



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 06:21 AM UTC

PDB ID : 8DUJ / pdb_00008duj
EMDB ID : EMD-27721
Title : Global map in C1 of RyR1 particles in complex with ImperaCalcin
Authors : Haji-Ghassemi, O.; Van Petegm, F.
Deposited on : 2022-07-27
Resolution : 3.70 Å(reported)
Based on initial model : 6M2W

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

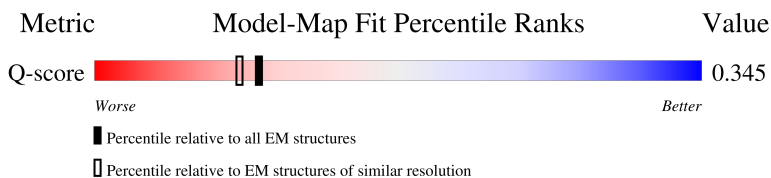
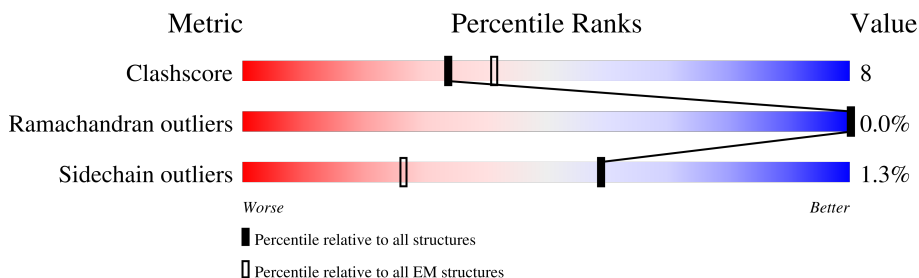
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

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	M	33	24% 67% 33%
2	A	5037	11% 64% 12% 24%
2	D	5037	15% 68% 8% 23%
2	G	5037	8% 66% 12% 22%

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Mol	Chain	Length	Quality of chain
2	J	5037	
3	B	107	
3	E	107	
3	H	107	
3	K	107	
4	C	149	
4	F	149	
4	I	149	
4	L	149	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 106156 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 Imperacalcin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	33	Total	C	N	O	S	33	0
			514	296	116	90	12		

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	3933	Total	C	N	O	S	0	0
			26285	16856	4666	4625	138		
2	A	3823	Total	C	N	O	S	1	0
			24845	15885	4439	4407	114		
2	D	3865	Total	C	N	O	S	1	0
			23336	14719	4259	4281	77		
2	J	3892	Total	C	N	O	S	0	0
			25245	16153	4530	4440	122		

- Molecule 3 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	107	Total	C	N	O	S	0	0
			759	483	134	138	4		
3	B	107	Total	C	N	O	S	0	0
			735	465	130	136	4		
3	E	106	Total	C	N	O	S	0	0
			657	415	115	125	2		
3	K	106	Total	C	N	O	S	0	0
			758	483	135	136	4		

- Molecule 4 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	138	Total	C	N	O	S	0	0
			711	431	139	139	2		

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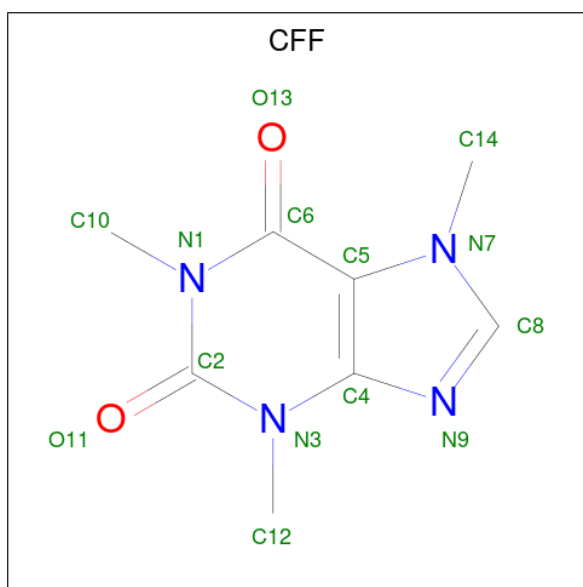
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Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	137	Total	C	N	O	S	0	0
			707	430	137	139	1		
4	F	137	Total	C	N	O		0	0
			710	434	137	139			
4	L	139	Total	C	N	O	S	0	0
			706	427	139	139	1		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	32	ALA	GLU	engineered mutation	UNP P0DP23
I	68	ALA	GLU	engineered mutation	UNP P0DP23
I	105	ALA	GLU	engineered mutation	UNP P0DP23
I	141	ALA	GLU	engineered mutation	UNP P0DP23
C	32	ALA	GLU	engineered mutation	UNP P0DP23
C	68	ALA	GLU	engineered mutation	UNP P0DP23
C	105	ALA	GLU	engineered mutation	UNP P0DP23
C	141	ALA	GLU	engineered mutation	UNP P0DP23
F	32	ALA	GLU	engineered mutation	UNP P0DP23
F	68	ALA	GLU	engineered mutation	UNP P0DP23
F	105	ALA	GLU	engineered mutation	UNP P0DP23
F	141	ALA	GLU	engineered mutation	UNP P0DP23
L	32	ALA	GLU	engineered mutation	UNP P0DP23
L	68	ALA	GLU	engineered mutation	UNP P0DP23
L	105	ALA	GLU	engineered mutation	UNP P0DP23
L	141	ALA	GLU	engineered mutation	UNP P0DP23

- Molecule 5 is CAFFEINE (CCD ID: CFF) (formula: $C_8H_{10}N_4O_2$).

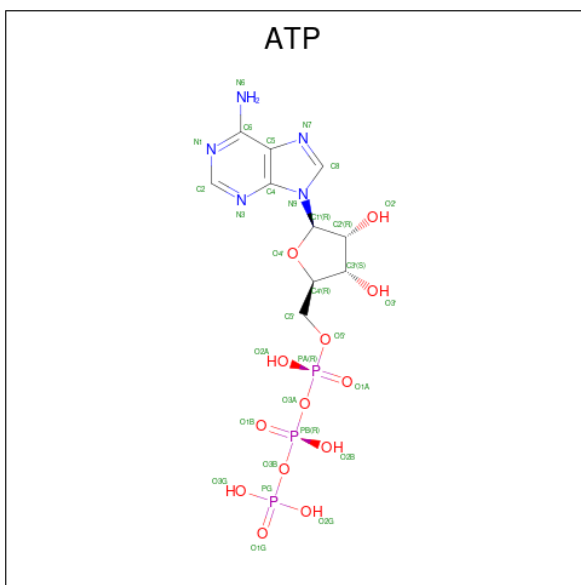


Mol	Chain	Residues	Atoms				AltConf
5	G	1	Total	C	N	O	0
			14	8	4	2	
5	A	1	Total	C	N	O	0
			14	8	4	2	
5	D	1	Total	C	N	O	0
			14	8	4	2	
5	J	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
6	G	1	Total	Ca	0
			1	1	
6	A	1	Total	Ca	0
			1	1	
6	D	1	Total	Ca	0
			1	1	
6	J	1	Total	Ca	0
			1	1	

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
7	G	1	Total 31	C 10	N 5	O 13	P 3	0
7	A	1	Total 31	C 10	N 5	O 13	P 3	0
7	D	1	Total 31	C 10	N 5	O 13	P 3	0
7	J	1	Total 31	C 10	N 5	O 13	P 3	0

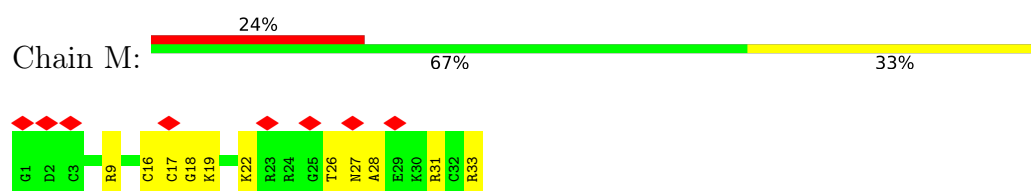
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
8	G	1	Total Zn 1 1	0
8	A	1	Total Zn 1 1	0
8	D	1	Total Zn 1 1	0
8	J	1	Total Zn 1 1	0

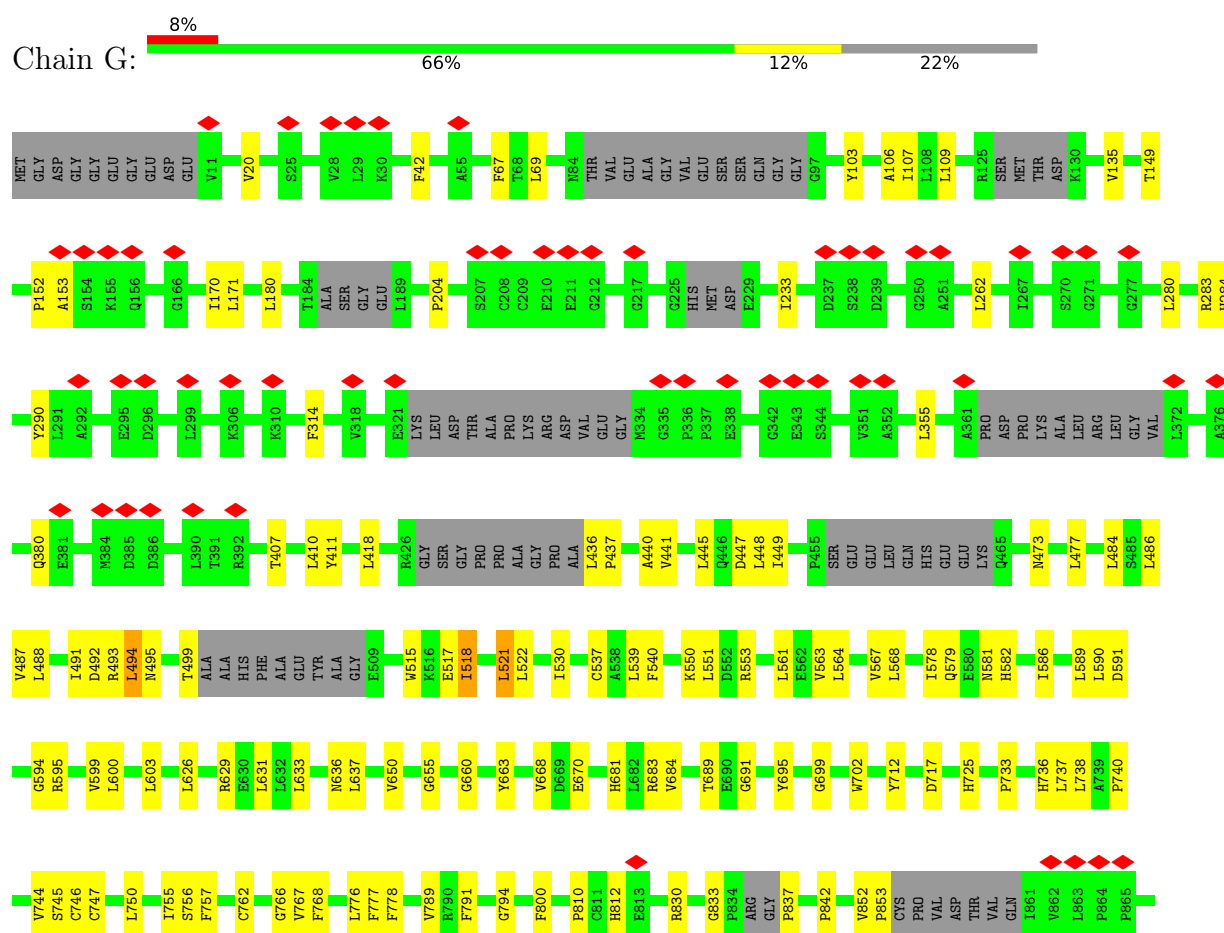
3 Residue-property plots

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: Imperacalcin

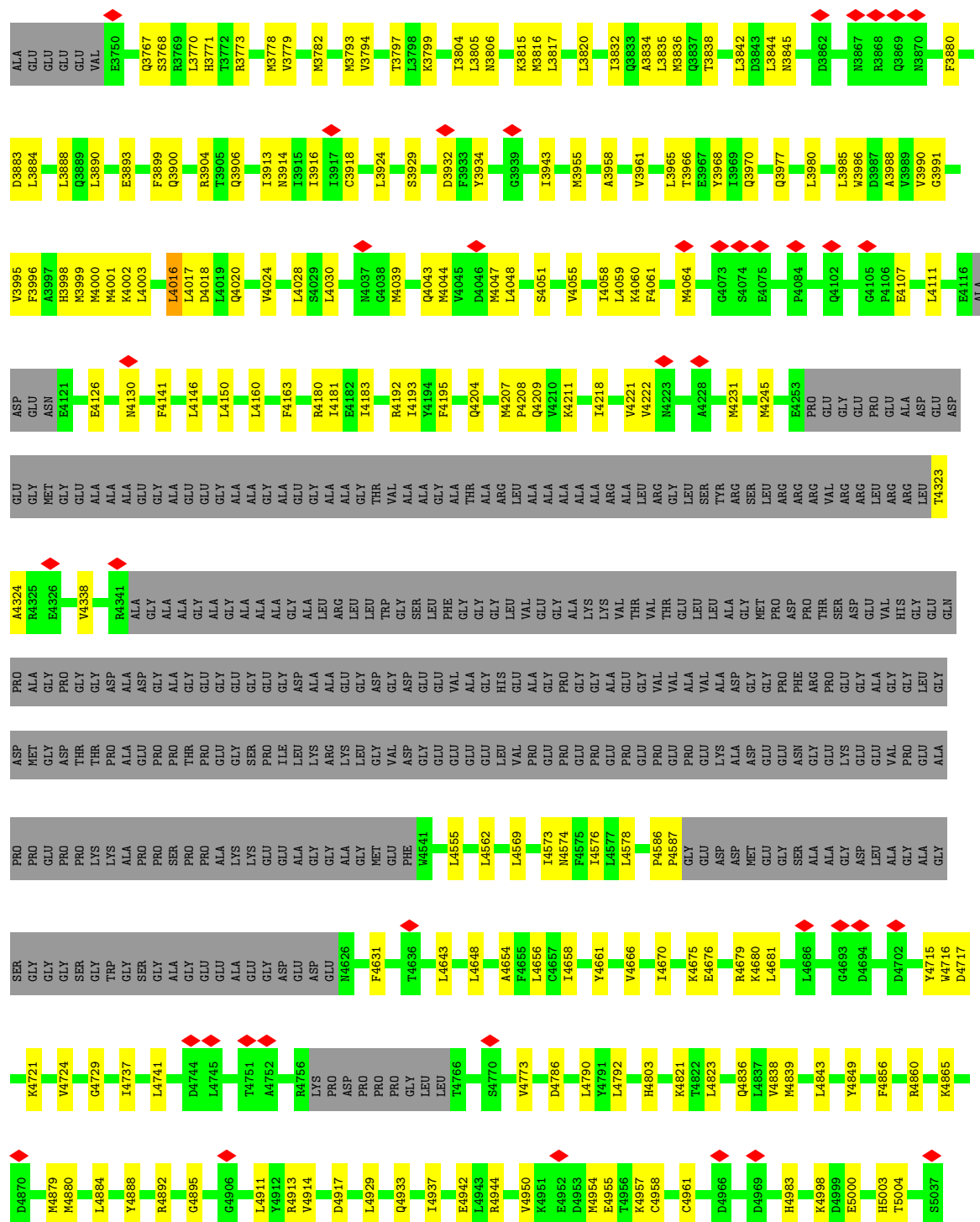


• Molecule 2: Ryanodine receptor 1

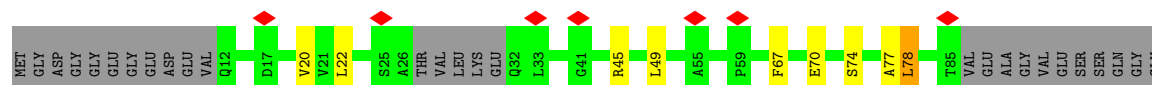




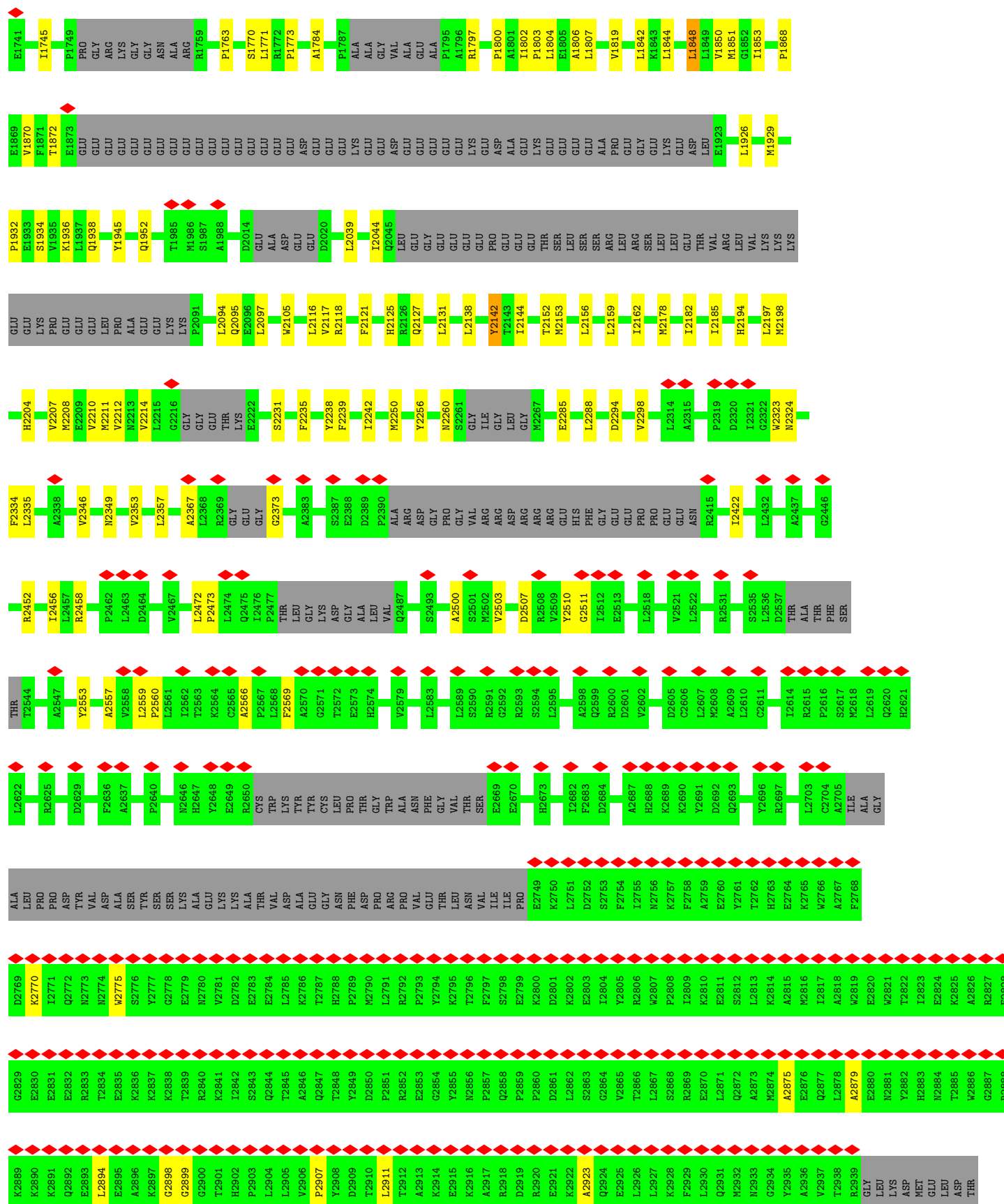




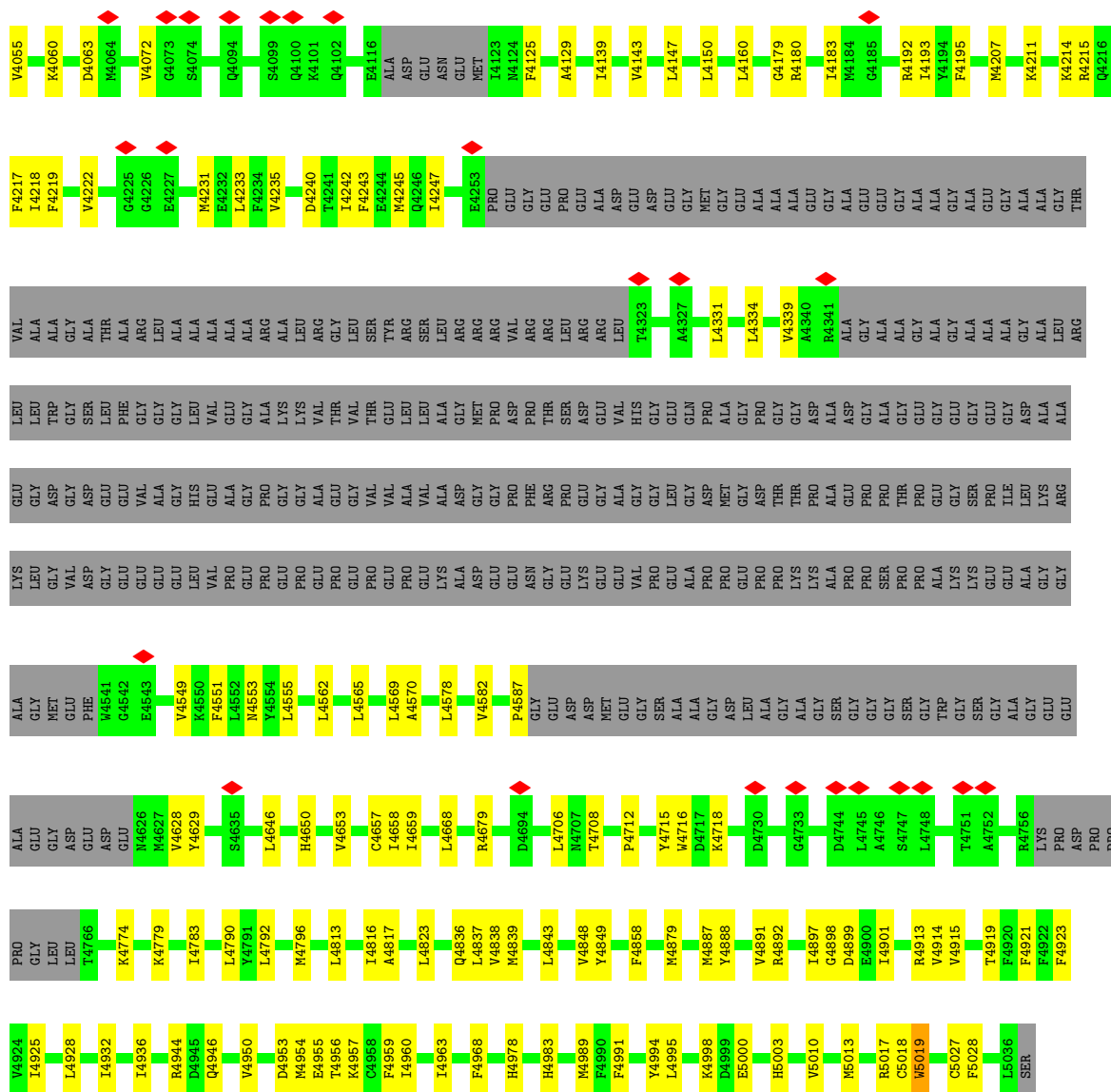
- Molecule 2: Ryanodine receptor 1



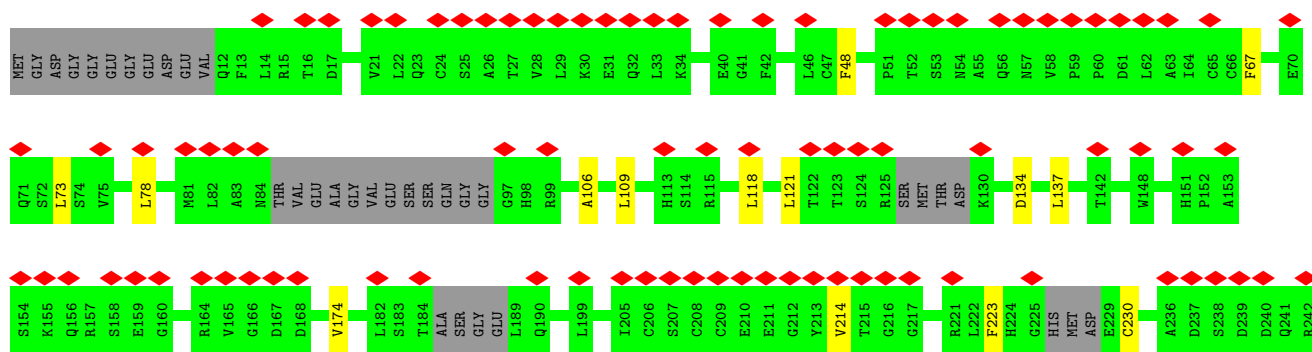








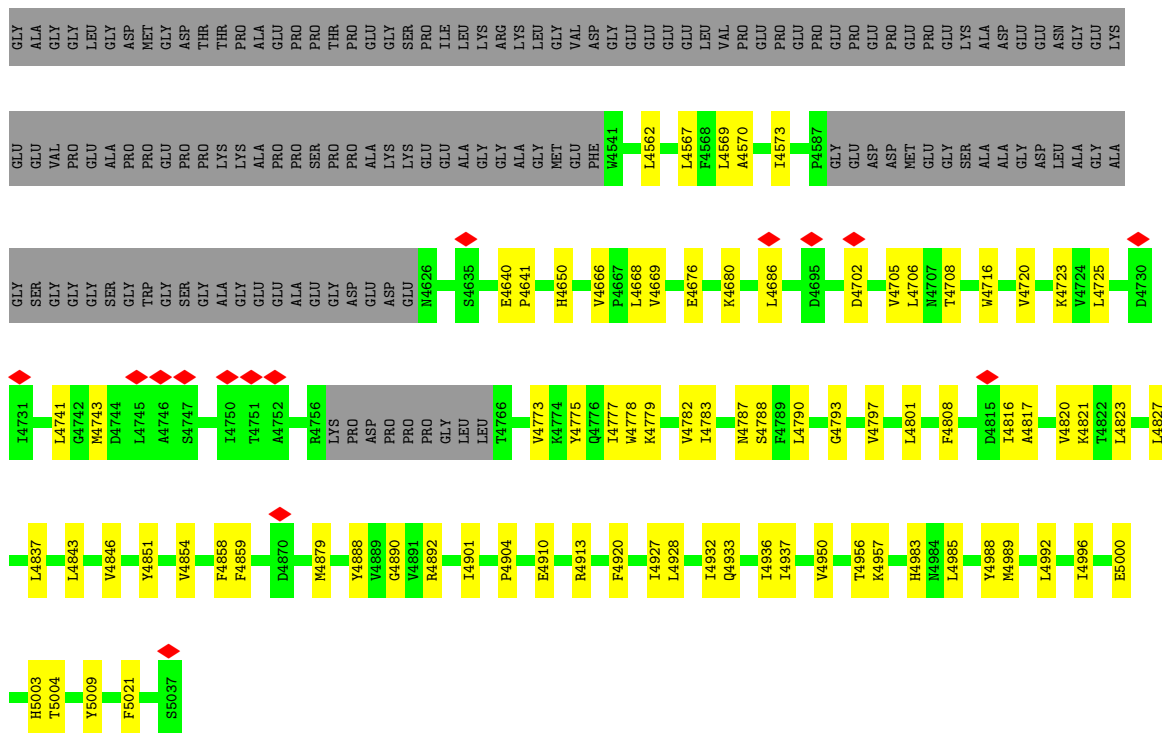
• Molecule 2: Ryanodine receptor 1



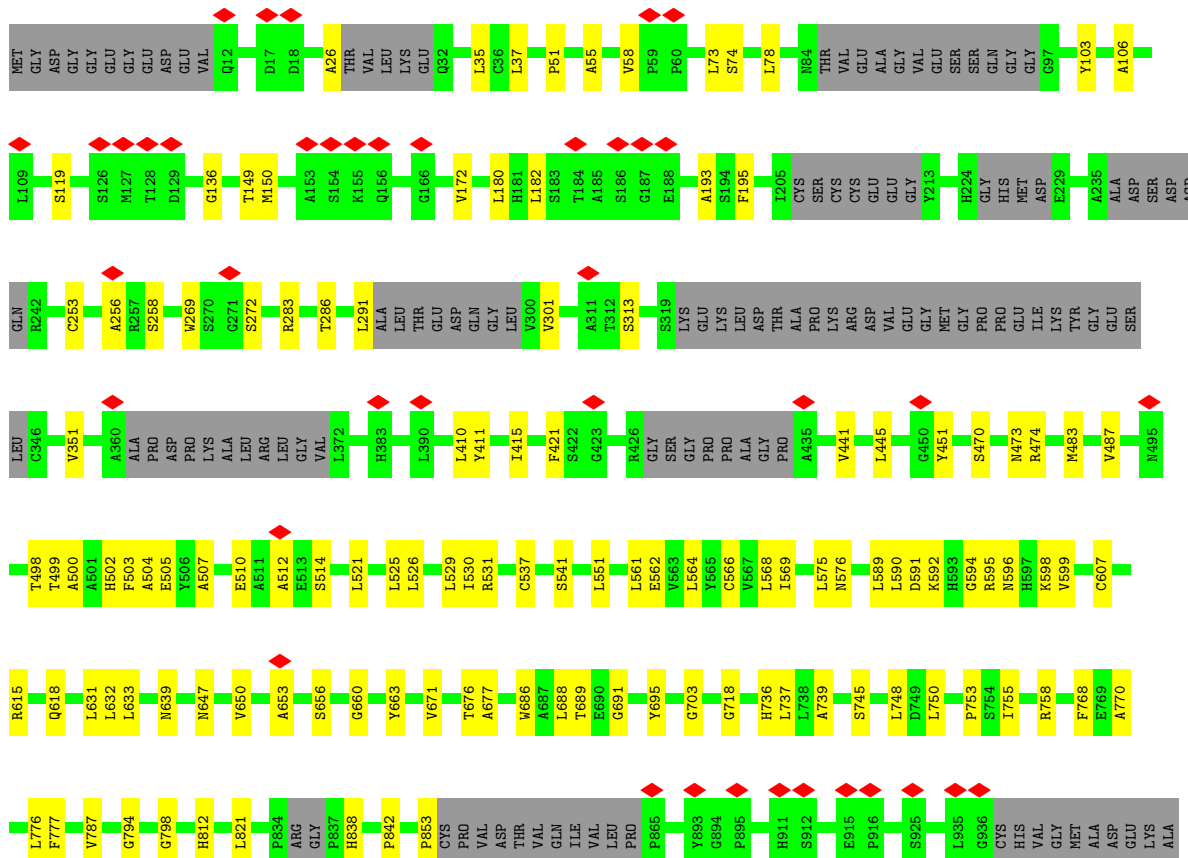






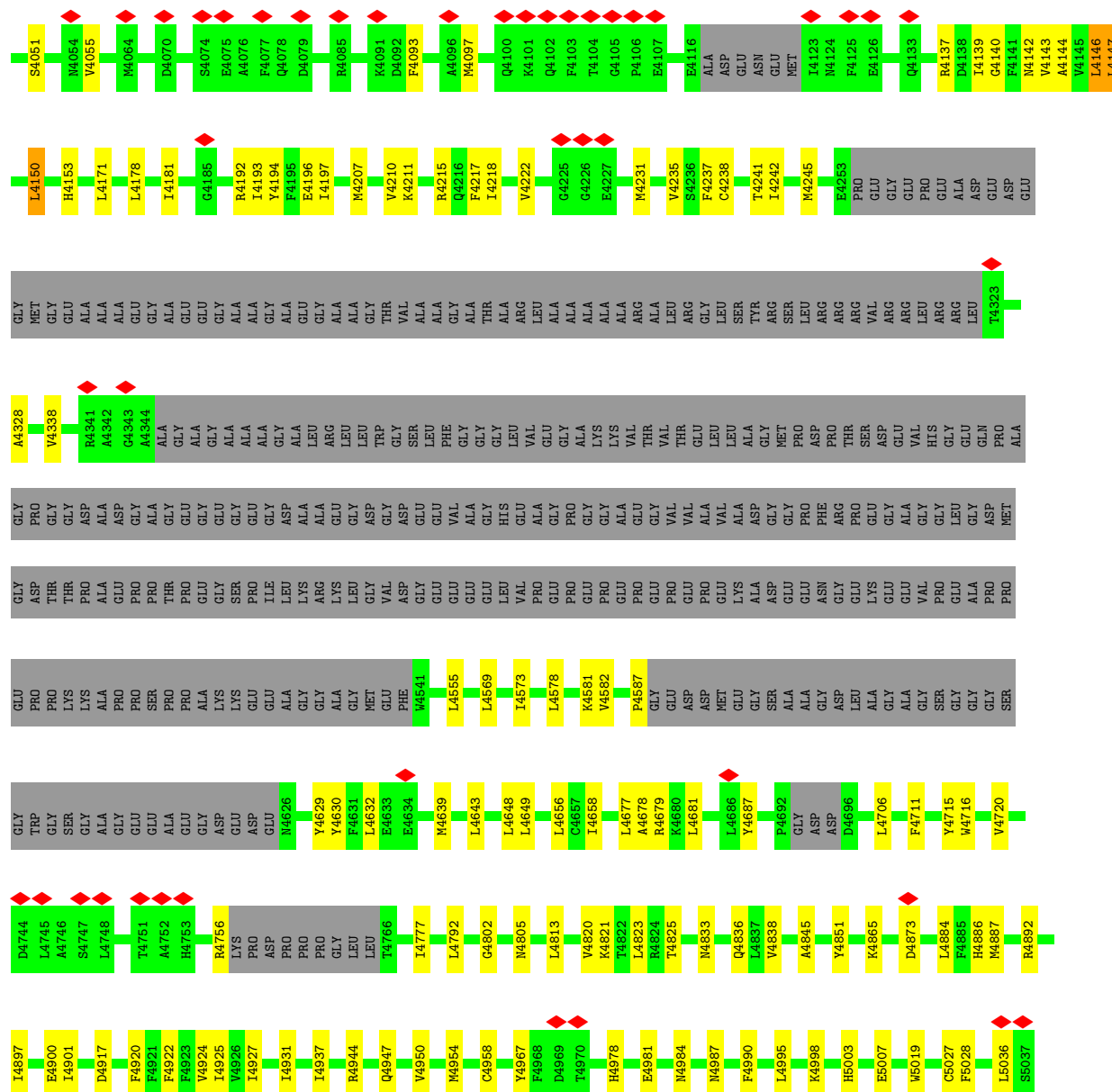


- Molecule 2: Ryanodine receptor 1





THR	LEU	ASN	VAL	ILE	ILE	P2748	E2749	K2750	L2751	D2752	S2753	F2754	I2755	N2756	K2757	F2758	A2759	E2760	I2761	T2762	H2763	E2764	K2765	N2766	A2767	F2768	D2769	K2770	I2771	Q2772	N2773	I2774	N2775	S2776	I2777	G2778	N2779	E2779	K2780	I2781	D2782	E2783	E2784	K2785	K2786	T2787	H2788	F2789	L2790	R2792	F2793	I2794	T2796	S2798	K2800	I2801		
K2802	E2803	I2804	Y2805	R2806	W2807	P2808	I2809	K2810	E2811	S2812	F2813	K2814	A2815	M2816	I2817	A2818	W2819	E2820	W2821	T2822	I2823	E2824	K2825	R2826	R2827	E2828	G2829	E2830	E2831	E2832	R2833	T2834	E2835	K2836	K2837	K2838	T2839	R2840	K2841	I2842	S2843	Q2844	T2845	A2846	Q2847	T2848	Y2849	D2850	P2851	R2852	E2853	G2854	Y2855	N2856	P2857	Q2858	P2859	D2860
L2862	S2863	Q2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	V2908	A2909	Q2910	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920	E2921	A2923
Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933	G2934	Y2935	A2936	V2937	T2938	R2939	GLY	LEU	LYS	ASP	MET	GLU	ALA	LEU	ASP	THR	SER	SER	I2961	S2970	A2979	VAL	VAL	SER	GLY	ARG	VAL	G2990	LYS	PRO	H2991	E2992	K3000	I3001	L3002	S3019	THR	PRO	ALA	LYS	VAL	LEU	GLY	SER	GLY				
GLY	HIS	ALA	SER	N3033	L3046	H3052	ARG	VAL	SER	PHE	GLY	THR	ASP	ALA	PRO	V3064	R3073	SER	ASP	GLU	ALA	ARG	THR	VAL	MET	LYS	SER	GLY	PRO	GLU	ILE	VAL	K3089	E3108	R3111	LEU	GLY	LYS	VAL	SER	GLN	ARG	THR	GLN	VAL	LYS	VAL	GLY	Q3127									
Y3131	T3132	T3133	V3134	A3135	L3136	L3140	H3150	PHE	GLY	ASP	ASP	VAL	ILE	LEU	ASP	D3160	L3175	THR	THR	LYS	ASN	THR	TYR	VAL	GLU	LYS	LEU	R3187	A3199	ALA	MET	PRO	VAL	ALA	PHE	LEU	GLU	PRO	GLN	LEU	ASN	GLY	ASN	CYS	SER	VAL	TYR	THR	LYS	SER								
PRO	ARG	GLU	ARG	ALA	ILE	LEU	GLY	PRO	ASN	SER	VAL	GLU	MET	CYS	PRO	ASP	ILE	VAL	R3248	L3249	M3250	A3251	A3257	GLU	SER	GLY	ALA	ARG	GLY	THR	GLU	MET	P3267	L3281	V3284	TRP	GLU	ARG	GLY	PRO	GLU	ALA	PRO	PRO	PRO	ALA	LEU	PRO	ALA	GLY	ALA							
PRO	PRO	CYS	THR	ALA	VAL	THR	S3309	H3326	LEU	GLY	ILE	ASP	GLU	ALA	THR	TRP	MET	LYS	R3337	A3342	P3351	A3369	Q3378	LEU	ARG	LEU	GLU	ALA	LYS	ALA	GLU	GLY	GLY	GLU	LEU	VAL	R3395	D3396	E3397	V3400	L3408	F3435	G3439	E3463	ILE													
ASN	ASN	MET	PHE	LEU	THR	ALA	ASP	LYS	SER	LYS	MET	ALA	LYS	GLY	ALA	GLN	SER	GLY	GLY	ASP	GLN	ARG	THR	LYS	LYS	LYS	ARG	ARG	GLY	VAL	GLN	THR	SER	LEU	I3510	V3511	L3514	K3515	L3522	A3526	D3529	L3532	L3535															
R3539	A3543	D3544	V3549	F3552	L3553	Q3554	N3555	ASN	LEU	HIS	LEU	LEU	GLN	GLY	VAL	GLY	GLY	SER	PRO	SER	LEU	TRP	GLN	MET	ALA	LEU	TYR	ARG	GLU	GLU	ASP	ALA	D3588	P3589	E3590	K3591	H3611	TYR	LYS	SER	LYS	LYS	ALA	VAL	TRP	HIS												
LYS	LEU	S3625	R3629	R3630	A3631	A3634	L3641	P3645	T3646	H3647	R3648	A3649	C3650	N3651	M3652	F3653	N3673	L3677	E3682	GLN	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	VAL	GLU	GLU	GLU	T3693	P3694	D3695	P3697	L3698	L3701	V3702	L3716	D3719	V3720	L3721	V3722	K3723	A3724	Y3725	A3726	D3727	L3728								
M3729	A3730	K3731	S3732	L3735	GLU	GLY	GLY	ASN	GLU	ALA	GLU	GLU	GLU	VAL	K3760	Q3761	R3762	S3768	H3771	T3772	R3773	E3777	Q3781	M3782	I3783	Q3788	T3965	E3966	Y3967	Y3968	S3796	S3803	I3804	L3805	K3815	M3816	L3817	L3820	L3832	L3835	M4026	L4027	L4028	S4029	V4035	V4036												
N3860	E3861	D3862	L3866	N3867	R3868	Q3869	N3870	G3871	L3884	F3885	R3886	Q3889	L3890	L3891	C3892	N3897	Q3900	N3901	Y3902	L3923	G3939	Q3960	F3962	N3963	S3964	L3965	T3966	E3967	Y3968	I3969	L3980	L3985	W3986	V3990	K4021	D4022	N4023	V4024	N4025	N4026	L4027	L4028	S4029	V4035	V4036													



• Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H: 71% 28%

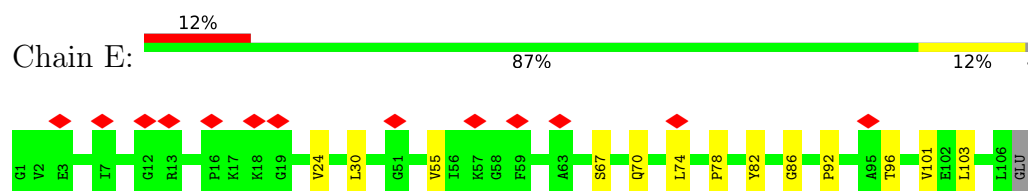


• Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B

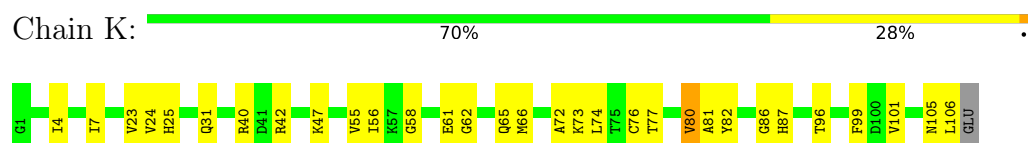
Chain B: 85% 15%



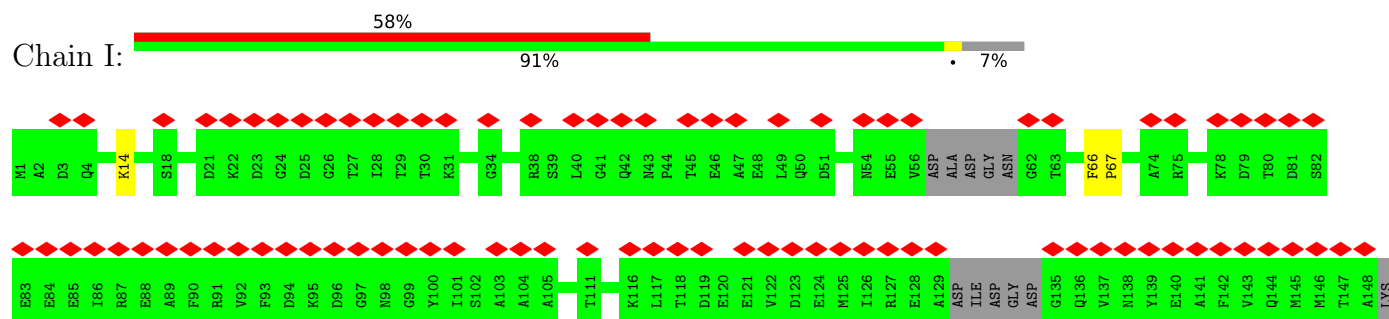
- Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B



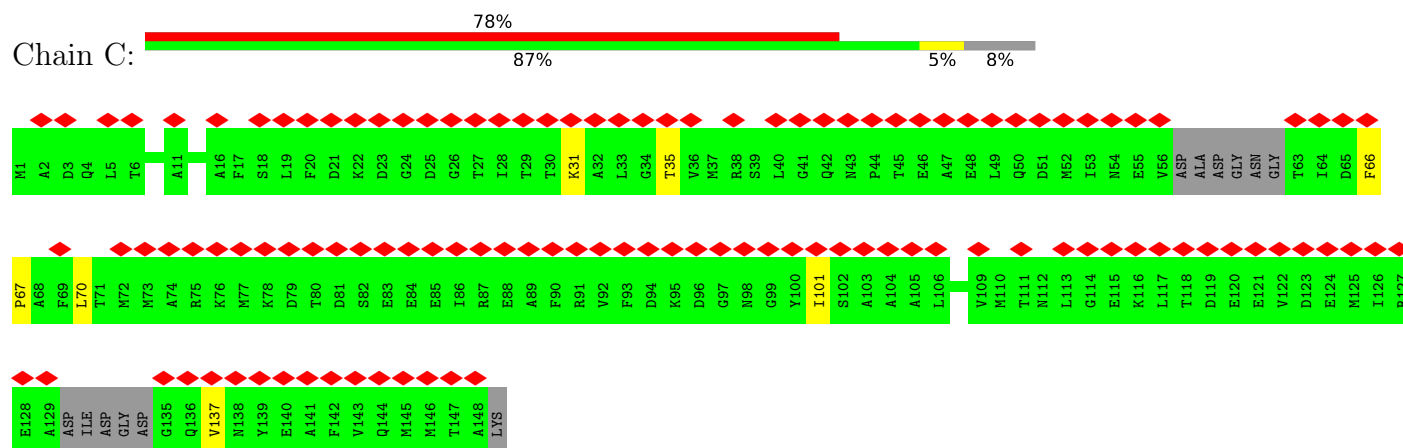
- Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B



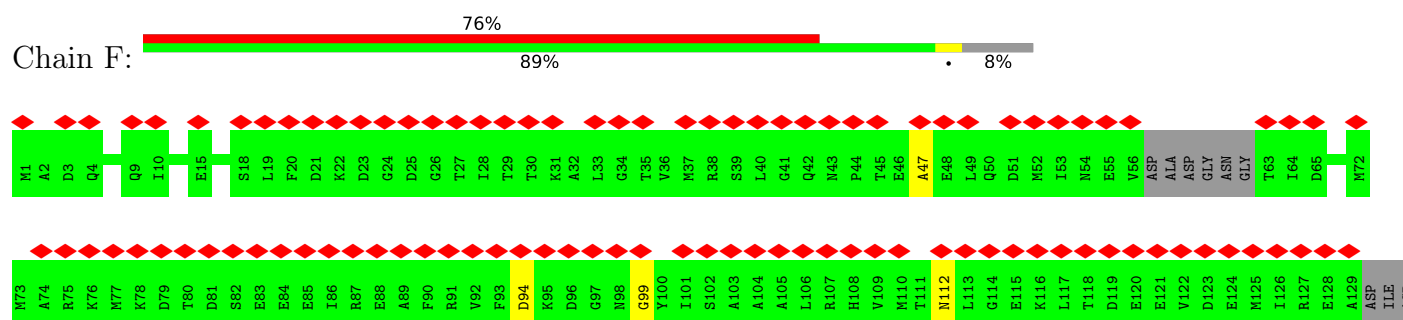
- Molecule 4: Calmodulin-1



- Molecule 4: Calmodulin-1

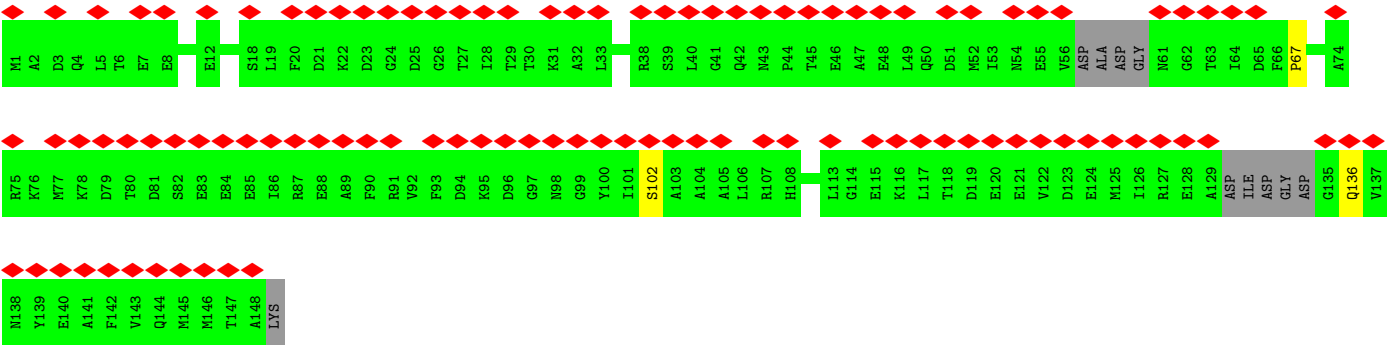
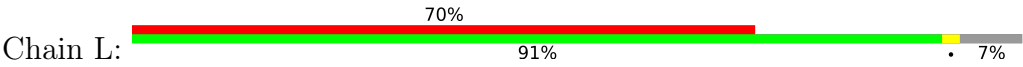


- Molecule 4: Calmodulin-1





• Molecule 4: Calmodulin-1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	144529	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.559	Depositor
Minimum map value	-1.060	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.066	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	479.36002, 479.36002, 479.36002	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	M	0.10	0/516	0.27	0/672
2	A	0.20	0/25342	0.37	6/34836 (0.0%)
2	D	0.21	0/23698	0.37	4/32668 (0.0%)
2	G	0.13	0/26809	0.30	3/36763 (0.0%)
2	J	0.16	0/25729	0.31	0/35328
3	B	0.14	0/751	0.38	0/1025
3	E	0.07	0/671	0.23	0/926
3	H	0.11	0/775	0.30	0/1054
3	K	0.37	0/774	0.54	0/1051
4	C	0.08	0/707	0.22	0/978
4	F	0.07	0/711	0.16	0/984
4	I	0.07	0/711	0.18	0/981
4	L	0.07	0/706	0.18	0/976
All	All	0.17	0/107900	0.34	13/148242 (0.0%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2125	HIS	N-CA-C	-8.15	102.47	111.36
2	A	4045	VAL	N-CA-C	-8.03	102.71	110.42
2	A	494	LEU	N-CA-C	-7.49	103.12	111.28
2	D	3671	ASP	N-CA-C	-7.35	103.35	111.36
2	G	4018	ASP	N-CA-C	-7.04	103.53	111.14
2	G	4016	LEU	N-CA-C	6.79	118.68	111.28
2	A	77	ALA	N-CA-C	-6.75	103.92	111.28
2	G	4018	ASP	N-CA-CB	6.32	119.23	110.07
2	A	3989	VAL	N-CA-C	-5.96	104.70	110.42
2	D	2127	GLN	N-CA-C	5.22	116.65	111.07
2	A	1548	LEU	CA-C-N	5.03	131.19	122.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1548	LEU	C-N-CA	5.03	131.19	122.28
2	D	4235	VAL	N-CA-C	-5.00	105.52	110.62

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	M	514	0	522	9	0
2	A	24845	0	19916	455	0
2	D	23336	0	16446	311	0
2	G	26285	0	21941	417	0
2	J	25245	0	20257	342	0
3	B	735	0	669	11	0
3	E	657	0	537	7	0
3	H	759	0	724	21	0
3	K	758	0	735	21	0
4	C	707	0	386	5	0
4	F	710	0	386	3	0
4	I	711	0	383	4	0
4	L	706	0	363	2	0
5	A	14	0	10	0	0
5	D	14	0	10	0	0
5	G	14	0	10	0	0
5	J	14	0	10	0	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
6	G	1	0	0	0	0
6	J	1	0	0	0	0
7	A	31	0	12	2	0
7	D	31	0	12	1	0
7	G	31	0	12	3	0
7	J	31	0	12	1	0
8	A	1	0	0	0	0
8	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	G	1	0	0	0	0
8	J	1	0	0	0	0
All	All	106156	0	83353	1556	0

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

All (1556) 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)
2:A:415:ILE:CD1	2:A:493:ARG:HD2	1.68	1.23
2:A:415:ILE:HD11	2:A:493:ARG:CD	1.68	1.21
2:D:4055:VAL:HG11	2:D:4163:PHE:CZ	1.91	1.05
2:A:4048:LEU:HD11	2:A:4055:VAL:HG21	1.36	1.03
2:A:357:LEU:HB2	2:A:378:LEU:HA	1.45	0.98
2:D:4055:VAL:HG11	2:D:4163:PHE:HZ	1.30	0.94
2:A:359:TYR:HA	2:A:376:ALA:HA	1.52	0.92
2:G:2198:MET:HB3	2:G:2203:MET:HE1	1.51	0.92
2:A:4048:LEU:HD11	2:A:4055:VAL:CG2	2.00	0.90
2:J:4024:VAL:HA	2:J:4027:LEU:HD12	1.51	0.89
2:G:2155:LEU:HD21	2:G:2198:MET:HE1	1.54	0.89
2:D:4044:MET:SD	2:D:4047:MET:HE2	2.12	0.89
2:D:4183:ILE:HG23	2:D:5021:PHE:HB2	1.52	0.89
2:A:478:PHE:HE1	2:A:483:MET:HE3	1.37	0.89
2:D:4037:ASN:HD21	2:D:4155:PRO:HD2	1.37	0.88
2:A:3980:LEU:HD12	2:A:3985:LEU:HD22	1.55	0.87
2:D:3677:LEU:HD21	2:D:3698:LEU:HD21	1.58	0.84
2:D:4059:LEU:HD21	2:D:4167:ALA:HA	1.60	0.82
2:D:3989:VAL:HG11	2:D:4027:LEU:HD21	1.62	0.82
2:D:4059:LEU:HD11	2:D:4167:ALA:HB2	1.58	0.82
2:G:3648:ARG:HG3	2:G:3652:MET:HE1	1.62	0.82
2:A:273:HIS:H	2:A:335:GLY:HA3	1.43	0.81
2:A:489:ASN:HB3	2:A:493:ARG:HH12	1.45	0.80
2:A:483:MET:HE1	2:A:529:LEU:HD11	1.63	0.80
2:A:3981:ALA:HA	2:A:3986:TRP:CH2	2.17	0.79
2:J:3723:MET:HE1	2:J:3793:MET:HA	1.63	0.79
2:J:1699:GLU:HG2	2:J:1814:MET:HE1	1.64	0.79
2:G:2559:LEU:HD23	2:G:2602:VAL:HG12	1.64	0.79
2:J:1943:LEU:HD13	2:J:2098:VAL:HG22	1.65	0.79
2:J:498:THR:HG22	2:J:499:THR:H	1.48	0.79
2:D:4055:VAL:CG1	2:D:4163:PHE:CZ	2.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4055:VAL:CG1	2:D:4163:PHE:CE1	2.67	0.78
2:D:2159:LEU:O	2:D:2162:ILE:HG22	1.84	0.78
2:A:4048:LEU:HD11	2:A:4055:VAL:CB	2.14	0.77
2:J:2170:MET:HE3	2:J:2171:GLY:H	1.50	0.77
2:A:1870:VAL:HG11	2:A:2097:LEU:HD22	1.65	0.77
2:D:3677:LEU:HD11	2:D:3698:LEU:HD23	1.64	0.77
2:D:4052:SER:HA	2:D:4055:VAL:CG1	2.15	0.77
3:H:78:PRO:HD3	3:H:96:THR:HG22	1.67	0.77
2:G:3980:LEU:HD12	2:G:3985:LEU:HD22	1.65	0.76
2:J:4222:VAL:HB	2:J:4950:VAL:HG22	1.67	0.76
2:J:35:LEU:HD22	2:J:51:PRO:HG3	1.66	0.76
2:J:1494:MET:HE3	2:J:1495:VAL:H	1.50	0.75
2:D:4022:ASP:O	2:D:4025:VAL:HG22	1.87	0.75
2:A:4048:LEU:CD1	2:A:4055:VAL:HG11	2.16	0.74
2:J:3783:ILE:HD11	2:J:3832:ILE:HD13	1.69	0.74
2:A:357:LEU:CB	2:A:378:LEU:HA	2.17	0.74
2:D:4055:VAL:CG2	2:D:4163:PHE:CE1	2.70	0.74
3:B:66:MET:HE3	3:B:67:SER:H	1.53	0.73
2:A:224:HIS:HA	2:A:388:LEU:HD22	1.68	0.73
2:G:3835:LEU:HD21	2:G:3880:PHE:CZ	2.23	0.73
2:A:475:GLN:NE2	2:A:531:ARG:O	2.21	0.73
1:M:27[A]:ASN:OD1	1:M:28[A]:ALA:N	2.22	0.73
2:A:478:PHE:CE1	2:A:483:MET:HE3	2.22	0.73
2:A:223:PHE:HD2	2:A:389:PHE:HE1	1.37	0.72
2:D:4936:ILE:HG21	2:J:4927:ILE:HD12	1.72	0.72
3:H:66:MET:HE1	3:H:72:ALA:HB3	1.69	0.72
2:J:576:ASN:OD1	2:J:2169:GLN:NE2	2.22	0.72
2:G:2298:VAL:HG11	2:G:2335:LEU:HD21	1.71	0.72
2:G:4231:MET:HE3	2:G:4231:MET:HA	1.73	0.71
3:B:25:HIS:HB3	3:B:40:ARG:HE	1.55	0.71
2:D:3842:LEU:HB2	2:D:3929:SER:HB2	1.72	0.71
2:G:2522:LEU:HA	2:G:2526:PHE:HB2	1.73	0.71
2:A:445:LEU:HD23	2:A:521:LEU:HB3	1.72	0.71
2:A:1257:VAL:HG21	2:A:1597:VAL:HG21	1.72	0.71
2:A:4991:PHE:HE2	2:A:5010:VAL:HG11	1.56	0.71
2:J:2198:MET:SD	2:J:2203:MET:HE1	2.30	0.71
2:D:4044:MET:SD	2:D:4047:MET:CE	2.79	0.71
3:E:82:TYR:HB3	3:E:86:GLY:HA2	1.73	0.70
2:J:3701:LEU:HD21	2:J:3725:TYR:HD2	1.56	0.70
2:D:67:PHE:HB3	2:D:109:LEU:HD12	1.71	0.70
2:J:2248:ARG:HG2	2:J:2286:LEU:HD21	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:483:MET:SD	2:A:484:LEU:N	2.64	0.70
2:A:1929:MET:HE3	2:A:1929:MET:H	1.57	0.70
2:G:2193:GLN:O	2:G:2195:PRO:HD3	1.92	0.69
2:A:1291:LEU:HD12	2:A:1595:LEU:HD12	1.72	0.69
2:D:3927:GLN:HB2	2:D:3992:PHE:CE1	2.27	0.69
2:D:4052:SER:HA	2:D:4055:VAL:HG12	1.74	0.69
2:A:3767:GLN:NE2	2:A:3806:ASN:O	2.23	0.69
3:K:82:TYR:HB3	3:K:86:GLY:HA2	1.75	0.69
2:A:2452:ARG:NH2	2:D:174:VAL:O	2.26	0.69
2:D:2128:TYR:HD2	2:D:3669:PHE:HD2	1.41	0.69
2:D:565:TYR:HB2	2:D:602:VAL:HG22	1.75	0.68
2:D:4021:LYS:O	2:D:4025:VAL:HG13	1.94	0.68
2:G:445:LEU:HB3	2:G:521:LEU:HD22	1.76	0.68
2:A:1804:LEU:HD12	2:A:1853:ILE:HD13	1.75	0.68
2:D:4207:MET:HE3	2:D:4207:MET:HA	1.75	0.67
2:G:1106:ARG:HH21	2:G:1185:GLY:HA3	1.59	0.67
2:D:2299:VAL:HG21	2:D:2356:LEU:HB3	1.77	0.67
2:D:3989:VAL:O	2:D:3993:LEU:HG	1.94	0.67
2:D:4037:ASN:ND2	2:D:4155:PRO:HD2	2.09	0.67
2:G:2298:VAL:HA	2:G:2331:TYR:OH	1.95	0.67
2:A:1724:CYS:HA	2:A:1851:MET:HE1	1.76	0.67
2:A:4150:LEU:HB3	2:A:4160:LEU:HD21	1.77	0.67
2:G:3943:ILE:HD11	2:G:4002:LYS:HZ1	1.60	0.66
2:D:4231:MET:HE3	2:D:4231:MET:HA	1.76	0.66
2:J:4139:ILE:O	2:J:4143:VAL:HG13	1.95	0.66
2:G:3768:SER:HA	2:G:3771:HIS:HB3	1.77	0.66
2:D:3640:PRO:HG2	2:D:3643:ASN:HB2	1.77	0.66
3:H:68:LEU:HD12	3:H:106:LEU:HD23	1.77	0.66
2:D:4787:ASN:OD1	2:D:4788:SER:N	2.28	0.66
2:A:3820:LEU:HD23	2:A:3902:TYR:HE2	1.59	0.66
2:G:1708:ARG:HH12	2:G:1814:MET:HE1	1.59	0.66
2:A:575:LEU:HD13	2:A:609:CYS:HB2	1.78	0.66
2:G:1454:THR:HG22	2:G:1456:ASP:H	1.60	0.66
2:A:3951:PHE:O	2:A:3955:MET:HG3	1.95	0.66
2:D:4055:VAL:CG2	2:D:4163:PHE:HE1	2.09	0.66
2:A:488:LEU:HD11	2:A:540:PHE:HE1	1.60	0.65
2:A:1639:LEU:HB3	2:A:1648:MET:HB3	1.78	0.65
2:J:3768:SER:HA	2:J:3771:HIS:HB3	1.78	0.65
2:D:4055:VAL:HG11	2:D:4163:PHE:CE1	2.29	0.65
1:M:26[A]:THR:HG22	2:J:4937:ILE:HG23	1.79	0.65
2:D:4037:ASN:HA	2:D:4154:VAL:HG22	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4059:LEU:HD21	2:D:4167:ALA:CA	2.27	0.65
2:D:4177:TYR:O	2:D:4197:ILE:HD12	1.97	0.65
2:A:3953:LYS:O	2:A:3957:VAL:HG23	1.96	0.65
2:G:1653:LEU:HB3	2:G:1660:GLN:HB2	1.77	0.65
2:J:4687:TYR:HD2	2:J:4706:LEU:HD11	1.61	0.65
2:G:2354:VAL:O	2:G:2358:ILE:HG22	1.97	0.65
2:A:625:LEU:HD21	2:A:632:LEU:HD11	1.78	0.65
2:A:4716:TRP:H	2:A:4716:TRP:CD1	2.13	0.65
2:G:755:ILE:HB	2:G:768:PHE:HB2	1.79	0.64
2:A:3981:ALA:HA	2:A:3986:TRP:HH2	1.60	0.64
2:A:655:GLY:H	2:A:852:VAL:HG22	1.62	0.64
2:D:3990:VAL:HG13	2:D:4051:SER:HB3	1.79	0.64
2:D:4055:VAL:HG21	2:D:4163:PHE:CE1	2.32	0.64
2:J:4958:CYS:SG	2:J:4978:HIS:CD2	2.89	0.64
2:G:590:LEU:HD23	2:G:631:LEU:HD12	1.79	0.64
2:G:4020:GLN:O	2:G:4024:VAL:HG23	1.98	0.64
2:A:3788:GLY:HA2	2:A:3835:LEU:HG	1.78	0.64
2:G:1093:GLU:HB3	2:G:1201:HIS:HB3	1.79	0.64
3:H:8:SER:HB3	3:H:71:ARG:HB2	1.80	0.64
2:J:4027:LEU:HB2	2:J:4146:LEU:HD21	1.77	0.64
2:G:2301:TYR:CE2	2:G:2331:TYR:HD2	2.15	0.64
2:G:4001:MET:HE1	2:G:4061:PHE:HB2	1.80	0.64
2:D:4153:HIS:O	2:D:4155:PRO:HD3	1.97	0.64
2:J:4140:GLY:O	2:J:4143:VAL:HG22	1.98	0.64
2:A:489:ASN:HB3	2:A:493:ARG:NH1	2.12	0.64
2:J:1704:PRO:HG2	2:J:1707:LEU:HB2	1.80	0.64
2:G:4821:LYS:HE2	2:G:4821:LYS:HA	1.80	0.64
2:A:633:LEU:HD23	2:A:1639:LEU:HD11	1.80	0.64
2:A:1679:ASN:ND2	2:A:1797:ARG:O	2.31	0.64
2:A:3719:ASP:H	2:A:3793:MET:HE1	1.62	0.64
2:A:4020:GLN:O	2:A:4024:VAL:HG23	1.98	0.64
2:A:4207:MET:HE2	2:A:4207:MET:HA	1.80	0.64
2:G:842:PRO:HD3	2:G:1073:ARG:HG3	1.80	0.63
2:G:3722:TYR:CZ	2:G:3782:MET:HE1	2.34	0.63
2:A:3918:CYS:HA	2:A:3921:ASP:OD2	1.99	0.63
2:A:4549:VAL:O	2:A:4553:ASN:ND2	2.31	0.63
2:J:1700:ASP:HB3	2:J:1703:LEU:HB2	1.79	0.63
3:K:56:ILE:HD12	3:K:81:ALA:HB2	1.80	0.63
2:G:2024:PRO:HG2	2:G:2027:ILE:HG12	1.81	0.63
2:G:2512:ILE:HG21	2:G:2518:LEU:HB2	1.81	0.63
2:A:3775:ALA:O	2:A:3778:MET:HG3	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:419:ASP:OD1	2:A:493:ARG:HD3	1.99	0.63
2:A:4240:ASP:HB3	2:A:4668:LEU:HD11	1.81	0.63
2:A:4796:MET:HA	2:A:4796:MET:HE2	1.81	0.63
2:D:3955:MET:HE1	2:D:4016:LEU:HD13	1.81	0.63
2:G:3767:GLN:NE2	2:G:3806:ASN:O	2.27	0.63
2:J:1494:MET:HE3	2:J:1495:VAL:N	2.13	0.63
2:G:1730:MET:HE1	2:G:2159:LEU:HD22	1.81	0.62
2:A:3832:ILE:O	2:A:3836:MET:HG2	1.99	0.62
2:D:938:HIS:H	2:D:1054:GLU:H	1.46	0.62
2:J:2288:LEU:O	2:J:3849:ARG:NH1	2.31	0.62
2:A:645:ARG:HD2	2:A:826:ILE:HG13	1.80	0.62
2:G:1851:MET:HB2	2:G:1853:ILE:HG13	1.82	0.62
2:G:3698:LEU:HB3	2:G:3773:ARG:HD3	1.81	0.62
2:D:4055:VAL:CG1	2:D:4163:PHE:HE1	2.12	0.62
2:J:3723:MET:CE	2:J:3793:MET:HA	2.29	0.62
3:E:24:VAL:HG12	3:E:103:LEU:HA	1.80	0.62
2:D:2302:LEU:HB3	2:D:2363:CYS:HB3	1.80	0.62
2:D:4046:ASP:O	2:D:4049:VAL:HG22	2.00	0.62
4:F:94:ASP:HA	4:F:99:GLY:HA2	1.81	0.62
2:G:488:LEU:HD21	2:G:540:PHE:HE1	1.65	0.62
2:D:2346:VAL:HG12	2:D:2349:ASN:H	1.64	0.62
2:D:3889:GLN:HG3	2:D:3967:GLU:HG3	1.82	0.62
2:J:3732:SER:O	2:J:3735:LEU:HB2	1.99	0.62
2:D:2163:ARG:NH2	2:D:2201:LEU:O	2.32	0.61
2:J:1733:GLU:HG2	2:J:2201:LEU:HD23	1.81	0.61
2:A:1848:LEU:HD12	2:A:1853:ILE:HD11	1.82	0.61
2:J:1784:ALA:HA	3:K:55:VAL:HA	1.82	0.61
2:G:4913:ARG:NH2	2:G:4917:ASP:OD2	2.34	0.61
3:H:37:ASP:OD1	3:H:38:SER:N	2.33	0.61
2:A:3829:PHE:HD1	2:A:3832:ILE:HD11	1.65	0.61
2:A:4837:LEU:HD11	2:A:4932:ILE:HG23	1.81	0.61
1:M:26[B]:THR:O	2:A:4944:ARG:NH2	2.33	0.61
2:G:67:PHE:HB3	2:G:109:LEU:HD12	1.82	0.61
2:G:683:ARG:NH1	2:G:717:ASP:OD2	2.34	0.61
2:G:3934:TYR:OH	2:G:3998:HIS:ND1	2.34	0.61
2:G:2116:LEU:O	2:G:2120:MET:HG3	2.01	0.61
2:G:2642:LYS:O	2:G:2646:ASN:ND2	2.34	0.61
2:D:4983:HIS:O	7:D:5103:ATP:N6	2.29	0.61
2:G:2495:VAL:HG12	2:G:2497:ASP:H	1.65	0.61
2:G:2005:GLN:O	2:G:2009:LEU:HD12	2.00	0.61
2:D:4241:THR:HG22	2:D:4245:MET:HE2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4218:ILE:O	2:D:4222:VAL:HG23	2.01	0.61
2:J:4181:ILE:HD11	2:J:4987:ASN:HB3	1.83	0.61
2:G:4884:LEU:HD11	2:A:4914:VAL:HG21	1.83	0.61
2:G:411:TYR:HB2	2:G:486:LEU:HD21	1.82	0.60
2:G:3906:GLN:NE2	2:G:3913:ILE:O	2.28	0.60
2:A:2500:ALA:N	2:A:2553:TYR:HE2	1.99	0.60
2:A:3981:ALA:HA	2:A:3986:TRP:CZ3	2.36	0.60
2:J:2158:CYS:O	2:J:2162:ILE:HD12	2.01	0.60
2:A:1454:THR:HG22	2:A:1456:ASP:H	1.66	0.60
2:D:4175:ARG:N	2:D:4176:PRO:HD2	2.16	0.60
2:G:1257:VAL:HG21	2:G:1597:VAL:HG21	1.82	0.60
2:G:3844:LEU:HD21	2:G:3932:ASP:HB3	1.83	0.60
2:J:4995:LEU:HD21	2:J:5007:GLU:HB3	1.84	0.60
2:D:4055:VAL:HG13	2:D:4163:PHE:CE1	2.36	0.60
2:J:106:ALA:HA	2:J:149:THR:HA	1.83	0.60
2:J:4023:MET:O	2:J:4027:LEU:HG	2.01	0.60
2:J:4231:MET:HE3	2:J:4231:MET:HA	1.84	0.60
2:G:581:ASN:OD1	2:G:582:HIS:N	2.35	0.60
2:J:689:THR:HG22	2:J:776:LEU:H	1.67	0.60
2:A:1730:MET:HE3	2:A:1730:MET:HA	1.84	0.59
2:A:3959:LYS:NZ	2:A:4022:ASP:OD2	2.34	0.59
2:D:4680:LYS:HG3	2:D:4686:LEU:HD11	1.83	0.59
2:G:4126:GLU:O	2:G:4130:ASN:ND2	2.36	0.59
2:A:4956:THR:HG23	2:A:4957:LYS:HG3	1.84	0.59
2:D:4027:LEU:O	2:D:4031:LEU:HG	2.03	0.59
2:A:830:ARG:HA	2:A:839:LEU:HA	1.84	0.59
3:B:27:THR:HB	3:B:100:ASP:HB3	1.85	0.59
2:D:2894:LEU:O	2:D:2899:GLY:N	2.32	0.59
2:D:4183:ILE:HD12	2:D:5021:PHE:HD1	1.67	0.59
2:G:594:GLY:HA2	2:G:1594:ARG:HD2	1.83	0.59
2:G:1678:ASN:OD1	2:G:1681:VAL:HG23	2.02	0.59
2:G:4044:MET:HE3	2:G:4044:MET:HA	1.85	0.59
2:A:347:PHE:CD1	2:A:387:ALA:HB2	2.37	0.59
2:A:4888:TYR:OH	2:D:4913:ARG:NH2	2.36	0.59
2:D:583:ILE:HD12	2:D:583:ILE:H	1.67	0.59
2:D:4055:VAL:HG22	2:D:4163:PHE:HE1	1.68	0.59
2:J:2471:SER:HA	2:J:2525:GLY:HA3	1.84	0.59
2:G:418:LEU:HD11	2:G:494:LEU:HD22	1.85	0.59
2:G:578:ILE:H	2:G:578:ILE:HD12	1.67	0.59
2:D:4024:VAL:HA	2:D:4027:LEU:HD12	1.83	0.59
2:J:526:LEU:O	2:J:530:ILE:HG12	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1966:VAL:HG21	2:J:3650:CYS:HA	1.84	0.59
2:A:4813:LEU:HD13	2:D:4846:VAL:HG13	1.85	0.59
2:D:2128:TYR:HB3	2:D:3673:MET:HE2	1.84	0.59
2:G:668:VAL:HG21	2:G:738:LEU:HD12	1.84	0.59
2:G:3900:GLN:NE2	2:G:3968:TYR:O	2.35	0.59
2:A:1717:SER:HA	2:A:1721:GLU:HB2	1.85	0.59
2:D:4851:TYR:HD2	2:D:4920:PHE:HD1	1.51	0.59
2:J:2295:LEU:O	2:J:2299:VAL:HG12	2.02	0.59
2:J:2894:LEU:O	2:J:2899:GLY:N	2.31	0.59
2:D:3670:GLU:HA	2:D:3728:ILE:HD12	1.85	0.58
2:G:1931:LEU:HD13	2:G:1939:MET:HE1	1.84	0.58
2:G:4059:LEU:HD12	2:G:4163:PHE:HE1	1.67	0.58
2:A:3812:VAL:O	2:A:3816:MET:HG2	2.03	0.58
2:A:4048:LEU:HD11	2:A:4055:VAL:HG11	1.84	0.58
2:D:1995:THR:HA	4:F:112:ASN:HA	1.85	0.58
2:J:4984:ASN:HB3	2:J:4987:ASN:HB2	1.85	0.58
2:J:595:ARG:NH2	2:J:631:LEU:O	2.36	0.58
2:A:3891:LEU:HD11	2:A:3899:PHE:CZ	2.39	0.58
2:A:3916:ILE:O	2:A:3920:VAL:HG23	2.04	0.58
2:G:2138:LEU:HB3	2:G:3658:LYS:HD3	1.86	0.58
2:G:4204:GLN:O	2:G:4207:MET:HG2	2.03	0.58
3:H:40:ARG:NH2	3:H:102:GLU:OE2	2.36	0.58
2:A:414:PHE:HD2	2:A:441:VAL:HG21	1.68	0.58
2:A:3722:TYR:HD2	2:A:3782:MET:HE1	1.67	0.58
2:A:3805:LEU:HD21	2:A:3891:LEU:HA	1.84	0.58
2:D:3767:GLN:NE2	2:D:3806:ASN:O	2.36	0.58
2:G:1293:LEU:HG	2:G:1580:PHE:HE1	1.68	0.58
2:J:4036:VAL:HA	2:J:4153:HIS:O	2.03	0.58
2:G:699:GLY:H	2:G:1647:CYS:HB3	1.68	0.58
2:G:2305:CYS:O	2:G:2324:ASN:ND2	2.36	0.58
2:G:3844:LEU:HD12	2:G:3844:LEU:H	1.69	0.58
2:A:4051:SER:O	2:A:4052:SER:C	2.46	0.58
2:A:4551:PHE:O	2:A:4555:LEU:HD13	2.04	0.58
2:J:2499:LYS:O	2:J:2503:VAL:HG12	2.04	0.58
2:G:794:GLY:HA3	2:G:812:HIS:HB3	1.85	0.58
2:G:4823:LEU:HD12	2:A:4843:LEU:HD22	1.86	0.58
2:A:1819:VAL:HG23	2:A:1926:LEU:HD13	1.85	0.58
2:D:3647:HIS:O	2:D:3651:ASN:ND2	2.37	0.58
2:J:445:LEU:HD13	2:J:525:LEU:HD12	1.86	0.58
2:A:4231:MET:O	2:A:4235:VAL:HG23	2.04	0.58
2:D:2596:THR:HA	4:F:47:ALA:HB1	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3890:LEU:HA	2:G:3893:GLU:HB2	1.86	0.58
2:G:4836:GLN:HE21	2:J:4944:ARG:HH12	1.52	0.58
2:A:478:PHE:HD1	2:A:483:MET:SD	2.27	0.58
2:D:4145:VAL:HG13	2:D:4194:TYR:HD2	1.67	0.58
2:J:2208:MET:O	2:J:2212:VAL:HG23	2.03	0.58
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.87	0.57
2:G:106:ALA:HA	2:G:149:THR:HA	1.86	0.57
2:A:2142:TYR:CD1	2:A:2197:LEU:HD21	2.39	0.57
2:D:2271:THR:HG23	2:D:2274:ASP:H	1.69	0.57
2:D:2382:GLU:O	2:D:2386:ILE:HG12	2.03	0.57
2:A:483:MET:HE1	2:A:529:LEU:CD1	2.34	0.57
2:A:663:TYR:HE1	2:A:745:SER:HB2	1.69	0.57
3:K:105:ASN:OD1	3:K:106:LEU:N	2.37	0.57
2:G:2000:SER:O	2:G:2005:GLN:NE2	2.36	0.57
2:G:2298:VAL:HG22	2:G:2331:TYR:OH	2.04	0.57
2:J:1291:LEU:HD12	2:J:1550:PRO:HG2	1.86	0.57
2:J:4569:LEU:HD11	2:J:4649:LEU:HD22	1.86	0.57
2:G:4675:LYS:HD2	2:G:4679:ARG:HH21	1.70	0.57
2:A:2894:LEU:O	2:A:2898:GLY:N	2.37	0.57
2:A:3768:SER:HA	2:A:3771:HIS:CE1	2.39	0.57
2:A:4587:PRO:HD3	2:A:4628:VAL:HG21	1.85	0.57
2:D:1103:GLY:HA3	2:D:1123:VAL:HA	1.86	0.57
2:D:4741:LEU:HD22	2:D:4743:MET:HG3	1.85	0.57
2:G:3647:HIS:O	2:G:3651:ASN:ND2	2.37	0.57
2:G:3991:GLY:O	2:G:3995:VAL:HG12	2.04	0.57
2:J:688:LEU:HD23	2:J:691:GLY:H	1.69	0.57
2:G:2349:ASN:O	2:G:2353:VAL:HG12	2.05	0.57
2:A:2238:TYR:HE2	4:C:67:PRO:HB2	1.70	0.57
2:G:2559:LEU:HD21	2:G:2603:ILE:HD13	1.87	0.57
2:A:1072:VAL:HG12	2:A:1195:GLY:HA2	1.87	0.57
2:J:103:TYR:HA	2:J:150:MET:HE1	1.86	0.57
2:G:2239:PHE:HD2	2:G:2250:MET:HE1	1.69	0.57
2:G:2294:ASP:O	2:G:2298:VAL:HG23	2.04	0.57
2:D:3695:PRO:O	2:D:3700:GLN:NE2	2.38	0.57
2:J:590:LEU:HD23	2:J:631:LEU:HD13	1.87	0.57
2:J:2477:PRO:HD2	2:J:2536:LEU:HD11	1.86	0.57
2:A:22:LEU:HD23	2:A:22:LEU:H	1.70	0.57
2:A:1737:PRO:HD3	2:A:1771:LEU:HG	1.87	0.57
2:A:1850:VAL:HG23	2:A:1851:MET:HE3	1.86	0.57
2:A:4139:ILE:O	2:A:4143:VAL:HG22	2.04	0.57
2:D:3836:MET:HB2	2:D:3884:LEU:HD21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4716:TRP:H	2:G:4716:TRP:CD1	2.22	0.57
2:D:3986:TRP:HA	2:D:3986:TRP:CE3	2.39	0.57
2:D:4779:LYS:O	2:D:4783:ILE:HG12	2.05	0.56
2:J:3647:HIS:O	2:J:3651:ASN:ND2	2.37	0.56
2:G:2522:LEU:HD11	2:G:2582:MET:HG3	1.88	0.56
2:A:2194:HIS:CB	2:A:2197:LEU:HD23	2.36	0.56
2:J:1780:PRO:HG2	3:K:42:ARG:HD3	1.86	0.56
2:G:3799:LYS:NZ	2:G:3883:ASP:OD2	2.38	0.56
2:G:4843:LEU:HD22	2:J:4823:LEU:HD12	1.87	0.56
2:A:478:PHE:CD1	2:A:483:MET:SD	2.98	0.56
2:A:3806:ASN:HA	2:A:3890:LEU:HD23	1.87	0.56
2:A:4195:PHE:HD2	2:A:4991:PHE:HD1	1.53	0.56
2:A:4562:LEU:HG	2:A:4657:CYS:SG	2.45	0.56
2:D:418:LEU:HA	2:D:421:PHE:CE1	2.41	0.56
2:J:1644:GLU:HB3	2:J:1646:ARG:HG3	1.88	0.56
2:J:3788:GLY:HA2	2:J:3835:LEU:HG	1.87	0.56
2:J:3980:LEU:HD22	2:J:3985:LEU:HD22	1.87	0.56
2:A:4954:MET:HE2	2:A:4954:MET:HA	1.86	0.56
2:D:1679:ASN:ND2	2:D:1797:ARG:O	2.33	0.56
2:D:4037:ASN:HD22	2:D:4154:VAL:HG13	1.71	0.56
2:D:4159:ARG:HA	2:D:4162:ASN:ND2	2.20	0.56
2:J:411:TYR:O	2:J:415:ILE:HG12	2.06	0.56
2:G:883:ALA:HB1	2:G:907:LEU:HA	1.88	0.56
2:G:1653:LEU:HD12	2:G:1707:LEU:HD11	1.87	0.56
2:A:2144:ILE:HG12	2:A:2152:THR:HG21	1.87	0.56
3:B:37:ASP:OD1	3:B:38:SER:N	2.39	0.56
2:D:2254:LEU:HG	2:D:2258:LEU:HD23	1.86	0.56
2:D:4222:VAL:HB	2:D:4950:VAL:HG22	1.87	0.56
2:J:4021:LYS:O	2:J:4024:VAL:HG22	2.04	0.56
2:A:1773:PRO:HD3	2:A:2156:LEU:HB3	1.88	0.56
2:J:596:ASN:HB3	2:J:599:VAL:HG23	1.88	0.56
2:J:1450:VAL:N	2:J:1494:MET:HE1	2.21	0.56
2:G:3834:ALA:O	2:G:3838:THR:HG23	2.06	0.56
2:D:1962:ALA:HA	2:D:3653:PHE:HE2	1.70	0.56
2:J:1663:HIS:HB3	2:J:1707:LEU:HD21	1.88	0.56
2:A:2894:LEU:O	2:A:2899:GLY:N	2.32	0.56
2:G:2512:ILE:HG23	2:G:2517:PHE:HD2	1.71	0.56
2:A:1730:MET:HE2	2:A:2156:LEU:HD22	1.88	0.56
2:D:4037:ASN:ND2	2:D:4154:VAL:HA	2.21	0.56
2:G:2308:GLN:O	2:G:2324:ASN:ND2	2.32	0.56
2:G:2520:HIS:O	2:G:2524:VAL:HG12	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:4072:VAL:HG22	2:A:4125:PHE:HD2	1.71	0.56
2:A:4915:VAL:O	2:A:4919:THR:HG22	2.06	0.56
2:D:3674:ILE:O	2:D:3678:SER:HB3	2.06	0.56
2:J:4981:GLU:O	2:J:4987:ASN:ND2	2.39	0.56
2:D:2680:TRP:HA	2:D:2683:PHE:CE2	2.40	0.55
2:D:4024:VAL:HG23	2:D:4146:LEU:HD22	1.89	0.55
2:D:4028:LEU:HA	2:D:4031:LEU:HD12	1.87	0.55
2:D:4055:VAL:HG22	2:D:4163:PHE:CE1	2.41	0.55
2:G:684:VAL:HG21	2:G:744:VAL:HG11	1.87	0.55
2:G:1833:SER:HB3	2:G:1836:PHE:HD2	1.71	0.55
2:A:647:ASN:ND2	2:A:820:ARG:O	2.39	0.55
2:D:4904:PRO:HG3	2:D:4913:ARG:HE	1.71	0.55
3:H:41:ASP:OD1	3:H:41:ASP:N	2.40	0.55
2:A:4048:LEU:HD11	2:A:4055:VAL:CG1	2.36	0.55
2:G:3943:ILE:HD11	2:G:4002:LYS:NZ	2.21	0.55
2:A:22:LEU:HA	2:A:202:MET:HA	1.88	0.55
2:A:4243:PHE:O	2:A:4247:ILE:HG12	2.07	0.55
2:D:1131:ARG:N	2:D:1137:GLU:O	2.39	0.55
2:J:2349:ASN:O	2:J:2353:VAL:HG12	2.06	0.55
2:J:2546:MET:HA	2:J:2546:MET:HE2	1.88	0.55
2:J:2680:TRP:HA	2:J:2683:PHE:CE2	2.42	0.55
2:J:3722:TYR:OH	2:J:3782:MET:HG2	2.06	0.55
2:A:218:HIS:ND1	2:A:218:HIS:C	2.65	0.55
2:A:484:LEU:HG	2:A:485:SER:N	2.21	0.55
2:G:3924:LEU:HD12	2:G:3988:ALA:HB2	1.88	0.55
2:G:4555:LEU:HD11	2:G:4656:LEU:HB3	1.88	0.55
2:G:4578:LEU:HD12	2:A:4879:MET:HG3	1.88	0.55
2:A:495:ASN:HD22	2:A:550:LYS:HE2	1.71	0.55
2:A:853:PRO:HA	2:A:1023:PRO:HB3	1.88	0.55
2:D:3963:ASN:O	2:D:3966:THR:OG1	2.20	0.55
2:G:171:LEU:HD13	2:G:180:LEU:HD23	1.87	0.55
2:G:2332:LEU:HA	2:G:2335:LEU:HD12	1.89	0.55
2:A:2346:VAL:HG12	2:A:2349:ASN:H	1.72	0.55
2:D:3767:GLN:NE2	2:D:3804:ILE:O	2.39	0.55
2:D:4037:ASN:HD22	2:D:4154:VAL:HA	1.71	0.55
2:J:291:LEU:HA	2:J:301:VAL:HA	1.88	0.55
3:K:56:ILE:HD12	3:K:81:ALA:CB	2.37	0.55
2:A:3767:GLN:NE2	2:A:3804:ILE:O	2.40	0.55
1:M:27[A]:ASN:ND2	2:G:4942:GLU:OE2	2.40	0.55
2:G:153:ALA:HB2	2:G:170:ILE:HG12	1.89	0.55
2:J:1639:LEU:HD21	2:J:1650:ILE:HD13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4211:LYS:NZ	7:G:5103:ATP:O3G	2.40	0.55
3:H:56:ILE:HG21	3:H:81:ALA:HA	1.88	0.55
2:A:3640:PRO:HD2	2:A:3643:ASN:HB2	1.89	0.55
2:D:2237:CYS:O	2:D:2241:ARG:HG3	2.06	0.55
2:J:4658:ILE:HD13	2:J:4792:LEU:HB3	1.88	0.55
2:G:4562:LEU:HD21	2:G:4656:LEU:HB2	1.89	0.54
2:A:223:PHE:O	2:A:388:LEU:HB3	2.07	0.54
2:A:4708:THR:HG22	2:A:4774:LYS:HB3	1.90	0.54
2:G:1847:THR:O	2:G:1851:MET:HG2	2.07	0.54
2:J:755:ILE:HB	2:J:768:PHE:HB2	1.88	0.54
2:J:1716:ILE:HD11	2:J:1844:LEU:HA	1.89	0.54
2:G:1735:ILE:HD11	2:G:2197:LEU:HD13	1.90	0.54
2:A:1694:LEU:O	2:A:1698:LEU:HG	2.07	0.54
2:A:4679:ARG:NH2	2:A:4715:TYR:OH	2.40	0.54
3:B:105:ASN:OD1	3:B:105:ASN:N	2.40	0.54
2:J:2502:MET:HE3	2:J:2502:MET:HA	1.89	0.54
2:G:3835:LEU:HD22	2:G:3884:LEU:HD22	1.88	0.54
2:G:4222:VAL:HG12	2:G:4950:VAL:HG22	1.89	0.54
2:J:2286:LEU:HD12	2:J:2286:LEU:H	1.71	0.54
2:J:4865:LYS:HE2	2:J:4900:GLU:HB3	1.90	0.54
2:G:1649:ASP:HB3	2:G:1652:GLU:HG3	1.88	0.54
2:G:2435:ARG:HG2	2:G:2504:LEU:HD21	1.89	0.54
2:A:4041:ALA:O	2:A:4045:VAL:HG23	2.07	0.54
2:D:2552:ARG:HA	2:D:2599:GLN:HE22	1.72	0.54
2:A:1601:MET:HE3	2:A:1601:MET:HA	1.88	0.54
2:A:411:TYR:CB	2:A:486:LEU:HD11	2.38	0.54
2:A:2182:ILE:O	2:A:2185:ILE:HG22	2.08	0.54
2:A:4048:LEU:CD1	2:A:4055:VAL:CG1	2.86	0.54
2:G:561:LEU:HD11	2:G:599:VAL:HB	1.89	0.54
2:G:1580:PHE:CE2	2:G:1592:PRO:HG2	2.43	0.54
2:G:1760:HIS:HE1	2:G:2095:GLN:HE22	1.54	0.54
2:G:2128:TYR:CD2	2:G:3673:MET:HG2	2.43	0.54
2:A:437:PRO:HB2	2:A:440:ALA:HB3	1.90	0.54
2:A:505:GLU:HA	2:A:512:ALA:HB2	1.90	0.54
2:D:3986:TRP:CE3	2:D:4047:MET:SD	3.01	0.54
1:M:16[A]:CYS:SG	1:M:17[A]:CYS:N	2.81	0.54
2:A:493:ARG:O	2:A:496:VAL:HB	2.08	0.54
2:D:3992:PHE:O	2:D:3995:VAL:HG13	2.08	0.54
2:J:607:CYS:HB3	2:J:618:GLN:HE21	1.73	0.54
2:G:42:PHE:HD1	2:G:447:ASP:HB3	1.71	0.54
2:G:3904:ARG:O	2:G:3914:ASN:ND2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1648:MET:HE1	2:A:1656:ARG:HD2	1.89	0.54
2:D:661:LYS:HA	2:D:749:ASP:HA	1.89	0.54
2:D:4041:ALA:O	2:D:4045:VAL:HG23	2.08	0.54
2:D:4174:PHE:HA	2:D:4177:TYR:HD2	1.72	0.54
2:A:551:LEU:HD11	2:A:589:LEU:HD22	1.90	0.53
2:D:1844:LEU:O	2:D:1848:LEU:HG	2.08	0.53
2:D:3725:TYR:O	2:D:3729:MET:HG2	2.09	0.53
2:D:4055:VAL:HG13	2:D:4163:PHE:HE1	1.72	0.53
2:J:1819:VAL:HG22	2:J:1926:LEU:HD13	1.90	0.53
2:J:4238:CYS:O	2:J:4242:ILE:HG12	2.08	0.53
3:B:25:HIS:HB3	3:B:40:ARG:NE	2.20	0.53
2:J:4821:LYS:O	2:J:4825:THR:HG23	2.09	0.53
2:A:348:VAL:HG22	2:A:357:LEU:HD21	1.90	0.53
2:A:488:LEU:HD11	2:A:540:PHE:CE1	2.43	0.53
2:D:2128:TYR:HD2	2:D:3669:PHE:CD2	2.25	0.53
2:J:564:LEU:O	2:J:568:LEU:HG	2.08	0.53
2:J:1944:GLU:HB2	2:J:2123:LEU:HD21	1.90	0.53
2:G:4823:LEU:HD21	2:A:4839:MET:HB3	1.91	0.53
2:A:349:GLN:HB2	2:A:356:TRP:CE3	2.44	0.53
2:A:4968:PHE:HE2	2:A:4978:HIS:CG	2.27	0.53
2:J:2116:LEU:O	2:J:2120:MET:HG3	2.08	0.53
2:J:3698:LEU:O	2:J:3702:VAL:HG23	2.09	0.53
2:A:45:ARG:HG2	2:A:443:LEU:HD21	1.91	0.53
2:A:3722:TYR:CE1	2:A:3726:ALA:HB2	2.44	0.53
2:D:283:ARG:HA	2:D:290:TYR:HA	1.89	0.53
3:H:61:GLU:O	3:H:65:GLN:HG3	2.09	0.53
2:A:273:HIS:N	2:A:335:GLY:HA3	2.19	0.53
2:A:495:ASN:ND2	2:A:550:LYS:HE2	2.24	0.53
3:B:91:ILE:HD12	3:B:97:LEU:HD11	1.91	0.53
2:D:1684:ALA:O	2:D:1688:HIS:ND1	2.38	0.53
2:J:1123:VAL:HG23	2:J:1132:TRP:HB2	1.90	0.53
2:J:2203:MET:O	2:J:2207:VAL:HG23	2.09	0.53
2:G:4892:ARG:NH2	2:A:4899:ASP:OD1	2.42	0.53
2:A:2194:HIS:HB2	2:A:2197:LEU:HD23	1.90	0.53
2:D:1651:LEU:H	2:D:1651:LEU:HD12	1.72	0.53
2:A:1096:THR:HB	2:A:1199:VAL:H	1.73	0.53
2:A:4650:HIS:HA	2:A:4653:VAL:HG12	1.90	0.53
2:A:4978:HIS:HE1	2:A:4983:HIS:CE1	2.26	0.53
2:G:637:LEU:HD12	2:G:1635:THR:HB	1.90	0.53
2:A:4179:GLY:HA3	2:A:4195:PHE:CE1	2.43	0.53
2:D:2159:LEU:O	2:D:2162:ILE:CG2	2.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2825:LYS:HA	2:D:2935:TYR:HA	1.89	0.53
2:D:4140:GLY:O	2:D:4143:VAL:HG12	2.09	0.53
2:J:575:LEU:HD12	2:J:575:LEU:H	1.74	0.53
2:J:3696:ASP:OD1	2:J:3696:ASP:N	2.37	0.53
2:G:1087:ARG:HG2	2:G:1154:ASP:HA	1.91	0.52
2:G:2377:LEU:HG	2:G:2465:ASP:HA	1.90	0.52
2:A:223:PHE:CD2	2:A:389:PHE:HE1	2.23	0.52
2:A:4217:PHE:HE1	2:A:4233:LEU:HB3	1.73	0.52
2:D:1288:PHE:HA	2:D:1553:PHE:HA	1.91	0.52
2:G:1104:TRP:CD1	2:G:1190:PRO:HA	2.45	0.52
2:G:1206:GLN:NE2	2:G:1230:MET:O	2.39	0.52
2:D:770:ALA:HB3	2:D:1473:THR:H	1.73	0.52
2:D:3927:GLN:HB2	2:D:3992:PHE:HE1	1.73	0.52
2:D:3997:ALA:O	2:D:4001:MET:HG2	2.09	0.52
2:D:4793:GLY:O	2:D:4797:VAL:HG23	2.09	0.52
2:G:484:LEU:HD13	2:G:539:LEU:HD11	1.91	0.52
2:G:2104:ARG:O	2:G:2108:GLU:HG2	2.10	0.52
2:G:4208:PRO:HD2	2:G:4209:GLN:OE1	2.09	0.52
2:A:2142:TYR:CE1	2:A:2197:LEU:HD21	2.45	0.52
2:A:3798:LEU:O	2:A:3802:ILE:HG23	2.10	0.52
2:A:4968:PHE:CE2	2:A:4978:HIS:CG	2.97	0.52
2:J:2434:GLY:O	2:J:2508:ARG:NE	2.43	0.52
2:G:4024:VAL:O	2:G:4028:LEU:HG	2.10	0.52
2:A:414:PHE:CD2	2:A:441:VAL:HG21	2.45	0.52
2:J:1701:ALA:O	2:J:1830:VAL:HG23	2.09	0.52
2:A:4051:SER:O	2:A:4054:ASN:N	2.39	0.52
2:A:4901:ILE:HD12	2:A:4913:ARG:HH21	1.73	0.52
2:J:1694:LEU:HD22	2:J:1715:LEU:HB2	1.92	0.52
2:J:4677:LEU:HD23	2:J:4711:PHE:HE1	1.74	0.52
2:G:3999:MET:O	2:G:4003:LEU:HG	2.10	0.52
2:G:4338:VAL:HG21	2:A:4838:VAL:HG11	1.91	0.52
2:A:2211:MET:HE3	2:A:2212:VAL:N	2.24	0.52
2:J:653:ALA:HB3	2:J:656:SER:HB3	1.91	0.52
2:J:2144:ILE:HG12	2:J:2152:THR:HG21	1.90	0.52
2:J:2354:VAL:O	2:J:2358:ILE:HG12	2.10	0.52
2:J:4215:ARG:O	2:J:4218:ILE:HG13	2.09	0.52
2:G:4661:TYR:OH	2:G:4786:ASP:OD2	2.27	0.52
2:A:1434:TYR:HB3	2:A:1572:ILE:HG21	1.92	0.52
2:A:3705:PHE:HB3	2:A:3778:MET:CE	2.39	0.52
2:A:4936:ILE:HD13	2:D:4927:ILE:HG12	1.91	0.52
2:D:1105:ALA:HA	2:D:1122:TYR:H	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2128:TYR:CB	2:D:3673:MET:HE2	2.39	0.52
2:J:253:CYS:HA	2:J:258:SER:HB3	1.92	0.52
2:J:2894:LEU:O	2:J:2898:GLY:N	2.43	0.52
2:J:3805:LEU:HB3	2:J:3890:LEU:HB3	1.92	0.52
2:J:4687:TYR:CD2	2:J:4706:LEU:HD11	2.42	0.52
2:G:441:VAL:HG23	2:G:518:ILE:HD11	1.91	0.52
2:A:565:TYR:HE2	2:A:601:ASP:HB3	1.74	0.52
2:A:2559:LEU:HG	2:A:2560:PRO:HD3	1.92	0.52
2:A:4219:PHE:HD1	2:A:4950:VAL:HG21	1.75	0.52
4:C:31:LYS:O	4:C:35:THR:HG23	2.10	0.52
2:D:3674:ILE:HD11	2:D:3698:LEU:HD11	1.91	0.52
2:D:3986:TRP:CH2	2:D:4044:MET:HG2	2.45	0.52
2:J:3701:LEU:HD21	2:J:3725:TYR:CD2	2.40	0.52
2:G:4838:VAL:HG11	2:J:4338:VAL:HG21	1.92	0.52
2:A:1476:MET:O	2:A:1484:HIS:N	2.43	0.52
2:D:4059:LEU:HD21	2:D:4166:LEU:C	2.35	0.52
2:J:3889:GLN:HG3	2:J:3967:GLU:HG3	1.92	0.52
3:K:76:CYS:SG	3:K:80:VAL:HG11	2.50	0.52
2:G:1476:MET:O	2:G:1484:HIS:N	2.43	0.51
2:J:3723:MET:HE2	2:J:3796:SER:HB2	1.92	0.51
1:M:9[B]:ARG:HA	1:M:31[B]:ARG:HG2	1.91	0.51
3:H:22:CYS:N	3:H:48:PHE:O	2.39	0.51
2:D:3888:LEU:HD13	2:D:3968:TYR:OH	2.10	0.51
2:D:4242:ILE:HD11	2:D:4989:MET:HE1	1.93	0.51
2:G:449:ILE:HD12	2:G:521:LEU:HD23	1.92	0.51
2:A:500:ALA:HB2	2:A:515:TRP:CE3	2.45	0.51
2:J:1551:ALA:HB1	2:J:1553:PHE:CE2	2.46	0.51
2:J:1708:ARG:HH12	2:J:1837:GLN:HA	1.75	0.51
2:J:3719:ASP:OD1	2:J:3719:ASP:N	2.44	0.51
2:A:499:THR:HB	2:A:502:HIS:CB	2.40	0.51
2:A:1844:LEU:HD12	2:A:1848:LEU:HD23	1.93	0.51
2:A:4195:PHE:CE2	2:A:4991:PHE:HB2	2.45	0.51
2:D:3962:PHE:O	2:D:3966:THR:HG23	2.11	0.51
2:D:4888:TYR:OH	2:J:4917:ASP:OD2	2.24	0.51
2:J:3820:LEU:HD13	2:J:3902:TYR:HE2	1.75	0.51
2:G:591:ASP:O	2:G:1594:ARG:NH1	2.43	0.51
2:J:4927:ILE:O	2:J:4931:ILE:HG12	2.10	0.51
2:G:1580:PHE:HE2	2:G:1592:PRO:HG2	1.75	0.51
2:A:3828:PHE:O	2:A:3832:ILE:HG12	2.10	0.51
2:D:2350:ALA:HB1	2:D:2436:CYS:HB3	1.93	0.51
2:G:3673:MET:HE2	2:G:3728:ILE:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:66:PHE:CZ	4:C:70:LEU:HD11	2.46	0.51
2:D:4181:ILE:HG22	2:D:4182:GLU:H	1.74	0.51
2:J:498:THR:HG22	2:J:499:THR:N	2.22	0.51
3:K:24:VAL:HB	3:K:101:VAL:HG23	1.91	0.51
2:G:4849:TYR:CE1	2:J:4578:LEU:HD13	2.46	0.51
2:A:1868:PRO:O	2:A:1872:THR:OG1	2.23	0.51
2:J:269:TRP:CE2	2:J:272:SER:HB3	2.45	0.51
2:G:4059:LEU:HD12	2:G:4163:PHE:CE1	2.45	0.51
2:A:591:ASP:OD1	2:A:1594:ARG:NH1	2.44	0.51
2:A:3900:GLN:HB3	2:A:3976:ASN:HD21	1.76	0.51
2:J:3723:MET:CE	2:J:3796:SER:HB2	2.41	0.51
3:K:58:GLY:HA3	3:K:80:VAL:CG1	2.41	0.51
2:G:683:ARG:HG2	2:G:717:ASP:HB3	1.92	0.51
2:G:1947:CYS:HB2	2:G:2126:ARG:NH2	2.26	0.51
2:G:3638:MET:C	2:G:3638:MET:HE2	2.36	0.51
2:A:3927:GLN:HE21	2:A:3991:GLY:HA3	1.76	0.51
2:D:3798:LEU:HD12	2:D:3884:LEU:HA	1.93	0.51
2:D:4854:VAL:HG13	2:D:4858:PHE:CE1	2.46	0.51
2:J:470:SER:HA	2:J:473:ASN:HD21	1.76	0.51
2:G:487:VAL:HG13	2:G:522:LEU:HD11	1.93	0.50
2:G:1931:LEU:HD22	2:G:1935:VAL:HG11	1.92	0.50
2:G:2248:ARG:HD3	2:G:2286:LEU:HD22	1.91	0.50
2:G:4961:CYS:SG	2:G:4983:HIS:HE1	2.30	0.50
2:A:561:LEU:HD11	2:A:599:VAL:HG22	1.93	0.50
2:A:633:LEU:HB3	2:A:1639:LEU:HD11	1.93	0.50
2:D:2094:LEU:O	2:D:2098:VAL:HG22	2.10	0.50
2:D:4890:GLY:O	2:D:4892:ARG:N	2.42	0.50
2:J:1577:ALA:O	2:J:1584:ARG:NE	2.40	0.50
2:J:4028:LEU:HG	2:J:4146:LEU:HD22	1.92	0.50
2:G:579:GLN:H	2:G:582:HIS:HD2	1.59	0.50
2:G:4888:TYR:CD1	2:A:4914:VAL:HG22	2.45	0.50
2:A:232:THR:OG1	2:A:257:ARG:O	2.27	0.50
2:A:790:ARG:NH1	2:A:1624:LEU:O	2.44	0.50
2:A:1802:ILE:HD13	2:A:1807:LEU:HD22	1.92	0.50
2:D:3986:TRP:HE3	2:D:4047:MET:SD	2.34	0.50
2:G:800:PHE:HE2	2:G:810:PRO:HB3	1.76	0.50
2:A:684:VAL:HG12	2:A:781:VAL:HG22	1.94	0.50
2:J:4825:THR:HG22	2:J:4947:GLN:HE22	1.75	0.50
2:G:1772:ARG:NH2	2:G:1952:GLN:OE1	2.40	0.50
2:G:2238:TYR:CE2	4:I:67:PRO:HB2	2.47	0.50
2:A:668:VAL:HA	2:A:789:VAL:HG23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1650:ILE:HG22	2:A:1651:LEU:HD12	1.92	0.50
2:A:3790:THR:HG22	2:A:3835:LEU:HD23	1.93	0.50
2:D:3729:MET:HA	2:D:3732:SER:HB3	1.92	0.50
2:J:2377:LEU:HD21	2:J:2468:GLY:HA3	1.93	0.50
2:G:492:ASP:HA	2:G:550:LYS:HZ1	1.76	0.50
2:G:746:CYS:HA	2:G:757:PHE:HA	1.93	0.50
2:J:4845:ALA:HA	2:J:4887:MET:HE1	1.94	0.50
2:G:629:ARG:NH2	3:H:90:VAL:O	2.44	0.50
2:G:3990:VAL:HG13	2:G:4051:SER:HB3	1.94	0.50
2:D:1839:VAL:HG21	2:D:1934:SER:HB2	1.94	0.50
2:D:3674:ILE:HG21	2:D:3732:SER:HB2	1.94	0.50
2:J:1473:THR:HA	2:J:1488:LYS:HA	1.94	0.50
2:A:596:ASN:HB3	2:A:599:VAL:HG23	1.94	0.50
2:A:4048:LEU:CD1	2:A:4055:VAL:CB	2.87	0.50
2:A:4921:PHE:HD1	2:A:4925:ILE:HD13	1.75	0.50
2:D:2463:LEU:O	2:D:2467:VAL:HG23	2.11	0.50
2:J:595:ARG:NH1	2:J:1643:GLU:OE2	2.44	0.50
2:J:1835:GLU:HB2	2:J:1932:PRO:HG3	1.94	0.50
2:J:4873:ASP:N	2:J:4873:ASP:OD1	2.43	0.50
2:G:495:ASN:HD21	2:G:553:ARG:NH1	2.10	0.50
2:A:2125:HIS:NE2	2:A:3724:ALA:HB1	2.27	0.50
2:D:1007:TYR:HE2	2:D:1022:VAL:HG22	1.77	0.50
2:D:2377:LEU:HD23	2:D:2378:ALA:H	1.77	0.50
2:D:4017:LEU:HD12	2:D:4139:ILE:HG21	1.93	0.50
2:D:4045:VAL:O	2:D:4049:VAL:HG13	2.12	0.50
2:D:4716:TRP:H	2:D:4716:TRP:CD1	2.29	0.50
2:G:1653:LEU:HD13	2:G:1660:GLN:HA	1.94	0.50
2:G:4914:VAL:HG21	2:J:4884:LEU:HD21	1.93	0.50
2:A:248:GLU:HA	2:A:372:LEU:O	2.12	0.50
2:A:4211:LYS:O	2:A:4215:ARG:HG2	2.11	0.50
2:A:4848:VAL:HG11	2:A:4887:MET:HG2	1.93	0.50
2:J:3900:GLN:NE2	2:J:3968:TYR:O	2.45	0.50
2:G:473:ASN:O	2:G:477:LEU:HG	2.12	0.49
2:G:2195:PRO:HB3	2:G:2242:ILE:CG2	2.41	0.49
2:A:639:ASN:HD22	2:A:676:THR:HG21	1.77	0.49
2:A:3768:SER:HA	2:A:3771:HIS:ND1	2.27	0.49
2:A:3991:GLY:O	2:A:3995:VAL:HG12	2.12	0.49
2:A:4331:LEU:HD12	2:A:4334:LEU:HD21	1.93	0.49
2:A:5017:ARG:NH1	2:A:5019:TRP:HZ2	2.10	0.49
2:D:1218:GLY:O	2:D:1223:PHE:N	2.34	0.49
2:D:3669:PHE:CZ	2:D:3728:ILE:HD11	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:3832:ILE:HD11	2:J:3884:LEU:HD11	1.94	0.49
2:G:689:THR:HA	2:G:778:PHE:HE2	1.76	0.49
2:G:1732:SER:OG	2:G:1733:GLU:OE2	2.27	0.49
2:G:3955:MET:HE1	2:G:4016:LEU:HA	1.93	0.49
2:G:4181:ILE:HG23	2:G:4193:ILE:HB	1.95	0.49
2:G:4823:LEU:HD12	2:A:4843:LEU:HD13	1.94	0.49
2:A:67:PHE:HB3	2:A:109:LEU:HD12	1.94	0.49
2:A:3890:LEU:HA	2:A:3893:GLU:HB2	1.95	0.49
2:J:1091:GLU:HA	2:J:1150:GLY:HA2	1.94	0.49
2:J:4581:LYS:HD2	2:J:4632:LEU:HD22	1.93	0.49
4:L:102:SER:HA	4:L:136:GLN:HA	1.94	0.49
2:G:2155:LEU:CD2	2:G:2198:MET:HE1	2.36	0.49
3:H:77:THR:HG23	3:H:80:VAL:HG12	1.94	0.49
2:A:1434:TYR:HB2	2:A:1519:LEU:HB3	1.94	0.49
2:A:3897:ASN:O	2:A:3901:ASN:ND2	2.45	0.49
2:D:2212:VAL:HG22	2:D:2256:TYR:CZ	2.47	0.49
2:J:551:LEU:HD21	2:J:589:LEU:HD12	1.94	0.49
2:J:561:LEU:HD21	2:J:598:LYS:HB3	1.94	0.49
2:J:591:ASP:O	2:J:1594:ARG:NH1	2.44	0.49
2:G:1713:ASP:HA	2:G:1716:ILE:HG12	1.94	0.49
2:G:3977:GLN:HG2	2:G:4030:LEU:HD23	1.93	0.49
2:G:4574:ASN:O	2:A:4849:TYR:OH	2.29	0.49
2:A:273:HIS:HB2	2:A:335:GLY:C	2.38	0.49
2:D:666:VAL:HA	2:D:791:PHE:HA	1.94	0.49
2:D:2238:TYR:O	2:D:2242:ILE:HG12	2.11	0.49
2:J:537:CYS:O	2:J:541:SER:OG	2.29	0.49
2:G:233:ILE:HD13	2:G:284:HIS:CE1	2.47	0.49
2:G:3641:LEU:HA	2:G:3644:LEU:HD23	1.95	0.49
2:A:1719:HIS:CD2	2:A:1800:PRO:HB2	2.48	0.49
2:A:4923:PHE:O	2:A:4928:LEU:HD23	2.11	0.49
2:D:1639:LEU:N	2:D:1648:MET:O	2.46	0.49
2:D:4837:LEU:HD11	2:D:4932:ILE:HG23	1.94	0.49
2:J:4920:PHE:CZ	2:J:4924:VAL:HG11	2.47	0.49
2:G:4024:VAL:HG13	2:G:4146:LEU:HD22	1.93	0.49
3:H:71:ARG:HG2	3:H:102:GLU:HB2	1.92	0.49
2:A:3992:PHE:HB3	2:A:3996:PHE:CE2	2.47	0.49
2:A:4817:ALA:HA	2:A:4823:LEU:HD12	1.94	0.49
2:D:2000:SER:O	2:D:2005:GLN:NE2	2.37	0.49
2:D:3677:LEU:HD12	2:D:3697:PRO:HB2	1.95	0.49
2:J:283:ARG:HA	2:J:291:LEU:H	1.77	0.49
2:J:4679:ARG:NH1	2:J:4715:TYR:OH	2.34	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1859:VAL:O	2:G:1863:LEU:HD23	2.11	0.49
2:D:2868:SER:O	2:D:2872:GLN:N	2.42	0.49
2:D:3732:SER:OG	2:D:3733:CYS:N	2.45	0.49
2:A:173:SER:HB3	2:A:178:ARG:H	1.78	0.49
4:C:101:ILE:O	4:C:137:VAL:N	2.46	0.49
2:D:2283:ASN:HB3	2:D:2286:LEU:HD12	1.93	0.49
2:D:4126:GLU:O	2:D:4130:ASN:ND2	2.46	0.49
2:J:4093:PHE:O	2:J:4097:MET:HG3	2.13	0.49
2:G:1097:THR:HA	2:G:1143:TRP:HZ3	1.77	0.49
2:A:1607:ARG:NH2	2:A:1610:ASN:OD1	2.46	0.49
2:A:4898:GLY:HA2	2:A:4913:ARG:HH22	1.77	0.49
2:A:4953:ASP:HA	2:A:4956:THR:HG22	1.93	0.49
2:D:280:LEU:N	2:D:314:PHE:O	2.45	0.49
2:J:2294:ASP:O	2:J:2298:VAL:HG23	2.13	0.49
2:G:262:LEU:H	2:G:262:LEU:HD23	1.77	0.49
2:G:499:THR:HA	2:G:515:TRP:CZ3	2.48	0.49
2:G:1104:TRP:CH2	2:G:1153:ILE:HB	2.48	0.49
2:G:1232:ARG:NH2	2:G:1828:ASP:O	2.45	0.49
2:G:1673:VAL:HG12	2:G:1681:VAL:HG11	1.95	0.49
2:G:4218:ILE:HD11	2:G:4954:MET:SD	2.53	0.49
2:A:2198:MET:N	2:A:2198:MET:HE2	2.27	0.49
2:D:2894:LEU:O	2:D:2898:GLY:N	2.46	0.49
2:D:3985:LEU:O	2:D:3989:VAL:HG23	2.12	0.49
2:D:3998:HIS:O	2:D:3999:MET:C	2.52	0.49
2:D:4773:VAL:O	2:D:4777:ILE:HG23	2.13	0.49
2:G:2247:GLN:HG2	2:G:2279:SER:HA	1.94	0.48
2:A:222:LEU:HD12	2:A:388:LEU:HB2	1.95	0.48
2:A:478:PHE:CE1	2:A:483:MET:HG2	2.47	0.48
2:A:637:LEU:HD13	2:A:1635:THR:HG21	1.94	0.48
2:A:1143:TRP:CD1	2:A:1164:LEU:HD21	2.48	0.48
2:A:2500:ALA:HB2	2:A:2553:TYR:CD2	2.48	0.48
2:G:1115:LEU:HG	2:G:1123:VAL:HG11	1.95	0.48
2:D:864:PRO:O	2:D:868:GLU:N	2.44	0.48
2:J:842:PRO:HG2	2:J:1196:PRO:HA	1.95	0.48
2:J:1270:LEU:HD21	2:J:1591:CYS:SG	2.53	0.48
2:G:2461:VAL:O	2:G:2510:TYR:OH	2.29	0.48
2:A:247:TYR:CE2	2:A:359:TYR:HB3	2.48	0.48
2:A:1235:THR:HG22	2:A:1610:ASN:HD21	1.76	0.48
2:A:4222:VAL:HG11	2:A:4950:VAL:HA	1.95	0.48
2:J:5027:CYS:SG	2:J:5028:PHE:N	2.86	0.48
2:G:3698:LEU:O	2:G:3702:VAL:HG23	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1784:ALA:O	3:B:82:TYR:OH	2.23	0.48
2:A:4143:VAL:O	2:A:4147:LEU:HG	2.13	0.48
2:D:3998:HIS:O	2:D:4001:MET:N	2.45	0.48
2:G:530:ILE:HD11	2:G:537:CYS:HA	1.96	0.48
2:G:1297:PHE:HE2	2:G:1525:GLY:HA2	1.78	0.48
2:G:2254:LEU:O	2:G:2258:LEU:HG	2.14	0.48
2:G:2509:VAL:HG13	2:G:2510:TYR:HD1	1.79	0.48
3:E:74:LEU:HD12	3:E:101:VAL:HB	1.96	0.48
2:A:1932:PRO:O	2:A:1936:LYS:HG3	2.14	0.48
2:G:909:ASN:HA	2:G:967:PRO:HA	1.96	0.48
2:A:265:LEU:HD12	2:A:279:PRO:HB2	1.95	0.48
2:A:2503:VAL:HG11	2:A:2557:ALA:HB1	1.96	0.48
2:D:1784:ALA:HA	3:E:55:VAL:HA	1.95	0.48
2:J:1849:LEU:HB2	2:J:1854:PHE:HD2	1.78	0.48
3:H:62:GLY:HA3	3:H:74:LEU:HD11	1.94	0.48
2:A:5017:ARG:HH11	2:A:5019:TRP:HZ2	1.62	0.48
2:D:118:LEU:HA	2:D:137:LEU:HA	1.96	0.48
2:D:2247:GLN:NE2	2:D:2281:ILE:O	2.37	0.48
2:J:2281:ILE:HB	2:J:2337:PHE:HD2	1.77	0.48
2:J:3892:CYS:SG	2:J:3968:TYR:HA	2.54	0.48
2:G:355:LEU:HD22	2:G:380:GLN:HA	1.96	0.48
2:G:1104:TRP:HA	2:G:1191:VAL:HG12	1.95	0.48
2:G:2125:HIS:NE2	2:G:3724:ALA:HB1	2.28	0.48
2:G:3648:ARG:HA	2:G:3651:ASN:HD22	1.78	0.48
2:A:223:PHE:HD2	2:A:389:PHE:CE1	2.26	0.48
2:A:4217:PHE:CE1	2:A:4233:LEU:HB3	2.48	0.48
2:G:4839:MET:HB3	2:J:4823:LEU:HD21	1.96	0.47
3:H:10:GLY:HA3	3:H:70:GLN:HB2	1.95	0.47
2:A:500:ALA:O	2:A:504:ALA:HB3	2.14	0.47
2:A:590:LEU:HB2	2:A:599:VAL:HG11	1.95	0.47
2:A:752:VAL:HG22	2:A:754:SER:H	1.78	0.47
2:A:3782:MET:CE	2:A:3793:MET:HG3	2.44	0.47
2:A:4658:ILE:HD13	2:A:4792:LEU:HB3	1.95	0.47
2:D:4567:LEU:HD21	2:D:4816:ILE:HG13	1.95	0.47
2:D:4985:LEU:HD12	2:D:4985:LEU:H	1.78	0.47
2:G:1289:LEU:HD22	2:G:1552:VAL:HG13	1.96	0.47
2:A:618:GLN:NE2	2:A:1673:VAL:O	2.47	0.47
2:A:3782:MET:HE2	2:A:3793:MET:HG3	1.96	0.47
2:A:4219:PHE:CD1	2:A:4950:VAL:HG21	2.49	0.47
2:A:4991:PHE:CE2	2:A:5010:VAL:HG11	2.44	0.47
2:J:842:PRO:O	2:J:1197:GLY:N	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:2006:ILE:HD13	2:J:2009:LEU:HD21	1.96	0.47
3:H:28:GLY:HA2	3:H:99:PHE:HA	1.96	0.47
2:A:350:HIS:H	2:A:357:LEU:HD23	1.79	0.47
2:A:2472:LEU:HD23	2:A:2473:PRO:HD2	1.96	0.47
2:D:3881:THR:HG21	2:D:3922:TYR:OH	2.14	0.47
2:D:4179:GLY:HA3	2:D:4197:ILE:HD11	1.95	0.47
2:J:445:LEU:CD1	2:J:525:LEU:HD12	2.42	0.47
2:J:2040:ALA:HA	2:J:2045:GLN:HA	1.96	0.47
2:J:2287:ALA:O	2:J:2349:ASN:ND2	2.44	0.47
2:J:2335:LEU:HB3	2:J:2432:LEU:HD13	1.96	0.47
2:J:2500:ALA:HB2	2:J:2553:TYR:HD1	1.79	0.47
2:G:1093:GLU:HG3	2:G:1148:VAL:HG12	1.95	0.47
2:G:1848:LEU:HD13	2:G:1853:ILE:HD12	1.95	0.47
2:A:1451:GLY:HA3	2:A:1494:MET:HA	1.95	0.47
2:A:2367:ALA:O	2:A:2373:GLY:N	2.48	0.47
2:A:3800:LEU:O	2:A:3804:ILE:HG22	2.14	0.47
2:A:4193:ILE:H	2:A:4193:ILE:HD12	1.79	0.47
2:J:1698:LEU:HD12	2:J:1712:TYR:CZ	2.49	0.47
2:J:3967:GLU:OE1	2:J:3967:GLU:HA	2.15	0.47
2:G:2006:ILE:HG21	2:G:3653:PHE:HA	1.95	0.47
2:G:4998:LYS:HG2	2:G:5003:HIS:CE1	2.49	0.47
2:A:3809:ASN:ND2	2:A:3812:VAL:HG23	2.29	0.47
2:A:4968:PHE:HE2	2:A:4978:HIS:ND1	2.12	0.47
2:D:3677:LEU:HD11	2:D:3698:LEU:CD2	2.40	0.47
2:D:3966:THR:O	2:D:3970:GLN:N	2.48	0.47
2:J:753:PRO:HB2	2:J:770:ALA:H	1.79	0.47
2:J:1926:LEU:HG	2:J:1939:MET:CE	2.44	0.47
2:J:2868:SER:O	2:J:2872:GLN:N	2.46	0.47
2:J:4021:LYS:HG3	2:J:4142:ASN:ND2	2.29	0.47
2:G:681:HIS:CE1	2:G:683:ARG:HE	2.32	0.47
2:G:3771:HIS:NE2	2:G:3815:LYS:HE2	2.29	0.47
2:A:546:TRP:O	2:A:550:LYS:HG2	2.13	0.47
2:A:626:LEU:HD12	2:A:1688:HIS:CE1	2.50	0.47
2:A:2182:ILE:HD11	2:A:2231:SER:OG	2.13	0.47
2:A:2566:ALA:HA	2:A:2569:PHE:HD2	1.79	0.47
2:D:1962:ALA:HA	2:D:3653:PHE:CE2	2.49	0.47
2:D:4108:ILE:O	2:D:4112:LEU:HD23	2.14	0.47
2:J:632:LEU:HD13	2:J:1666:THR:HG23	1.96	0.47
2:J:1962:ALA:HA	2:J:3653:PHE:CE2	2.50	0.47
2:A:1936:LYS:HZ1	2:A:2105:TRP:CG	2.33	0.47
2:A:4045:VAL:O	2:A:4049:VAL:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:4215:ARG:NH1	7:A:5103:ATP:O1A	2.47	0.47
2:D:1638:ALA:HA	2:D:1649:ASP:HA	1.97	0.47
2:D:3674:ILE:HA	2:D:3677:LEU:HD23	1.96	0.47
2:J:35:LEU:HD12	2:J:182:LEU:HD21	1.97	0.47
2:J:483:MET:O	2:J:487:VAL:HG12	2.14	0.47
2:J:618:GLN:OE1	2:J:1678:ASN:ND2	2.43	0.47
2:J:736:HIS:HB2	2:J:739:ALA:HB2	1.96	0.47
2:J:794:GLY:O	2:J:798:GLY:N	2.47	0.47
2:J:2107:GLN:O	2:J:3694:LYS:NZ	2.47	0.47
2:J:5036:LEU:H	2:J:5036:LEU:HD12	1.80	0.47
3:K:25:HIS:HB3	3:K:40:ARG:HH21	1.78	0.47
3:K:86:GLY:O	3:K:87:HIS:C	2.57	0.47
2:G:4569:LEU:O	2:G:4573:ILE:HG22	2.14	0.47
2:J:180:LEU:HA	2:J:193:ALA:HA	1.96	0.47
2:J:650:VAL:O	2:J:777:PHE:N	2.44	0.47
2:J:4207:MET:HB2	2:J:4210:VAL:HG22	1.97	0.47
2:J:4218:ILE:HB	2:J:4954:MET:HE1	1.97	0.47
2:G:689:THR:HG22	2:G:776:LEU:H	1.79	0.47
2:A:3891:LEU:HD12	2:A:3891:LEU:O	2.14	0.47
2:D:4031:LEU:HD21	2:D:4044:MET:HG3	1.96	0.47
2:J:3723:MET:SD	2:J:3793:MET:HE2	2.55	0.47
2:J:4218:ILE:O	2:J:4222:VAL:HG23	2.14	0.47
3:K:58:GLY:HA3	3:K:80:VAL:HG13	1.97	0.47
2:G:791:PHE:N	2:G:1626:TRP:O	2.39	0.47
2:G:3996:PHE:HD2	2:G:4020:GLN:HG2	1.80	0.47
2:A:672:VAL:HB	2:A:675:LEU:HB2	1.97	0.47
2:A:2138:LEU:HD13	2:A:3658:LYS:CB	2.45	0.47
2:A:3985:LEU:HG	2:A:3986:TRP:N	2.30	0.47
2:D:667:MET:N	2:D:790:ARG:O	2.47	0.47
2:D:3989:VAL:CG1	2:D:4027:LEU:HD21	2.39	0.47
2:J:35:LEU:CD1	2:J:182:LEU:HD21	2.45	0.47
2:G:1099:GLU:C	2:G:1100:MET:HE2	2.39	0.46
2:G:4933:GLN:O	2:G:4937:ILE:HG12	2.15	0.46
2:G:5000:GLU:HA	2:G:5003:HIS:CD2	2.50	0.46
3:H:4:ILE:HD13	3:H:65:GLN:OE1	2.15	0.46
2:A:281:ARG:HB3	2:A:290:TYR:HD2	1.80	0.46
2:A:2298:VAL:HG21	2:A:2334:PHE:HE2	1.80	0.46
2:A:3836:MET:HA	2:A:3839:CYS:SG	2.55	0.46
2:A:4214:LYS:O	2:A:4218:ILE:HG22	2.15	0.46
2:D:78:LEU:HD21	2:D:174:VAL:HG11	1.97	0.46
2:D:2098:VAL:O	2:D:2102:VAL:HG12	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4186:ALA:HB2	2:D:5009:TYR:CE2	2.50	0.46
2:D:4705:VAL:HB	2:D:4778:TRP:CD1	2.50	0.46
2:J:647:ASN:HD21	2:J:821:LEU:HA	1.78	0.46
2:G:853:PRO:HA	2:G:1023:PRO:HB3	1.97	0.46
2:G:3986:TRP:O	2:G:3990:VAL:HG23	2.14	0.46
2:G:4060:LYS:C	2:G:4064:MET:HE3	2.41	0.46
2:A:516:LYS:O	2:A:519:VAL:HG12	2.15	0.46
2:D:1237:TRP:CD1	2:D:1607:ARG:HA	2.50	0.46
2:D:2506:LEU:HD23	2:D:2510:TYR:HB2	1.98	0.46
2:J:421:PHE:CZ	2:J:507:ALA:HA	2.51	0.46
2:J:745:SER:O	2:J:758:ARG:N	2.48	0.46
2:G:600:LEU:HD23	2:G:600:LEU:HA	1.78	0.46
2:A:2458:ARG:HH21	2:A:2510:TYR:HA	1.81	0.46
2:A:3809:ASN:OD1	2:A:3811:GLU:N	2.48	0.46
2:A:3996:PHE:HB3	2:A:4020:GLN:NE2	2.30	0.46
2:D:1694:LEU:HA	2:D:1711:TYR:HD2	1.80	0.46
2:J:1076:ARG:HB3	2:J:1191:VAL:HG23	1.97	0.46
2:J:4178:LEU:HD11	2:J:4194:TYR:HB3	1.96	0.46
2:A:2323:TRP:CH2	2:A:2422:ILE:HG12	2.49	0.46
2:A:2324:ASN:ND2	2:A:2324:ASN:O	2.48	0.46
2:A:4991:PHE:O	2:A:4995:LEU:HD13	2.14	0.46
4:C:67:PRO:HA	4:C:70:LEU:HD12	1.98	0.46
2:D:666:VAL:HB	2:D:744:VAL:HB	1.98	0.46
2:D:1855:GLY:O	2:D:1859:VAL:HG13	2.15	0.46
2:D:2128:TYR:HB2	2:D:3673:MET:CE	2.46	0.46
2:D:2280:VAL:HG11	2:D:2338:ALA:HA	1.97	0.46
2:D:4702:ASP:O	2:D:4706:LEU:HG	2.16	0.46
2:J:500:ALA:HA	2:J:504:ALA:HB3	1.97	0.46
2:J:1575:LEU:HD23	2:J:1575:LEU:H	1.81	0.46
2:G:4150:LEU:HB3	2:G:4160:LEU:HD21	1.96	0.46
2:G:4729:GLY:HA2	2:G:4737:ILE:HG13	1.97	0.46
2:A:225:GLY:HA2	2:A:389:PHE:CZ	2.51	0.46
2:A:2153:MET:HE2	2:A:2153:MET:HA	1.97	0.46
2:A:5027:CYS:SG	2:A:5028:PHE:N	2.88	0.46
2:D:1164:LEU:N	2:D:1167:GLU:O	2.48	0.46
2:D:4031:LEU:HD11	2:D:4146:LEU:CD1	2.46	0.46
2:J:256:ALA:HB1	2:J:286:THR:HG21	1.96	0.46
2:J:591:ASP:HA	2:J:631:LEU:HD21	1.97	0.46
2:J:1717:SER:HA	2:J:1721:GLU:HB2	1.96	0.46
2:G:842:PRO:HG2	2:G:1196:PRO:HA	1.97	0.46
2:G:2527:LEU:HA	2:G:2582:MET:HE1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1116:GLY:H	2:A:1121:ALA:HB3	1.80	0.46
2:A:1842:LEU:HD23	2:A:1938:GLN:HB2	1.97	0.46
2:D:668:VAL:N	2:D:742:ASP:O	2.49	0.46
2:J:3815:LYS:HE3	2:J:3815:LYS:HB2	1.67	0.46
2:J:4150:LEU:HD13	2:J:4150:LEU:HA	1.72	0.46
3:K:62:GLY:O	3:K:66:MET:HG2	2.15	0.46
2:G:487:VAL:O	2:G:491:ILE:HG22	2.15	0.46
2:G:668:VAL:HG22	2:G:789:VAL:HG23	1.96	0.46
2:G:1667:LEU:O	2:G:1671:ARG:HG3	2.16	0.46
2:G:3719:ASP:H	2:G:3793:MET:HE1	1.81	0.46
2:G:3722:TYR:CE2	2:G:3782:MET:HE1	2.50	0.46
2:D:1689:VAL:HG13	2:D:1691:GLN:H	1.79	0.46
2:J:1291:LEU:HD13	2:J:1595:LEU:HD11	1.98	0.46
2:J:3677:LEU:HD11	2:J:3698:LEU:HD13	1.97	0.46
2:G:733:PRO:HG2	2:G:762:CYS:HB3	1.98	0.46
2:G:1637:MET:HB3	2:G:1637:MET:HE2	1.55	0.46
2:G:1717:SER:HA	2:G:1721:GLU:HB2	1.97	0.46
2:G:3934:TYR:HB2	2:G:3999:MET:HE3	1.98	0.46
2:A:49:LEU:HD23	2:A:49:LEU:H	1.80	0.46
2:A:4231:MET:N	2:A:4231:MET:HE2	2.31	0.46
2:D:2155:LEU:HD22	2:D:2190:VAL:HB	1.98	0.46
2:D:3771:HIS:CE1	2:D:3815:LYS:HD3	2.51	0.46
2:J:566:CYS:HA	2:J:569:ILE:HG22	1.98	0.46
2:J:2191:PHE:HA	2:J:2198:MET:HE3	1.97	0.46
2:J:3793:MET:HA	2:J:3793:MET:HE2	1.97	0.46
2:G:2295:LEU:O	2:G:2299:VAL:HG23	2.15	0.46
2:G:4039:MET:O	2:G:4043:GLN:HG3	2.15	0.46
2:G:4060:LYS:O	2:G:4064:MET:HE3	2.16	0.46
2:A:401:ALA:HA	2:A:404:ILE:HD12	1.97	0.46
2:A:2178:MET:O	2:A:2182:ILE:HG23	2.16	0.46
2:D:1526:LEU:HA	2:D:1541:GLN:HA	1.97	0.46
2:D:4055:VAL:CG1	2:D:4163:PHE:HZ	2.11	0.46
3:E:30:LEU:HD11	3:E:92:PRO:HD2	1.98	0.46
2:J:703:GLY:N	2:J:1647:CYS:SG	2.89	0.46
2:J:3645:PRO:HG2	2:J:3648:ARG:HD3	1.96	0.46
3:K:61:GLU:O	3:K:65:GLN:HG3	2.16	0.46
3:K:74:LEU:HB2	3:K:99:PHE:HB2	1.98	0.46
2:G:1802:ILE:HG13	2:G:1803:PRO:HD2	1.98	0.46
2:G:4849:TYR:HE1	2:J:4578:LEU:HD13	1.80	0.46
2:A:461:HIS:ND1	2:A:3707:ARG:HG2	2.31	0.46
2:D:2307:LEU:N	2:D:2322:GLY:O	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2696:TYR:HE2	2:D:2997:PHE:HA	1.80	0.46
2:D:3805:LEU:HD23	2:D:3890:LEU:HB3	1.97	0.46
2:J:2126:ARG:HE	2:J:2126:ARG:HB3	1.62	0.46
2:J:2159:LEU:HA	2:J:2162:ILE:HD12	1.98	0.46
2:J:3986:TRP:O	2:J:3990:VAL:HG12	2.16	0.46
2:G:2499:LYS:C	2:G:2553:TYR:HE2	2.23	0.45
2:G:3817:LEU:HD22	2:G:3899:PHE:HD1	1.81	0.45
2:G:4141:PHE:HZ	2:G:4195:PHE:O	1.99	0.45
2:A:842:PRO:HD3	2:A:1073:ARG:HD2	1.98	0.45
2:A:3841:VAL:HG21	2:A:3925:ARG:HD2	1.98	0.45
2:A:4031:LEU:HD12	2:A:4031:LEU:O	2.16	0.45
2:D:2207:VAL:HA	2:D:2210:VAL:HG12	1.99	0.45
2:D:4181:ILE:HG22	2:D:4182:GLU:N	2.31	0.45
2:J:149:THR:N	2:J:172:VAL:O	2.48	0.45
2:J:2458:ARG:NE	2:J:2510:TYR:HA	2.31	0.45
2:J:3762:ARG:HH12	2:J:4756:ARG:H	1.63	0.45
2:J:4231:MET:O	2:J:4235:VAL:HG13	2.16	0.45
2:G:551:LEU:HD12	2:G:551:LEU:O	2.16	0.45
2:G:551:LEU:HD11	2:G:589:LEU:HD13	1.98	0.45
2:G:4856:PHE:CD2	2:G:4879:MET:HE1	2.51	0.45
2:A:2285:GLU:HA	2:A:2288:LEU:HD12	1.97	0.45
2:D:784:SER:OG	2:D:785:ALA:N	2.49	0.45
2:D:1848:LEU:HB2	2:D:1854:PHE:CZ	2.52	0.45
2:D:4181:ILE:HG23	2:D:4988:TYR:CE1	2.51	0.45
3:E:67:SER:H	3:E:70:GLN:HE21	1.63	0.45
2:J:3673:MET:HE2	2:J:3728:ILE:HG21	1.98	0.45
2:J:4024:VAL:HG21	2:J:4142:ASN:HB2	1.97	0.45
2:G:563:VAL:O	2:G:567:VAL:HG12	2.15	0.45
2:A:414:PHE:CD1	2:A:414:PHE:C	2.94	0.45
2:A:414:PHE:O	2:A:414:PHE:HD1	1.98	0.45
2:A:2121:PHE:HB3	2:A:3725:TYR:HE2	1.82	0.45
2:A:3990:VAL:HG13	2:A:4051:SER:HB2	1.98	0.45
2:D:418:LEU:HA	2:D:421:PHE:HE1	1.81	0.45
2:D:3794:VAL:HG11	2:D:3835:LEU:HD11	1.97	0.45
2:J:445:LEU:HB3	2:J:521:LEU:HD12	1.97	0.45
2:J:1683:HIS:NE2	2:J:1798:LEU:O	2.50	0.45
2:G:2463:LEU:O	2:G:2467:VAL:HG23	2.15	0.45
2:G:4654:ALA:O	2:G:4658:ILE:HG22	2.17	0.45
2:A:345:LEU:C	2:A:387:ALA:HB1	2.42	0.45
2:A:4994:TYR:CZ	2:A:4998:LYS:HD3	2.51	0.45
2:D:2358:ILE:HD11	2:J:195:PHE:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4338:VAL:HG21	2:J:4838:VAL:HG11	1.97	0.45
2:G:2680:TRP:HA	2:G:2683:PHE:CE2	2.51	0.45
2:G:3805:LEU:HD11	2:G:3816:MET:HE1	1.99	0.45
2:G:4944:ARG:HD2	2:A:4836:GLN:HE22	1.81	0.45
2:A:1194:LEU:HD12	2:A:1194:LEU:HA	1.85	0.45
2:A:2095:GLN:O	2:A:2127:GLN:NE2	2.50	0.45
2:J:74:SER:O	2:J:78:LEU:N	2.42	0.45
2:J:2159:LEU:HD12	2:J:2201:LEU:HD13	1.99	0.45
2:G:1870:VAL:HG11	2:G:2097:LEU:HD22	1.97	0.45
2:G:2301:TYR:CE2	2:G:2331:TYR:CD2	3.02	0.45
2:G:3966:THR:O	2:G:3970:GLN:HG2	2.16	0.45
2:G:4666:VAL:O	2:G:4670:ILE:HG12	2.16	0.45
2:A:651:GLY:HA3	2:A:776:LEU:HG	1.98	0.45
2:D:73:LEU:O	2:D:106:ALA:N	2.39	0.45
2:J:4241:THR:O	2:J:4245:MET:HE3	2.16	0.45
2:G:518:ILE:HD13	2:G:518:ILE:HA	1.80	0.45
2:A:597:HIS:HB2	2:A:1665:HIS:ND1	2.32	0.45
2:A:1290:ARG:NH2	2:A:1598:GLN:OE1	2.33	0.45
2:A:1770:SER:HB2	2:A:1952:GLN:NE2	2.31	0.45
2:A:4582:VAL:HG11	2:A:4629:TYR:HD1	1.81	0.45
2:A:4823:LEU:HD13	2:D:4843:LEU:HD22	1.98	0.45
2:D:997:ALA:HB1	2:D:1021:LEU:HA	1.99	0.45
2:D:2354:VAL:O	2:D:2358:ILE:HG22	2.17	0.45
2:D:3661:TRP:O	2:D:3665:GLU:N	2.50	0.45
2:D:3986:TRP:HA	2:D:3986:TRP:HE3	1.79	0.45
2:J:37:LEU:HD12	2:J:37:LEU:HA	1.80	0.45
2:G:691:GLY:HA3	2:G:712:TYR:CD1	2.52	0.45
2:G:1593:PRO:O	2:G:1596:GLU:HG2	2.16	0.45
2:G:2500:ALA:HB2	2:G:2553:TYR:HD2	1.82	0.45
2:A:2294:ASP:O	2:A:2298:VAL:HG23	2.17	0.45
2:D:593:HIS:HA	2:D:1593:PRO:HD2	1.99	0.45
2:D:4904:PRO:HB3	2:D:4910:GLU:HA	1.99	0.45
2:J:531:ARG:NH2	2:J:562:GLU:OE1	2.50	0.45
2:J:633:LEU:HD23	2:J:1639:LEU:HD12	1.99	0.45
2:J:2156:LEU:HD23	2:J:2156:LEU:HA	1.79	0.45
2:J:2312:MET:SD	2:J:2313:LEU:N	2.90	0.45
2:J:3136:LEU:O	2:J:3140:LEU:N	2.41	0.45
2:J:3698:LEU:HB3	2:J:3773:ARG:HG2	1.97	0.45
2:J:4924:VAL:HG13	2:J:4925:ILE:HG13	1.99	0.45
2:G:564:LEU:O	2:G:568:LEU:HG	2.17	0.45
2:G:1996:ARG:NH2	2:G:1997:GLU:OE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:638:ILE:HG12	2:A:703:GLY:HA2	1.99	0.45
2:D:223:PHE:HA	2:D:230:CYS:HA	1.99	0.45
2:D:1007:TYR:CE2	2:D:1022:VAL:HG22	2.52	0.45
2:J:1634:LEU:HD23	2:J:1634:LEU:HA	1.86	0.45
2:J:4820:VAL:CG1	2:J:4823:LEU:HD23	2.47	0.45
2:G:3674:ILE:O	2:G:3678:SER:OG	2.23	0.45
2:G:3842:LEU:O	2:G:3929:SER:OG	2.34	0.45
2:G:4204:GLN:C	2:G:4245:MET:HE1	2.41	0.45
2:A:2208:MET:HE2	2:A:2250:MET:HE1	1.98	0.45
2:D:2128:TYR:CE2	2:D:3669:PHE:HB2	2.51	0.45
2:D:4851:TYR:HE2	2:D:4920:PHE:HA	1.82	0.45
2:J:3889:GLN:HB2	2:J:3964:SER:HA	1.97	0.45
2:G:69:LEU:HD21	2:G:107:ILE:HD11	1.98	0.44
2:G:283:ARG:HB3	2:G:290:TYR:CD1	2.53	0.44
2:G:2384:ILE:HD11	2:G:2494:PHE:HD1	1.82	0.44
2:G:4721:LYS:HB3	2:G:4741:LEU:HD23	1.99	0.44
2:D:214:VAL:N	2:D:341:TYR:H	2.15	0.44
2:J:1720:LEU:HD23	2:J:1720:LEU:H	1.83	0.44
2:J:1763:PRO:HG3	2:J:2094:LEU:HD22	2.00	0.44
2:J:3886:ARG:HG2	2:J:3960:GLN:CD	2.42	0.44
3:K:73:LYS:HB3	3:K:73:LYS:HE2	1.72	0.44
2:G:1731:LEU:HD12	2:G:1772:ARG:HH21	1.82	0.44
2:G:4180:ARG:HB3	2:G:4192:ARG:HH21	1.82	0.44
2:A:1437:VAL:HG11	2:A:1450:VAL:HG11	1.99	0.44
2:A:2507:ASP:HA	2:A:2511:GLY:HA2	1.99	0.44
2:D:3889:GLN:HB2	2:D:3964:SER:HA	2.00	0.44
2:J:55:ALA:HA	2:J:58:VAL:O	2.17	0.44
2:G:2500:ALA:N	2:G:2553:TYR:HE2	2.16	0.44
2:A:172:VAL:HG22	2:A:179:TYR:CD1	2.52	0.44
2:A:355:LEU:CB	2:A:380:GLN:HA	2.47	0.44
2:A:483:MET:HE2	2:A:483:MET:C	2.42	0.44
2:A:4959:PHE:HD2	2:A:4960:ILE:HD13	1.81	0.44
2:A:5013:MET:HE3	2:A:5018:CYS:O	2.18	0.44
2:D:2156:LEU:HD22	2:D:2201:LEU:HD21	1.99	0.44
2:J:718:GLY:HA3	2:J:737:LEU:HA	1.99	0.44
2:J:4820:VAL:HG13	2:J:4823:LEU:HD23	1.99	0.44
2:G:2159:LEU:HA	2:G:2162:ILE:HG22	1.99	0.44
2:G:4218:ILE:HA	2:G:4221:VAL:HG12	1.99	0.44
2:G:4888:TYR:O	2:G:4892:ARG:NH1	2.39	0.44
2:A:488:LEU:HD13	2:A:488:LEU:HA	1.81	0.44
2:A:2039:LEU:HD13	2:A:2044:ILE:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3722:TYR:CD2	2:A:3782:MET:HE1	2.49	0.44
2:A:3722:TYR:HE2	2:A:3782:MET:SD	2.41	0.44
2:A:3914:ASN:OD1	2:A:3917:ILE:HG12	2.17	0.44
2:A:4183:ILE:HG13	2:A:4193:ILE:HD13	1.99	0.44
2:A:4817:ALA:HA	2:A:4823:LEU:HB3	1.99	0.44
2:D:121:LEU:N	2:D:134:ASP:O	2.51	0.44
2:J:3702:VAL:HG21	2:J:3773:ARG:HB3	1.99	0.44
2:J:4897:ILE:HG23	2:J:4901:ILE:HD12	2.00	0.44
2:G:1827:ARG:HE	2:G:1827:ARG:HB2	1.64	0.44
2:G:2012:PHE:HZ	2:G:2031:LEU:HD13	1.82	0.44
2:G:4648:LEU:HD22	2:G:4803:HIS:HE1	1.81	0.44
2:A:723:THR:O	2:A:723:THR:OG1	2.33	0.44
2:A:2879:ALA:HB2	2:A:2923:ALA:HB2	1.98	0.44
2:D:4820:VAL:HB	2:D:4823:LEU:HG	1.98	0.44
2:J:2251:PHE:CD2	2:J:2286:LEU:HB3	2.52	0.44
2:J:4922:PHE:O	2:J:4927:ILE:HG12	2.17	0.44
2:G:1006:SER:O	2:G:1018:ASN:N	2.50	0.44
2:G:3698:LEU:HD23	2:G:3701:LEU:HD12	2.00	0.44
2:G:3955:MET:HE1	2:G:4016:LEU:CA	2.48	0.44
2:G:4957:LYS:HB3	2:G:4957:LYS:HE3	1.85	0.44
2:A:78:LEU:HD11	2:A:147:TRP:CE3	2.53	0.44
2:A:906:CYS:HA	2:A:913:LEU:HA	1.98	0.44
2:A:3780:LEU:HD11	2:A:3819:TYR:CD1	2.53	0.44
2:A:3974:THR:O	2:A:3978:GLN:HG2	2.17	0.44
2:A:4955:GLU:N	2:A:4955:GLU:OE1	2.51	0.44
2:D:3875:MET:HE2	2:D:3875:MET:HA	1.99	0.44
2:J:35:LEU:HA	2:J:51:PRO:HA	1.99	0.44
2:J:1641:ILE:HB	2:J:1644:GLU:HB2	2.00	0.44
2:G:1735:ILE:HG22	2:G:1771:LEU:HB3	1.99	0.44
2:G:3705:PHE:HB3	2:G:3778:MET:HG3	2.00	0.44
2:A:273:HIS:N	2:A:334:MET:O	2.51	0.44
2:A:411:TYR:HB3	2:A:486:LEU:HD11	1.99	0.44
2:A:3992:PHE:O	2:A:3995:VAL:HG13	2.18	0.44
2:D:3729:MET:O	2:D:3730:ALA:C	2.61	0.44
2:D:4778:TRP:O	2:D:4782:VAL:HG23	2.18	0.44
2:J:73:LEU:HD23	2:J:73:LEU:H	1.82	0.44
2:J:1211:LEU:HD13	2:J:1214:PHE:HB2	2.00	0.44
2:A:358:THR:HG21	2:A:383:HIS:O	2.18	0.44
2:A:1763:PRO:HG3	2:A:2094:LEU:HD13	2.00	0.44
2:A:2204:HIS:HA	2:A:2207:VAL:HG12	2.00	0.44
2:D:4105:GLY:O	2:D:4108:ILE:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2299:VAL:HG21	2:G:2356:LEU:HB3	2.00	0.44
2:G:2430:ILE:HD12	2:G:2502:MET:HE1	2.00	0.44
2:G:2616:PRO:HG2	2:G:2664:PHE:CG	2.53	0.44
2:G:3888:LEU:HD12	2:G:3968:TYR:OH	2.18	0.44
2:G:4715:TYR:CE2	2:G:4717:ASP:HB3	2.53	0.44
2:A:106:ALA:HA	2:A:149:THR:HA	2.00	0.44
2:A:1452:TRP:HB3	2:A:1548:LEU:HD13	2.00	0.44
2:G:2110:TYR:HA	2:G:3700:GLN:HE21	1.83	0.43
2:G:4323:THR:OG1	2:G:4324:ALA:N	2.49	0.43
2:A:178:ARG:HG3	2:A:195:PHE:CE2	2.53	0.43
2:A:206:CYS:O	2:A:334:MET:HA	2.17	0.43
2:A:1092:PHE:HB3	2:A:1149:VAL:HG12	1.99	0.43
2:A:4712:PRO:HB3	2:A:4718:LYS:HA	1.99	0.43
2:D:4640:GLU:HB3	2:D:4641:PRO:HD3	1.99	0.43
2:D:4933:GLN:O	2:D:4937:ILE:HG12	2.18	0.43
2:G:2202:GLY:HA2	2:G:2204:HIS:CE1	2.53	0.43
2:G:3701:LEU:HD11	2:G:3725:TYR:CD2	2.54	0.43
2:G:4895:GLY:O	2:J:4892:ARG:NH1	2.51	0.43
2:A:2875:ALA:HB1	2:A:2923:ALA:HB1	2.00	0.43
2:A:4193:ILE:HD12	2:A:4193:ILE:N	2.33	0.43
2:D:4179:GLY:C	2:D:4195:PHE:CE1	2.96	0.43
2:D:4198:SER:HB3	2:D:4201:ASN:OD1	2.19	0.43
2:J:26:ALA:C	2:J:182:LEU:HD13	2.44	0.43
2:J:2283:ASN:CB	2:J:2286:LEU:HD13	2.49	0.43
2:J:3730:ALA:HB1	2:J:3803:SER:OG	2.19	0.43
2:J:4217:PHE:CD1	2:J:4217:PHE:C	2.97	0.43
2:G:626:LEU:HD23	2:G:626:LEU:HA	1.83	0.43
2:G:1153:ILE:HD11	2:G:1160:ILE:HG23	2.00	0.43
2:G:1862:ILE:O	2:G:1866:ILE:HG22	2.18	0.43
2:A:20:VAL:HG12	2:A:204:PRO:HA	1.99	0.43
2:A:2159:LEU:HA	2:A:2162:ILE:HG22	2.00	0.43
2:A:3886:ARG:NH1	2:A:3890:LEU:HD11	2.33	0.43
2:A:4790:LEU:HD23	2:A:4790:LEU:HA	1.87	0.43
2:D:4901:ILE:HD13	2:D:4913:ARG:NH1	2.33	0.43
2:J:451:TYR:CE2	2:J:474:ARG:HD2	2.53	0.43
2:J:525:LEU:HD23	2:J:529:LEU:HD23	1.99	0.43
2:J:677:ALA:HA	3:K:40:ARG:HG2	1.99	0.43
2:G:655:GLY:HA3	2:G:852:VAL:HG13	2.00	0.43
2:G:670:GLU:HA	2:G:740:PRO:HB3	1.99	0.43
2:G:4676:GLU:HG3	2:G:4680:LYS:HE2	1.99	0.43
2:A:578:ILE:C	2:A:578:ILE:HD12	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:4242:ILE:HA	2:A:4245:MET:HE3	2.00	0.43
2:J:3962:PHE:O	2:J:3966:THR:HG23	2.18	0.43
2:J:4639:MET:O	2:J:4643:LEU:N	2.43	0.43
2:G:747:CYS:N	2:G:756:SER:O	2.42	0.43
2:G:2166:LEU:HD12	2:G:2210:VAL:HG23	2.00	0.43
2:G:3779:VAL:HG13	2:G:3797:THR:HG22	2.00	0.43
2:A:1687:SER:OG	3:B:90:VAL:HG13	2.18	0.43
2:A:2553:TYR:CD1	2:A:2553:TYR:C	2.95	0.43
2:D:1296:GLN:HA	2:D:1547:LYS:HA	1.99	0.43
2:D:4801:LEU:HB3	2:D:4808:PHE:CG	2.54	0.43
2:J:505:GLU:HA	2:J:512:ALA:HB2	2.00	0.43
2:J:1291:LEU:HD23	2:J:1291:LEU:HA	1.88	0.43
2:J:1815:LEU:HD13	2:J:1841:VAL:HG12	2.00	0.43
2:G:170:ILE:HD13	2:G:170:ILE:HA	1.89	0.43
2:G:553:ARG:CZ	2:G:553:ARG:HB2	2.48	0.43
2:G:695:TYR:HH	2:G:1241:SER:HG	1.63	0.43
2:G:830:ARG:HE	2:G:830:ARG:HB3	1.72	0.43
2:G:1076:ARG:HD3	2:G:1109:LEU:HD23	2.00	0.43
2:G:1160:ILE:HD12	2:G:1179:PHE:HB2	1.99	0.43
2:G:3832:ILE:HD13	2:G:3832:ILE:HA	1.90	0.43
2:G:4955:GLU:OE2	7:G:5103:ATP:O3'	2.35	0.43
2:A:279:PRO:HA	2:A:315:CYS:HA	2.00	0.43
2:A:468:LEU:HD12	2:A:468:LEU:HA	1.85	0.43
2:A:2907:PRO:O	2:A:2911:LEU:N	2.47	0.43
2:A:4044:MET:HB3	2:A:4044:MET:HE3	1.72	0.43
2:A:4339:VAL:HG11	2:A:4816:ILE:HD11	2.01	0.43
2:A:4897:ILE:HD12	2:A:4897:ILE:HA	1.88	0.43
2:D:2240:CYS:SG	2:D:2241:ARG:N	2.90	0.43
2:D:3924:LEU:O	2:D:3928:GLU:HG2	2.18	0.43
2:D:4003:LEU:HD21	2:D:4012:LEU:HB3	2.01	0.43
2:D:4569:LEU:O	2:D:4573:ILE:HG22	2.18	0.43
2:J:2534:ALA:HB2	2:J:2589:LEU:HG	1.99	0.43
2:J:4235:VAL:HG21	2:J:5019:TRP:CH2	2.54	0.43
2:J:4716:TRP:CD1	2:J:4716:TRP:H	2.35	0.43
2:G:636:ASN:CG	2:G:702:TRP:HE1	2.27	0.43
2:G:833:GLY:H	2:G:837:PRO:HD2	1.83	0.43
2:G:947:GLU:HA	2:G:1049:TYR:HA	2.01	0.43
2:G:2295:LEU:O	2:G:2298:VAL:HB	2.19	0.43
2:G:4047:MET:SD	2:G:4048:LEU:HD22	2.58	0.43
2:G:4681:LEU:HD21	2:G:4724:VAL:HG11	2.00	0.43
2:A:359:TYR:HA	2:A:376:ALA:CA	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:500:ALA:O	2:A:505:GLU:N	2.50	0.43
2:A:1745:ILE:O	2:A:1745:ILE:HG13	2.19	0.43
2:D:2159:LEU:C	2:D:2162:ILE:HG22	2.43	0.43
2:D:4992:LEU:O	2:D:4996:ILE:HG12	2.19	0.43
2:J:1087:ARG:HG2	2:J:1154:ASP:HA	2.00	0.43
2:J:1130:GLN:HA	2:J:1138:PRO:HA	1.99	0.43
2:J:1636:MET:HE1	2:J:1649:ASP:OD1	2.19	0.43
2:G:2596:THR:HB	2:G:2599:GLN:HB2	2.01	0.43
2:G:3794:VAL:HG11	2:G:3835:LEU:HD11	2.01	0.43
2:G:4860:ARG:NH2	2:J:4629:TYR:OH	2.52	0.43
2:A:342:GLY:N	2:A:390:LEU:O	2.51	0.43
2:A:360:ALA:H	2:A:376:ALA:C	2.26	0.43
2:A:483:MET:CE	2:A:529:LEU:HD11	2.43	0.43
2:A:5000:GLU:HA	2:A:5003:HIS:CD2	2.54	0.43
2:D:2128:TYR:CB	2:D:3673:MET:CE	2.96	0.43
2:D:2277:ALA:HB2	2:D:2334:PHE:HD1	1.84	0.43
2:J:3760:LYS:HE3	2:J:3760:LYS:HB2	1.80	0.43
2:J:4144:ALA:O	2:J:4147:LEU:HG	2.18	0.43
2:G:418:LEU:HD13	2:G:493:ARG:HB3	2.01	0.43
2:G:1270:LEU:O	2:G:1564:PHE:N	2.37	0.43
2:G:1595:LEU:HD23	2:G:1595:LEU:HA	1.88	0.43
2:G:2495:VAL:O	2:G:2498:HIS:ND1	2.52	0.43
2:G:4879:MET:HB3	2:J:4578:LEU:O	2.19	0.43
2:D:4790:LEU:HD23	2:D:4790:LEU:HA	1.84	0.43
2:J:695:TYR:HE2	2:J:1241:SER:H	1.66	0.43
2:J:2125:HIS:HB2	2:J:3725:TYR:HE1	1.83	0.43
2:G:1125:ASN:HD22	2:G:1132:TRP:HE1	1.66	0.43
2:G:1130:GLN:HA	2:G:1138:PRO:HA	2.01	0.43
2:G:2495:VAL:HB	2:G:2498:HIS:CE1	2.53	0.43
2:G:3673:MET:HE3	2:G:3673:MET:HB3	1.89	0.43
2:G:4017:LEU:HA	2:G:4020:GLN:HB2	2.00	0.43
2:A:2353:VAL:O	2:A:2357:LEU:HG	2.19	0.43
2:D:3990:VAL:HG22	2:D:4047:MET:HG3	2.00	0.43
2:D:4702:ASP:HA	2:D:4705:VAL:HG12	2.01	0.43
2:J:470:SER:HA	2:J:473:ASN:ND2	2.34	0.43
2:J:688:LEU:CD2	2:J:691:GLY:H	2.31	0.43
2:G:1692:ALA:HB3	3:H:41:ASP:HB2	2.00	0.42
2:G:3698:LEU:HD23	2:G:3698:LEU:HA	1.89	0.42
2:G:4048:LEU:HD12	2:G:4163:PHE:CE2	2.54	0.42
2:G:4658:ILE:HB	2:G:4792:LEU:HD12	2.01	0.42
2:A:411:TYR:HB2	2:A:486:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:600:LEU:HB3	2:A:1665:HIS:HB3	2.01	0.42
2:A:3886:ARG:CZ	2:A:3890:LEU:HD11	2.49	0.42
2:A:4565:LEU:CD2	2:A:4653:VAL:HG21	2.49	0.42
2:A:4963:ILE:HG21	2:A:4968:PHE:HE1	1.83	0.42
2:D:4179:GLY:HA3	2:D:4195:PHE:CZ	2.53	0.42
2:D:4720:VAL:HA	2:D:4723:LYS:HE2	2.01	0.42
2:J:794:GLY:HA3	2:J:812:HIS:HB3	2.01	0.42
2:J:2194:HIS:HB2	2:J:2197:LEU:HB3	1.99	0.42
2:J:3817:LEU:HD12	2:J:3817:LEU:HA	1.83	0.42
2:G:579:GLN:H	2:G:582:HIS:CD2	2.35	0.42
2:G:629:ARG:HE	2:G:1688:HIS:CD2	2.37	0.42
2:G:1927:LEU:HD13	2:G:2101:MET:HG3	2.01	0.42
2:G:3820:LEU:HD12	2:G:3820:LEU:HA	1.91	0.42
2:G:3845:ASN:OD1	2:G:3845:ASN:N	2.52	0.42
2:D:2128:TYR:CD2	2:D:3669:PHE:HB2	2.53	0.42
2:J:410:LEU:HG	2:J:441:VAL:HG12	2.00	0.42
2:J:1243:PRO:HB3	2:J:1602:PRO:HA	2.02	0.42
2:J:4197:ILE:HD12	2:J:4990:PHE:HB3	2.02	0.42
2:J:4218:ILE:HB	2:J:4954:MET:CE	2.49	0.42
2:G:660:GLY:O	2:G:750:LEU:N	2.39	0.42
2:G:1229:ASN:HB2	2:G:1827:ARG:HG2	2.02	0.42
2:G:1733:GLU:OE2	2:G:1733:GLU:N	2.52	0.42
4:I:14:LYS:HA	4:I:66:PHE:HZ	1.85	0.42
2:A:150:MET:HE3	2:A:150:MET:HB3	1.77	0.42
2:A:4983:HIS:O	7:A:5103:ATP:N6	2.45	0.42
2:D:1454:THR:HA	2:D:1548:LEU:HA	2.00	0.42
2:J:1149:VAL:HG13	2:J:1164:LEU:HG	1.99	0.42
2:J:1733:GLU:N	2:J:1733:GLU:OE2	2.52	0.42
2:J:1863:LEU:HD23	2:J:1863:LEU:HA	1.81	0.42
1:M:18[B]:GLY:O	1:M:19[B]:LYS:HG2	2.19	0.42
2:G:2228:MET:HE3	2:G:2228:MET:HB3	1.90	0.42
2:A:707:VAL:HG12	2:A:782:SER:OG	2.19	0.42
2:A:721:LEU:N	2:A:728:ARG:O	2.53	0.42
2:A:804:PRO:HA	2:A:805:PRO:HD3	1.94	0.42
2:A:3658:LYS:HA	2:A:3662:ILE:HD11	2.01	0.42
2:A:4017:LEU:HD12	2:A:4139:ILE:HG21	2.01	0.42
2:A:4659:ILE:HD12	2:A:4659:ILE:HA	1.86	0.42
2:D:3978:GLN:OE1	2:D:4040:ILE:HD11	2.19	0.42
2:D:4956:THR:HG22	2:D:4957:LYS:HG2	2.01	0.42
2:J:4813:LEU:HD23	2:J:4813:LEU:HA	1.86	0.42
2:G:582:HIS:O	2:G:586:ILE:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:736:HIS:ND1	2:G:737:LEU:O	2.53	0.42
2:G:1943:LEU:HD13	2:G:2098:VAL:HG22	2.01	0.42
2:G:2427:ALA:HB1	2:G:2498:HIS:HA	2.02	0.42
2:G:4929:LEU:HD12	2:G:4929:LEU:HA	1.84	0.42
2:A:638:ILE:HD12	2:A:638:ILE:HA	1.86	0.42
2:A:2239:PHE:O	2:A:2242:ILE:HG22	2.19	0.42
2:A:3888:LEU:HD23	2:A:3888:LEU:HA	1.85	0.42
2:A:3924:LEU:HD21	2:A:3984:ARG:HE	1.83	0.42
2:A:4183:ILE:C	2:A:4183:ILE:HD12	2.45	0.42
2:D:1729:SER:O	2:D:2163:ARG:NH1	2.53	0.42
2:D:4708:THR:HG21	2:D:4775:TYR:HB2	2.00	0.42
2:D:4821:LYS:HE2	2:D:4821:LYS:HB2	1.80	0.42
2:J:663:TYR:HE1	2:J:745:SER:HB3	1.84	0.42
2:J:4023:MET:HE3	2:J:4027:LEU:HD21	2.01	0.42
2:G:280:LEU:N	2:G:314:PHE:O	2.51	0.42
2:G:1671:ARG:HG2	2:G:1714:LEU:HA	2.00	0.42
2:G:2201:LEU:HD23	2:G:2201:LEU:HA	1.83	0.42
2:G:2210:VAL:O	2:G:2214:VAL:HG12	2.19	0.42
2:G:2472:LEU:HD23	2:G:2472:LEU:HA	1.86	0.42
2:G:3958:ALA:HA	2:G:3961:VAL:HG12	2.02	0.42
2:G:4183:ILE:HD12	2:G:4183:ILE:C	2.44	0.42
2:A:221:ARG:HG2	2:A:393:CYS:SG	2.60	0.42
2:A:637:LEU:HD23	2:A:637:LEU:HA	1.83	0.42
2:A:1850:VAL:HG12	2:A:1945:TYR:CD1	2.54	0.42
2:A:3798:LEU:HD23	2:A:3798:LEU:HA	1.80	0.42
2:D:790:ARG:HA	2:D:1627:ALA:HA	2.02	0.42
2:D:2525:GLY:C	2:D:2528:PRO:HD2	2.44	0.42
2:D:3970:GLN:HE22	2:D:5004:THR:HA	1.84	0.42
2:D:4052:SER:CA	2:D:4055:VAL:HG12	2.45	0.42
2:D:4928:LEU:HA	2:D:4928:LEU:HD12	1.83	0.42
2:D:5000:GLU:HA	2:D:5003:HIS:CD2	2.54	0.42
2:J:1804:LEU:HD23	2:J:1805:GLU:H	1.84	0.42
2:J:1962:ALA:HA	2:J:3653:PHE:HE2	1.85	0.42
2:G:595:ARG:HH12	2:G:633:LEU:HD21	1.85	0.42
2:G:663:TYR:CE2	2:G:745:SER:HB2	2.55	0.42
2:G:766:GLY:HA2	2:G:1476:MET:HA	2.02	0.42
2:G:1143:TRP:HB3	2:G:1164:LEU:HD21	2.00	0.42
2:G:4911:LEU:HD11	2:D:4324:ALA:H	1.83	0.42
2:A:1803:PRO:HB2	2:A:1806:ALA:HB3	2.02	0.42
2:D:48:PHE:CD1	2:D:48:PHE:C	2.97	0.42
2:D:1218:GLY:O	2:D:1222:GLY:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3729:MET:O	2:D:3732:SER:N	2.53	0.42
2:D:4666:VAL:HA	2:D:4669:VAL:HG12	2.01	0.42
2:J:3923:LEU:HD12	2:J:3923:LEU:HA	1.84	0.42
2:J:4573:ILE:HD12	2:J:4573:ILE:HA	1.92	0.42
3:K:4:ILE:HG23	3:K:72:ALA:HB1	2.02	0.42
2:G:517:GLU:O	2:G:521:LEU:HD12	2.20	0.42
2:G:589:LEU:C	2:G:589:LEU:HD23	2.45	0.42
2:G:626:LEU:HD22	2:G:1688:HIS:CE1	2.55	0.42
2:G:1153:ILE:CD1	2:G:1160:ILE:HA	2.49	0.42
2:G:3649:ALA:HA	2:G:3652:MET:HE2	2.02	0.42
3:H:56:ILE:H	3:H:56:ILE:HG13	1.59	0.42
3:H:63:ALA:HA	3:H:66:MET:HB2	2.00	0.42
2:A:442:ILE:HD13	2:A:442:ILE:HA	1.94	0.42
2:A:4180:ARG:HB3	2:A:4192:ARG:NE	2.35	0.42
2:A:4569:LEU:HG	2:A:4646:LEU:HD13	2.01	0.42
2:A:4779:LYS:O	2:A:4783:ILE:HG23	2.20	0.42
2:D:3780:LEU:HD23	2:D:3780:LEU:HA	1.83	0.42
2:J:686:TRP:CD1	2:J:748:LEU:HD13	2.54	0.42
2:J:1205:GLY:HA3	2:J:1225:PRO:HB3	2.01	0.42
3:K:7:ILE:H	3:K:7:ILE:HG13	1.66	0.42
1:M:22[A]:LYS:HG3	1:M:33[A]:ARG:HD3	2.02	0.42
2:A:111:HIS:CE1	2:A:113:HIS:HB3	2.55	0.42
2:A:247:TYR:N	2:A:374:LYS:O	2.48	0.42
2:A:582:HIS:O	2:A:586:ILE:HG12	2.20	0.42
2:A:655:GLY:HA3	2:A:852:VAL:HA	2.01	0.42
2:A:766:GLY:HA2	2:A:1476:MET:HA	2.02	0.42
2:A:4570:ALA:HB2	2:A:4650:HIS:HE1	1.85	0.42
2:A:4578:LEU:O	2:D:4879:MET:HB3	2.20	0.42
2:J:686:TRP:CE3	2:J:777:PHE:HB3	2.54	0.42
2:J:2012:PHE:HZ	2:J:2031:LEU:HD13	1.85	0.42
2:J:4051:SER:O	2:J:4055:VAL:HG12	2.19	0.42
2:G:2384:ILE:HD13	2:G:2384:ILE:HA	1.88	0.42
2:G:4107:GLU:O	2:G:4111:LEU:HG	2.20	0.42
4:I:14:LYS:HA	4:I:66:PHE:CZ	2.55	0.42
2:A:592:LYS:HA	2:A:1580:PHE:CE2	2.55	0.42
2:A:1936:LYS:HD3	2:A:2116:LEU:HD21	2.02	0.42
2:D:291:LEU:HA	2:D:301:VAL:HA	2.02	0.42
2:D:839:LEU:O	2:D:1200:GLY:N	2.41	0.42
2:D:3920:VAL:O	2:D:3924:LEU:HD13	2.19	0.42
2:D:4027:LEU:HD23	2:D:4047:MET:HE1	2.02	0.42
2:J:1097:THR:HG23	2:J:1143:TRP:HE1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:2142:TYR:HB3	2:J:2197:LEU:HD13	2.02	0.42
2:J:4681:LEU:HD11	2:J:4706:LEU:HD22	2.02	0.42
2:G:20:VAL:HA	2:G:204:PRO:HA	2.01	0.41
2:G:591:ASP:HA	2:G:631:LEU:HD11	2.02	0.41
2:G:2377:LEU:HD21	2:G:2468:GLY:HA3	2.02	0.41
2:G:4051:SER:O	2:G:4051:SER:OG	2.33	0.41
2:A:560:ILE:HA	2:A:563:VAL:HG12	2.02	0.41
2:A:1079:LYS:NZ	2:A:1107:PRO:O	2.53	0.41
2:A:3989:VAL:O	2:A:3993:LEU:HG	2.20	0.41
2:A:4060:LYS:O	2:A:4063:ASP:N	2.52	0.41
2:A:4180:ARG:HB3	2:A:4192:ARG:HE	1.85	0.41
2:D:884:LEU:HA	2:D:960:MET:O	2.20	0.41
2:D:2225:PHE:O	2:D:2229:VAL:HG23	2.20	0.41
2:D:4570:ALA:HB2	2:D:4650:HIS:CE1	2.55	0.41
2:J:269:TRP:CZ2	2:J:272:SER:HB3	2.55	0.41
2:J:592:LYS:O	2:J:1592:PRO:HB2	2.19	0.41
2:J:4587:PRO:HG3	2:J:4630:TYR:HB3	2.01	0.41
2:G:1492:CYS:HB2	2:G:1494:MET:HE1	2.01	0.41
2:G:1636:MET:HG2	2:G:1637:MET:N	2.35	0.41
2:G:2466:LEU:O	2:G:2470:ILE:HG22	2.20	0.41
3:H:37:ASP:OD1	3:H:37:ASP:C	2.63	0.41
2:A:529:LEU:HD23	2:A:529:LEU:HA	1.92	0.41
2:A:548:VAL:HG11	2:A:582:HIS:CD2	2.55	0.41
2:A:575:LEU:HD21	2:A:606:LEU:HA	2.02	0.41
2:A:1771:LEU:HD23	2:A:1771:LEU:HA	1.89	0.41
2:A:2770:LYS:O	2:A:2775:TRP:N	2.52	0.41
2:D:643:SER:HA	2:D:782:SER:HA	2.02	0.41
2:D:2490:MET:HE2	2:D:2490:MET:HB2	1.98	0.41
2:D:3984:ARG:O	2:D:3985:LEU:C	2.63	0.41
2:J:615:ARG:CZ	2:J:2168:VAL:HG21	2.50	0.41
2:J:853:PRO:HB3	2:J:1023:PRO:HA	2.01	0.41
2:J:2226:PRO:HA	2:J:2229:VAL:HG12	2.02	0.41
2:J:3969:ILE:HD13	2:J:3980:LEU:HD12	2.02	0.41
2:J:4833:ASN:ND2	2:J:4836:GLN:OE1	2.46	0.41
2:G:1293:LEU:HD21	2:G:1594:ARG:HG2	2.02	0.41
2:G:1694:LEU:HD23	2:G:1694:LEU:HA	1.94	0.41
2:G:2131:LEU:HD22	2:G:2131:LEU:HA	1.94	0.41
2:G:2197:LEU:O	2:G:2201:LEU:N	2.36	0.41
2:G:4715:TYR:HE2	2:G:4717:ASP:HB3	1.84	0.41
2:A:2211:MET:HE3	2:A:2211:MET:C	2.46	0.41
2:D:4668:LEU:HD12	2:D:4668:LEU:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:2236:LEU:HD23	2:J:2236:LEU:HA	1.83	0.41
2:J:2505:PHE:O	2:J:2509:VAL:HG12	2.20	0.41
2:J:3777:GLU:O	2:J:3781:GLN:HG2	2.21	0.41
2:J:4802:GLY:HA2	2:J:4805:ASN:O	2.20	0.41
2:G:1760:HIS:CE1	2:G:2095:GLN:HE22	2.35	0.41
2:G:2299:VAL:HG11	2:G:2356:LEU:O	2.20	0.41
2:A:2156:LEU:HD23	2:A:2156:LEU:HA	1.81	0.41
2:A:2456:ILE:HD13	2:A:2456:ILE:HA	1.93	0.41
2:A:4047:MET:HE3	2:A:4047:MET:HB3	1.76	0.41
2:A:4879:MET:HE2	2:A:4879:MET:HA	2.01	0.41
2:D:3924:LEU:HD12	2:D:3988:ALA:HB2	2.03	0.41
2:D:3984:ARG:O	2:D:3987:ASP:N	2.54	0.41
2:J:594:GLY:HA2	2:J:1594:ARG:HD2	2.03	0.41
2:J:1148:VAL:HG21	2:J:1212:ARG:HD2	2.00	0.41
2:J:1674:CYS:HB2	2:J:1685:LEU:HD22	2.02	0.41
2:J:2155:LEU:HB2	2:J:2188:ASN:HD22	1.84	0.41
2:J:4147:LEU:HD11	2:J:4171:LEU:HD13	2.02	0.41
2:J:4211:LYS:NZ	7:J:5103:ATP:O1B	2.43	0.41
2:G:410:LEU:HD21	2:G:441:VAL:HG12	2.02	0.41
2:G:1731:LEU:HA	2:G:1772:ARG:HH21	1.86	0.41
2:G:2238:TYR:CD2	4:I:67:PRO:HB2	2.56	0.41
2:G:3644:LEU:HD12	2:G:3645:PRO:O	2.21	0.41
2:A:288:GLY:HA3	2:A:405:HIS:CE1	2.56	0.41
2:A:1148:VAL:HG21	2:A:1213:PHE:CD2	2.56	0.41
2:A:2095:GLN:HA	2:A:2127:GLN:CD	2.46	0.41
2:A:4706:LEU:HD23	2:A:4706:LEU:HA	1.93	0.41
2:D:1160:ILE:O	2:D:1178:ALA:N	2.53	0.41
2:J:510:GLU:O	2:J:514:SER:OG	2.33	0.41
2:J:2418:LEU:O	2:J:2422:ILE:HG13	2.20	0.41
2:J:4137:ARG:NH1	2:J:4196:GLU:OE1	2.51	0.41
2:G:407:THR:HG21	2:G:448:LEU:HD11	2.02	0.41
2:G:1771:LEU:HD11	2:G:2153:MET:SD	2.61	0.41
2:G:3970:GLN:HE22	2:G:5004:THR:HG22	1.85	0.41
2:G:4222:VAL:CG1	2:G:4950:VAL:HG22	2.50	0.41
2:G:4576:ILE:HG21	2:G:4643:LEU:HB2	2.03	0.41
2:G:4843:LEU:HD13	2:J:4823:LEU:HD12	2.01	0.41
2:G:4880:MET:CE	2:J:4328:ALA:HB2	2.51	0.41
2:A:358:THR:HA	2:A:386:ASP:OD2	2.20	0.41
2:A:1297:PHE:HA	2:A:1522:LEU:HD12	2.02	0.41
2:A:4960:ILE:H	2:A:4960:ILE:HG12	1.71	0.41
3:B:28:GLY:HA2	3:B:99:PHE:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3735:LEU:O	2:D:3736:GLU:C	2.62	0.41
2:D:4242:ILE:CD1	2:D:4989:MET:HE1	2.50	0.41
2:G:1838:PHE:O	2:G:1842:LEU:HB2	2.21	0.41
2:G:1934:SER:O	2:G:1938:GLN:HG2	2.20	0.41
2:G:2250:MET:HE2	2:G:2250:MET:HB2	1.89	0.41
2:G:2442:LEU:HA	2:G:2442:LEU:HD23	1.81	0.41
2:G:4865:LYS:HA	2:G:4865:LYS:HD2	1.90	0.41
2:A:359:TYR:CA	2:A:376:ALA:HA	2.38	0.41
2:A:2207:VAL:HG21	2:A:2235:PHE:CD2	2.55	0.41
2:A:2210:VAL:O	2:A:2214:VAL:HG12	2.21	0.41
2:A:3722:TYR:CE2	2:A:3782:MET:SD	3.14	0.41
2:D:3896:ASN:O	2:D:3900:GLN:HG3	2.21	0.41
2:D:4028:LEU:HD21	2:D:4146:LEU:HA	2.02	0.41
2:J:1438:ARG:HB3	2:J:1515:VAL:HG13	2.01	0.41
2:J:2142:TYR:OH	2:J:2194:HIS:ND1	2.53	0.41
2:J:3716:LEU:HD23	2:J:3716:LEU:H	1.85	0.41
2:G:436:LEU:HD23	2:G:436:LEU:HA	1.91	0.41
2:G:1160:ILE:HG21	2:G:1179:PHE:HD2	1.85	0.41
2:G:1492:CYS:HB2	2:G:1494:MET:CE	2.51	0.41
2:G:1747:LEU:HB3	2:G:2041:HIS:HD2	1.86	0.41
2:A:102:LEU:HA	2:A:162:LYS:HA	2.02	0.41
2:A:2194:HIS:HB3	2:A:2197:LEU:HD23	2.03	0.41
2:D:2325:PRO:HB2	2:D:2421:ALA:HB1	2.01	0.41
3:E:78:PRO:HD3	3:E:96:THR:HA	2.02	0.41
2:J:119:SER:N	2:J:136:GLY:O	2.43	0.41
2:J:1762:LEU:O	2:J:1765:VAL:HG22	2.21	0.41
2:J:2281:ILE:HD12	2:J:2282:ASP:H	1.84	0.41
2:G:107:ILE:HD12	2:G:107:ILE:HA	1.99	0.41
2:G:1863:LEU:HD21	2:G:1946:PHE:CE1	2.56	0.41
2:G:2211:MET:HE3	2:G:2211:MET:HB3	1.86	0.41
2:G:4055:VAL:HG13	2:G:4163:PHE:HZ	1.86	0.41
2:A:419:ASP:OD1	2:A:493:ARG:CD	2.67	0.41
2:A:527:ALA:O	2:A:530:ILE:HG22	2.21	0.41
2:A:1076:ARG:HG3	2:A:1077:ALA:O	2.20	0.41
2:A:1530:THR:HA	2:A:1535:GLU:HA	2.03	0.41
2:A:3842:LEU:HD21	2:A:3933:PHE:CD1	2.56	0.41
2:A:4016:LEU:O	2:A:4020:GLN:HG2	2.20	0.41
2:A:4048:LEU:CD1	2:A:4055:VAL:HB	2.51	0.41
2:D:665:GLU:H	2:D:793:LEU:HA	1.86	0.41
2:D:1667:LEU:O	2:D:1714:LEU:HD11	2.21	0.41
2:D:2683:PHE:CD1	2:D:2683:PHE:C	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3136:LEU:O	2:D:3140:LEU:N	2.41	0.41
2:D:4904:PRO:HD3	2:D:4913:ARG:HH21	1.86	0.41
2:J:1294:PRO:HB3	2:J:1549:PHE:CZ	2.56	0.41
2:J:1492:CYS:SG	2:J:1494:MET:HB2	2.61	0.41
2:J:2355:ARG:O	2:J:2359:ARG:HG2	2.21	0.41
2:J:4967:TYR:CD1	2:J:4967:TYR:C	2.98	0.41
2:J:4998:LYS:HD2	2:J:5003:HIS:CD2	2.56	0.41
3:K:31:GLN:HB2	3:K:96:THR:OG1	2.21	0.41
1:M:18[A]:GLY:O	1:M:19[A]:LYS:HG2	2.20	0.41
2:G:1460:HIS:HD2	2:G:1602:PRO:HB3	1.85	0.41
2:G:3675:ASP:OD1	2:G:3675:ASP:C	2.64	0.41
2:G:3782:MET:HE2	2:G:3782:MET:HB2	1.85	0.41
2:D:1105:ALA:N	2:D:1189:LEU:O	2.54	0.41
2:D:4183:ILE:HD13	2:D:4183:ILE:N	2.35	0.41
2:D:4817:ALA:HB1	2:D:4827:LEU:HD11	2.01	0.41
2:J:313:SER:O	2:J:351:VAL:HG12	2.21	0.41
2:J:639:ASN:ND2	2:J:676:THR:OG1	2.54	0.41
2:J:1229:ASN:HB2	2:J:1827:ARG:H	1.86	0.41
2:J:1466:LEU:HD12	2:J:1496:TRP:HB2	2.02	0.41
2:J:4217:PHE:CD2	2:J:4237:PHE:HB2	2.56	0.41
2:J:4777:ILE:HD13	2:J:4777:ILE:HA	1.91	0.41
2:G:437:PRO:HB2	2:G:440:ALA:HB3	2.03	0.40
2:G:767:VAL:O	2:G:1475:THR:OG1	2.37	0.40
2:G:1721:GLU:OE2	2:G:1725:ARG:NH1	2.54	0.40
2:G:1777:PHE:HB3	2:G:1801:ALA:HA	2.03	0.40
2:G:1839:VAL:HG23	2:G:1935:VAL:HG22	2.03	0.40
2:A:1237:TRP:CH2	2:A:1652:GLU:HG3	2.56	0.40
2:A:1934:SER:O	2:A:1938:GLN:HG2	2.21	0.40
2:A:2256:TYR:O	2:A:2260:ASN:ND2	2.55	0.40
2:D:1748:PHE:HA	2:D:1749:PRO:HD3	1.97	0.40
2:D:3980:LEU:HD13	2:D:3980:LEU:HA	1.71	0.40
2:J:671:VAL:HG12	2:J:787:VAL:HA	2.02	0.40
2:J:838:HIS:ND1	2:J:1201:HIS:HB2	2.35	0.40
2:J:2238:TYR:CE1	4:L:67:PRO:HB2	2.55	0.40
2:G:1719:HIS:CD2	2:G:1802:ILE:HD12	2.55	0.40
2:G:2460:LEU:HA	2:G:2460:LEU:HD23	1.89	0.40
2:A:118:LEU:HA	2:A:137:LEU:HA	2.03	0.40
2:A:621:ILE:HG21	2:A:1673:VAL:HG11	2.04	0.40
2:A:2117:VAL:HG23	2:A:3704:HIS:CD2	2.56	0.40
2:A:4843:LEU:HD12	2:A:4843:LEU:HA	1.86	0.40
2:A:4891:VAL:HG13	2:A:4892:ARG:HG3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3882:GLN:OE1	2:D:3960:GLN:NE2	2.46	0.40
2:D:4077:PHE:HE1	2:D:4093:PHE:HD1	1.68	0.40
2:D:4676:GLU:O	2:D:4680:LYS:HG2	2.21	0.40
2:J:4192:ARG:C	2:J:4193:ILE:HD13	2.45	0.40
2:G:1699:GLU:HG2	2:G:1810:LYS:HD3	2.02	0.40
2:G:3836:MET:HE3	2:G:3918:CYS:SG	2.61	0.40
2:G:4586:PRO:HA	2:G:4587:PRO:HD3	1.91	0.40
2:G:4958:CYS:HA	7:G:5103:ATP:N7	2.36	0.40
2:A:2335:LEU:HD23	2:A:2335:LEU:HA	1.88	0.40
2:A:3882:GLN:HA	2:A:3960:GLN:HG2	2.02	0.40
2:A:4072:VAL:HG21	2:A:4129:ALA:HB2	2.03	0.40
2:D:2159:LEU:HA	2:D:2162:ILE:HG22	2.02	0.40
2:J:502:HIS:C	2:J:503:PHE:HD1	2.29	0.40
2:J:660:GLY:O	2:J:750:LEU:N	2.48	0.40
2:J:3966:THR:HG22	2:J:4026:MET:HA	2.02	0.40
3:K:23:VAL:HG12	3:K:47:LYS:HG2	2.02	0.40
2:G:603:LEU:HB3	2:G:1669:LEU:HD13	2.03	0.40
2:G:650:VAL:O	2:G:777:PHE:N	2.53	0.40
2:G:3767:GLN:NE2	2:G:3804:ILE:O	2.55	0.40
2:G:4000:MET:HE1	2:G:4058:ILE:HG12	2.03	0.40
2:G:4790:LEU:HD13	2:G:4790:LEU:HA	1.95	0.40
2:A:70:GLU:HG3	2:A:117:TYR:HE2	1.85	0.40
2:A:758:ARG:HA	2:A:763:PRO:HA	2.04	0.40
2:A:1719:HIS:ND1	2:A:1802:ILE:HD12	2.37	0.40
2:A:2250:MET:HA	2:A:2250:MET:HE3	2.04	0.40
2:A:3986:TRP:O	2:A:3990:VAL:HG23	2.22	0.40
2:A:4233:LEU:HD13	2:A:4233:LEU:HA	1.97	0.40
2:A:4946:GLN:O	2:A:4950:VAL:HG23	2.21	0.40
2:D:350:HIS:CE1	2:D:352:ALA:HB3	2.57	0.40
2:D:4117:ALA:HB2	2:D:4123:ILE:HG22	2.03	0.40
2:D:4725:LEU:CD1	2:D:4743:MET:HE1	2.51	0.40
2:G:1161:ILE:HG23	2:G:1176:GLU:O	2.21	0.40
2:G:1202:LEU:HD12	2:G:1203:ASN:N	2.36	0.40
2:G:1763:PRO:HG3	2:G:2094:LEU:HD22	2.03	0.40
2:G:4051:SER:O	2:G:4055:VAL:HG12	2.22	0.40
2:G:4856:PHE:HZ	2:J:4582:VAL:HB	1.85	0.40
2:A:526:LEU:CD2	2:A:563:VAL:HG21	2.50	0.40
2:A:1290:ARG:HG3	2:A:1551:ALA:HB2	2.03	0.40
2:A:1784:ALA:HA	3:B:55:VAL:HA	2.03	0.40
2:A:2118:ARG:HB2	2:A:3704:HIS:NE2	2.36	0.40
2:A:2131:LEU:HD12	2:A:2131:LEU:HA	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3889:GLN:NE2	2:A:3963:ASN:HB3	2.37	0.40
2:A:4245:MET:HE1	2:A:4989:MET:CE	2.51	0.40
2:A:4650:HIS:O	2:A:4653:VAL:HG12	2.22	0.40
2:D:2278:ALA:HA	2:D:2281:ILE:HG12	2.03	0.40
2:J:1850:VAL:HA	2:J:1945:TYR:CE1	2.57	0.40
2:J:4555:LEU:HD21	2:J:4656:LEU:HD22	2.03	0.40
2:J:4678:ALA:HB1	2:J:4720:VAL:HG21	2.04	0.40
2:J:4851:TYR:CD2	2:J:4920:PHE:HD1	2.39	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	M	62/33 (188%)	56 (90%)	6 (10%)	0	100	100
2	A	3718/5037 (74%)	3668 (99%)	48 (1%)	2 (0%)	48	78
2	D	1943/5037 (39%)	1917 (99%)	26 (1%)	0	100	100
2	G	3827/5037 (76%)	3774 (99%)	53 (1%)	0	100	100
2	J	3786/5037 (75%)	3726 (98%)	60 (2%)	0	100	100
3	B	58/107 (54%)	56 (97%)	2 (3%)	0	100	100
3	E	104/107 (97%)	100 (96%)	4 (4%)	0	100	100
3	H	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
3	K	104/107 (97%)	100 (96%)	4 (4%)	0	100	100
4	F	131/149 (88%)	130 (99%)	1 (1%)	0	100	100
4	I	132/149 (89%)	132 (100%)	0	0	100	100
4	L	133/149 (89%)	131 (98%)	2 (2%)	0	100	100
All	All	14103/21056 (67%)	13889 (98%)	212 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	4052	SER
2	A	614	VAL

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	M	56/28 (200%)	56 (100%)	0	100	100
2	A	1728/4276 (40%)	1705 (99%)	23 (1%)	61	71
2	D	1204/4276 (28%)	1180 (98%)	24 (2%)	48	64
2	G	1976/4276 (46%)	1958 (99%)	18 (1%)	70	75
2	J	1721/4276 (40%)	1703 (99%)	18 (1%)	68	74
3	B	67/88 (76%)	67 (100%)	0	100	100
3	E	49/88 (56%)	49 (100%)	0	100	100
3	H	73/88 (83%)	71 (97%)	2 (3%)	39	59
3	K	74/88 (84%)	72 (97%)	2 (3%)	39	59
4	C	9/123 (7%)	9 (100%)	0	100	100
4	F	9/123 (7%)	9 (100%)	0	100	100
4	I	8/123 (6%)	8 (100%)	0	100	100
4	L	5/123 (4%)	5 (100%)	0	100	100
All	All	6979/17976 (39%)	6892 (99%)	87 (1%)	59	72

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	135	VAL
2	G	494	LEU
2	G	518	ILE
2	G	521	LEU
2	G	725	HIS
2	G	1552	VAL

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Mol	Chain	Res	Type
2	G	1693	GLN
2	G	2131	LEU
2	G	2197	LEU
2	G	2281	ILE
2	G	2368	LEU
2	G	2613	TYR
2	G	3018	LEU
2	G	3770	LEU
2	G	3916	ILE
2	G	3965	LEU
2	G	4631	PHE
2	G	4773	VAL
3	H	56	ILE
3	H	87	HIS
2	A	74	SER
2	A	78	LEU
2	A	218	HIS
2	A	334	MET
2	A	357	LEU
2	A	389	PHE
2	A	484	LEU
2	A	486	LEU
2	A	488	LEU
2	A	491	ILE
2	A	494	LEU
2	A	498	THR
2	A	1254	HIS
2	A	1454	THR
2	A	1549	PHE
2	A	1848	LEU
2	A	2142	TYR
2	A	3722	TYR
2	A	3985	LEU
2	A	3995	VAL
2	A	4049	VAL
2	A	4858	PHE
2	A	5019	TRP
2	D	2125	HIS
2	D	3674	ILE
2	D	3677	LEU
2	D	3732	SER
2	D	3733	CYS

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Mol	Chain	Res	Type
2	D	3980	LEU
2	D	3984	ARG
2	D	3985	LEU
2	D	3995	VAL
2	D	4025	VAL
2	D	4036	VAL
2	D	4044	MET
2	D	4048	LEU
2	D	4128	PHE
2	D	4142	ASN
2	D	4147	LEU
2	D	4162	ASN
2	D	4169	SER
2	D	4182	GLU
2	D	4183	ILE
2	D	4190	ILE
2	D	4238	CYS
2	D	4562	LEU
2	D	4859	PHE
2	J	1204	LEU
2	J	2128	TYR
2	J	3641	LEU
2	J	3696	ASP
2	J	3721	LEU
2	J	3723	MET
2	J	3727	ASP
2	J	3728	ILE
2	J	3735	LEU
2	J	3897	ASN
2	J	4023	MET
2	J	4029	SER
2	J	4035	VAL
2	J	4146	LEU
2	J	4147	LEU
2	J	4150	LEU
2	J	4648	LEU
2	J	4886	HIS
3	K	77	THR
3	K	80	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
2	G	79	GLN
2	G	113	HIS
2	G	151	HIS
2	G	412	ASN
2	G	647	ASN
2	G	838	HIS
2	G	1458	HIS
2	G	1614	GLN
2	G	1645	ASN
2	G	1660	GLN
2	G	1663	HIS
2	G	1683	HIS
2	G	1696	HIS
2	G	2095	GLN
2	G	2107	GLN
2	G	2184	ASN
2	G	2204	HIS
2	G	2283	ASN
2	G	2498	HIS
2	G	2646	ASN
2	G	3813	GLN
2	G	3889	GLN
2	G	3909	ASN
2	G	3960	GLN
2	G	4005	GLN
2	G	4130	ASN
2	G	4776	GLN
2	G	4806	ASN
2	G	5003	HIS
2	G	5006	GLN
3	H	70	GLN
2	A	71	GLN
2	A	495	ASN
2	A	838	HIS
2	A	1084	GLN
2	A	1130	GLN
2	A	1201	HIS
2	A	1206	GLN
2	A	1660	GLN
2	A	1678	ASN
2	A	1952	GLN
2	A	2127	GLN
2	A	2260	ASN

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Mol	Chain	Res	Type
2	A	2324	ASN
2	A	2599	GLN
2	A	3813	GLN
2	A	3977	GLN
2	A	3982	HIS
2	A	4043	GLN
2	A	4142	ASN
2	A	4216	GLN
2	A	4558	ASN
2	A	4574	ASN
2	A	4857	ASN
3	B	94	ASN
2	D	576	ASN
2	D	2029	GLN
2	D	2441	HIS
2	D	3813	GLN
2	D	3833	GLN
2	D	4037	ASN
3	E	43	ASN
2	J	543	ASN
2	J	576	ASN
2	J	581	ASN
2	J	639	ASN
2	J	720	HIS
2	J	1201	HIS
2	J	1458	HIS
2	J	1569	GLN
2	J	1660	GLN
2	J	1691	GLN
2	J	1702	HIS
2	J	1952	GLN
2	J	2095	GLN
2	J	2169	GLN
2	J	2204	HIS
2	J	3700	GLN
2	J	3813	GLN
2	J	4142	ASN
2	J	4776	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	CFF	J	5101	-	15,15,15	0.63	0	23,23,23	0.49	0
5	CFF	A	5101	-	15,15,15	0.62	0	23,23,23	0.49	0
5	CFF	D	5101	-	15,15,15	0.62	0	23,23,23	0.48	0
7	ATP	G	5103	-	32,33,33	0.25	0	48,52,52	0.28	0
7	ATP	D	5103	-	32,33,33	0.25	0	48,52,52	0.28	0
5	CFF	G	5101	-	15,15,15	0.62	0	23,23,23	0.48	0
7	ATP	J	5103	-	32,33,33	0.26	0	48,52,52	0.29	0
7	ATP	A	5103	-	32,33,33	0.25	0	48,52,52	0.29	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CFF	J	5101	-	-	-	0/2/2/2
5	CFF	A	5101	-	-	-	0/2/2/2
5	CFF	D	5101	-	-	-	0/2/2/2
7	ATP	D	5103	-	-	12/22/38/38	0/3/3/3
7	ATP	G	5103	-	-	8/22/38/38	0/3/3/3
5	CFF	G	5101	-	-	-	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ATP	J	5103	-	-	10/22/38/38	0/3/3/3
7	ATP	A	5103	-	-	6/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	5103	ATP	PB-O3B-PG-O2G
7	G	5103	ATP	C5'-O5'-PA-O2A
7	G	5103	ATP	C4'-C5'-O5'-PA
7	A	5103	ATP	PB-O3A-PA-O5'
7	A	5103	ATP	C5'-O5'-PA-O2A
7	A	5103	ATP	C5'-O5'-PA-O3A
7	A	5103	ATP	C4'-C5'-O5'-PA
7	D	5103	ATP	C5'-O5'-PA-O3A
7	D	5103	ATP	C4'-C5'-O5'-PA
7	J	5103	ATP	C5'-O5'-PA-O1A
7	J	5103	ATP	C5'-O5'-PA-O2A
7	J	5103	ATP	C5'-O5'-PA-O3A
7	D	5103	ATP	C3'-C4'-C5'-O5'
7	J	5103	ATP	C3'-C4'-C5'-O5'
7	J	5103	ATP	C4'-C5'-O5'-PA
7	D	5103	ATP	O4'-C4'-C5'-O5'
7	J	5103	ATP	O4'-C4'-C5'-O5'
7	D	5103	ATP	PB-O3B-PG-O1G
7	J	5103	ATP	PB-O3B-PG-O1G
7	D	5103	ATP	PG-O3B-PB-O2B
7	D	5103	ATP	PA-O3A-PB-O2B
7	G	5103	ATP	C5'-O5'-PA-O1A
7	G	5103	ATP	C5'-O5'-PA-O3A
7	D	5103	ATP	C5'-O5'-PA-O1A
7	A	5103	ATP	PG-O3B-PB-O2B
7	J	5103	ATP	PG-O3B-PB-O2B
7	G	5103	ATP	O4'-C1'-N9-C8
7	G	5103	ATP	O4'-C1'-N9-C4
7	J	5103	ATP	O4'-C1'-N9-C4
7	J	5103	ATP	O4'-C1'-N9-C8
7	G	5103	ATP	PB-O3B-PG-O1G

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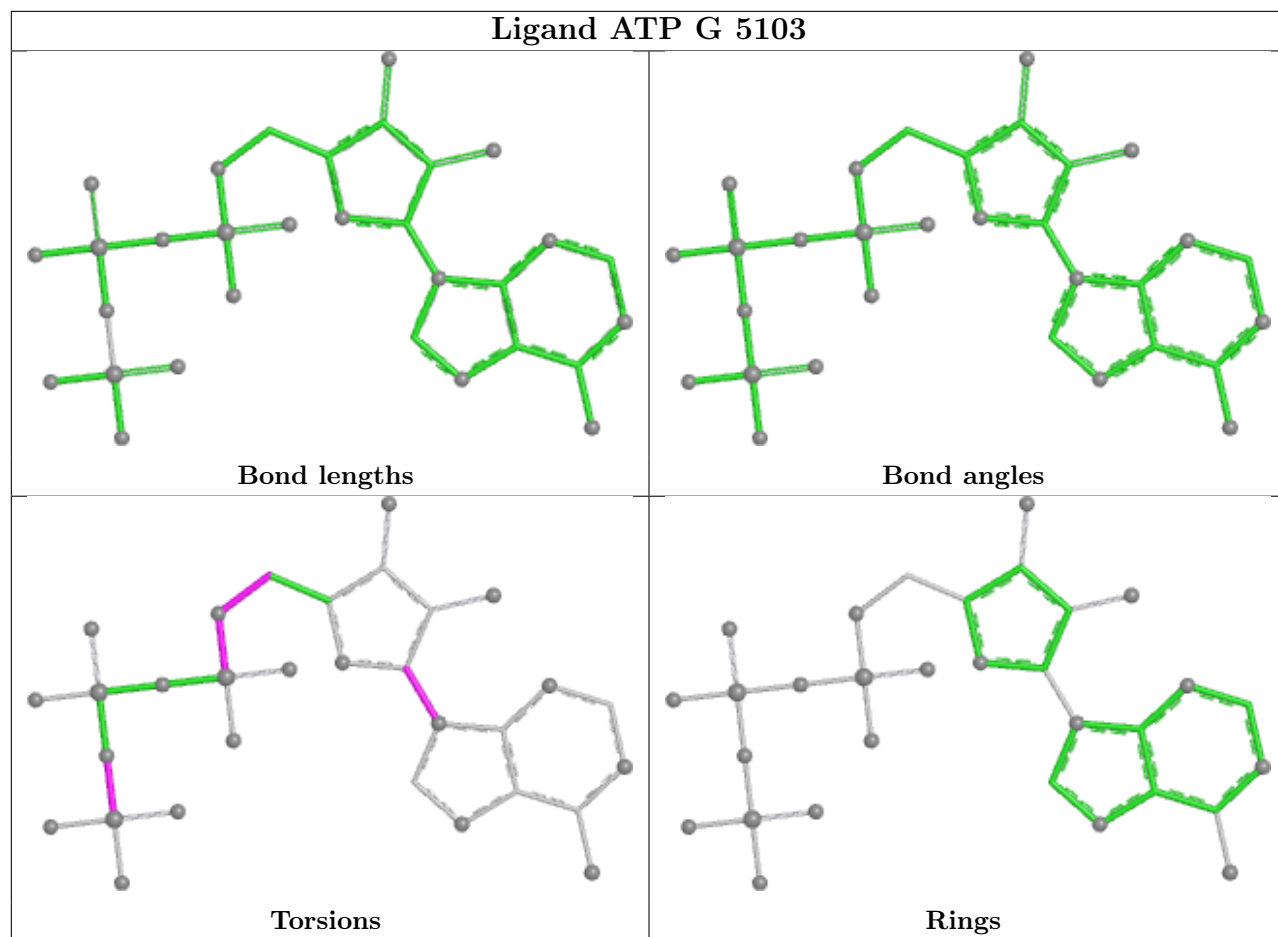
Mol	Chain	Res	Type	Atoms
7	D	5103	ATP	PB-O3B-PG-O2G
7	D	5103	ATP	PB-O3B-PG-O3G
7	A	5103	ATP	PB-O3A-PA-O2A
7	D	5103	ATP	PG-O3B-PB-O1B
7	D	5103	ATP	PA-O3A-PB-O1B

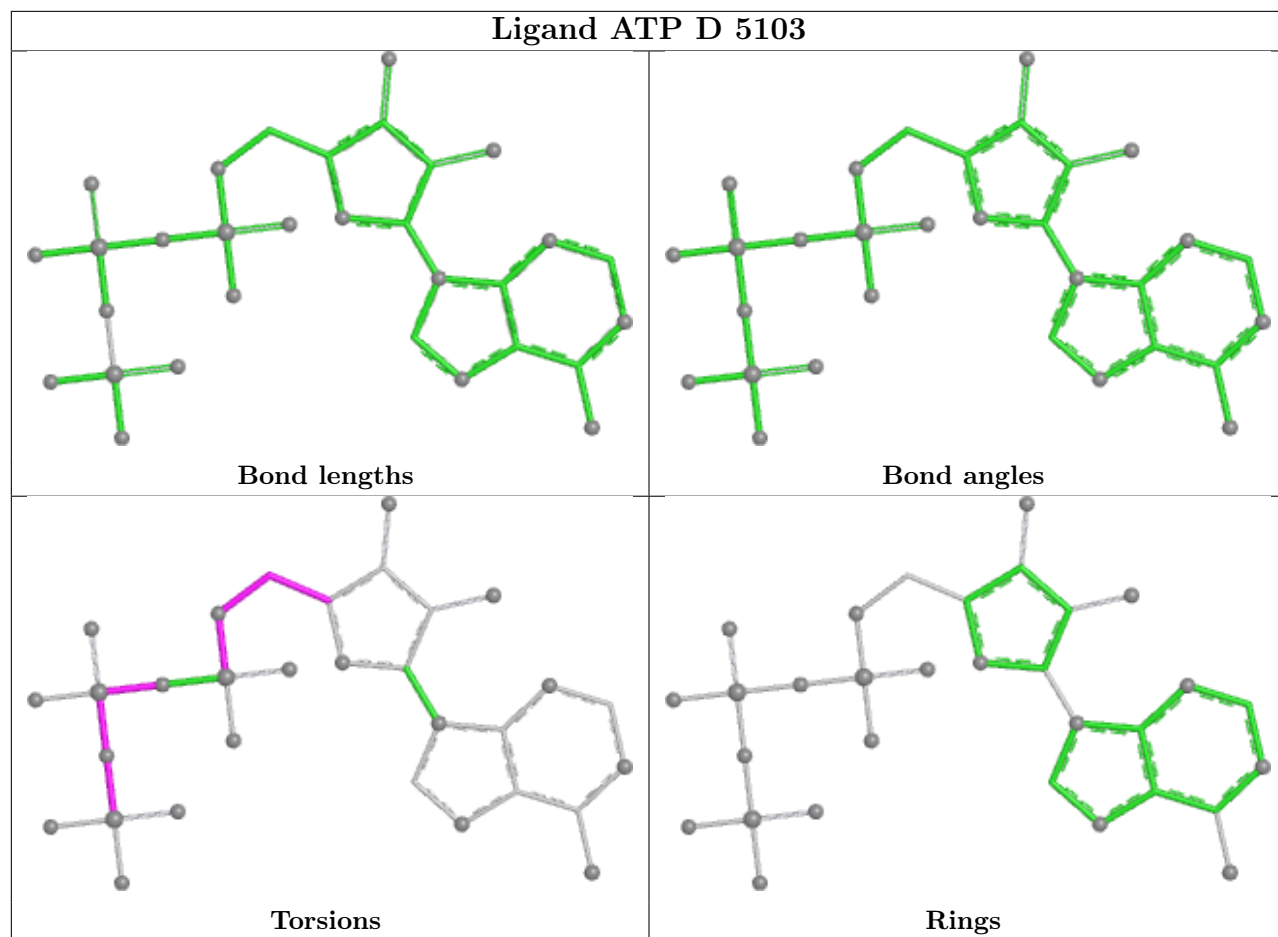
There are no ring outliers.

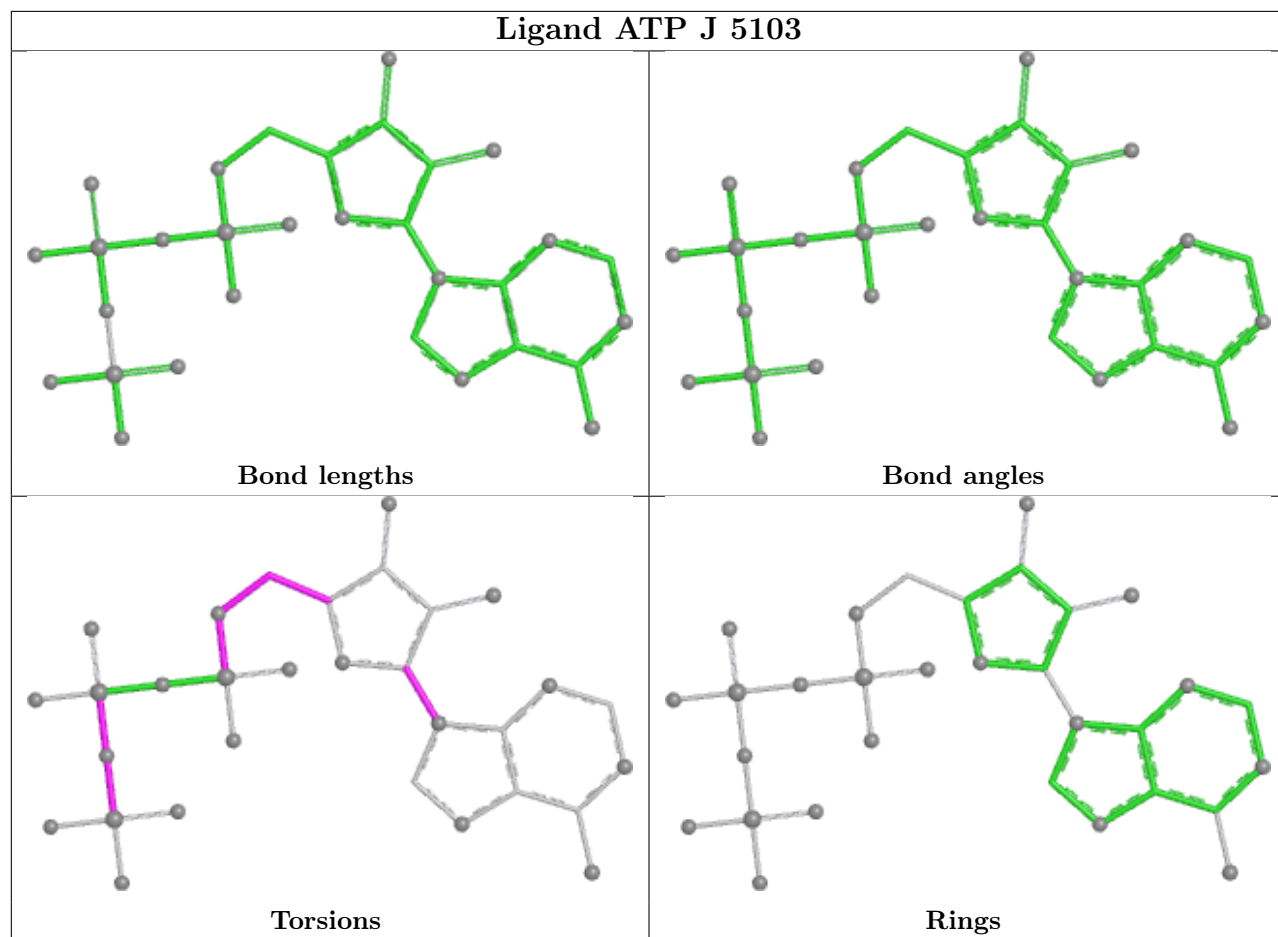
4 monomers are involved in 7 short contacts:

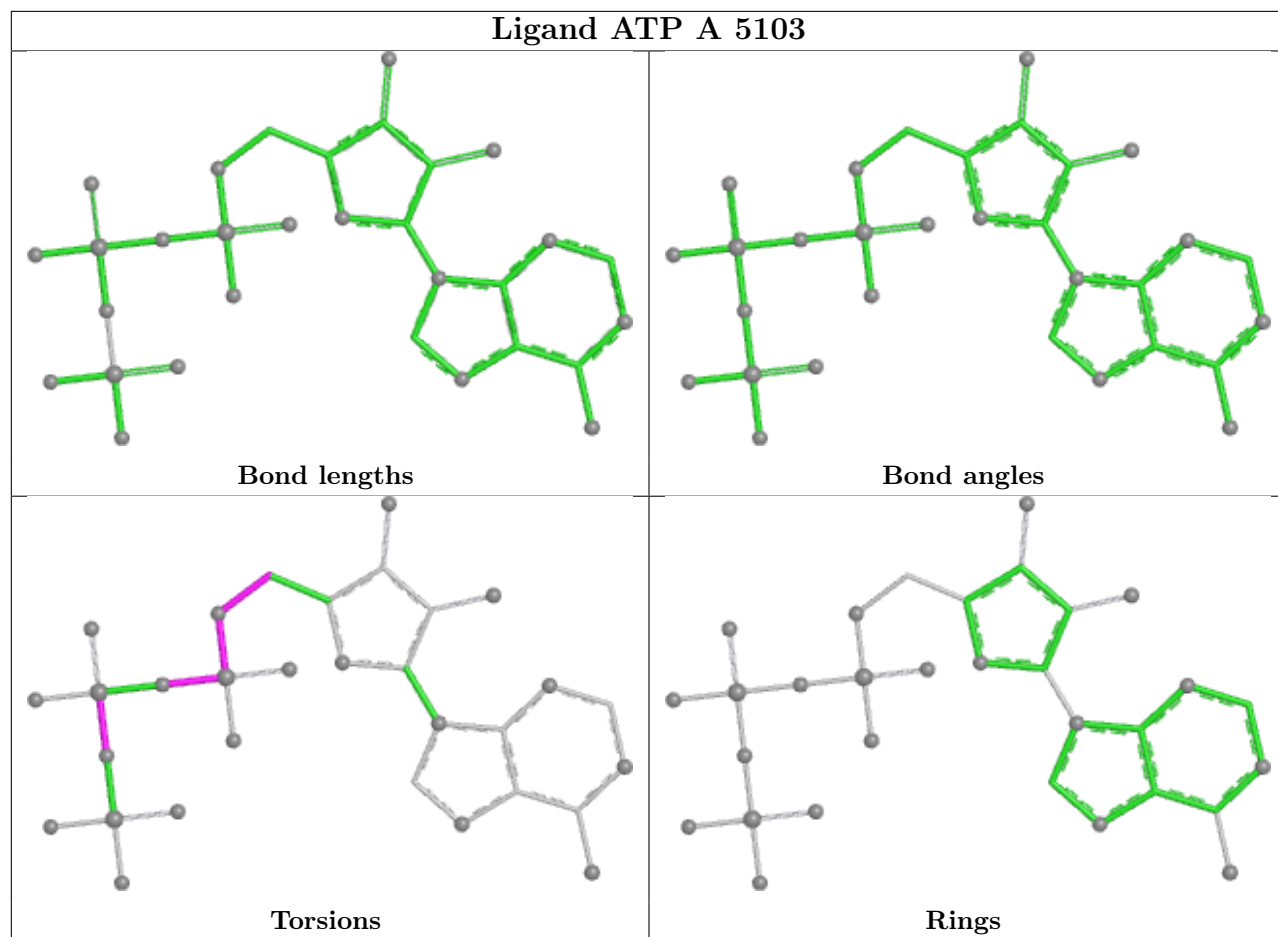
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	5103	ATP	3	0
7	D	5103	ATP	1	0
7	J	5103	ATP	1	0
7	A	5103	ATP	2	0

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.









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.

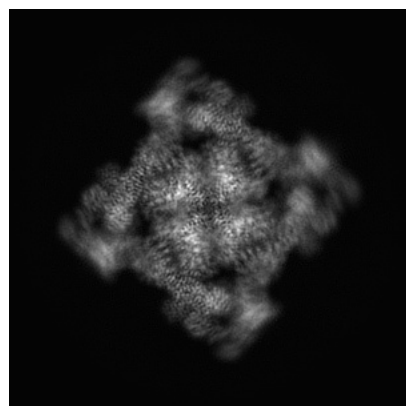
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27721. These allow visual inspection of the internal detail of the map and identification of artifacts.

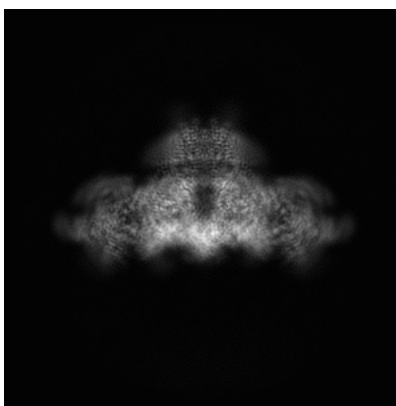
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

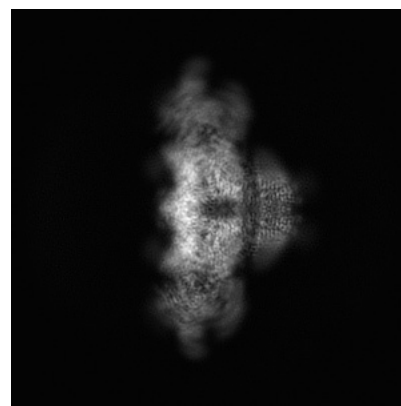
6.1.1 Primary map



X

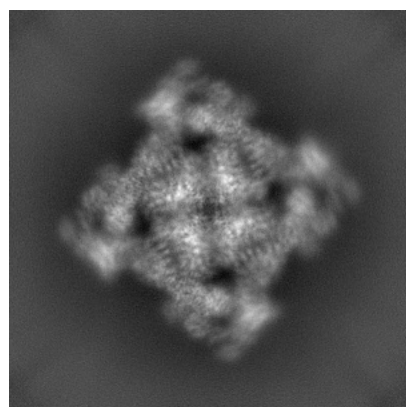


Y

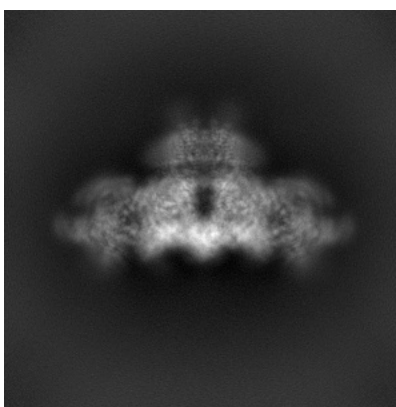


Z

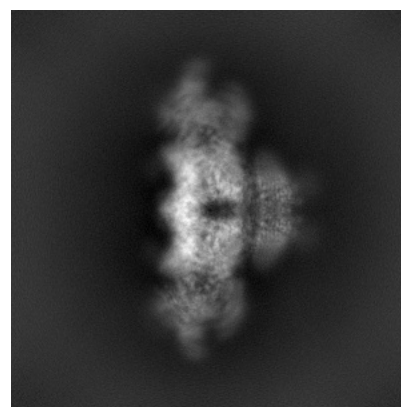
6.1.2 Raw map



X



Y

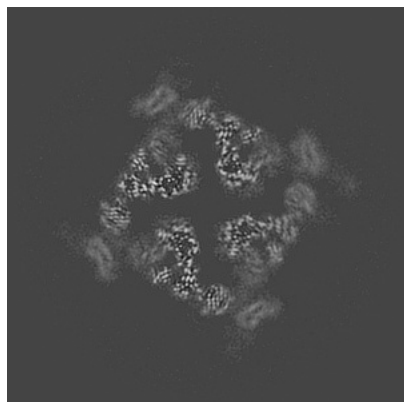


Z

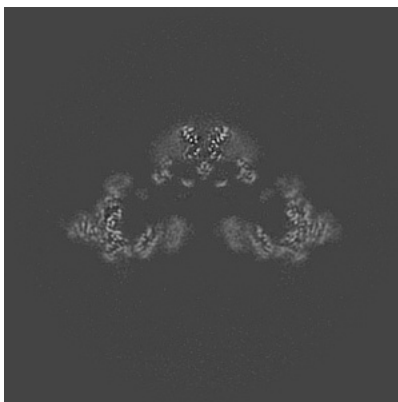
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

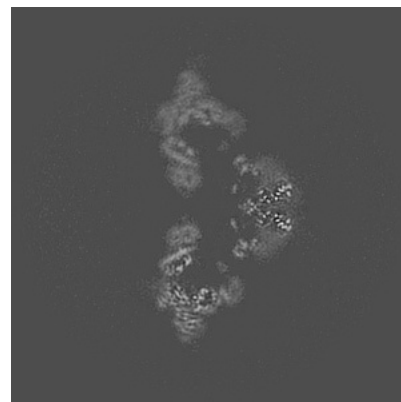
6.2.1 Primary map



X Index: 224

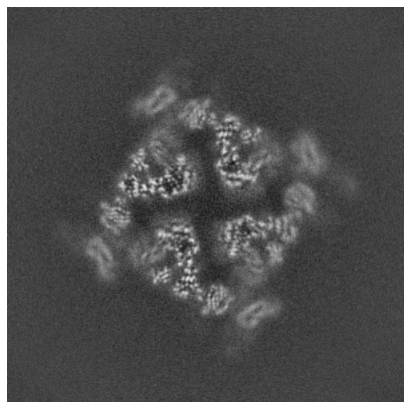


Y Index: 224

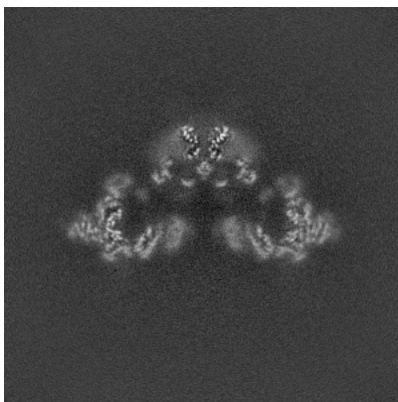


Z Index: 224

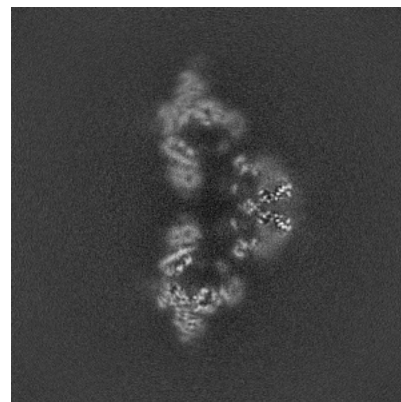
6.2.2 Raw map



X Index: 224



Y Index: 224

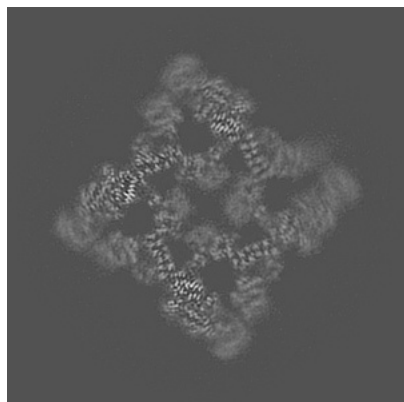


Z Index: 224

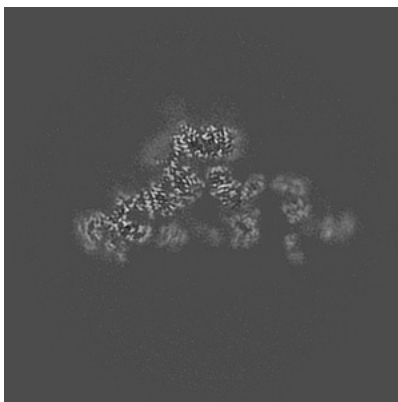
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

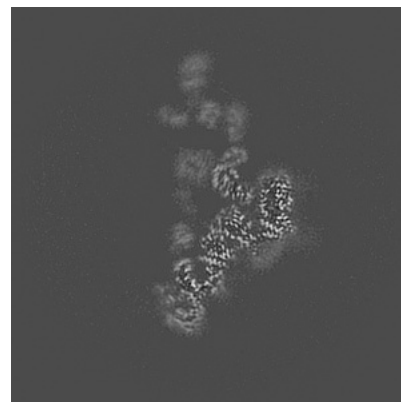
6.3.1 Primary map



X Index: 203

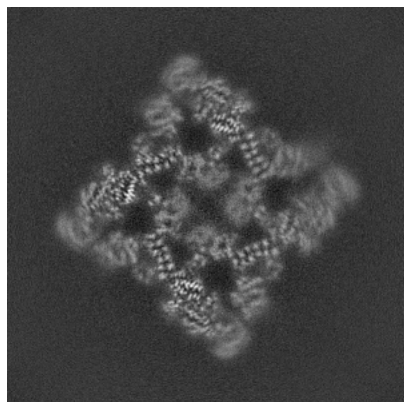


Y Index: 205

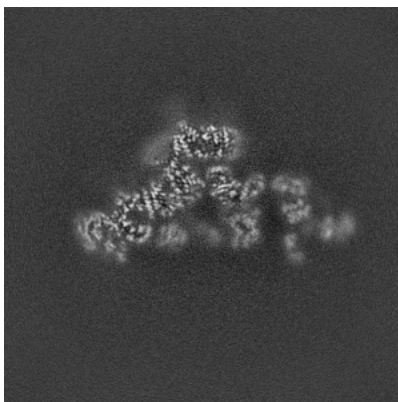


Z Index: 242

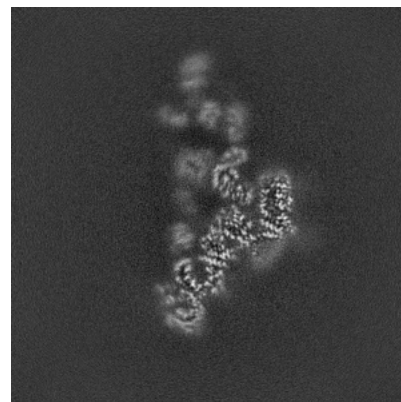
6.3.2 Raw map



X Index: 203



Y Index: 205

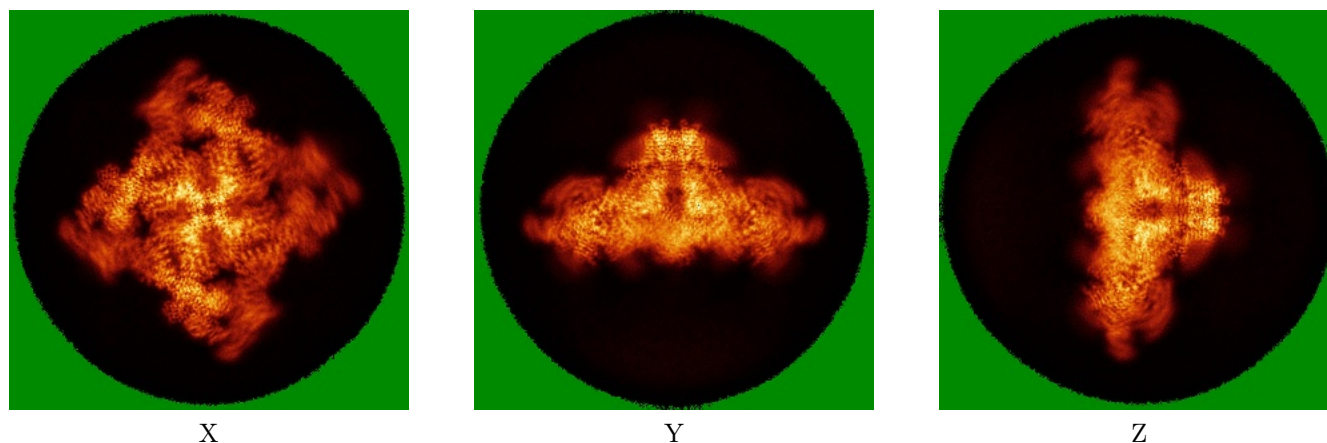


Z Index: 242

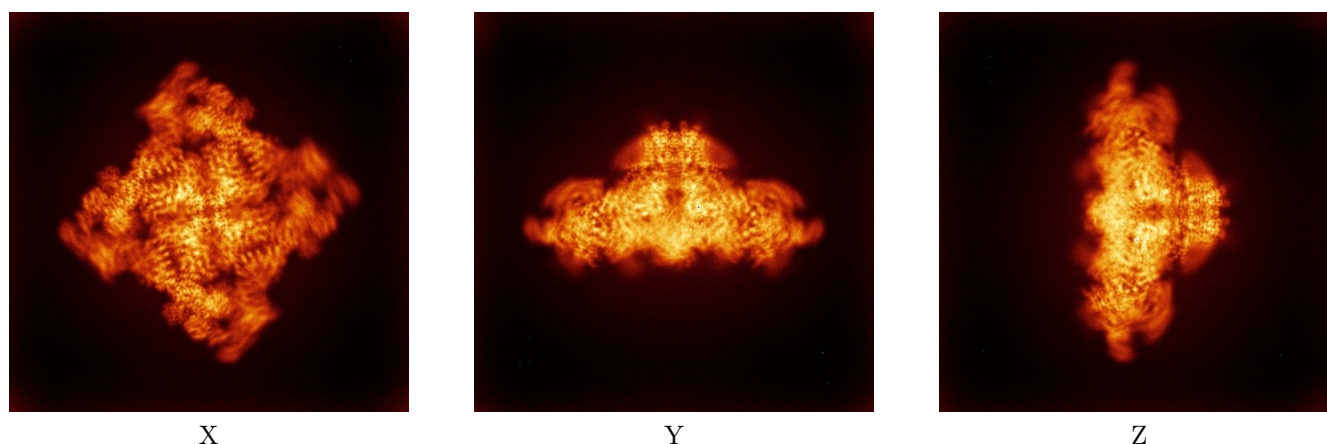
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

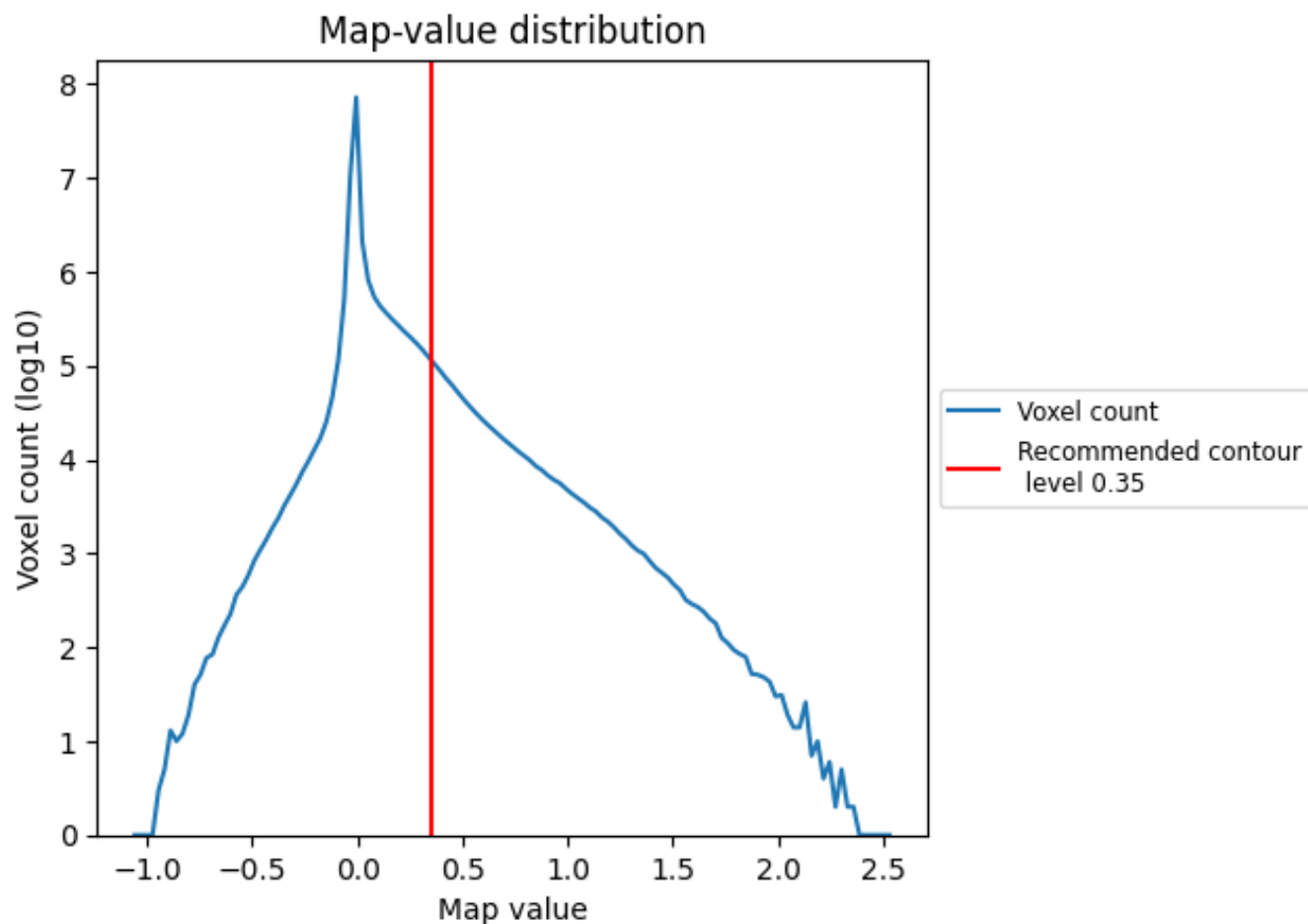
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

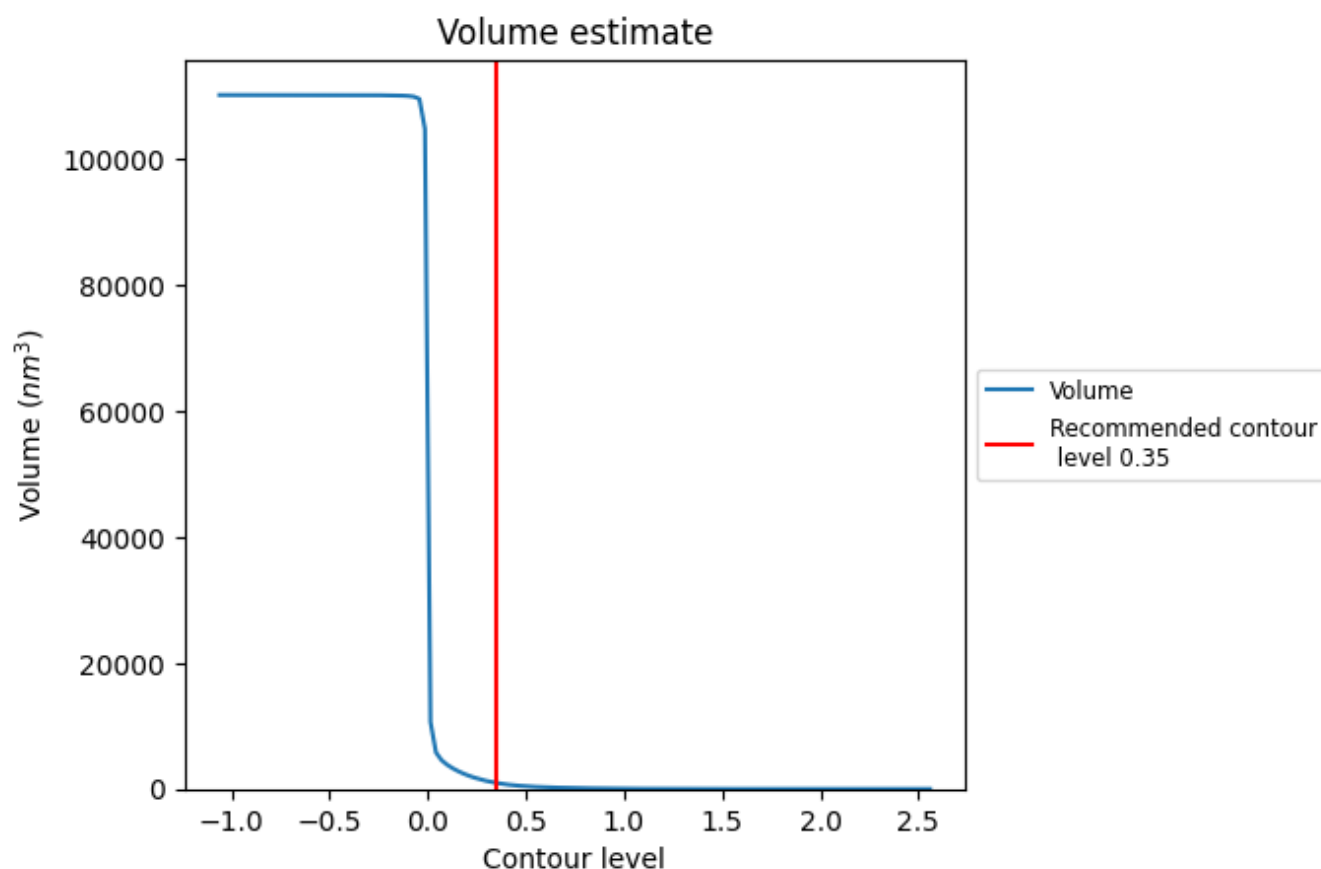
This section contains the results of statistical analysis of the map.

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.

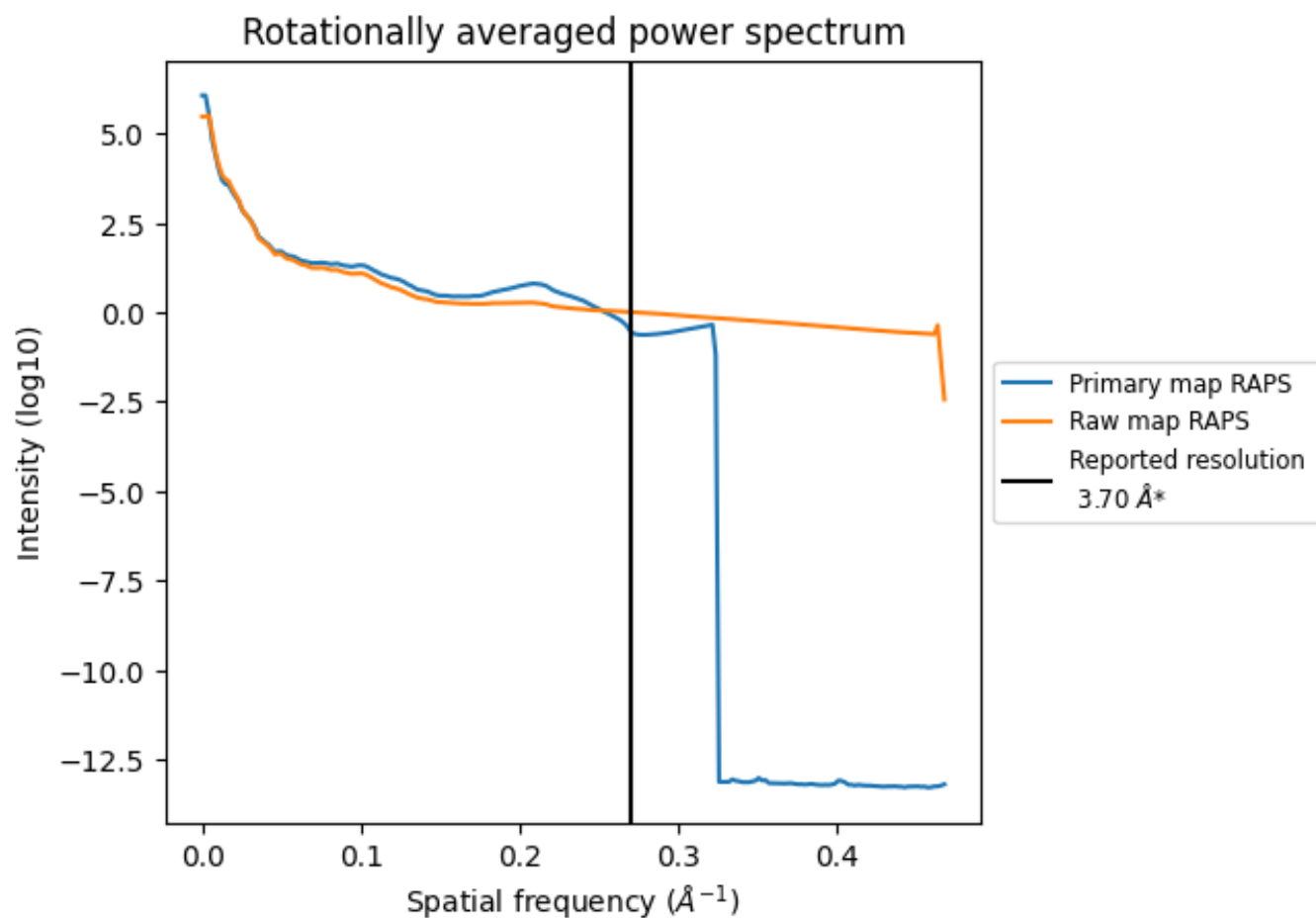
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 957 nm^3 ; this corresponds to an approximate mass of 865 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 ⓘ

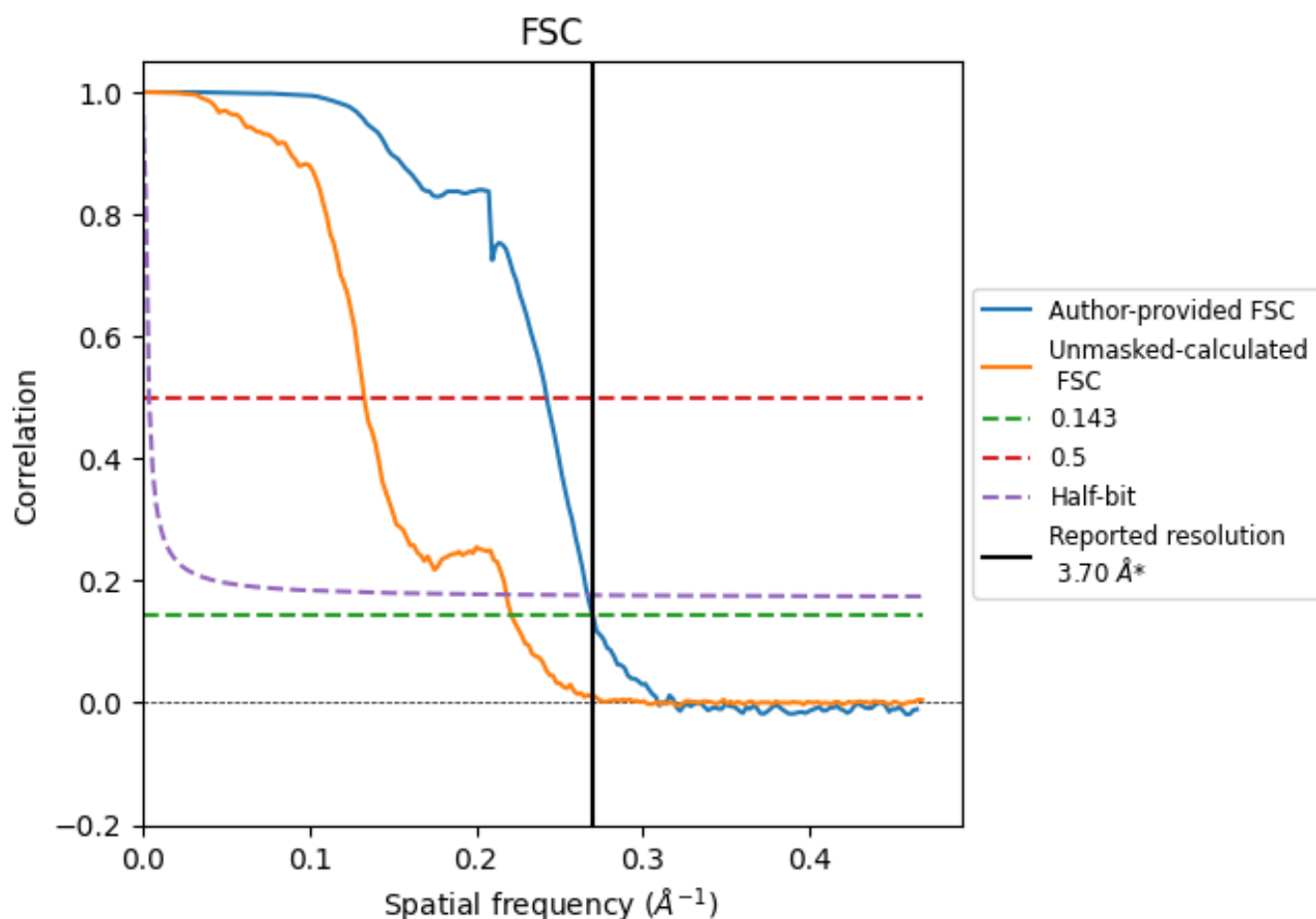


*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.71	4.13	3.75
Unmasked-calculated*	4.52	7.52	4.58

*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 4.52 differs from the reported value 3.7 by more than 10 %

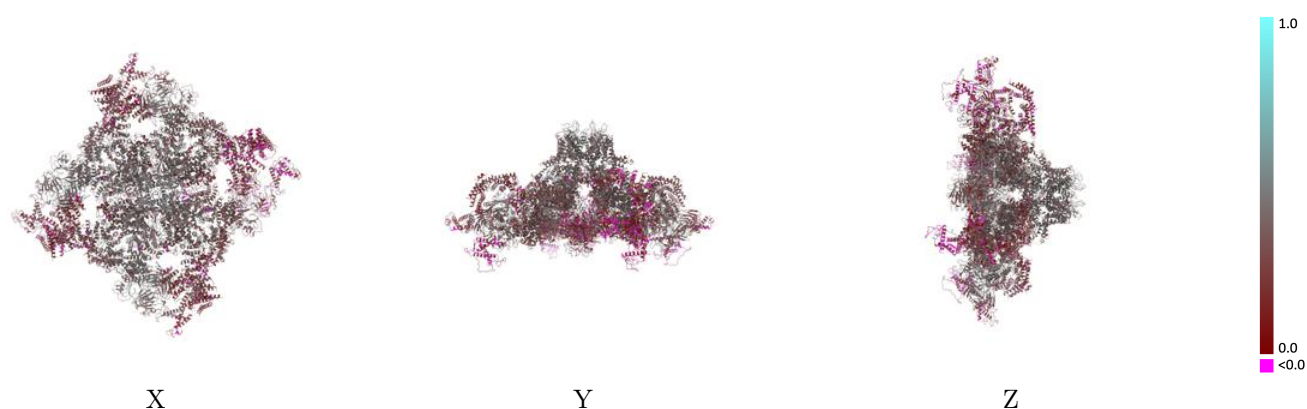
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27721 and PDB model 8DUJ. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

This section was not generated.

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

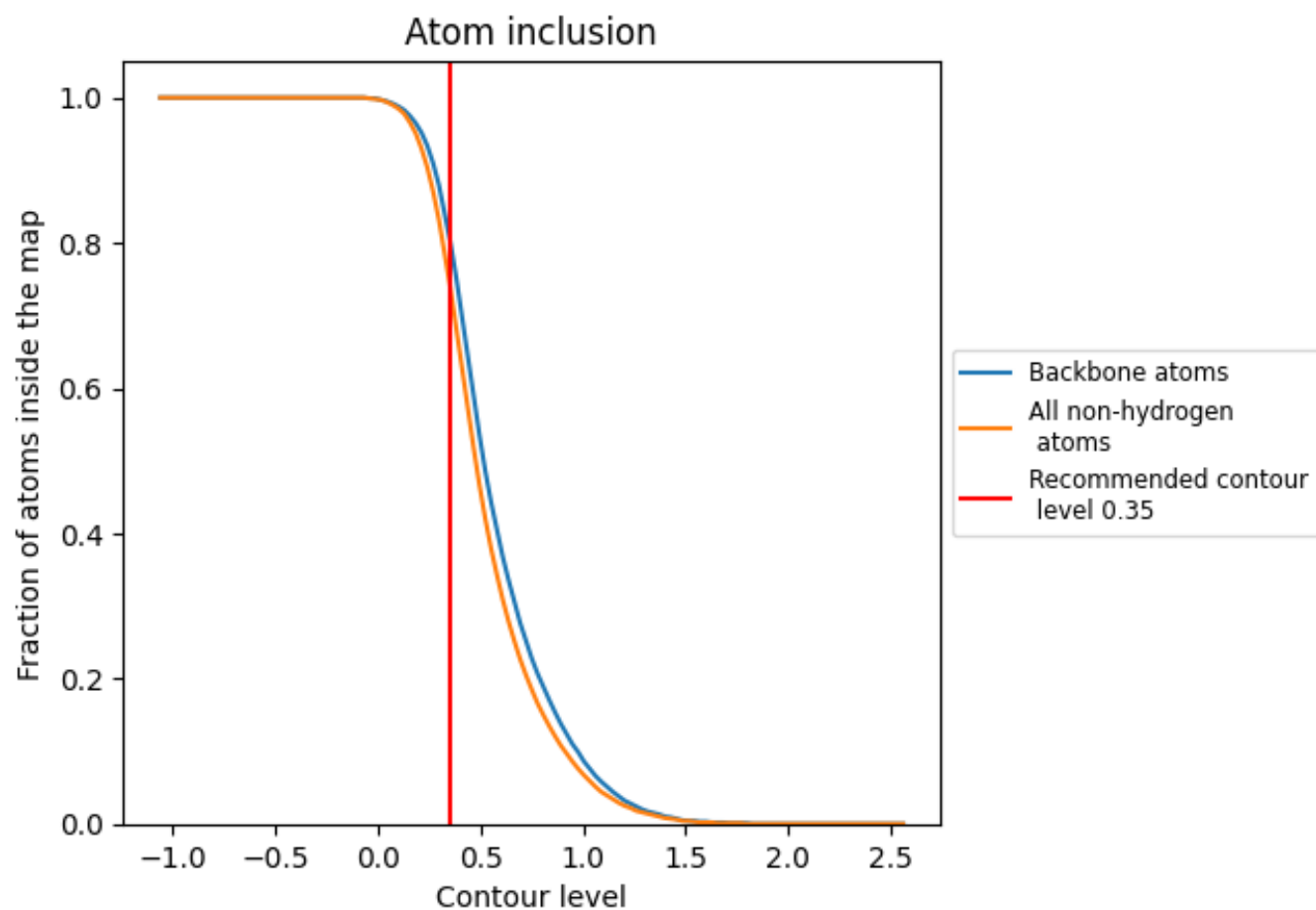


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 81% of all backbone atoms, 74% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7430	 0.3450
A	 0.7390	 0.3470
B	 0.8290	 0.3980
C	 0.1920	 0.2430
D	 0.7080	 0.3050
E	 0.7030	 0.2960
F	 0.1970	 0.2240
G	 0.7760	 0.3660
H	 0.8610	 0.4330
I	 0.3760	 0.2800
J	 0.7910	 0.3640
K	 0.8640	 0.4400
L	 0.2950	 0.2410
M	 0.6070	 0.3960

