1	C	3614	LYS
1	C	3622	LYS
1	C	3688	GLU
1	C	4178	LEU
1	C	4180	ARG
1	C	4181	ILE
1	C	4183	ILE
1	C	4188	ARG
1	C	4190	ILE
1	C	4192	ARG

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Mol	Chain	Res	Type
1	C	4196	GLU
1	C	4209	GLN
1	C	4212	GLU
1	C	4215	ARG
1	C	4224	GLU
1	C	4227	GLU
1	C	4230	LYS
1	C	4231	MET
1	C	4244	GLU
1	C	4252	SER
1	C	4543	GLU
1	C	4544	LEU
1	C	4550	LYS
1	C	4555	LEU
1	C	4561	THR
1	C	4577	LEU
1	C	4578	LEU
1	C	4580	TYR
1	C	4581	LYS
1	C	4583	SER
1	C	4584	ASP
1	C	4627	MET
1	C	4628	VAL
1	C	4633	GLU
1	C	4635	SER
1	C	4639	MET
1	C	4645	CYS
1	C	4651	THR
1	C	4665	LYS
1	C	4667	PRO
1	C	4673	ARG
1	C	4679	ARG
1	C	4680	LYS
1	C	4689	THR
1	C	4695	ASP
1	C	4697	VAL
1	C	4704	LEU
1	C	4706	LEU
1	C	4707	ASN
1	C	4708	THR
1	C	4710	SER
1	C	4711	PHE

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Mol	Chain	Res	Type
1	C	4713	SER
1	C	4716	TRP
1	C	4721	LYS
1	C	4730	ASP
1	C	4731	ILE
1	C	4735	GLU
1	C	4743	MET
1	C	4745	LEU
1	C	4747	SER
1	C	4749	GLU
1	C	4772	ASP
1	C	4773	VAL
1	C	4774	LYS
1	C	4777	ILE
1	C	4788	SER
1	C	4809	PHE
1	C	4818	MET
1	C	4821	LYS
1	C	4822	THR
1	C	4824	ARG
1	C	4835	LYS
1	C	4837	LEU
1	C	4844	LEU
1	C	4861	LYS
1	C	4865	LYS
1	C	4869	GLU
1	C	4871	GLU
1	C	4876	CYS
1	C	4887	MET
1	C	4889	VAL
1	C	4908	GLU
1	C	4913	ARG
1	C	4920	PHE
1	C	4927	ILE
1	C	4933	GLN
1	C	4945	ASP
1	C	4949	GLN
1	C	4951	LYS
1	C	4957	LYS
1	C	4966	ASP
1	C	4976	GLU
1	C	4980	LEU

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Mol	Chain	Res	Type
1	C	4985	LEU
1	C	4989	MET
1	C	4992	LEU
1	C	4995	LEU
1	C	4997	ASN
1	C	4998	LYS
1	C	5004	THR
1	C	5006	GLN
1	C	5012	LYS
1	C	5028	PHE
1	C	5030	LYS
1	C	5034	ASP
1	D	125	ARG
1	D	373	LYS
1	D	392	ARG
1	D	846	LEU
1	D	1534	LYS
1	D	1743[A]	ARG
1	D	1743[B]	ARG
1	D	1752	ARG
1	D	2100[A]	HIS
1	D	2100[B]	HIS
1	D	2336	ARG
1	D	2369[A]	ARG
1	D	2369[B]	ARG
1	D	2690	LYS
1	D	2786	LYS
1	D	2827	ARG
1	D	2870[A]	GLU
1	D	2870[B]	GLU
1	D	2914	LYS
1	D	2985	ARG
1	D	3053	ARG
1	D	3185	LYS
1	D	3325	ASN
1	D	3453	ARG
1	D	3577	ARG
1	D	3614	LYS
1	D	3622	LYS
1	D	3688	GLU
1	D	4178	LEU
1	D	4180	ARG

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Mol	Chain	Res	Type
1	D	4181	ILE
1	D	4183	ILE
1	D	4188	ARG
1	D	4190	ILE
1	D	4192	ARG
1	D	4196	GLU
1	D	4209	GLN
1	D	4212	GLU
1	D	4215	ARG
1	D	4224	GLU
1	D	4227	GLU
1	D	4230	LYS
1	D	4231	MET
1	D	4244	GLU
1	D	4252	SER
1	D	4543	GLU
1	D	4544	LEU
1	D	4550	LYS
1	D	4555	LEU
1	D	4561	THR
1	D	4577	LEU
1	D	4578	LEU
1	D	4580	TYR
1	D	4581	LYS
1	D	4583	SER
1	D	4584	ASP
1	D	4627	MET
1	D	4628	VAL
1	D	4633	GLU
1	D	4635	SER
1	D	4639	MET
1	D	4645	CYS
1	D	4651	THR
1	D	4665	LYS
1	D	4667	PRO
1	D	4673	ARG
1	D	4679	ARG
1	D	4680	LYS
1	D	4689	THR
1	D	4695	ASP
1	D	4697	VAL
1	D	4704	LEU

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Mol	Chain	Res	Type
1	D	4706	LEU
1	D	4707	ASN
1	D	4708	THR
1	D	4710	SER
1	D	4711	PHE
1	D	4713	SER
1	D	4716	TRP
1	D	4721	LYS
1	D	4730	ASP
1	D	4731	ILE
1	D	4735	GLU
1	D	4743	MET
1	D	4745	LEU
1	D	4747	SER
1	D	4749	GLU
1	D	4772	ASP
1	D	4773	VAL
1	D	4774	LYS
1	D	4777	ILE
1	D	4788	SER
1	D	4809	PHE
1	D	4818	MET
1	D	4821	LYS
1	D	4822	THR
1	D	4824	ARG
1	D	4835	LYS
1	D	4837	LEU
1	D	4844	LEU
1	D	4861	LYS
1	D	4865	LYS
1	D	4869	GLU
1	D	4871	GLU
1	D	4876	CYS
1	D	4887	MET
1	D	4889	VAL
1	D	4908	GLU
1	D	4913	ARG
1	D	4920	PHE
1	D	4927	ILE
1	D	4933	GLN
1	D	4945	ASP
1	D	4949	GLN

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Mol	Chain	Res	Type
1	D	4951	LYS
1	D	4957	LYS
1	D	4966	ASP
1	D	4976	GLU
1	D	4980	LEU
1	D	4985	LEU
1	D	4989	MET
1	D	4992	LEU
1	D	4995	LEU
1	D	4997	ASN
1	D	4998	LYS
1	D	5004	THR
1	D	5006	GLN
1	D	5012	LYS
1	D	5028	PHE
1	D	5030	LYS
1	D	5034	ASP
2	E	17	LYS
2	F	17	LYS
2	G	17	LYS
2	H	17	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	475	GLN
1	A	479	GLN
1	A	533	ASN
1	A	877	ASN
1	A	2127	GLN
1	A	2498	HIS
1	A	2877	GLN
1	A	2962	GLN
1	A	4133	GLN
1	A	4700	GLN
1	A	4707	ASN
1	A	4728	HIS
1	A	4886	HIS
1	B	475	GLN
1	B	479	GLN
1	B	533	ASN
1	B	877	ASN

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Mol	Chain	Res	Type
1	B	2127	GLN
1	B	2498	HIS
1	B	2877	GLN
1	B	2962	GLN
1	B	4133	GLN
1	B	4700	GLN
1	B	4707	ASN
1	B	4728	HIS
1	B	4886	HIS
1	C	475	GLN
1	C	479	GLN
1	C	533	ASN
1	C	877	ASN
1	C	2498	HIS
1	C	2877	GLN
1	C	2962	GLN
1	C	4133	GLN
1	C	4700	GLN
1	C	4728	HIS
1	C	4886	HIS
1	D	475	GLN
1	D	479	GLN
1	D	533	ASN
1	D	877	ASN
1	D	2127	GLN
1	D	2498	HIS
1	D	2877	GLN
1	D	2962	GLN
1	D	4133	GLN
1	D	4700	GLN
1	D	4728	HIS
1	D	4886	HIS

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	AMP	B	5101	-	21,25,25	0.74	0	23,38,38	1.26	2 (8%)
3	AMP	C	5101	-	21,25,25	0.74	0	23,38,38	1.26	2 (8%)
3	AMP	A	5101	-	21,25,25	0.74	0	23,38,38	1.26	2 (8%)
3	AMP	D	5101	-	21,25,25	0.74	0	23,38,38	1.26	2 (8%)

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	AMP	B	5101	-	-	2/6/26/26	0/3/3/3
3	AMP	C	5101	-	-	2/6/26/26	0/3/3/3
3	AMP	A	5101	-	-	2/6/26/26	0/3/3/3
3	AMP	D	5101	-	-	2/6/26/26	0/3/3/3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5101	AMP	N3-C2-N1	-3.81	123.50	128.67
3	D	5101	AMP	N3-C2-N1	-3.81	123.50	128.67
3	C	5101	AMP	N3-C2-N1	-3.81	123.50	128.67
3	A	5101	AMP	N3-C2-N1	-3.81	123.51	128.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	5101	AMP	C4-C5-N7	-2.20	107.01	109.34
3	D	5101	AMP	C4-C5-N7	-2.20	107.02	109.34
3	B	5101	AMP	C4-C5-N7	-2.19	107.02	109.34
3	C	5101	AMP	C4-C5-N7	-2.19	107.02	109.34

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

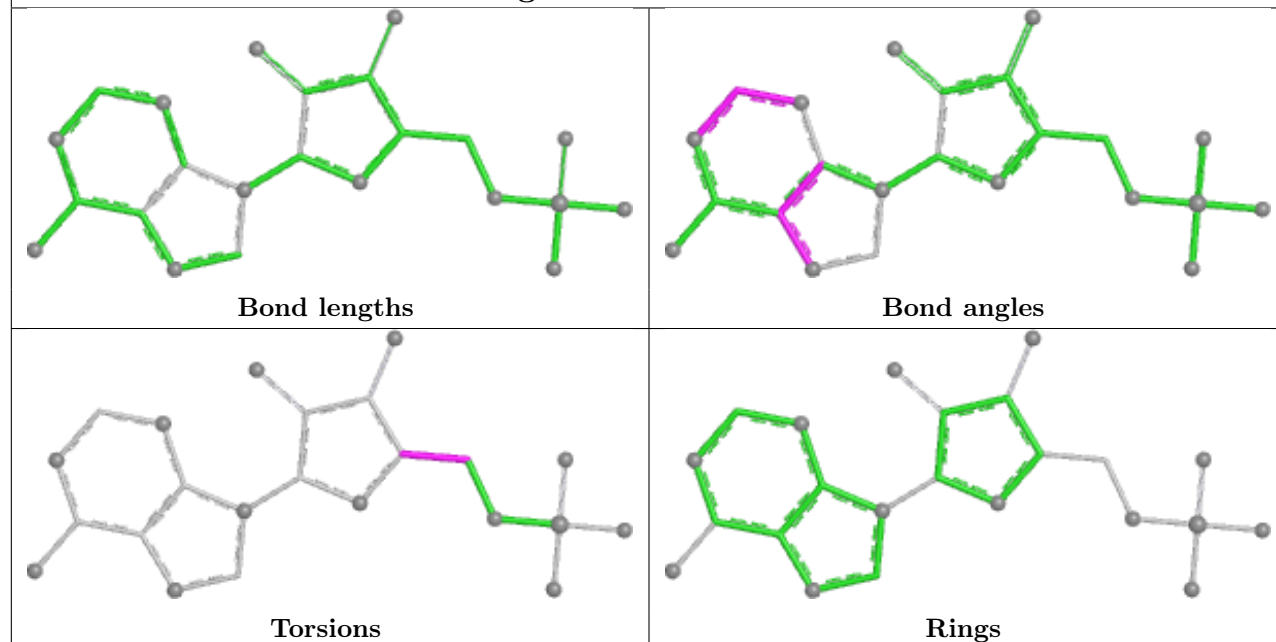
There are no ring outliers.

4 monomers are involved in 4 short contacts:

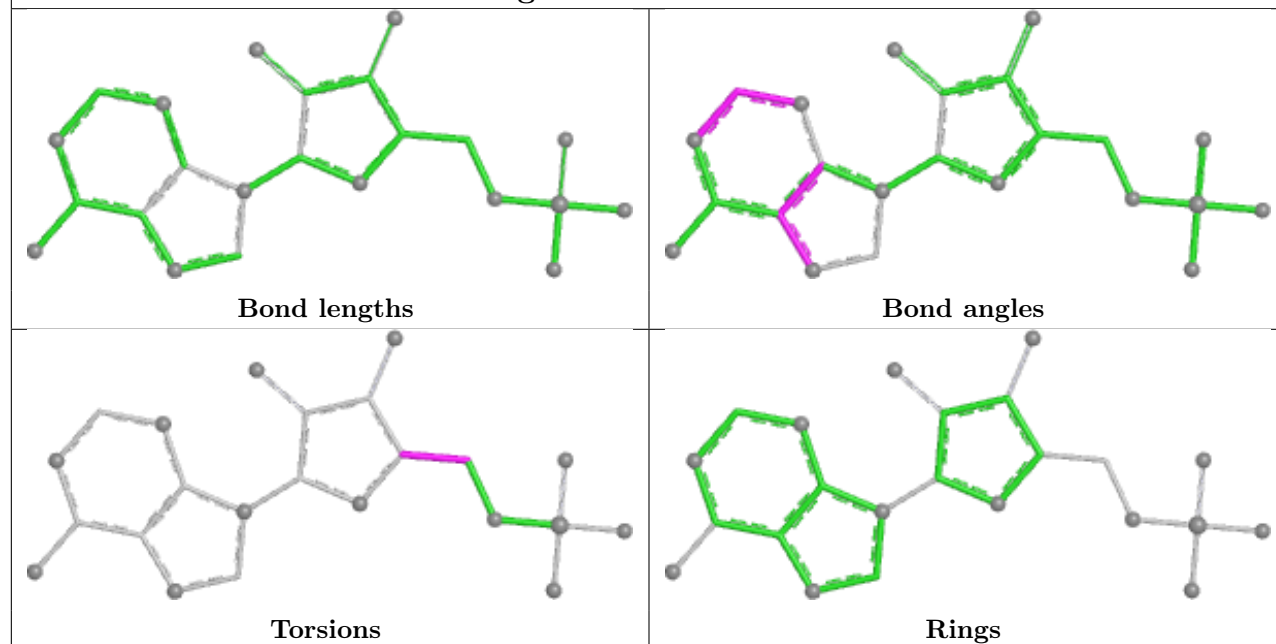
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5101	AMP	1	0
3	C	5101	AMP	1	0
3	A	5101	AMP	1	0
3	D	5101	AMP	1	0

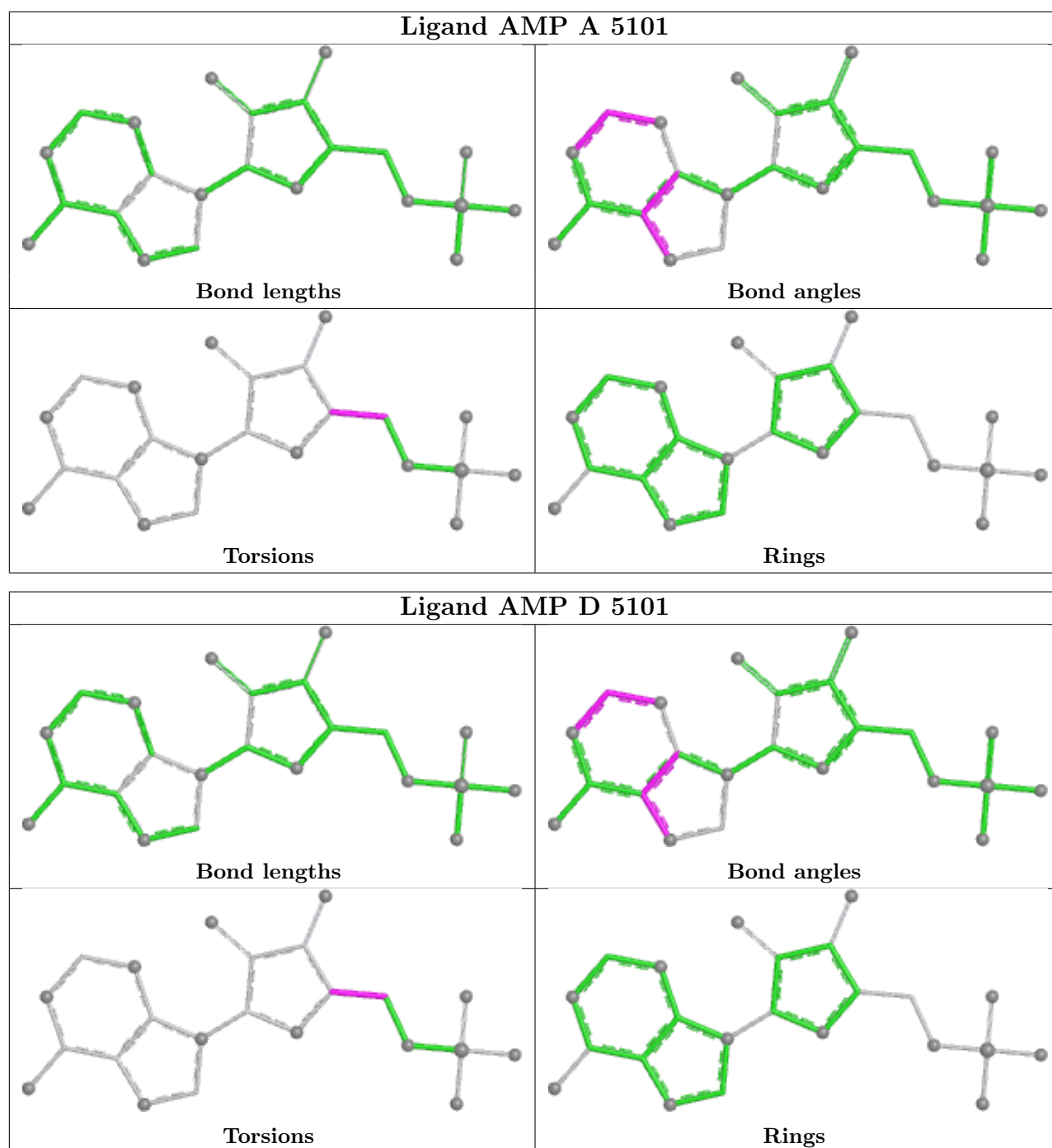
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand AMP B 5101



Ligand AMP C 5101





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.

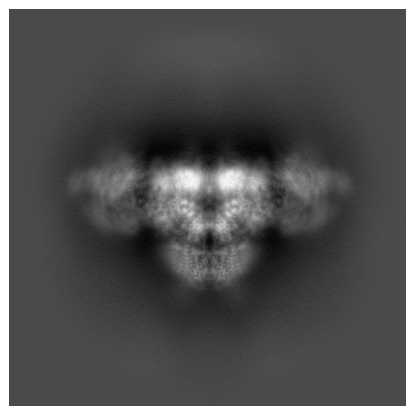
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40425. These allow visual inspection of the internal detail of the map and identification of artifacts.

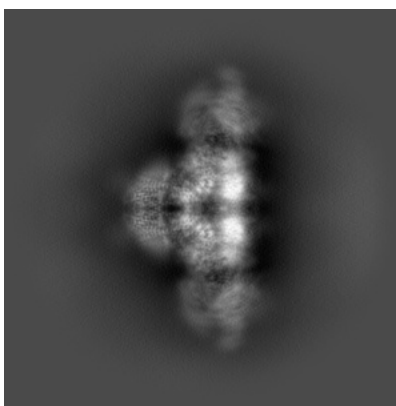
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

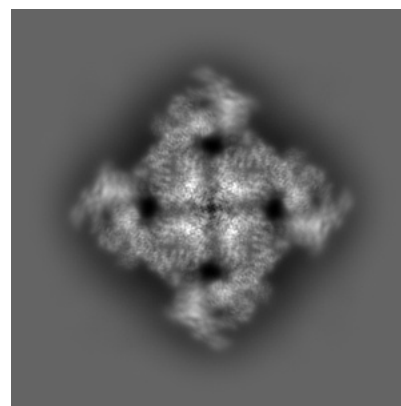
6.1.1 Primary map



X

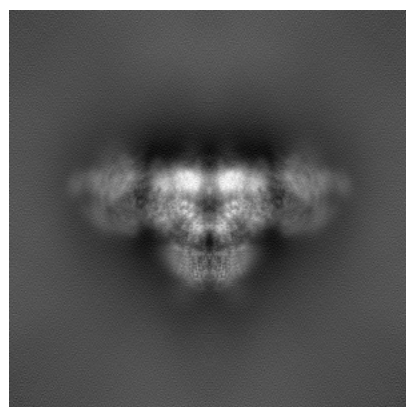


Y

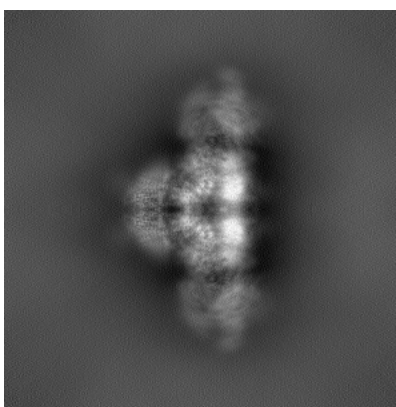


Z

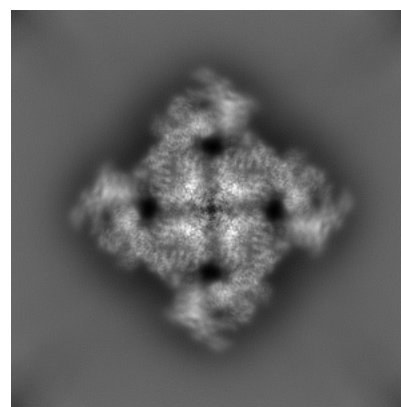
6.1.2 Raw map



X



Y

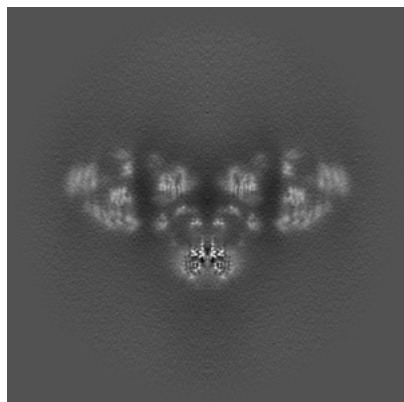


Z

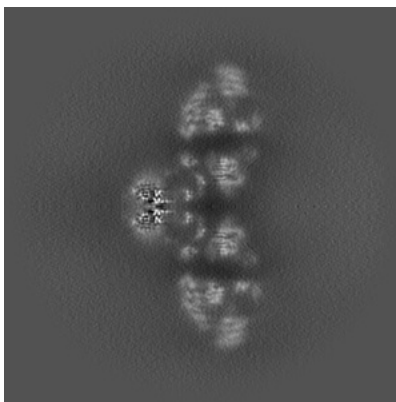
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

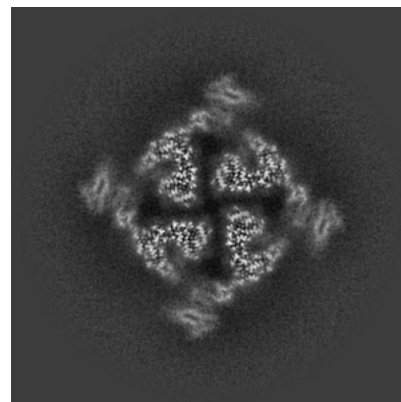
6.2.1 Primary map



X Index: 200

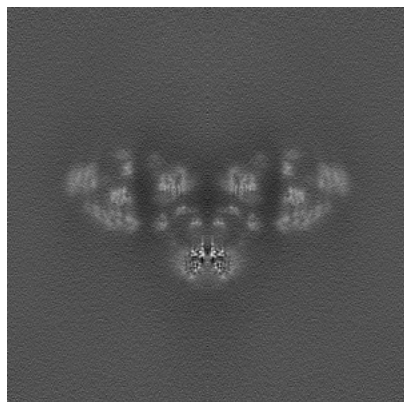


Y Index: 200

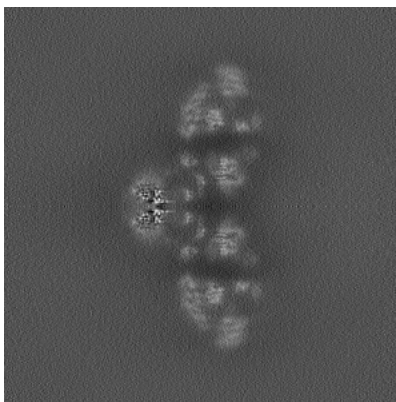


Z Index: 200

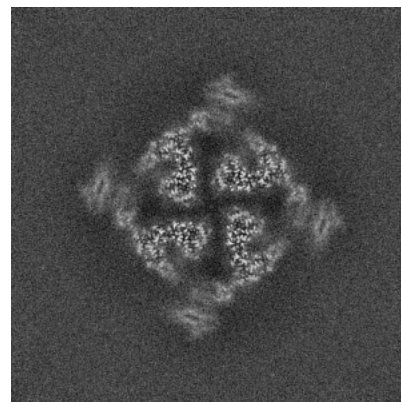
6.2.2 Raw map



X Index: 200



Y Index: 200

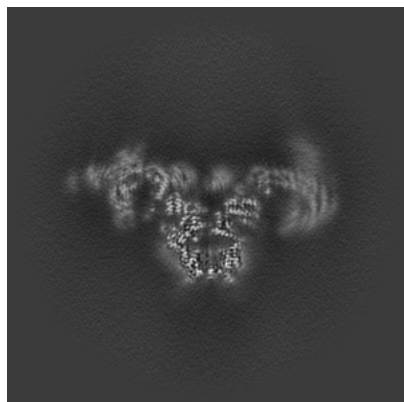


Z Index: 200

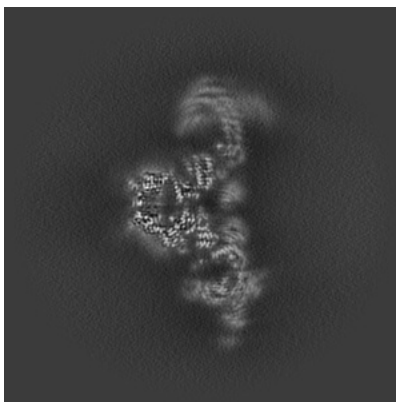
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

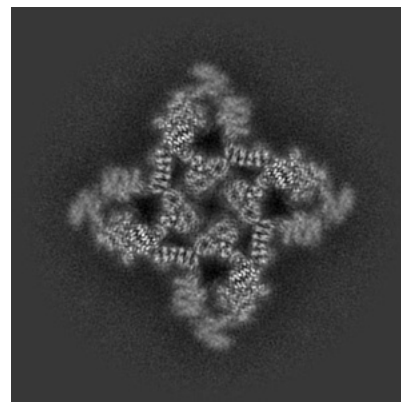
6.3.1 Primary map



X Index: 218

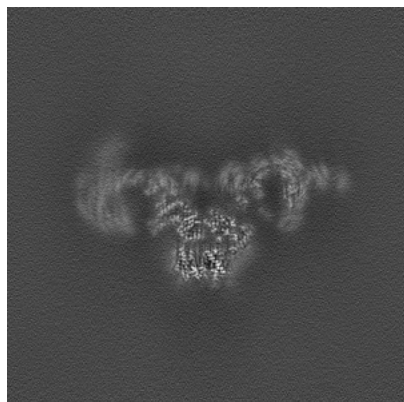


Y Index: 182

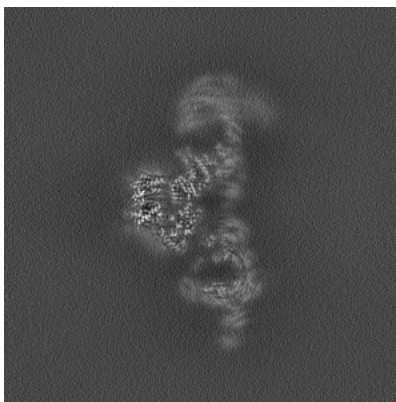


Z Index: 223

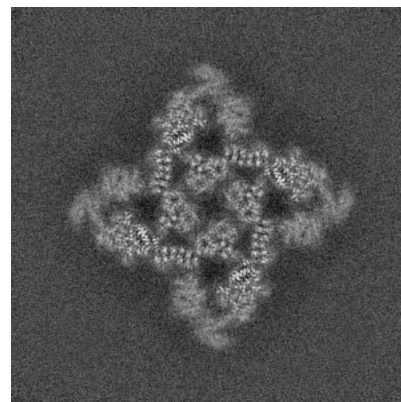
6.3.2 Raw map



X Index: 186



Y Index: 186

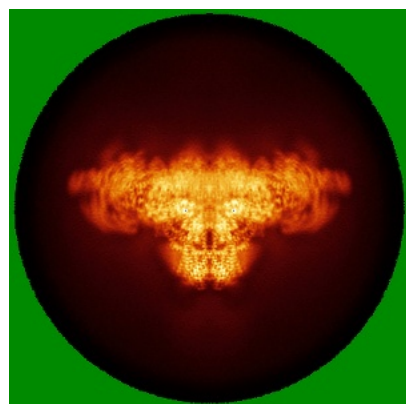


Z Index: 222

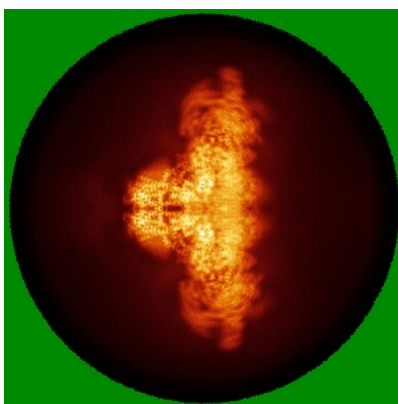
The images above show the largest variance slices of the map in three orthogonal directions.

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

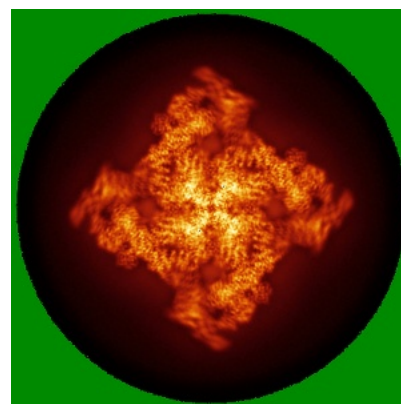
6.4.1 Primary map



X

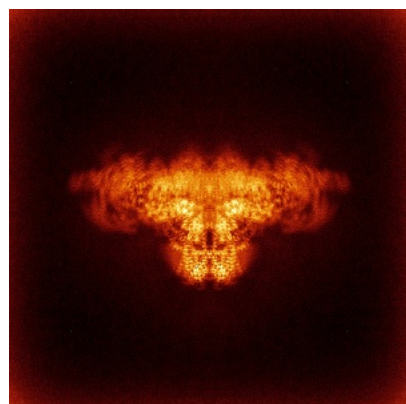


Y

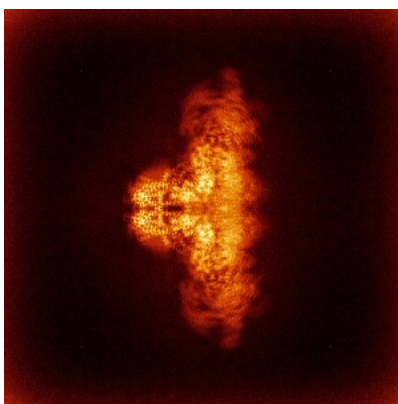


Z

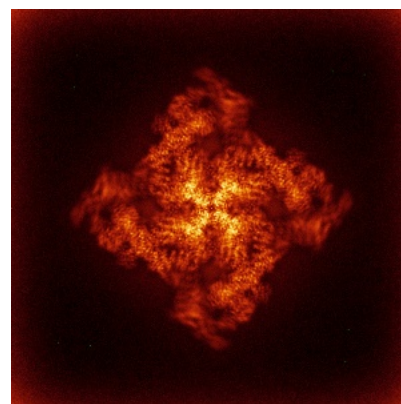
6.4.2 Raw map



X



Y

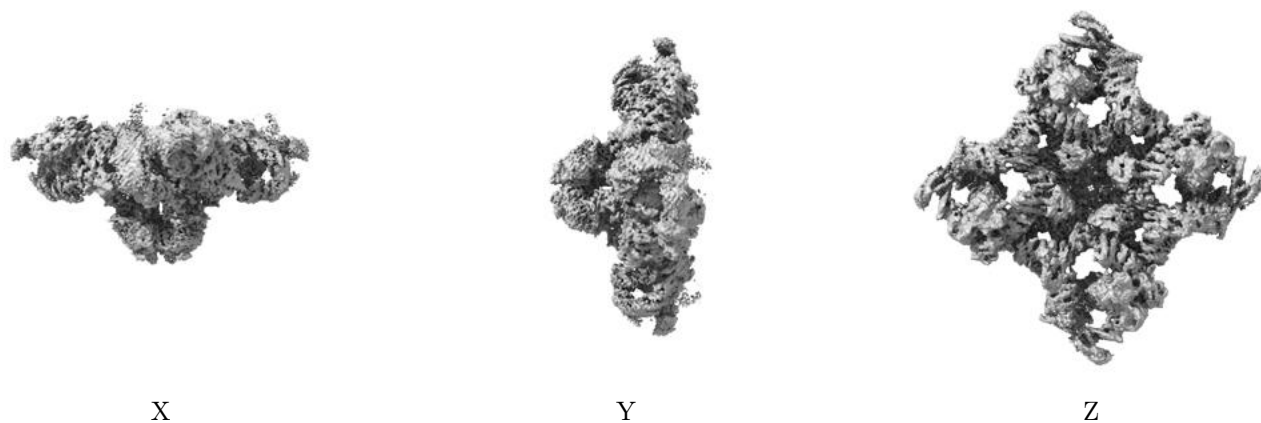


Z

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.

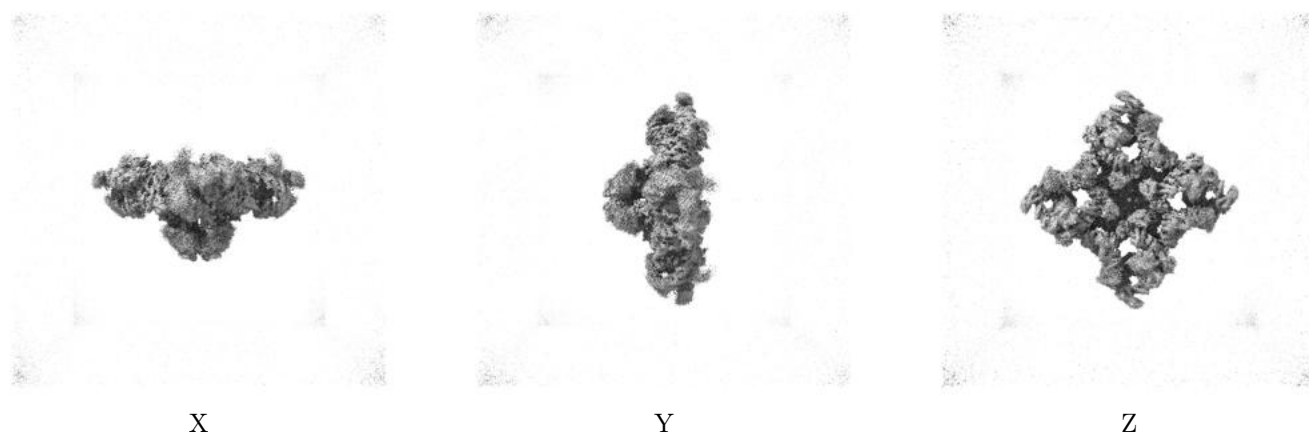
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.132. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

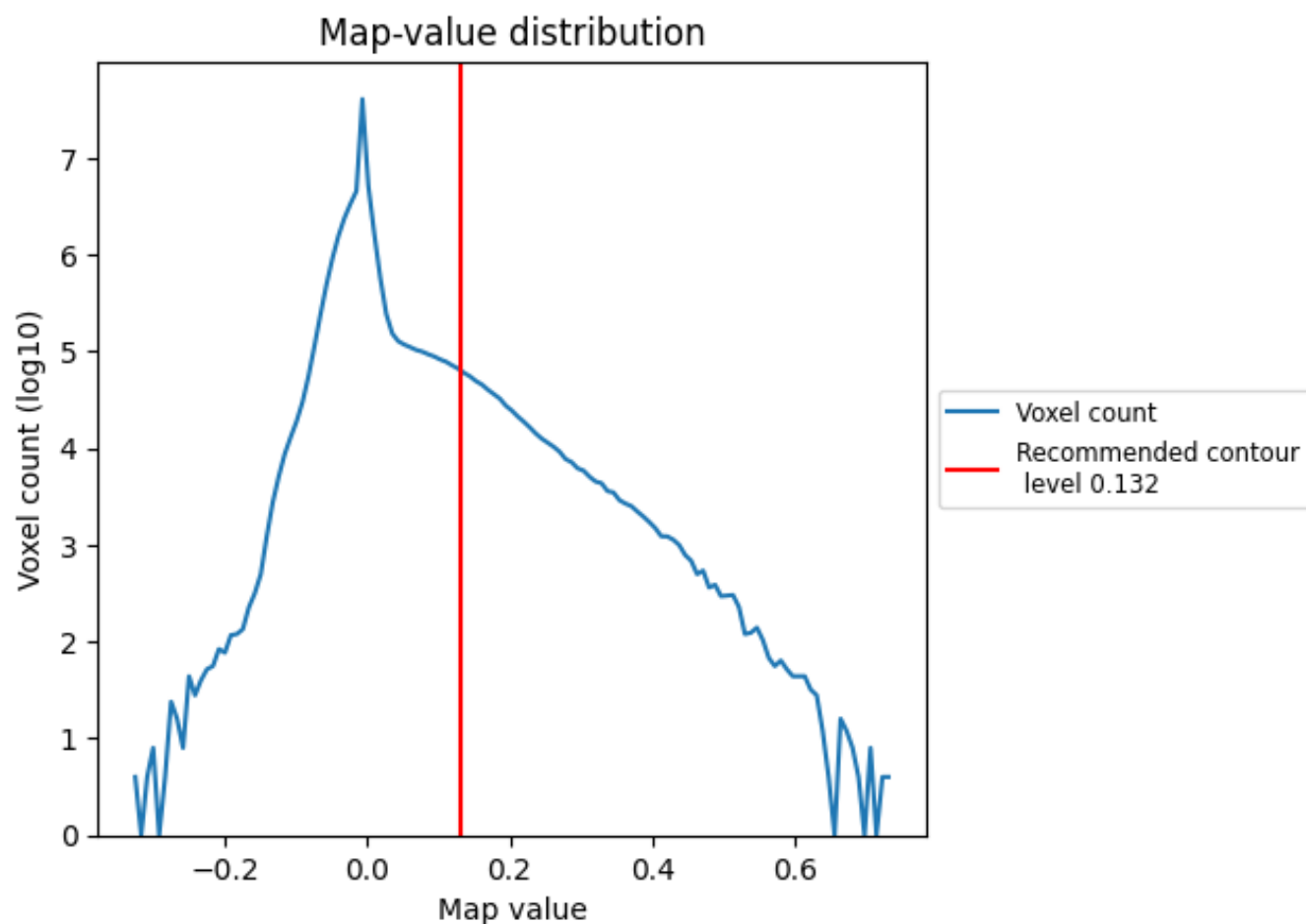
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

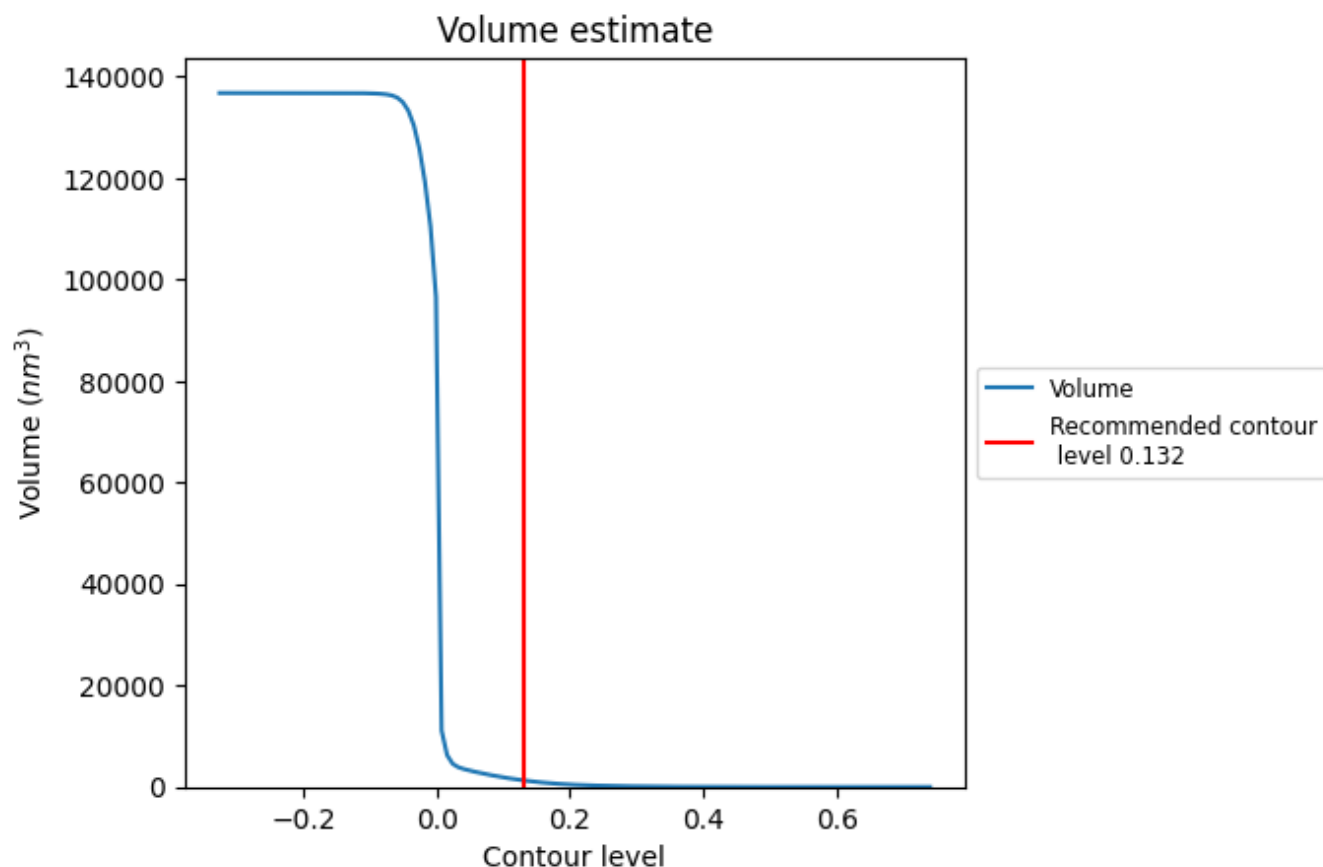
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

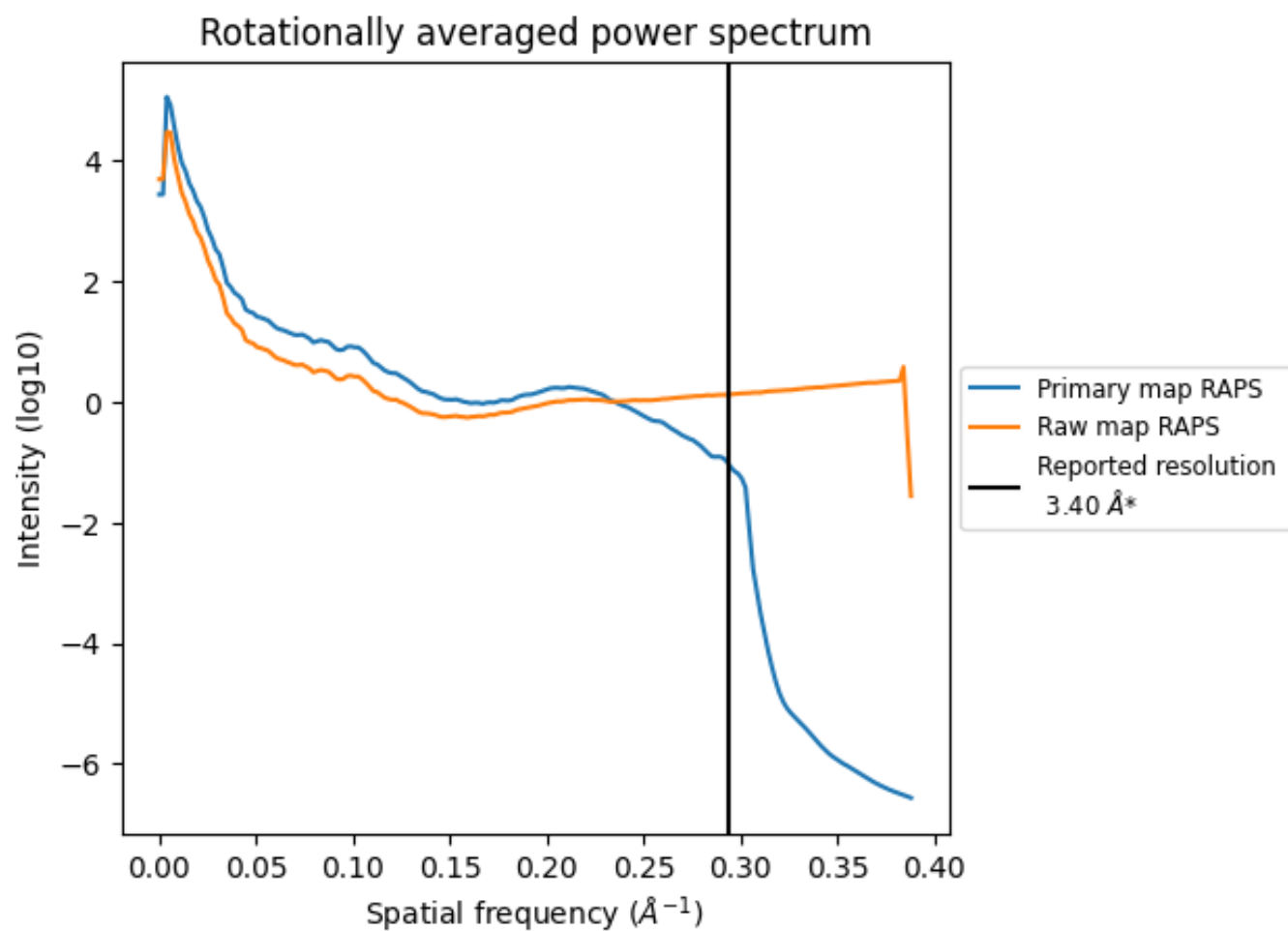
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1261 nm^3 ; this corresponds to an approximate mass of 1139 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 ⓘ

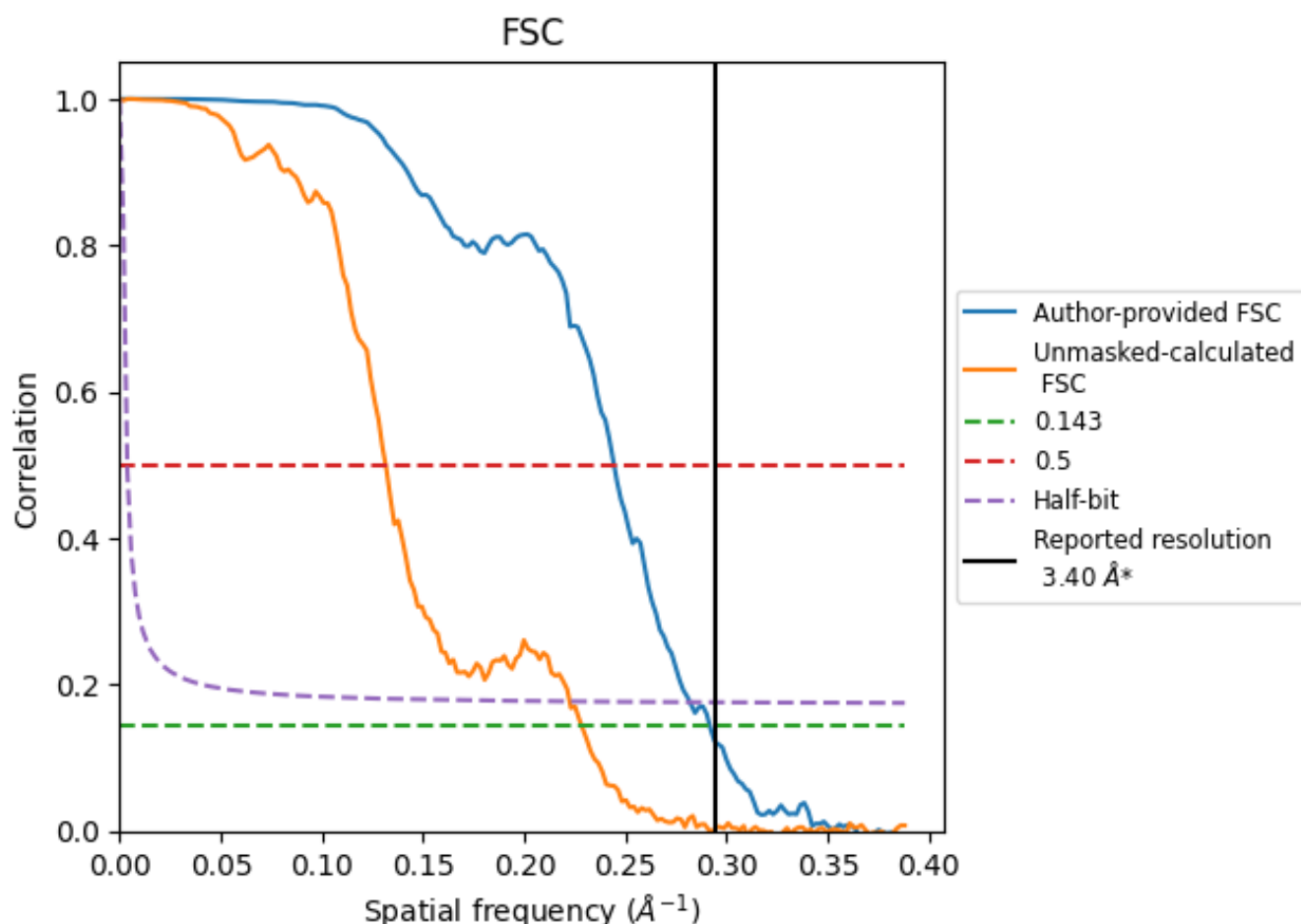


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 \AA^{-1}

8.2 Resolution estimates [i](#)

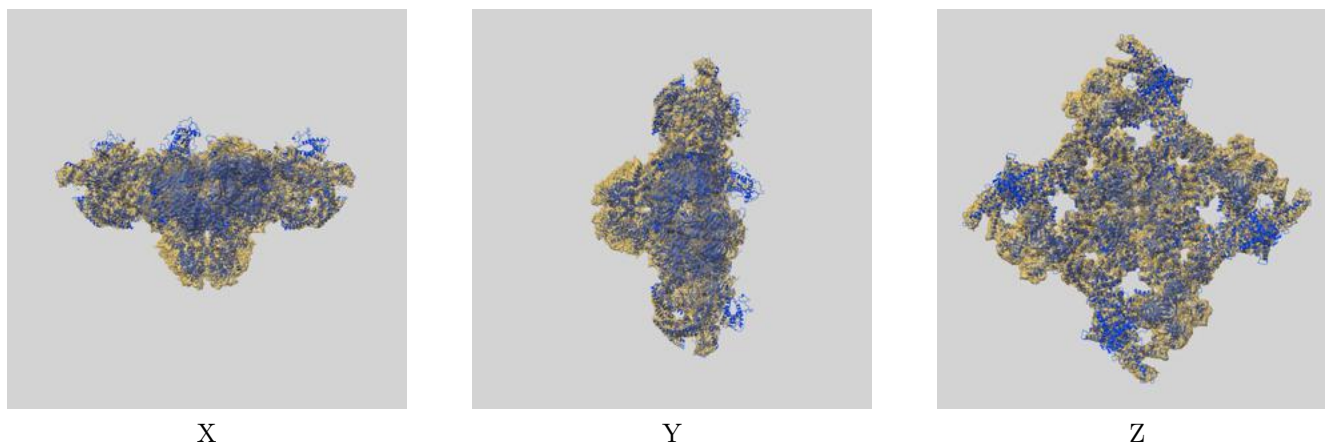
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.43	4.09	3.55
Unmasked-calculated*	4.37	7.60	4.49

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.37 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

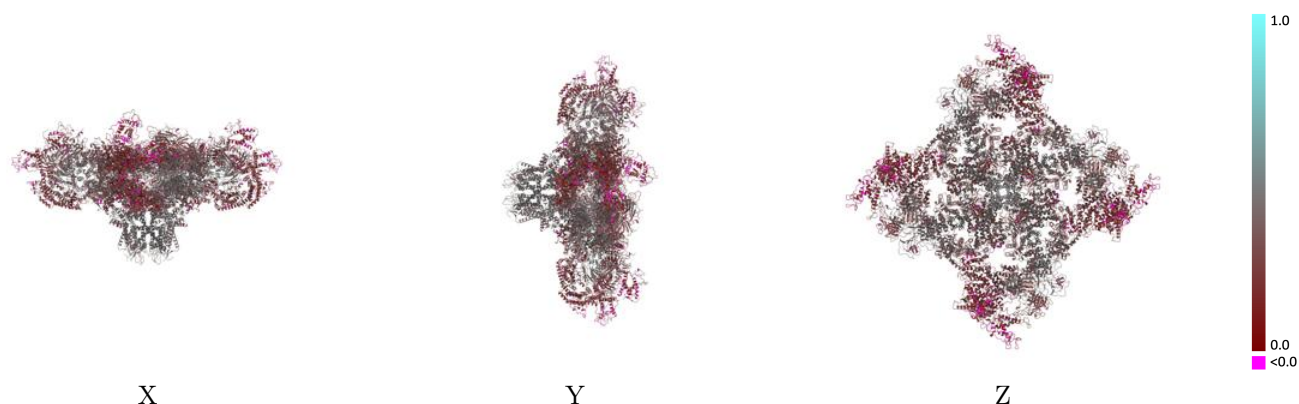
This section contains information regarding the fit between EMDB map EMD-40425 and PDB model 8SEQ. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



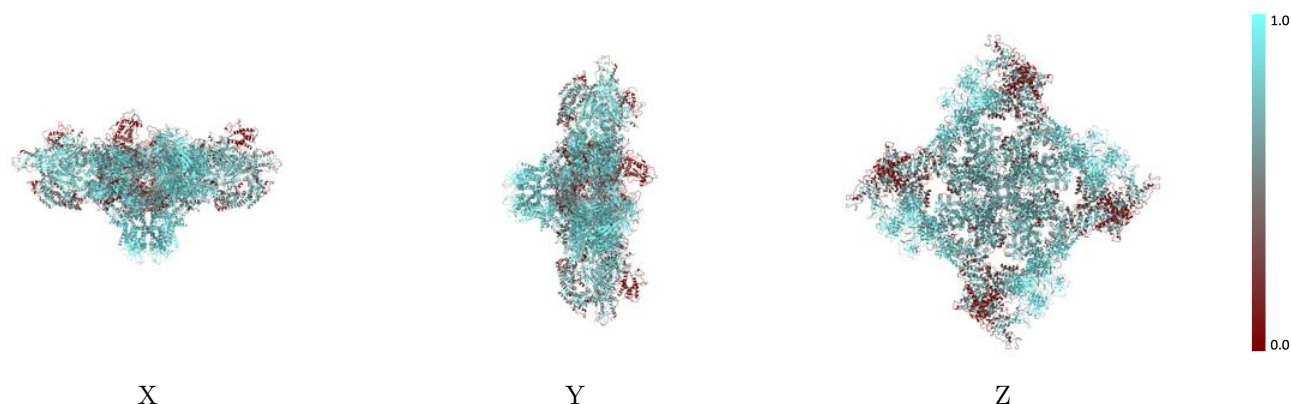
The images above show the 3D surface view of the map at the recommended contour level 0.132 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



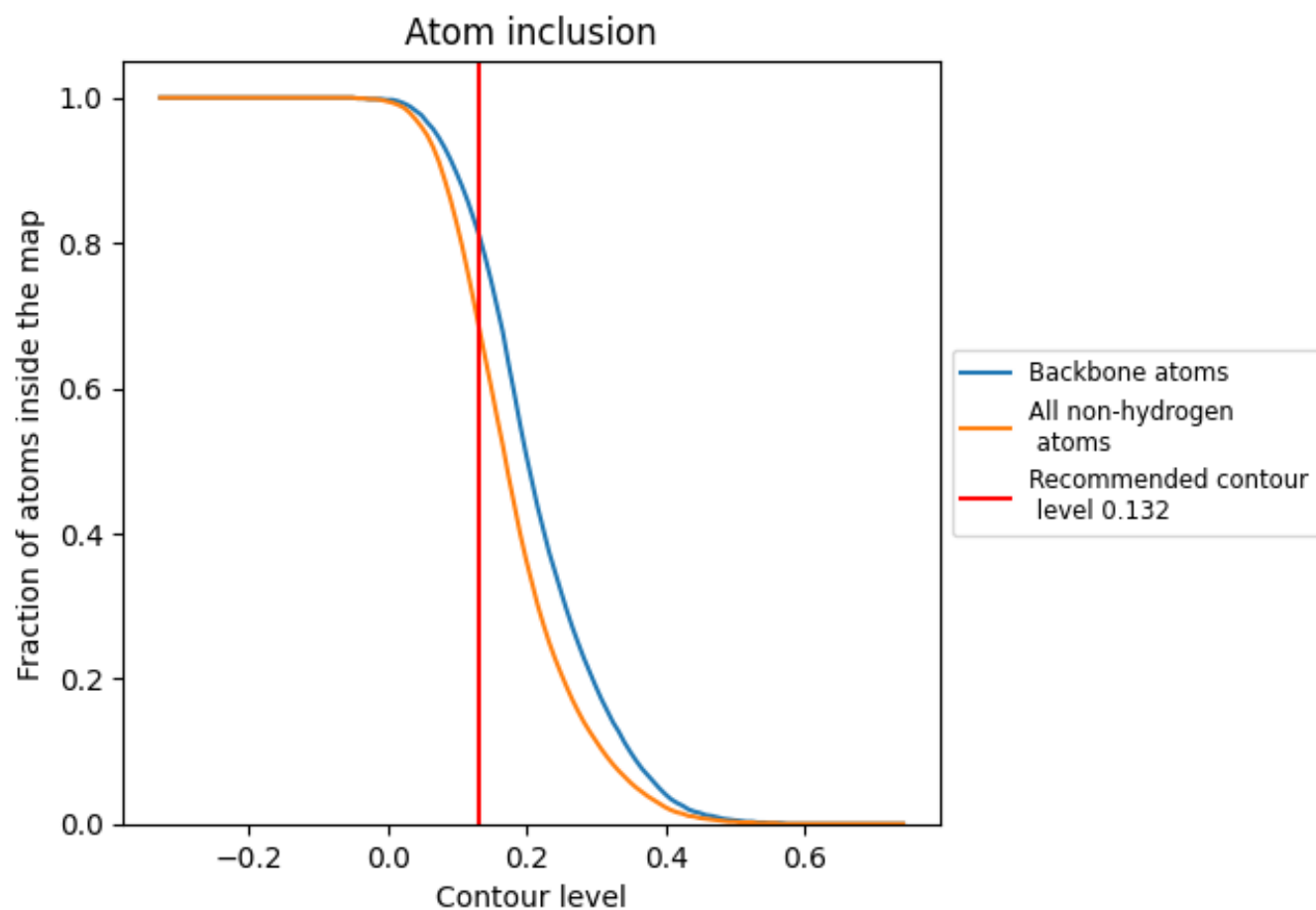
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.132).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 68% 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 (0.132) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6820	<div></div> 0.3220
A	<div></div> 0.6780	<div></div> 0.3210
B	<div></div> 0.6790	<div></div> 0.3200
C	<div></div> 0.6790	<div></div> 0.3200
D	<div></div> 0.6790	<div></div> 0.3200
E	<div></div> 0.8500	<div></div> 0.3890
F	<div></div> 0.8500	<div></div> 0.3880
G	<div></div> 0.8500	<div></div> 0.3900
H	<div></div> 0.8500	<div></div> 0.3920

1.0

0.0

<0.0