



Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 07:05 PM UTC

PDB ID : 9R8O / pdb_00009r8o
EMDB ID : EMD-53834
Title : Primed-state RyR1 in 0.05% POPC micelles, in complex with a nanobody and FKBP
Authors : Li, C.; Efremov, R.G.
Deposited on : 2025-05-16
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

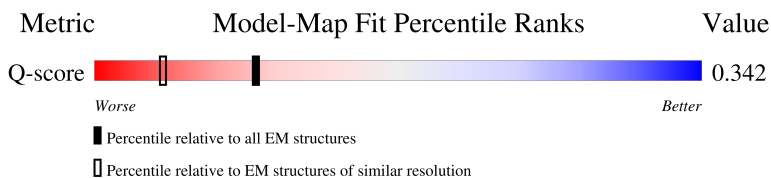
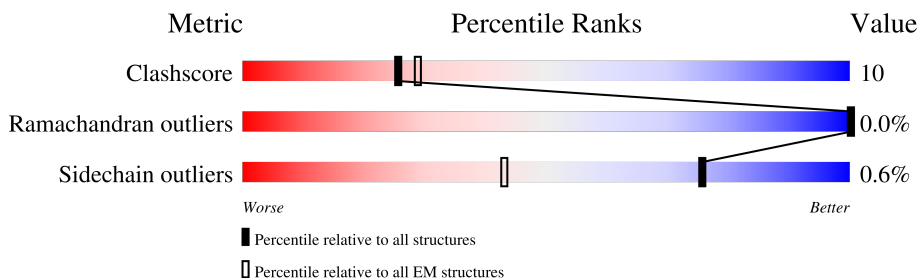
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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

Mol	Chain	Length	Quality of chain
1	A	126	30% 50% 49%
1	D	126	30% 50% 49%
1	G	126	31% 52% 48%
1	K	126	30% 51% 48%

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Mol	Chain	Length	Quality of chain
2	B	107	33%62%37%
2	E	107	33%64%36%
2	H	107	32%63%36%
2	L	107	35%60%39%
3	C	5027	65%21%14%
3	F	5027	65%21%14%
3	I	5027	65%21%14%
3	J	5027	65%21%14%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 145532 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 Nanobody 9657.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	126	Total	C	N	O	S	0	0
			967	597	170	195	5		
1	A	126	Total	C	N	O	S	0	0
			967	597	170	195	5		
1	D	126	Total	C	N	O	S	0	0
			967	597	170	195	5		
1	G	126	Total	C	N	O	S	0	0
			967	597	170	195	5		

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

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

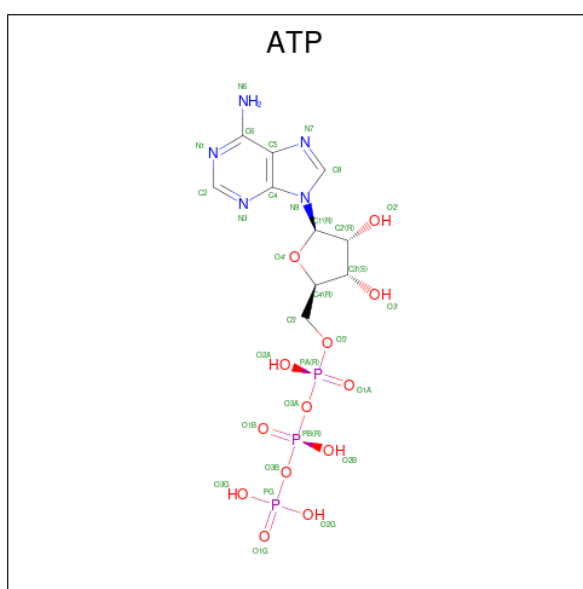
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	100	ASP	GLY	conflict	UNP Q8HYX6
B	100	ASP	GLY	conflict	UNP Q8HYX6
E	100	ASP	GLY	conflict	UNP Q8HYX6
H	100	ASP	GLY	conflict	UNP Q8HYX6

- Molecule 3 is a protein called Ryanodine receptor 1.

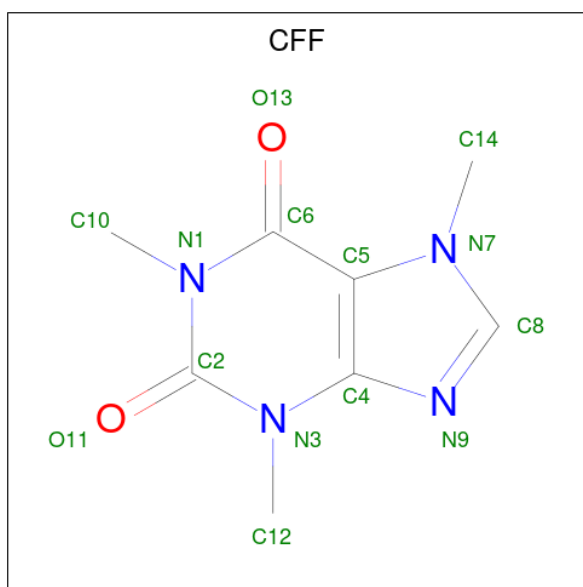
Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	4323	Total	C	N	O	S	0	0
			34214	21785	5897	6304	228		
3	C	4323	Total	C	N	O	S	0	0
			34214	21785	5897	6304	228		
3	F	4323	Total	C	N	O	S	0	0
			34214	21785	5897	6304	228		
3	I	4323	Total	C	N	O	S	0	0
			34214	21785	5897	6304	228		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	J	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	F	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	I	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 5 is CAFFEINE (CCD ID: CFF) (formula: $C_8H_{10}N_4O_2$) (labeled as "Ligand of Interest" by depositor).

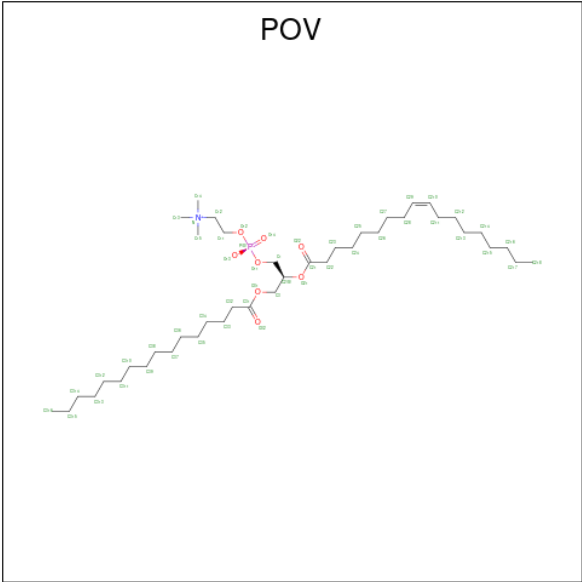


Mol	Chain	Residues	Atoms				AltConf
5	J	1	Total	C	N	O	0
			14	8	4	2	
5	C	1	Total	C	N	O	0
			14	8	4	2	
5	F	1	Total	C	N	O	0
			14	8	4	2	
5	I	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	J	1	Total	Ca	0
			1	1	
6	C	1	Total	Ca	0
			1	1	
6	F	1	Total	Ca	0
			1	1	
6	I	1	Total	Ca	0
			1	1	

- Molecule 7 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
7	J	1	Total	C	N	O	P	0
			35	25	1	8	1	
7	J	1	Total	C	N	O	P	0
			44	34	1	8	1	
7	J	1	Total	C	N	O	P	0
			26	16	1	8	1	
7	J	1	Total	C	N	O	P	0
			24	15	1	7	1	
7	J	1	Total	C	N	O	P	0
			34	24	1	8	1	
7	J	1	Total	C	N	O	P	0
			45	35	1	8	1	
7	J	1	Total	C	N	O	P	0
			32	22	1	8	1	
7	J	1	Total	C	N	O	P	0
			36	26	1	8	1	
7	J	1	Total	C				0
			13	13				
7	C	1	Total	C	N	O	P	0
			36	26	1	8	1	
7	C	1	Total	C				0
			13	13				
7	C	1	Total	C	N	O	P	0
			35	25	1	8	1	
7	C	1	Total	C	N	O	P	0
			44	34	1	8	1	
7	C	1	Total	C	N	O	P	0
			48	38	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
7	C	1	Total	C	N	O	P	0
			26	16	1	8	1	
7	C	1	Total	C	N	O	P	0
			24	15	1	7	1	
7	C	1	Total	C	N	O	P	0
			34	24	1	8	1	
7	C	1	Total	C	N	O	P	0
			48	38	1	8	1	
7	C	1	Total	C	N	O	P	0
			45	35	1	8	1	
7	C	1	Total	C	N	O	P	0
			32	22	1	8	1	
7	F	1	Total	C	N	O	P	0
			36	26	1	8	1	
7	F	1	Total	C				0
			13	13				
7	F	1	Total	C	N	O	P	0
			35	25	1	8	1	
7	F	1	Total	C	N	O	P	0
			44	34	1	8	1	
7	F	1	Total	C	N	O	P	0
			26	16	1	8	1	
7	F	1	Total	C	N	O	P	0
			24	15	1	7	1	
7	F	1	Total	C	N	O	P	0
			34	24	1	8	1	
7	F	1	Total	C	N	O	P	0
			48	38	1	8	1	
7	F	1	Total	C	N	O	P	0
			45	35	1	8	1	
7	F	1	Total	C	N	O	P	0
			32	22	1	8	1	
7	I	1	Total	C	N	O	P	0
			48	38	1	8	1	
7	I	1	Total	C	N	O	P	0
			45	35	1	8	1	
7	I	1	Total	C	N	O	P	0
			32	22	1	8	1	
7	I	1	Total	C	N	O	P	0
			36	26	1	8	1	
7	I	1	Total	C				0
			13	13				

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Mol	Chain	Residues	Atoms					AltConf
7	I	1	Total	C	N	O	P	0
			35	25	1	8	1	
7	I	1	Total	C	N	O	P	0
			44	34	1	8	1	
7	I	1	Total	C	N	O	P	0
			26	16	1	8	1	
7	I	1	Total	C	N	O	P	0
			24	15	1	7	1	
7	I	1	Total	C	N	O	P	0
			34	24	1	8	1	

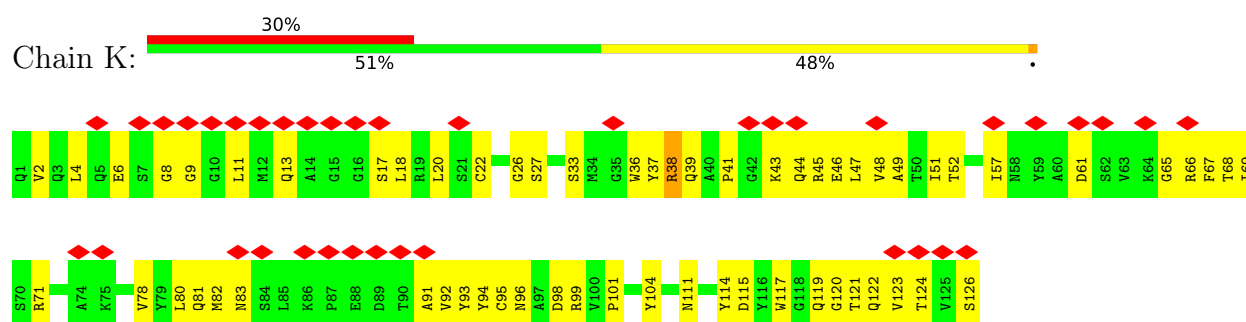
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
8	J	1	Total	Zn	0
			1	1	
8	C	1	Total	Zn	0
			1	1	
8	F	1	Total	Zn	0
			1	1	
8	I	1	Total	Zn	0
			1	1	

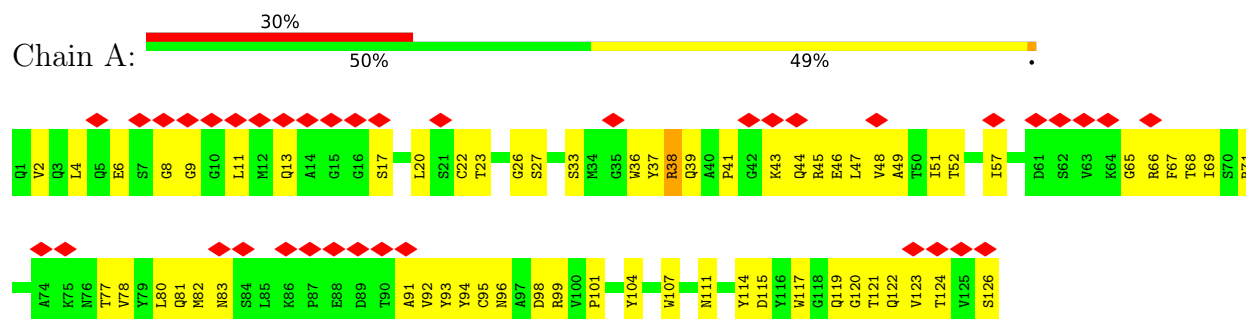
3 Residue-property plots [i](#)

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.

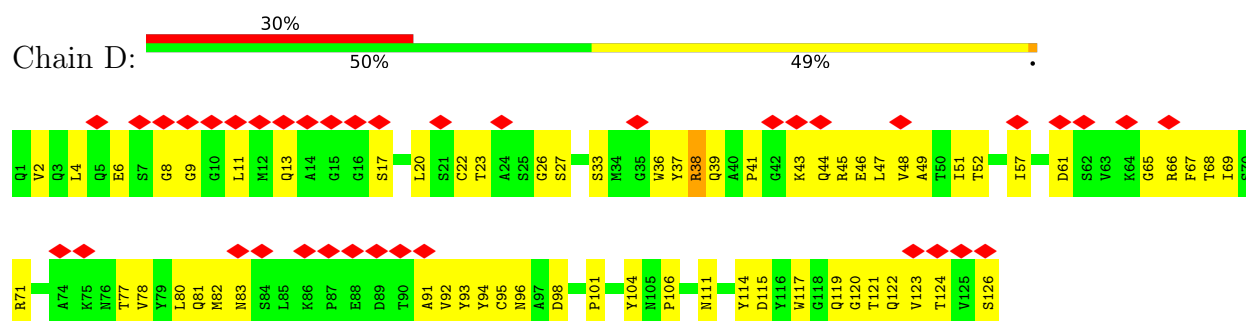
• Molecule 1: Nanobody 9657



• Molecule 1: Nanobody 9657

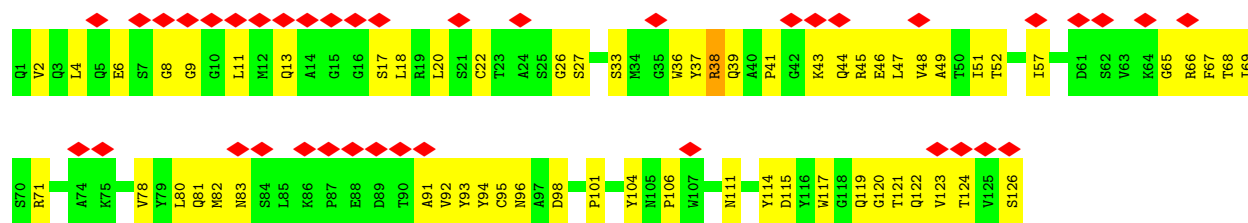


• Molecule 1: Nanobody 9657

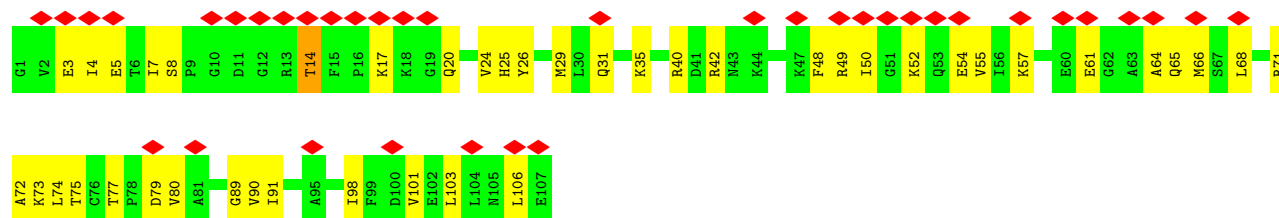


• Molecule 1: Nanobody 9657

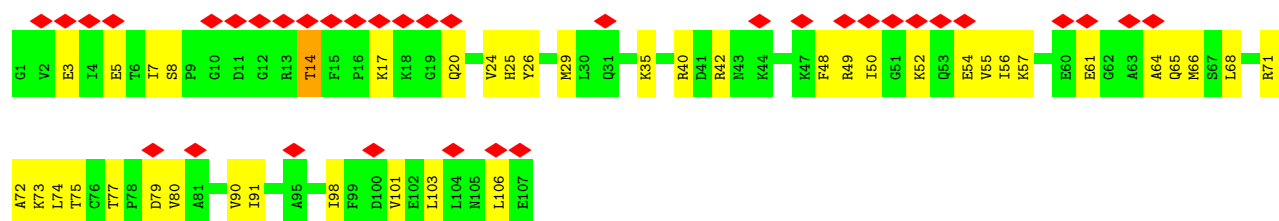




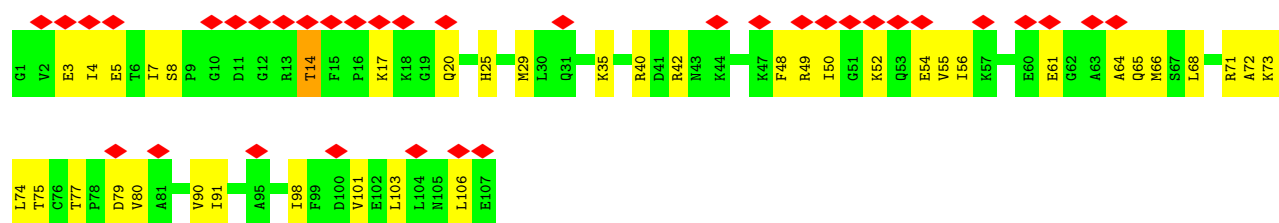
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



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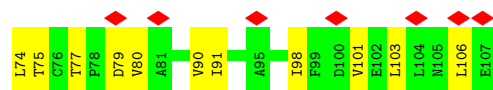


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



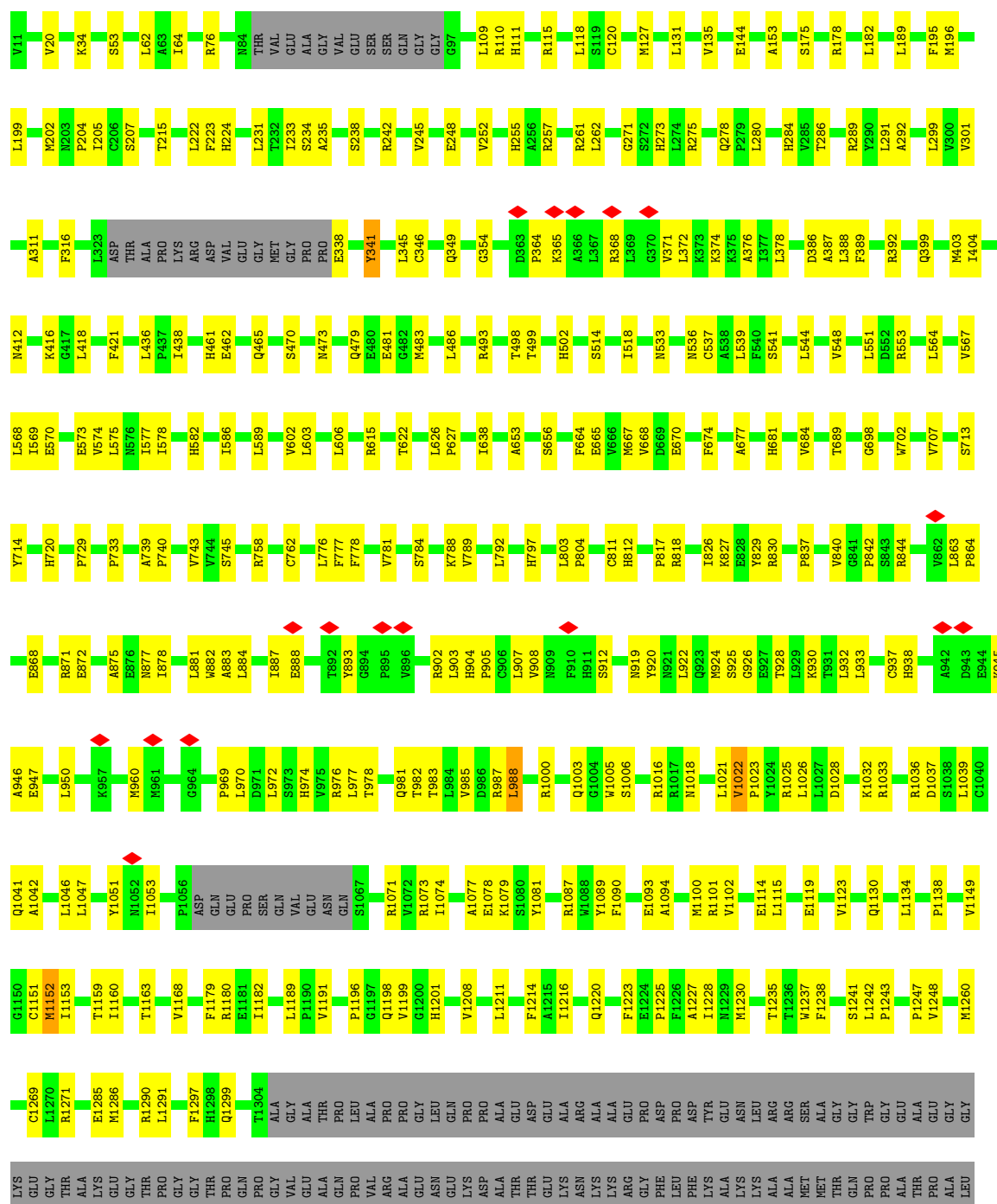
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B





• Molecule 3: Ryanodine receptor 1

Chain J: 65% 21% 14%

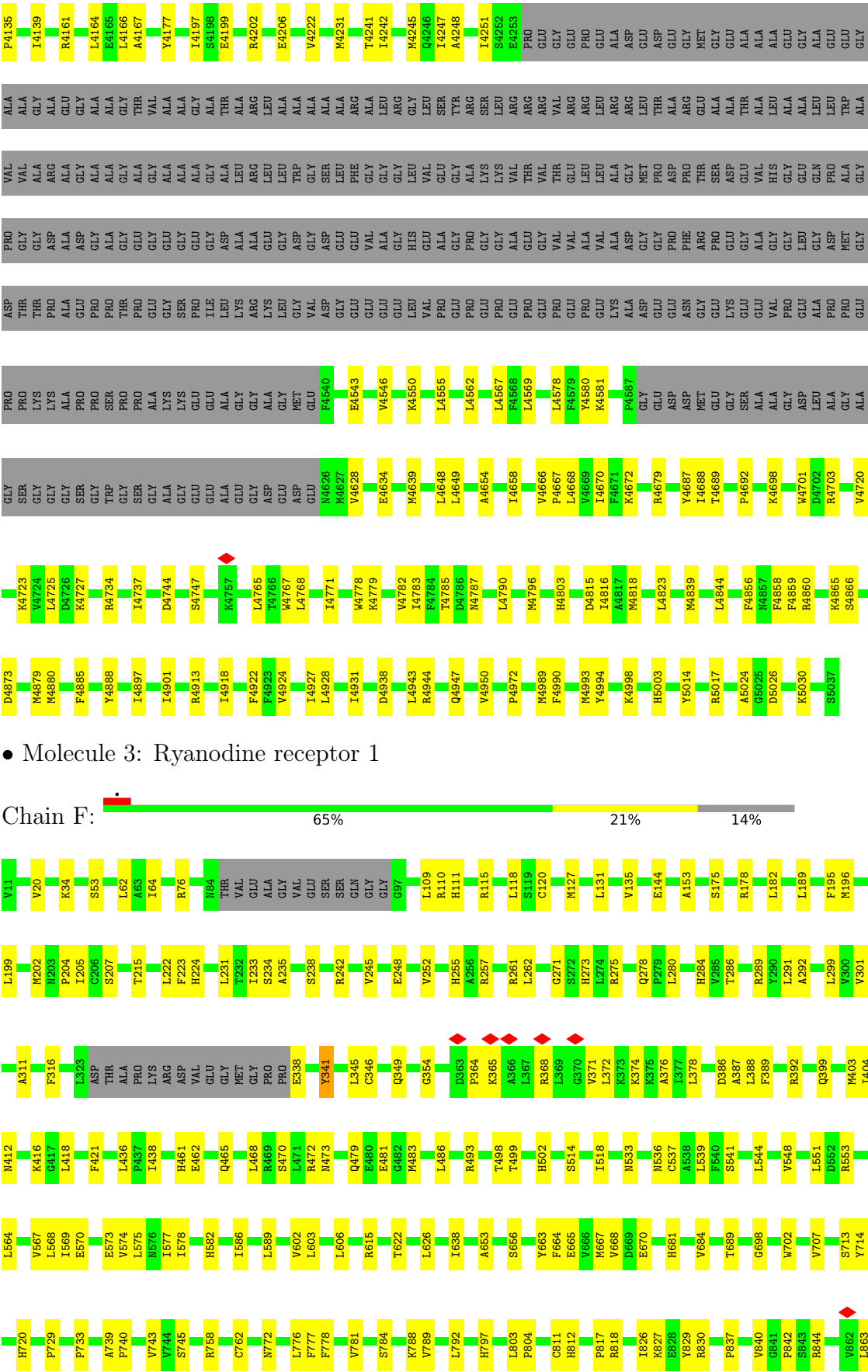


ALA	GLN	THR	THR	ASP	PRO	ARG	GLU	GLY	Y2855	Y2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	Q2864	V2865	T2866	L2867	S2868	P2869	E2870	L2871	Q2872	A2873	M2874	A2875	Q2876	Q2877	L2878	A2879	E2880	H2883	N2884	T2885	W2886	K2891	Q2892	E2893	L2894	E2895	A2896	L2897	G2898	G2899	Q2900	T2901	H2902	P2903	L2904	V2905	V2906	P2907	Y2908	D2909																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
K2786	T2787	H2788	P2789	M2790	L2791	R2792	P2793	Y2794	K2795	T2796	P2797	S2798	E2799	K2800	D2801	E2802	E2803	I2804	Y2805	W2806	W2807	P2808	I2809	K2810	E2811	S2812	L2813	K2814	A2815	N2816	L2817	A2818	N2819	E2820	V2821	T2822	E2823	E2824	K2825	A2826	E2827	E2828	E2829	G2830	GLU	GLU	ARG	THR	GLU	LYS	LYS	THR	ARG	LYS	ILE	GLN	THR																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
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Q2525	F2526	L2527	R2531	A2534	S2535	L2536	M2546	A2547	L2559	P2560	L2561	T2562	K2563	K2564	C2565	E2573	H2574	A2575	I2577	M2578	V2579	D2580	S2581	M2582	L2583	R2588	T2596	Q2599	R2600	I2603	E2604	D2605	C2606	L2607	M2608	A2609	L2610	R2615	P2616	S2617	M2618	L2619	L2622	L2623																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
PHE	GLY	GLU	PRO	PRO	GLU	GLU	H2414	L2418	G2419	H2420	A2421	I2422	M2423	L2429	I2430	D2431	T2453	R2454	R2458	S2459	L2460	D2465	L2466	V2467	G2468	I2469	S2470	L2472	P2473	D2482	G2483	K2489	M2490	S2491	A2492	S2501	Y2510	G2511	I2512	F2513	N2514	F2517	L2518	V2521	L2522																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
R2248	S2249	M2250	L2257	L2265	Q2268	G2269	S2270	T2271	P2272	V2275	V2299	C2310	N2324	P2325	N2329	C2332	N2349	R2355	R2359	K2360	P2361	R2369	G2372	L2380	E2381	I2384	D2393	G2394	P2395	GLY	VAL	ARG	ARG	ASP	ARG	ARG	ARG	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GL





V9989	L3817	L3654	L3542	L3424	V3284	E3184	P3085	V2966	T2901	LYS	S2776	L2703
V9995	K3821	E3655	E3547	N3428	R3287	L3186	V3088	M2967	H2902	LYS	Y2777	L2706
F9996	A3834	S3656	V3549	E3432	R3295	R3187	V3089	D2968	P2903	LYS	G2778	L2710
M4000	L3842	V3661	R3550	F3442	L3296	R3196	A3099	Q2971	L2905	ARG	E2779	P2711
K4014	L3854	H3667	E3551	F3459	P3297	L3197	S3100	F2972	V2906	LYS	N2780	P2712
L4017	E3854	S3668	F3552	V3459	A3298	A3198	E3101	F2973	P2907	ILE	N2781	
L4018	M3858	F3669	L3553	I3464	C3304	A3200	D3102	L2974	T2909	GLN	D2782	K2722
L4019	V3859	R3672	Q3560	I3464	C3304	M3201	E3104	L2977	D2909	THR	E2783	ALA
Q4020	N3860	Q3683	D3585	M3467	H3311	P3202	K3105	V2980	T2911	ALA	E2784	GLU
D4022	E3861	E3684	E3590	L3470	L3312	V3203	V3107	V2981	T2912	LYS	E2785	LYS
M4023	D3862	E3691	K3591	L3315	L3316	L3210	R3111	R2985	A2913	THR	K2786	THR
M4026	G3863	E3691	V3593	L3316	L3320	Y3213	GLY	V2986	K2914	PRO	T2787	ALA
M4034	T3864	E3691	R3594	L3316	L3320	N3214	LYS	E2987	E2915	ARG	H2788	VAL
G4038	V3865	E3691	R3594	L3316	L3320	S3217	GLN	E2987	E2915	ARG	P2789	ASP
E4056	I3866	E3691	R3594	L3316	L3320	Y3219	ARG	E2987	E2915	ARG	M2790	ALA
M4057	N3867	E3691	R3594	L3316	L3320	K3222	THR	E2987	E2915	ARG	L2791	GLY
I4058	M3875	E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	R2792	N2734
L4058	F3885	E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	P2793	F2735
L4058	Q3889	E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	Y2794	D2736
L4058	L3890	E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	K2795	P2737
V4072	H3895	E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	P2739	R2738
V4081	Q3900	E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	F2797	V2740
L4087	I3916	E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	S2798	E2741
L4088	T3919	E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	E2799	T2742
S4089	S3929	E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	K2800	L2743
K4090	I3930	E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	D2801	N2744
M4097	Y3936	E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	K2802	V2745
Q4100	Q3945	E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	E2803	I2746
T4104	F3951	E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	I2804	I2747
G4105	M3955	E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	Y2805	P2748
I4108	Q3960	E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	E2806	E2749
Q4109	L3965	E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	W2807	K2750
F4110	T3966	E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	P2808	L2751
L4112	E3967	E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	I2809	D2752
D4118	Y3968	E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	K2810	S2753
M4122	I3969	E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	F2754	F2754
A4129	Q3970	E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	E2811	K2755
		E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	S2812	I2755
		E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	L2813	K2756
		E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	K2814	K2757
		E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	A2815	F2758
		E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	M2816	A2759
		E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	I2817	E2760
		E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	A2818	E2764
		E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	W2819	K2765
		E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	E2820	W2766
		E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	W2821	A2767
		E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	I2823	F2768
		E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	E2824	D2769
		E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	K2825	K2770
		E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	I2771	I2771
		E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	R2827	Q2772
		E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	E2828	N2773
		E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	G2829	N2774
		E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	E2830	
		E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	GLU	
		E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	GLU	
		E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	THR	
		E3691	R3594	L3316	L3320	E3226	GLN	E2987	E2915	ARG	GLU	



R2104	R2234	Q2036	R2117	M2120	L2123	Q2127	Y2128	L2131	L2138	Y2142	P2146	L2156	E2157	C2158	I2162	L2166	E2175	M2178	I2179	I2182	V2190	Q2193	H2194	N2195	L2197	M2198	M2203	E2205	T2206	M2211	L2215	M2228	V2229	T2230	S2231	G2232	C2233												
GLU	GLY	GLU	LYS	ASP	L1922	G1925	L1926	M1929	F1930	L1931	S1934	V1935	Q1938	M1939	L1943	E1944	L1958	A1959	A1960	R1964	Y1965	Q1970	R1974	L1979	L1980	M1981	R1982	E1990	P2001	P2002	Q2005	L2010	H2011	F2012	K2013	C2021	E2025	R2028	M2101	V2102	V2103								
V1845	V1846	T1853	F1854	G1855	L1856	E1857	D1858	L1859	K1860	Q1861	L1862	M1865	V1870	E1874	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	PRO									
GLU	GLY	LYS	GLU	ASP	L1922	G1925	L1926	M1929	F1930	L1931	S1934	V1935	Q1938	M1939	L1943	E1944	L1958	A1959	A1960	R1964	Y1965	Q1970	R1974	L1979	L1980	M1981	R1982	E1990	P2001	P2002	Q2005	L2010	H2011	F2012	K2013	C2021	E2025	R2028	M2101	V2102	V2103								
V1845	V1846	T1853	F1854	G1855	L1856	E1857	D1858	L1859	K1860	Q1861	L1862	M1865	V1870	E1874	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	PRO									
L1885	V1689	D1690	Q1693	L1694	L1714	L1715	I1716	S1717	I1718	E1721	M1730	I1735	V1736	F1737	L1738	E1741	I1745	V1746	L1747	R1758	P1773	F1782	V1783	A1784	A1785	L1786	P1787	ALA	ALA	GLY	VAL	ALA	E1793	I1802	P1803	L1804	R1808	L1815	V1819	E1835	V1839	P1840							
L1526	M1527	T1530	E1535	F1540	L1548	F1549	P1550	A1551	V1552	F1553	V1554	L1555	V1561	I1562	Q1563	F1564	L1595	Q1598	M1599	L1600	V1603	L1613	T1617	R1618	R1619	V1626	A1627	V1628	L1634	T1635	M1636	H1637	A1638	L1639	E1644	C1647	M1648	E1655	C1674	R1680	V1681								
ARG	LEU	HIS	ASP	VAL	VAL	PRO	ALA	ASP	M1420	Y1435	S1436	V1437	E1444	C1447	V1448	W1449	Q1459	M1462	H1483	F1484	R1470	T1475	M1476	V1483	H1484	S1485	S1486	N1491	M1494	G1497	G1498	D1499	F1500	V1501	Q1505	Q1506	G1507	I1509	S1510	H1511	L1514	T1524	G1525						
GLU	GLY	THR	ALA	GLU	GLY	THR	PRO	THR	PRO	GLN	PRO	GLY	VAL	GLU	ALA	THR	PRO	LEU	ALA	PRO	GLY	GLU	ASN	GLU	GLN	LYS	LYS	ALA	ARG	GLY	PHE	PHE	LYS	ALA	LYS	ALA	MET	MET	THR	PRO	ALA	PRO	GLY	ALA	GLY	LEU	PRO		
C1269	L1270	R1271	E1285	M1286	L1287	F1288	L1289	R1290	L1291	F1297	T1304	ALA	GLY	ALA	THR	PRO	LEU	ALA	ALA	ALA	ALA	THR	ASP	GLU	GLN	LYS	LYS	ALA	ALA	ARG	ASP	PRO	ASP	TYR	GLU	ASN	LEU	ARG	ARG	SER	ALA	GLY	TRP	GLY	ALA	GLU	ALA	GLY	LYS
V1149	G1150	C1151	M1152	I1153	T1159	I1160	T1163	V1168	F1179	R1180	E1181	I1182	L1189	P1190	V1191	P1196	Q1198	V1199	V1208	L1211	F1214	A1215	I1216	Q1220	F1223	E1224	P1225	F1226	A1227	I1228	N1229	M1230	T1235	T1236	W1237	F1238	S1241	L1242	P1243	P1247	V1248	M1260							
Q1040	Q1041	A1042	L1046	L1047	Y1051	N1052	I1053	P1056	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	ASN	GLN	S1067	R1071	V1072	R1073	I1074	A1077	E1078	K1079	S1080	Y1081	R1087	W1088	Y1089	F1090	A1094	M1100	R1101	V1102	E1114	L1115	E1119	V1123	Q1130	R1131	L1134	P1138					
P864	Q1041	E947	L950	P956	K957	M960	M961	G964	P969	L970	D971	L972	S973	H974	Y975	R976	L977	T978	Q981	T982	L984	Y985	P986	R987	L988	R1000	Q1003	G1004	W1005	S1006	R1016	R1017	N1018	L1021	V1022	P1023	Y1024	R1025	L1026	L1027	D1028	K1032	R1033	R1036	D1037	S1038	L1039		





Frequency	Percentage
Daily	65%
Weekly	21%
Monthly	14%









4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39983	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.014	Depositor
Minimum map value	-0.135	Depositor
Average map value	0.066	Depositor
Map value standard deviation	0.134	Depositor
Recommended contour level	0.4	Depositor
Map size ($\text{\AA}$)	479.136, 479.136, 479.136	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.426, 1.426, 1.426	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CA, CFF, POV, 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	A	0.26	0/987	0.66	1/1340 (0.1%)
1	D	0.26	0/987	0.66	1/1340 (0.1%)
1	G	0.26	0/987	0.66	1/1340 (0.1%)
1	K	0.26	0/987	0.66	1/1340 (0.1%)
2	B	0.22	0/834	0.62	0/1123
2	E	0.22	0/834	0.62	0/1123
2	H	0.22	0/834	0.62	0/1123
2	L	0.22	0/834	0.62	0/1123
3	C	0.15	0/34990	0.39	1/47426 (0.0%)
3	F	0.15	0/34990	0.39	1/47426 (0.0%)
3	I	0.15	0/34990	0.39	1/47426 (0.0%)
3	J	0.15	0/34990	0.39	1/47426 (0.0%)
All	All	0.16	0/147244	0.41	8/199556 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
1	G	0	1
1	K	0	1
All	All	0	4

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	48	VAL	N-CA-C	-5.94	103.50	110.21
1	D	48	VAL	N-CA-C	-5.92	103.52	110.21
1	A	48	VAL	N-CA-C	-5.90	103.54	110.21
1	K	48	VAL	N-CA-C	-5.89	103.55	110.21
3	J	4122	MET	CB-CG-SD	5.57	129.41	112.70
3	F	4122	MET	CB-CG-SD	5.57	129.41	112.70
3	C	4122	MET	CB-CG-SD	5.56	129.39	112.70
3	I	4122	MET	CB-CG-SD	5.56	129.37	112.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	43	LYS	Peptide
1	D	43	LYS	Peptide
1	G	43	LYS	Peptide
1	K	43	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	967	0	916	41	0
1	D	967	0	916	40	0
1	G	967	0	916	41	0
1	K	967	0	916	43	0
2	B	818	0	824	25	0
2	E	818	0	824	24	0
2	H	818	0	824	25	0
2	L	818	0	824	29	0
3	C	34214	0	33622	691	0
3	F	34214	0	33622	683	0
3	I	34214	0	33622	680	0
3	J	34214	0	33622	687	0
4	C	31	0	12	0	0
4	F	31	0	12	0	0
4	I	31	0	12	0	0
4	J	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	14	0	10	0	0
5	F	14	0	10	0	0
5	I	14	0	10	0	0
5	J	14	0	10	0	0
6	C	1	0	0	0	0
6	F	1	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
7	C	385	0	508	24	0
7	F	337	0	437	22	0
7	I	337	0	437	21	0
7	J	289	0	366	18	0
8	C	1	0	0	0	0
8	F	1	0	0	0	0
8	I	1	0	0	0	0
8	J	1	0	0	0	0
All	All	145532	0	143284	2972	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 10.

All (2972) 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)
3:F:2759:ALA:HB1	3:F:2806:ARG:HB2	1.57	0.86
3:J:2759:ALA:HB1	3:J:2806:ARG:HB2	1.57	0.85
3:I:2759:ALA:HB1	3:I:2806:ARG:HB2	1.57	0.84
3:C:2759:ALA:HB1	3:C:2806:ARG:HB2	1.57	0.84
3:F:3036:LYS:HD3	3:F:3076:ASP:HB3	1.62	0.82
3:C:4839:MET:HE1	3:F:4823:LEU:HG	1.62	0.82
3:J:4823:LEU:HG	3:I:4839:MET:HE1	1.62	0.81
3:J:4839:MET:HE1	3:C:4823:LEU:HG	1.62	0.81
3:F:4839:MET:HE1	3:I:4823:LEU:HG	1.62	0.81
3:I:1153:ILE:HG22	3:I:1160:ILE:HG12	1.63	0.81
3:I:3036:LYS:HD3	3:I:3076:ASP:HB3	1.62	0.80
3:C:3036:LYS:HD3	3:C:3076:ASP:HB3	1.62	0.79
3:J:1153:ILE:HG22	3:J:1160:ILE:HG12	1.63	0.79
3:J:3036:LYS:HD3	3:J:3076:ASP:HB3	1.62	0.79
3:F:1153:ILE:HG22	3:F:1160:ILE:HG12	1.63	0.79
3:C:1153:ILE:HG22	3:C:1160:ILE:HG12	1.63	0.79
1:K:33:SER:H	1:K:52:THR:HA	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:SER:H	1:D:52:THR:HA	1.49	0.76
1:A:33:SER:H	1:A:52:THR:HA	1.49	0.76
1:G:33:SER:H	1:G:52:THR:HA	1.49	0.76
1:K:68:THR:HB	1:K:81:GLN:HB3	1.70	0.74
1:G:17:SER:HA	1:G:83:ASN:HA	1.71	0.73
3:I:3210:LEU:HB2	3:I:3304:CYS:HA	1.70	0.73
1:D:68:THR:HB	1:D:81:GLN:HB3	1.70	0.73
3:F:3210:LEU:HB2	3:F:3304:CYS:HA	1.70	0.73
1:K:17:SER:HA	1:K:83:ASN:HA	1.71	0.72
3:I:1943:LEU:HD13	3:I:2098:VAL:HG22	1.72	0.72
3:J:1943:LEU:HD13	3:J:2098:VAL:HG22	1.72	0.72
3:C:3210:LEU:HB2	3:C:3304:CYS:HA	1.70	0.72
1:D:17:SER:HA	1:D:83:ASN:HA	1.71	0.72
1:G:68:THR:HB	1:G:81:GLN:HB3	1.70	0.72
3:I:1115:LEU:HG	3:I:1123:VAL:HG11	1.71	0.72
3:F:2741:GLU:HB3	3:F:2744:ASN:HB2	1.72	0.72
3:F:1115:LEU:HG	3:F:1123:VAL:HG11	1.71	0.72
3:I:893:TYR:HB3	3:I:960:MET:HE1	1.72	0.71
3:J:1115:LEU:HG	3:J:1123:VAL:HG11	1.71	0.71
3:F:893:TYR:HB3	3:F:960:MET:HE1	1.72	0.71
1:A:17:SER:HA	1:A:83:ASN:HA	1.71	0.71
3:I:2741:GLU:HB3	3:I:2744:ASN:HB2	1.72	0.71
3:J:622:THR:HG23	3:J:626:LEU:HD22	1.73	0.71
3:F:34:LYS:H	3:F:53:SER:HB3	1.55	0.71
1:A:68:THR:HB	1:A:81:GLN:HB3	1.70	0.71
3:C:34:LYS:H	3:C:53:SER:HB3	1.55	0.71
3:I:622:THR:HG23	3:I:626:LEU:HD22	1.73	0.71
3:I:4241:THR:HB	3:I:4989:MET:HE1	1.72	0.71
3:J:3210:LEU:HB2	3:J:3304:CYS:HA	1.70	0.71
3:C:2741:GLU:HB3	3:C:2744:ASN:HB2	1.72	0.70
3:I:3889:GLN:HG3	3:I:3967:GLU:HG3	1.73	0.70
3:I:34:LYS:H	3:I:53:SER:HB3	1.55	0.70
3:C:1943:LEU:HD13	3:C:2098:VAL:HG22	1.72	0.70
3:J:893:TYR:HB3	3:J:960:MET:HE1	1.72	0.70
3:F:1943:LEU:HD13	3:F:2098:VAL:HG22	1.72	0.70
3:F:3889:GLN:HG3	3:F:3967:GLU:HG3	1.73	0.70
3:C:3889:GLN:HG3	3:C:3967:GLU:HG3	1.73	0.70
3:I:4034:ASN:HD21	3:I:4038:GLY:HA3	1.57	0.70
2:L:5:GLU:HB2	2:L:73:LYS:HB3	1.73	0.70
3:J:34:LYS:H	3:J:53:SER:HB3	1.55	0.70
3:C:1115:LEU:HG	3:C:1123:VAL:HG11	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:5:GLU:HB2	2:E:73:LYS:HB3	1.73	0.70
3:F:622:THR:HG23	3:F:626:LEU:HD22	1.73	0.70
3:J:4034:ASN:HD21	3:J:4038:GLY:HA3	1.57	0.70
3:F:4241:THR:HB	3:F:4989:MET:HE1	1.72	0.70
3:I:1926:LEU:HG	3:I:1939:MET:HE1	1.74	0.70
3:J:1241:SER:HA	3:J:1603:VAL:HG22	1.74	0.70
3:C:622:THR:HG23	3:C:626:LEU:HD22	1.73	0.70
3:F:4034:ASN:HD21	3:F:4038:GLY:HA3	1.56	0.70
3:C:893:TYR:HB3	3:C:960:MET:HE1	1.72	0.69
3:C:4034:ASN:HD21	3:C:4038:GLY:HA3	1.56	0.69
3:F:1241:SER:HA	3:F:1603:VAL:HG22	1.74	0.69
3:J:2741:GLU:HB3	3:J:2744:ASN:HB2	1.72	0.69
3:J:3889:GLN:HG3	3:J:3967:GLU:HG3	1.73	0.69
3:C:182:LEU:HD11	3:C:189:LEU:HB3	1.74	0.69
3:C:1476:MET:HB3	3:C:1484:HIS:HB3	1.74	0.69
3:C:1926:LEU:HG	3:C:1939:MET:HE1	1.74	0.69
3:C:4241:THR:HB	3:C:4989:MET:HE1	1.72	0.69
3:F:1926:LEU:HG	3:F:1939:MET:HE1	1.74	0.69
3:J:1078:GLU:HG3	3:J:1235:THR:HB	1.73	0.69
3:C:1241:SER:HA	3:C:1603:VAL:HG22	1.74	0.69
3:J:1926:LEU:HG	3:J:1939:MET:HE1	1.74	0.69
3:I:1241:SER:HA	3:I:1603:VAL:HG22	1.74	0.69
3:J:182:LEU:HD11	3:J:189:LEU:HB3	1.74	0.69
3:F:275:ARG:HB2	3:F:278:GLN:HB2	1.75	0.69
3:I:1476:MET:HB3	3:I:1484:HIS:HB3	1.74	0.69
3:C:1078:GLU:HG3	3:C:1235:THR:HB	1.73	0.69
2:B:5:GLU:HB2	2:B:73:LYS:HB3	1.73	0.69
3:J:4241:THR:HB	3:J:4989:MET:HE1	1.73	0.68
3:I:275:ARG:HB2	3:I:278:GLN:HB2	1.75	0.68
3:J:864:PRO:HD3	3:J:933:LEU:HD21	1.76	0.68
3:J:1476:MET:HB3	3:J:1484:HIS:HB3	1.74	0.68
3:F:1078:GLU:HG3	3:F:1235:THR:HB	1.73	0.68
2:H:5:GLU:HB2	2:H:73:LYS:HB3	1.73	0.68
3:F:1476:MET:HB3	3:F:1484:HIS:HB3	1.74	0.68
3:I:1078:GLU:HG3	3:I:1235:THR:HB	1.73	0.68
3:I:864:PRO:HD3	3:I:933:LEU:HD21	1.76	0.68
3:J:2243:SER:HB2	3:J:3861:GLU:HG2	1.76	0.68
3:F:182:LEU:HD11	3:F:189:LEU:HB3	1.74	0.68
3:F:864:PRO:HD3	3:F:933:LEU:HD21	1.76	0.67
3:J:275:ARG:HB2	3:J:278:GLN:HB2	1.75	0.67
3:C:864:PRO:HD3	3:C:933:LEU:HD21	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:2243:SER:HB2	3:I:3861:GLU:HG2	1.76	0.67
3:C:2243:SER:HB2	3:C:3861:GLU:HG2	1.76	0.67
3:I:182:LEU:HD11	3:I:189:LEU:HB3	1.74	0.67
3:I:1735:ILE:HD11	3:I:2156:LEU:HD11	1.77	0.67
3:J:3107:VAL:HG21	3:J:3171:SER:HB2	1.78	0.66
3:C:1980:LEU:HD11	3:C:1990:GLU:HA	1.77	0.66
3:C:2380:ILE:HG21	3:C:2469:ILE:HD13	1.78	0.66
2:E:68:LEU:HA	2:E:103:LEU:HB2	1.77	0.66
3:J:1735:ILE:HD11	3:J:2156:LEU:HD11	1.77	0.66
3:F:2243:SER:HB2	3:F:3861:GLU:HG2	1.76	0.66
3:F:1980:LEU:HD11	3:F:1990:GLU:HA	1.77	0.66
3:C:2700:MET:HE3	3:C:2701:PRO:HD3	1.78	0.66
2:H:68:LEU:HA	2:H:103:LEU:HB2	1.77	0.66
3:F:882:TRP:HZ3	3:F:905:PRO:HA	1.61	0.66
3:I:882:TRP:HZ3	3:I:905:PRO:HA	1.61	0.66
3:I:3107:VAL:HG21	3:I:3171:SER:HB2	1.78	0.66
3:J:882:TRP:HZ3	3:J:905:PRO:HA	1.61	0.66
3:F:2380:ILE:HG21	3:F:2469:ILE:HD13	1.78	0.66
3:J:2700:MET:HE3	3:J:2701:PRO:HD3	1.78	0.66
3:F:1735:ILE:HD11	3:F:2156:LEU:HD11	1.77	0.66
3:F:2700:MET:HE3	3:F:2701:PRO:HD3	1.78	0.66
3:J:2380:ILE:HG21	3:J:2469:ILE:HD13	1.78	0.65
3:C:275:ARG:HB2	3:C:278:GLN:HB2	1.75	0.65
3:C:1735:ILE:HD11	3:C:2156:LEU:HD11	1.77	0.65
3:C:3107:VAL:HG21	3:C:3171:SER:HB2	1.78	0.65
3:J:1980:LEU:HD11	3:J:1990:GLU:HA	1.77	0.65
2:B:68:LEU:HA	2:B:103:LEU:HB2	1.77	0.65
3:I:1980:LEU:HD11	3:I:1990:GLU:HA	1.77	0.65
3:C:882:TRP:HZ3	3:C:905:PRO:HA	1.61	0.65
3:F:3107:VAL:HG21	3:F:3171:SER:HB2	1.78	0.65
2:L:68:LEU:HA	2:L:103:LEU:HB2	1.77	0.65
3:F:569:ILE:HG13	3:F:570:GLU:HG2	1.79	0.65
3:I:2700:MET:HE3	3:I:2701:PRO:HD3	1.78	0.65
3:J:498:THR:HA	3:J:553:ARG:HH22	1.62	0.65
3:J:3102:ASP:HA	3:J:3105:LYS:HE2	1.79	0.64
3:I:498:THR:HA	3:I:553:ARG:HH22	1.62	0.64
3:J:438:ILE:HG23	3:J:518:ILE:HD11	1.80	0.64
3:C:3102:ASP:HA	3:C:3105:LYS:HE2	1.79	0.64
3:F:2712:PRO:HB2	3:F:3016:TYR:HE2	1.63	0.64
3:J:1870:VAL:HG21	3:J:2097:LEU:HD13	1.79	0.64
3:I:2380:ILE:HG21	3:I:2469:ILE:HD13	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:2642:LYS:HE3	3:J:2646:ASN:HD21	1.62	0.64
3:C:498:THR:HA	3:C:553:ARG:HH22	1.62	0.64
3:I:1870:VAL:HG21	3:I:2097:LEU:HD13	1.79	0.64
3:C:438:ILE:HG23	3:C:518:ILE:HD11	1.80	0.64
3:I:2642:LYS:HE3	3:I:2646:ASN:HD21	1.62	0.64
3:J:569:ILE:HG13	3:J:570:GLU:HG2	1.79	0.64
3:F:2642:LYS:HE3	3:F:2646:ASN:HD21	1.62	0.64
3:F:3102:ASP:HA	3:F:3105:LYS:HE2	1.79	0.64
3:I:3102:ASP:HA	3:I:3105:LYS:HE2	1.79	0.64
3:C:569:ILE:HG13	3:C:570:GLU:HG2	1.79	0.64
3:F:438:ILE:HG23	3:F:518:ILE:HD11	1.80	0.64
3:F:498:THR:HA	3:F:553:ARG:HH22	1.62	0.64
3:I:638:ILE:HD11	3:I:1636:MET:HE3	1.80	0.64
3:I:2712:PRO:HB2	3:I:3016:TYR:HE2	1.63	0.64
3:J:2630:VAL:HG13	3:J:2682:ILE:HD11	1.80	0.64
3:J:2712:PRO:HB2	3:J:3016:TYR:HE2	1.63	0.63
3:I:569:ILE:HG13	3:I:570:GLU:HG2	1.79	0.63
3:C:1870:VAL:HG21	3:C:2097:LEU:HD13	1.79	0.63
3:F:1870:VAL:HG21	3:F:2097:LEU:HD13	1.79	0.63
1:K:41:PRO:HD3	1:K:91:ALA:HA	1.81	0.63
3:C:2712:PRO:HB2	3:C:3016:TYR:HE2	1.63	0.63
3:C:2764:GLU:HB3	3:C:2857:PRO:HD3	1.81	0.63
1:D:41:PRO:HD3	1:D:91:ALA:HA	1.81	0.63
3:F:2764:GLU:HB3	3:F:2857:PRO:HD3	1.81	0.63
3:I:438:ILE:HG23	3:I:518:ILE:HD11	1.80	0.63
3:C:1089:TYR:HD2	3:C:1152:MET:HG2	1.64	0.63
1:D:93:TYR:O	1:D:120:GLY:HA3	1.99	0.63
1:G:41:PRO:HD3	1:G:91:ALA:HA	1.81	0.63
1:A:41:PRO:HD3	1:A:91:ALA:HA	1.81	0.63
1:A:93:TYR:O	1:A:120:GLY:HA3	1.99	0.63
3:C:638:ILE:HD11	3:C:1636:MET:HE3	1.80	0.63
3:C:2228:MET:HE2	3:C:2228:MET:HA	1.81	0.63
3:J:1089:TYR:HD2	3:J:1152:MET:HG2	1.64	0.63
3:I:2228:MET:HE2	3:I:2228:MET:HA	1.81	0.63
3:F:2630:VAL:HG13	3:F:2682:ILE:HD11	1.80	0.63
3:I:2764:GLU:HB3	3:I:2857:PRO:HD3	1.81	0.63
3:J:638:ILE:HD11	3:J:1636:MET:HE3	1.80	0.62
3:J:2178:MET:HB3	3:J:2228:MET:HE1	1.81	0.62
3:F:2228:MET:HE2	3:F:2228:MET:HA	1.81	0.62
3:F:2472:LEU:HD22	3:F:2473:PRO:HD2	1.81	0.62
1:G:93:TYR:O	1:G:120:GLY:HA3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2642:LYS:HE3	3:C:2646:ASN:HD21	1.62	0.62
1:D:39:GLN:HA	1:D:45:ARG:HA	1.81	0.62
1:K:39:GLN:HA	1:K:45:ARG:HA	1.81	0.62
3:J:2764:GLU:HB3	3:J:2857:PRO:HD3	1.81	0.62
1:A:39:GLN:HA	1:A:45:ARG:HA	1.81	0.62
3:C:2472:LEU:HD22	3:C:2473:PRO:HD2	1.81	0.62
3:F:109:LEU:HD12	3:F:118:LEU:HD23	1.81	0.62
3:F:1089:TYR:HD2	3:F:1152:MET:HG2	1.64	0.62
3:I:2211:MET:HE2	3:I:2211:MET:HA	1.82	0.62
3:J:2458:ARG:HG2	3:J:2510:TYR:HE1	1.65	0.62
3:C:2178:MET:HB3	3:C:2228:MET:HE1	1.81	0.62
3:C:2630:VAL:HG13	3:C:2682:ILE:HD11	1.80	0.62
3:F:638:ILE:HD11	3:F:1636:MET:HE3	1.80	0.62
3:F:2211:MET:HE2	3:F:2211:MET:HA	1.81	0.62
3:I:1089:TYR:HD2	3:I:1152:MET:HG2	1.64	0.62
3:I:2178:MET:HB3	3:I:2228:MET:HE1	1.81	0.62
3:J:2228:MET:HE2	3:J:2228:MET:HA	1.81	0.62
3:C:2458:ARG:HG2	3:C:2510:TYR:HE1	1.65	0.62
3:F:1470:ARG:HB2	3:F:1491:ASN:HB2	1.81	0.62
3:F:2178:MET:HB3	3:F:2228:MET:HE1	1.81	0.62
1:G:39:GLN:HA	1:G:45:ARG:HA	1.81	0.62
1:K:93:TYR:O	1:K:120:GLY:HA3	1.99	0.62
3:J:109:LEU:HD12	3:J:118:LEU:HD23	1.81	0.62
3:F:2624:ARG:HD3	3:F:2912:THR:HG23	1.82	0.62
3:F:3687:GLU:HG3	3:F:3690:VAL:HB	1.82	0.62
3:J:2522:LEU:HA	3:J:2526:PHE:HB2	1.81	0.62
3:F:3592:ILE:HG12	3:F:3595:ARG:HH21	1.65	0.62
3:I:3687:GLU:HG3	3:I:3690:VAL:HB	1.82	0.62
3:J:3687:GLU:HG3	3:J:3690:VAL:HB	1.82	0.62
3:C:1470:ARG:HB2	3:C:1491:ASN:HB2	1.81	0.62
3:F:830:ARG:HD2	3:F:837:PRO:HB3	1.82	0.62
3:I:2522:LEU:HA	3:I:2526:PHE:HB2	1.81	0.62
3:J:2472:LEU:HD22	3:J:2473:PRO:HD2	1.81	0.62
3:I:2095:GLN:HA	3:I:2127:GLN:HG3	1.82	0.62
3:J:830:ARG:HD2	3:J:837:PRO:HB3	1.82	0.62
3:C:830:ARG:HD2	3:C:837:PRO:HB3	1.82	0.62
3:C:1225:PRO:HG2	3:C:1228:ILE:HB	1.81	0.62
3:I:668:VAL:HG22	3:I:789:VAL:HG12	1.82	0.62
1:K:11:LEU:HD13	1:K:124:THR:HG22	1.81	0.61
3:C:2624:ARG:HD3	3:C:2912:THR:HG23	1.82	0.61
3:F:2095:GLN:HA	3:F:2127:GLN:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2458:ARG:HG2	3:F:2510:TYR:HE1	1.65	0.61
3:I:109:LEU:HD12	3:I:118:LEU:HD23	1.82	0.61
3:I:2272:PRO:HA	3:I:2275:VAL:HG12	1.82	0.61
3:J:668:VAL:HG22	3:J:789:VAL:HG12	1.82	0.61
3:C:231:LEU:HD11	3:C:245:VAL:HB	1.82	0.61
3:I:2472:LEU:HD22	3:I:2473:PRO:HD2	1.81	0.61
3:I:2624:ARG:HD3	3:I:2912:THR:HG23	1.82	0.61
3:C:668:VAL:HG22	3:C:789:VAL:HG12	1.82	0.61
3:F:2522:LEU:HA	3:F:2526:PHE:HB2	1.81	0.61
3:I:2198:MET:HE1	3:I:2203:MET:SD	2.40	0.61
3:I:2458:ARG:HG2	3:I:2510:TYR:HE1	1.65	0.61
3:J:1225:PRO:HG2	3:J:1228:ILE:HB	1.81	0.61
3:C:3687:GLU:HG3	3:C:3690:VAL:HB	1.82	0.61
3:F:231:LEU:HD11	3:F:245:VAL:HB	1.82	0.61
3:I:2630:VAL:HG13	3:I:2682:ILE:HD11	1.80	0.61
1:K:6:GLU:HB3	1:K:120:GLY:HA2	1.82	0.61
3:J:3592:ILE:HG12	3:J:3595:ARG:HH21	1.65	0.61
3:C:3592:ILE:HG12	3:C:3595:ARG:HH21	1.65	0.61
3:I:830:ARG:HD2	3:I:837:PRO:HB3	1.82	0.61
3:I:3442:PHE:HE2	3:I:3510:ILE:HA	1.65	0.61
3:J:2624:ARG:HD3	3:J:2912:THR:HG23	1.82	0.61
3:I:2534:ALA:HB1	3:I:2588:ARG:HE	1.66	0.61
3:C:109:LEU:HD12	3:C:118:LEU:HD23	1.82	0.61
3:C:2522:LEU:HA	3:C:2526:PHE:HB2	1.81	0.61
3:F:1225:PRO:HG2	3:F:1228:ILE:HB	1.81	0.61
1:G:6:GLU:HB3	1:G:120:GLY:HA2	1.82	0.61
3:J:1470:ARG:HB2	3:J:1491:ASN:HB2	1.81	0.61
1:A:11:LEU:HD13	1:A:124:THR:HG22	1.81	0.61
3:I:1023:PRO:HD2	3:I:1026:LEU:HD12	1.83	0.61
3:I:1470:ARG:HB2	3:I:1491:ASN:HB2	1.81	0.61
3:I:2712:PRO:HA	3:I:2955:PHE:HD2	1.66	0.61
3:J:231:LEU:HD11	3:J:245:VAL:HB	1.82	0.61
3:J:2095:GLN:HA	3:J:2127:GLN:HG3	1.82	0.61
3:C:3218:VAL:O	3:C:3222:LYS:HB2	2.01	0.61
3:F:2623:LEU:HA	3:F:2626:LEU:HD12	1.83	0.61
3:F:3442:PHE:HE2	3:F:3510:ILE:HA	1.65	0.61
3:J:2712:PRO:HA	3:J:2955:PHE:HD2	1.66	0.61
3:C:2095:GLN:HA	3:C:2127:GLN:HG3	1.82	0.61
3:C:2623:LEU:HA	3:C:2626:LEU:HD12	1.83	0.61
3:F:2272:PRO:HA	3:F:2275:VAL:HG12	1.82	0.61
3:I:2645:THR:HB	3:I:2702:CYS:HA	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:3442:PHE:HE2	3:J:3510:ILE:HA	1.65	0.60
1:A:6:GLU:HB3	1:A:120:GLY:HA2	1.82	0.60
3:C:1023:PRO:HD2	3:C:1026:LEU:HD12	1.83	0.60
1:G:11:LEU:HD13	1:G:124:THR:HG22	1.81	0.60
3:C:2211:MET:HE2	3:C:2211:MET:HA	1.82	0.60
3:C:3442:PHE:HE2	3:C:3510:ILE:HA	1.65	0.60
3:I:3592:ILE:HG12	3:I:3595:ARG:HH21	1.65	0.60
3:J:2198:MET:HE1	3:J:2203:MET:SD	2.40	0.60
3:J:2211:MET:HE2	3:J:2211:MET:HA	1.81	0.60
3:J:3218:VAL:O	3:J:3222:LYS:HB2	2.01	0.60
3:C:2980:VAL:HB	3:C:2986:VAL:HB	1.83	0.60
1:D:11:LEU:HD13	1:D:124:THR:HG22	1.81	0.60
3:C:4087:LEU:HB3	3:C:4122:MET:HE2	1.84	0.60
3:F:2198:MET:HE1	3:F:2203:MET:SD	2.40	0.60
3:F:2645:THR:HB	3:F:2702:CYS:HA	1.83	0.60
3:F:2980:VAL:HB	3:F:2986:VAL:HB	1.84	0.60
3:F:3218:VAL:O	3:F:3222:LYS:HB2	2.01	0.60
3:I:231:LEU:HD11	3:I:245:VAL:HB	1.82	0.60
3:I:1225:PRO:HG2	3:I:1228:ILE:HB	1.81	0.60
3:J:884:LEU:HB2	3:J:969:PRO:HG3	1.83	0.60
3:F:668:VAL:HG22	3:F:789:VAL:HG12	1.82	0.60
3:F:884:LEU:HB2	3:F:969:PRO:HG3	1.84	0.60
3:F:4087:LEU:HB3	3:F:4122:MET:HE2	1.84	0.60
3:I:3218:VAL:O	3:I:3222:LYS:HB2	2.01	0.60
3:J:1023:PRO:HD2	3:J:1026:LEU:HD12	1.83	0.60
3:C:2198:MET:HE1	3:C:2203:MET:SD	2.40	0.60
3:C:2645:THR:HB	3:C:2702:CYS:HA	1.83	0.60
3:C:2712:PRO:HA	3:C:2955:PHE:HD2	1.66	0.60
3:J:2534:ALA:HB1	3:J:2588:ARG:HE	1.66	0.60
3:C:2272:PRO:HA	3:C:2275:VAL:HG12	1.82	0.60
3:F:2534:ALA:HB1	3:F:2588:ARG:HE	1.66	0.60
3:F:2712:PRO:HA	3:F:2955:PHE:HD2	1.66	0.60
3:I:2928:LYS:O	3:I:2932:MET:HG3	2.02	0.60
3:J:2755:ILE:HD12	3:J:2813:LEU:HB3	1.84	0.60
3:J:2645:THR:HB	3:J:2702:CYS:HA	1.84	0.60
3:C:2755:ILE:HD12	3:C:2813:LEU:HB3	1.84	0.59
3:C:4059:LEU:HD13	3:C:4167:ALA:HB2	1.84	0.59
1:D:6:GLU:HB3	1:D:120:GLY:HA2	1.82	0.59
3:J:2980:VAL:HB	3:J:2986:VAL:HB	1.84	0.59
1:G:37:TYR:HB3	1:G:45:ARG:HB2	1.84	0.59
3:J:842:PRO:HD3	3:J:1073:ARG:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:2623:LEU:HA	3:J:2626:LEU:HD12	1.83	0.59
3:C:2490:MET:HE1	3:C:2546:MET:HB3	1.84	0.59
3:F:2928:LYS:O	3:F:2932:MET:HG3	2.02	0.59
3:J:2272:PRO:HA	3:J:2275:VAL:HG12	1.82	0.59
3:J:4087:LEU:HB3	3:J:4122:MET:HE2	1.84	0.59
3:F:4059:LEU:HD13	3:F:4167:ALA:HB2	1.84	0.59
1:K:37:TYR:HB3	1:K:45:ARG:HB2	1.84	0.59
3:C:842:PRO:HD3	3:C:1073:ARG:HB2	1.84	0.59
1:D:37:TYR:HB3	1:D:45:ARG:HB2	1.84	0.59
3:F:1023:PRO:HD2	3:F:1026:LEU:HD12	1.83	0.59
3:I:2980:VAL:HB	3:I:2986:VAL:HB	1.83	0.59
3:J:2928:LYS:O	3:J:2932:MET:HG3	2.02	0.59
3:C:4860:ARG:HH12	3:F:4628:VAL:HG11	1.68	0.59
3:I:884:LEU:HB2	3:I:969:PRO:HG3	1.83	0.59
3:I:2630:VAL:HG11	3:I:2644:LEU:HD11	1.85	0.59
3:J:2630:VAL:HG11	3:J:2644:LEU:HD11	1.85	0.59
3:I:2623:LEU:HA	3:I:2626:LEU:HD12	1.83	0.59
3:F:4860:ARG:HH12	3:I:4628:VAL:HG11	1.68	0.59
3:I:842:PRO:HD3	3:I:1073:ARG:HB2	1.84	0.59
3:I:4087:LEU:HB3	3:I:4122:MET:HE2	1.84	0.59
3:C:2971:GLN:HA	3:C:2974:ILE:HG12	1.85	0.59
3:C:2928:LYS:O	3:C:2932:MET:HG3	2.02	0.58
3:F:245:VAL:HG23	3:F:376:ALA:HB3	1.84	0.58
3:I:1835:GLU:O	3:I:1839:VAL:HG12	2.03	0.58
3:J:1835:GLU:O	3:J:1839:VAL:HG12	2.03	0.58
3:C:1835:GLU:O	3:C:1839:VAL:HG12	2.03	0.58
3:F:2490:MET:HE1	3:F:2546:MET:HB3	1.84	0.58
3:F:2755:ILE:HD12	3:F:2813:LEU:HB3	1.84	0.58
3:I:2490:MET:HE1	3:I:2546:MET:HB3	1.84	0.58
3:J:4546:VAL:HG22	3:J:4550:LYS:HE3	1.85	0.58
3:J:4628:VAL:HG11	3:I:4860:ARG:HH12	1.68	0.58
3:C:2534:ALA:HB1	3:C:2588:ARG:HE	1.66	0.58
3:I:2712:PRO:HB2	3:I:3016:TYR:CE2	2.38	0.58
3:F:842:PRO:HD3	3:F:1073:ARG:HB2	1.84	0.58
3:J:1449:TRP:HB3	3:J:1494:MET:HE3	1.86	0.58
3:J:4059:LEU:HD13	3:J:4167:ALA:HB2	1.84	0.58
3:C:1839:VAL:HG13	3:C:1840:PRO:HD3	1.86	0.58
3:C:2630:VAL:HG11	3:C:2644:LEU:HD11	1.85	0.58
3:F:2971:GLN:HA	3:F:2974:ILE:HG12	1.85	0.58
3:I:1839:VAL:HG13	3:I:1840:PRO:HD3	1.86	0.58
3:I:2755:ILE:HD12	3:I:2813:LEU:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:2490:MET:HE1	3:J:2546:MET:HB3	1.84	0.58
3:F:2712:PRO:HB2	3:F:3016:TYR:CE2	2.39	0.58
3:I:2098:VAL:HB	3:I:2127:GLN:HG2	1.86	0.58
3:I:3206:LEU:HD13	3:I:3246:LEU:HB3	1.86	0.58
3:J:3206:LEU:HD13	3:J:3246:LEU:HB3	1.86	0.58
3:J:4860:ARG:HH12	3:C:4628:VAL:HG11	1.67	0.58
3:C:245:VAL:HG23	3:C:376:ALA:HB3	1.84	0.58
3:C:1449:TRP:HB3	3:C:1494:MET:HE3	1.86	0.58
3:F:1449:TRP:HB3	3:F:1494:MET:HE3	1.86	0.58
3:I:3085:PRO:HB2	3:I:3088:VAL:HG12	1.86	0.58
3:I:4059:LEU:HD13	3:I:4167:ALA:HB2	1.84	0.58
3:J:2970:SER:HA	3:J:2973:PHE:CD2	2.39	0.58
3:C:884:LEU:HB2	3:C:969:PRO:HG3	1.83	0.58
3:I:4546:VAL:HG22	3:I:4550:LYS:HE3	1.85	0.58
3:J:1839:VAL:HG13	3:J:1840:PRO:HD3	1.86	0.58
3:F:2630:VAL:HG11	3:F:2644:LEU:HD11	1.85	0.58
3:F:2970:SER:HA	3:F:2973:PHE:CD2	2.39	0.58
3:I:2970:SER:HA	3:I:2973:PHE:CD2	2.39	0.58
3:J:2712:PRO:HB2	3:J:3016:TYR:CE2	2.39	0.58
1:A:37:TYR:HB3	1:A:45:ARG:HB2	1.84	0.58
3:I:1449:TRP:HB3	3:I:1494:MET:HE3	1.86	0.58
3:J:947:GLU:HA	3:J:950:LEU:HB2	1.86	0.57
3:J:2098:VAL:HB	3:J:2127:GLN:HG2	1.86	0.57
3:F:1835:GLU:O	3:F:1839:VAL:HG12	2.03	0.57
3:I:2971:GLN:HA	3:I:2974:ILE:HG12	1.85	0.57
1:K:38:ARG:HG3	1:K:46:GLU:HG2	1.86	0.57
3:C:653:ALA:HB3	3:C:656:SER:HB2	1.86	0.57
3:F:3270:ILE:HD12	3:F:3270:ILE:H	1.69	0.57
3:F:3768:SER:HA	3:F:3771:HIS:CD2	2.39	0.57
1:G:38:ARG:HG3	1:G:46:GLU:HG2	1.86	0.57
3:J:653:ALA:HB3	3:J:656:SER:HB2	1.86	0.57
3:J:3085:PRO:HB2	3:J:3088:VAL:HG12	1.85	0.57
3:C:2583:LEU:HB3	3:C:2622:LEU:HD22	1.86	0.57
3:C:2712:PRO:HB2	3:C:3016:TYR:CE2	2.38	0.57
3:C:2970:SER:HA	3:C:2973:PHE:CD2	2.39	0.57
3:J:245:VAL:HG23	3:J:376:ALA:HB3	1.84	0.57
1:A:38:ARG:HG3	1:A:46:GLU:HG2	1.86	0.57
3:C:3270:ILE:HD12	3:C:3270:ILE:H	1.69	0.57
3:J:2489:LYS:HB3	3:J:2492:ALA:HB3	1.86	0.57
3:J:2616:PRO:HA	3:J:2619:LEU:HD12	1.86	0.57
3:J:3768:SER:HA	3:J:3771:HIS:CD2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:245:VAL:HG23	3:I:376:ALA:HB3	1.84	0.57
3:I:653:ALA:HB3	3:I:656:SER:HB2	1.86	0.57
3:I:3768:SER:HA	3:I:3771:HIS:CD2	2.39	0.57
3:C:2582:MET:HE3	3:C:2610:LEU:HD21	1.86	0.57
3:F:1839:VAL:HG13	3:F:1840:PRO:HD3	1.86	0.57
3:F:3206:LEU:HD13	3:F:3246:LEU:HB3	1.86	0.57
3:F:3236:VAL:HA	3:F:3239:MET:SD	2.45	0.57
3:I:3144:PHE:HB2	3:I:3196:ARG:HB3	1.87	0.57
3:J:803:LEU:HD13	3:J:804:PRO:HD2	1.87	0.57
3:C:2616:PRO:HA	3:C:2619:LEU:HD12	1.86	0.57
3:F:947:GLU:HA	3:F:950:LEU:HB2	1.85	0.57
3:F:2583:LEU:HB3	3:F:2622:LEU:HD22	1.86	0.57
3:F:3085:PRO:HB2	3:F:3088:VAL:HG12	1.85	0.57
3:I:4725:LEU:HA	3:I:4737:ILE:HG21	1.87	0.57
3:F:3144:PHE:HB2	3:F:3196:ARG:HB3	1.87	0.57
3:I:2742:THR:HG22	3:I:2815:ALA:HB2	1.87	0.57
3:C:4546:VAL:HG22	3:C:4550:LYS:HE3	1.85	0.57
3:F:4546:VAL:HG22	3:F:4550:LYS:HE3	1.85	0.57
3:J:2742:THR:HG22	3:J:2815:ALA:HB2	1.87	0.56
3:J:2782:ASP:HB3	3:J:2785:LEU:HB2	1.87	0.56
3:J:2971:GLN:HA	3:J:2974:ILE:HG12	1.85	0.56
3:J:3270:ILE:H	3:J:3270:ILE:HD12	1.69	0.56
3:C:1979:LEU:HG	3:C:1982:ARG:HH21	1.70	0.56
3:C:2098:VAL:HB	3:C:2127:GLN:HG2	1.86	0.56
3:C:2489:LYS:HB3	3:C:2492:ALA:HB3	1.86	0.56
3:C:2742:THR:HG22	3:C:2815:ALA:HB2	1.87	0.56
3:C:3236:VAL:HA	3:C:3239:MET:SD	2.45	0.56
3:C:3768:SER:HA	3:C:3771:HIS:CD2	2.39	0.56
3:F:2742:THR:HG22	3:F:2815:ALA:HB2	1.87	0.56
3:I:947:GLU:HA	3:I:950:LEU:HB2	1.86	0.56
3:C:3206:LEU:HD13	3:C:3246:LEU:HB3	1.86	0.56
1:D:38:ARG:HG3	1:D:46:GLU:HG2	1.86	0.56
3:F:2616:PRO:HA	3:F:2619:LEU:HD12	1.86	0.56
3:F:4698:LYS:HB3	7:F:5110:POV:H13	1.87	0.56
3:J:2025:GLU:HA	3:J:2028:ARG:HD2	1.87	0.56
3:J:2965:ARG:HH22	3:J:2966:TRP:HE3	1.53	0.56
3:J:3236:VAL:HA	3:J:3239:MET:SD	2.45	0.56
3:J:4654:ALA:HB1	3:J:4796:MET:HE1	1.88	0.56
3:J:4725:LEU:HA	3:J:4737:ILE:HG21	1.87	0.56
3:C:399:GLN:O	3:C:403:MET:HG2	2.05	0.56
3:C:947:GLU:HA	3:C:950:LEU:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:878:ILE:HA	3:F:881:LEU:HD23	1.88	0.56
3:I:2583:LEU:HB3	3:I:2622:LEU:HD22	1.86	0.56
3:I:2616:PRO:HA	3:I:2619:LEU:HD12	1.86	0.56
3:I:3236:VAL:HA	3:I:3239:MET:SD	2.45	0.56
3:J:2583:LEU:HB3	3:J:2622:LEU:HD22	1.86	0.56
3:C:3085:PRO:HB2	3:C:3088:VAL:HG12	1.85	0.56
3:C:4725:LEU:HA	3:C:4737:ILE:HG21	1.87	0.56
3:F:2025:GLU:HA	3:F:2028:ARG:HD2	1.87	0.56
3:I:1747:LEU:HD11	3:I:2041:HIS:HB2	1.86	0.56
3:I:2489:LYS:HB3	3:I:2492:ALA:HB3	1.86	0.56
3:I:2883:HIS:HE1	3:I:2907:PRO:HA	1.71	0.56
3:I:4679:ARG:HH21	3:I:5017:ARG:HH21	1.52	0.56
3:J:878:ILE:HA	3:J:881:LEU:HD23	1.87	0.56
3:C:803:LEU:HD13	3:C:804:PRO:HD2	1.87	0.56
3:F:1747:LEU:HD11	3:F:2041:HIS:HB2	1.86	0.56
3:F:2098:VAL:HB	3:F:2127:GLN:HG2	1.86	0.56
3:I:1979:LEU:HG	3:I:1982:ARG:HH21	1.70	0.56
3:I:3270:ILE:H	3:I:3270:ILE:HD12	1.69	0.56
3:J:2582:MET:HE3	3:J:2610:LEU:HD21	1.86	0.56
1:A:9:GLY:HA2	1:A:123:VAL:HA	1.87	0.56
3:C:2211:MET:HE1	3:C:2229:VAL:HA	1.88	0.56
3:C:2782:ASP:HB3	3:C:2785:LEU:HB2	1.87	0.56
3:F:653:ALA:HB3	3:F:656:SER:HB2	1.86	0.56
3:F:1291:LEU:HD13	3:F:1595:LEU:HD11	1.88	0.56
3:F:4679:ARG:HH21	3:F:5017:ARG:HH21	1.52	0.56
3:I:4654:ALA:HB1	3:I:4796:MET:HE1	1.88	0.56
3:J:399:GLN:O	3:J:403:MET:HG2	2.05	0.56
3:J:1747:LEU:HD11	3:J:2041:HIS:HB2	1.86	0.56
3:J:2977:LEU:HA	3:J:2980:VAL:HG22	1.87	0.56
3:C:4679:ARG:HH21	3:C:5017:ARG:HH21	1.52	0.56
3:F:2965:ARG:HH22	3:F:2966:TRP:HE3	1.53	0.56
3:I:2582:MET:HE3	3:I:2610:LEU:HD21	1.87	0.56
3:I:2782:ASP:HB3	3:I:2785:LEU:HB2	1.87	0.56
3:J:2627:VAL:HG22	3:J:2678:LEU:HB2	1.87	0.56
3:F:2102:VAL:HG22	3:F:2120:MET:HG3	1.88	0.56
3:I:399:GLN:O	3:I:403:MET:HG2	2.05	0.56
3:I:2977:LEU:HA	3:I:2980:VAL:HG22	1.88	0.56
3:J:2211:MET:HE1	3:J:2229:VAL:HA	1.88	0.56
3:C:299:LEU:HD22	3:C:378:LEU:HG	1.88	0.56
3:C:2025:GLU:HA	3:C:2028:ARG:HD2	1.87	0.56
3:F:399:GLN:O	3:F:403:MET:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1979:LEU:HG	3:F:1982:ARG:HH21	1.70	0.56
3:F:2582:MET:HE3	3:F:2610:LEU:HD21	1.86	0.56
3:F:2627:VAL:HG22	3:F:2678:LEU:HB2	1.87	0.56
3:F:4654:ALA:HB1	3:F:4796:MET:HE1	1.88	0.56
3:I:2175:GLU:O	3:I:2179:ILE:HG12	2.06	0.56
3:I:3553:LEU:HG	3:I:3593:VAL:HG12	1.88	0.56
3:J:1291:LEU:HD13	3:J:1595:LEU:HD11	1.88	0.56
1:A:92:VAL:HA	1:A:122:GLN:HA	1.88	0.56
3:C:878:ILE:HA	3:C:881:LEU:HD23	1.87	0.56
3:F:2489:LYS:HB3	3:F:2492:ALA:HB3	1.86	0.56
3:F:2883:HIS:HE1	3:F:2907:PRO:HA	1.71	0.56
3:I:299:LEU:HD22	3:I:378:LEU:HG	1.88	0.56
3:I:2102:VAL:HG22	3:I:2120:MET:HG3	1.88	0.56
3:I:4698:LYS:HB3	7:I:5113:POV:H13	1.87	0.56
1:K:9:GLY:HA2	1:K:123:VAL:HA	1.87	0.55
3:J:681:HIS:HB3	3:J:784:SER:HB2	1.88	0.55
3:J:2974:ILE:HA	3:J:2977:LEU:HG	1.89	0.55
1:D:92:VAL:HA	1:D:122:GLN:HA	1.88	0.55
3:F:345:LEU:HB3	3:F:387:ALA:HB1	1.88	0.55
3:F:803:LEU:HD13	3:F:804:PRO:HD2	1.87	0.55
3:I:887:ILE:HG22	3:I:888:GLU:HG2	1.88	0.55
3:I:2965:ARG:HH22	3:I:2966:TRP:HE3	1.53	0.55
1:K:92:VAL:HA	1:K:122:GLN:HA	1.88	0.55
1:K:96:ASN:HB3	1:K:117:TRP:CD1	2.41	0.55
3:J:707:VAL:HG23	3:J:713:SER:HB2	1.88	0.55
3:C:292:ALA:HB1	3:C:311:ALA:HB1	1.89	0.55
3:C:2965:ARG:HH22	3:C:2966:TRP:HE3	1.53	0.55
3:C:4654:ALA:HB1	3:C:4796:MET:HE1	1.88	0.55
1:G:96:ASN:HB3	1:G:117:TRP:CD1	2.41	0.55
3:I:803:LEU:HD13	3:I:804:PRO:HD2	1.87	0.55
3:I:878:ILE:HA	3:I:881:LEU:HD23	1.87	0.55
3:J:2883:HIS:HE1	3:J:2907:PRO:HA	1.71	0.55
3:J:3144:PHE:HB2	3:J:3196:ARG:HB3	1.87	0.55
3:C:1498:GLY:HA2	3:C:1501:VAL:HG12	1.89	0.55
3:F:2974:ILE:HA	3:F:2977:LEU:HG	1.89	0.55
3:J:2175:GLU:O	3:J:2179:ILE:HG12	2.06	0.55
1:A:2:VAL:HA	1:A:26:GLY:HA3	1.89	0.55
3:C:707:VAL:HG23	3:C:713:SER:HB2	1.88	0.55
3:C:1747:LEU:HD11	3:C:2041:HIS:HB2	1.86	0.55
3:C:2627:VAL:HG22	3:C:2678:LEU:HB2	1.87	0.55
3:C:3144:PHE:HB2	3:C:3196:ARG:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2782:ASP:HB3	3:F:2785:LEU:HB2	1.87	0.55
3:I:2025:GLU:HA	3:I:2028:ARG:HD2	1.87	0.55
3:J:292:ALA:HB1	3:J:311:ALA:HB1	1.89	0.55
3:J:299:LEU:HD22	3:J:378:LEU:HG	1.88	0.55
3:J:3553:LEU:HG	3:J:3593:VAL:HG12	1.88	0.55
3:C:2651:CYS:HB3	3:C:2654:TYR:HB3	1.89	0.55
3:F:681:HIS:HB3	3:F:784:SER:HB2	1.88	0.55
3:F:1497:GLY:HA2	3:F:1500:PHE:HD2	1.72	0.55
3:F:2175:GLU:O	3:F:2179:ILE:HG12	2.06	0.55
3:F:2651:CYS:HB3	3:F:2654:TYR:HB3	1.89	0.55
3:J:1498:GLY:HA2	3:J:1501:VAL:HG12	1.89	0.55
3:J:1979:LEU:HG	3:J:1982:ARG:HH21	1.71	0.55
3:F:20:VAL:HG11	3:F:202:MET:HG3	1.88	0.55
3:F:292:ALA:HB1	3:F:311:ALA:HB1	1.89	0.55
3:F:2021:CYS:HB2	3:F:2028:ARG:HH12	1.72	0.55
1:G:92:VAL:HA	1:G:122:GLN:HA	1.88	0.55
3:I:292:ALA:HB1	3:I:311:ALA:HB1	1.89	0.55
3:I:2211:MET:HE1	3:I:2229:VAL:HA	1.88	0.55
3:C:681:HIS:HB3	3:C:784:SER:HB2	1.88	0.55
3:C:2977:LEU:HA	3:C:2980:VAL:HG22	1.88	0.55
3:F:299:LEU:HD22	3:F:378:LEU:HG	1.88	0.55
3:F:4725:LEU:HA	3:F:4737:ILE:HG21	1.87	0.55
1:G:9:GLY:HA2	1:G:123:VAL:HA	1.87	0.55
3:I:1497:GLY:HA2	3:I:1500:PHE:HD2	1.72	0.55
3:I:2675:THR:HG23	3:I:2710:LEU:HD13	1.89	0.55
3:I:2974:ILE:HA	3:I:2977:LEU:HG	1.89	0.55
3:J:4679:ARG:HH21	3:J:5017:ARG:HH21	1.52	0.55
3:C:2974:ILE:HA	3:C:2977:LEU:HG	1.89	0.55
3:F:2710:LEU:HD12	3:F:2711:PRO:HD2	1.89	0.55
3:J:4698:LYS:HB3	7:J:5108:POV:H13	1.87	0.55
3:C:985:VAL:HA	3:C:988:LEU:HD23	1.89	0.55
3:I:20:VAL:HG11	3:I:202:MET:HG3	1.88	0.55
3:J:887:ILE:HG22	3:J:888:GLU:HG2	1.88	0.55
3:C:887:ILE:HG22	3:C:888:GLU:HG2	1.88	0.55
3:C:2883:HIS:HE1	3:C:2907:PRO:HA	1.71	0.55
3:C:4698:LYS:HB3	7:C:5111:POV:H13	1.87	0.55
3:F:1498:GLY:HA2	3:F:1501:VAL:HG12	1.89	0.55
3:F:4056:GLU:HG2	3:F:4166:LEU:HD13	1.89	0.55
3:I:345:LEU:HB3	3:I:387:ALA:HB1	1.88	0.55
3:I:1498:GLY:HA2	3:I:1501:VAL:HG12	1.89	0.55
3:J:2102:VAL:HG22	3:J:2120:MET:HG3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:2299:VAL:HG12	3:J:2360:LYS:HD2	1.89	0.54
3:C:1291:LEU:HD13	3:C:1595:LEU:HD11	1.88	0.54
3:C:1497:GLY:HA2	3:C:1500:PHE:HD2	1.72	0.54
3:C:3553:LEU:HG	3:C:3593:VAL:HG12	1.88	0.54
1:D:96:ASN:HB3	1:D:117:TRP:CD1	2.41	0.54
3:F:2675:THR:HG23	3:F:2710:LEU:HD13	1.89	0.54
3:I:4056:GLU:HG2	3:I:4166:LEU:HD13	1.89	0.54
3:J:2536:LEU:HD22	3:J:2547:ALA:HB2	1.90	0.54
3:J:2675:THR:HG23	3:J:2710:LEU:HD13	1.89	0.54
7:J:5110:POV:H22A	7:F:5101:POV:H24	1.88	0.54
1:A:96:ASN:HB3	1:A:117:TRP:CD1	2.41	0.54
3:C:345:LEU:HB3	3:C:387:ALA:HB1	1.88	0.54
3:C:2021:CYS:HB2	3:C:2028:ARG:HH12	1.72	0.54
3:C:2299:VAL:HG12	3:C:2360:LYS:HD2	1.89	0.54
3:C:4785:THR:HG22	7:C:5110:POV:H23	1.89	0.54
1:D:8:GLY:HA3	1:D:20:LEU:HD23	1.90	0.54
1:D:9:GLY:HA2	1:D:123:VAL:HA	1.87	0.54
3:F:2977:LEU:HA	3:F:2980:VAL:HG22	1.87	0.54
3:J:2021:CYS:HB2	3:J:2028:ARG:HH12	1.72	0.54
3:J:4785:THR:HG22	7:J:5107:POV:H23	1.89	0.54
3:C:2102:VAL:HG22	3:C:2120:MET:HG3	1.88	0.54
3:C:2573:GLU:HG2	3:C:2618:MET:HE1	1.90	0.54
3:C:2710:LEU:HD12	3:C:2711:PRO:HD2	1.89	0.54
3:F:3730:ALA:O	3:F:3734:HIS:HB2	2.08	0.54
3:I:681:HIS:HB3	3:I:784:SER:HB2	1.88	0.54
3:I:707:VAL:HG23	3:I:713:SER:HB2	1.88	0.54
3:I:2573:GLU:HG2	3:I:2618:MET:HE1	1.90	0.54
3:I:2627:VAL:HG22	3:I:2678:LEU:HB2	1.87	0.54
3:J:698:GLY:H	3:J:1636:MET:HE1	1.73	0.54
3:J:3730:ALA:O	3:J:3734:HIS:HB2	2.08	0.54
3:C:698:GLY:H	3:C:1636:MET:HE1	1.73	0.54
3:F:698:GLY:H	3:F:1636:MET:HE1	1.73	0.54
3:F:2299:VAL:HG12	3:F:2360:LYS:HD2	1.89	0.54
3:I:985:VAL:HA	3:I:988:LEU:HD23	1.89	0.54
3:I:2299:VAL:HG12	3:I:2360:LYS:HD2	1.89	0.54
3:I:2710:LEU:HD12	3:I:2711:PRO:HD2	1.89	0.54
3:I:4231:MET:HA	3:I:4231:MET:HE3	1.90	0.54
3:C:365:LYS:HA	3:C:368:ARG:HE	1.73	0.54
3:C:4056:GLU:HG2	3:C:4166:LEU:HD13	1.89	0.54
7:C:5114:POV:H22A	7:I:5104:POV:H24	1.88	0.54
3:F:887:ILE:HG22	3:F:888:GLU:HG2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:3553:LEU:HG	3:F:3593:VAL:HG12	1.88	0.54
3:J:2651:CYS:HB3	3:J:2654:TYR:HB3	1.89	0.54
3:C:2536:LEU:HD22	3:C:2547:ALA:HB2	1.89	0.54
3:F:2211:MET:HE1	3:F:2229:VAL:HA	1.88	0.54
3:F:4818:MET:HB3	7:F:5108:POV:H14B	1.90	0.54
3:I:365:LYS:HA	3:I:368:ARG:HE	1.73	0.54
3:I:1291:LEU:HD13	3:I:1595:LEU:HD11	1.88	0.54
3:I:2021:CYS:HB2	3:I:2028:ARG:HH12	1.72	0.54
3:I:2032:GLN:O	3:I:2036:GLN:HG2	2.08	0.54
3:I:2536:LEU:HD22	3:I:2547:ALA:HB2	1.89	0.54
3:J:1497:GLY:HA2	3:J:1500:PHE:HD2	1.72	0.54
3:C:2175:GLU:O	3:C:2179:ILE:HG12	2.06	0.54
3:J:2573:GLU:HG2	3:J:2618:MET:HE1	1.90	0.54
3:J:4231:MET:HE3	3:J:4231:MET:HA	1.90	0.54
3:C:2381:GLU:HA	3:C:2384:ILE:HD12	1.90	0.54
3:F:365:LYS:HA	3:F:368:ARG:HE	1.73	0.54
3:F:707:VAL:HG23	3:F:713:SER:HB2	1.89	0.54
1:G:8:GLY:HA3	1:G:20:LEU:HD23	1.90	0.54
3:I:127:MET:H	3:I:127:MET:HE3	1.73	0.54
3:I:698:GLY:H	3:I:1636:MET:HE1	1.73	0.54
3:I:3068:LEU:HG	3:I:3139:VAL:HG11	1.89	0.54
3:J:365:LYS:HA	3:J:368:ARG:HE	1.73	0.54
3:J:985:VAL:HA	3:J:988:LEU:HD23	1.89	0.54
3:J:1444:GLU:HA	3:J:1508:ARG:HE	1.73	0.54
3:J:2381:GLU:HA	3:J:2384:ILE:HD12	1.90	0.54
3:J:4056:GLU:HG2	3:J:4166:LEU:HD13	1.89	0.54
3:C:1208:VAL:HA	3:C:1211:LEU:HB2	1.90	0.54
3:I:3147:ILE:HG23	3:I:3152:PHE:HB2	1.90	0.54
3:J:20:VAL:HG11	3:J:202:MET:HG3	1.88	0.54
3:J:345:LEU:HB3	3:J:387:ALA:HB1	1.88	0.54
3:C:2675:THR:HG23	3:C:2710:LEU:HD13	1.89	0.54
3:C:3730:ALA:O	3:C:3734:HIS:HB2	2.08	0.54
3:F:2573:GLU:HG2	3:F:2618:MET:HE1	1.90	0.54
1:G:2:VAL:HA	1:G:26:GLY:HA3	1.89	0.54
3:I:1444:GLU:HA	3:I:1508:ARG:HE	1.73	0.54
1:K:2:VAL:HA	1:K:26:GLY:HA3	1.89	0.53
2:B:17:LYS:HB2	2:B:20:GLN:HG3	1.90	0.53
3:C:20:VAL:HG11	3:C:202:MET:HG3	1.88	0.53
1:D:2:VAL:HA	1:D:26:GLY:HA3	1.89	0.53
3:F:985:VAL:HA	3:F:988:LEU:HD23	1.89	0.53
3:F:1738:LEU:HB2	3:F:2146:PRO:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:4634:GLU:HG2	3:F:4639:MET:HG3	1.91	0.53
3:I:224:HIS:HA	3:I:388:LEU:HD22	1.90	0.53
3:I:2644:LEU:HD13	3:I:2678:LEU:HD21	1.90	0.53
3:I:2755:ILE:HG22	3:I:2810:LYS:HD3	1.90	0.53
3:J:4818:MET:HB3	7:J:5106:POV:H14B	1.90	0.53
1:A:8:GLY:HA3	1:A:20:LEU:HD23	1.90	0.53
3:C:3068:LEU:HG	3:C:3139:VAL:HG11	1.89	0.53
7:C:5101:POV:H24	7:I:5102:POV:H22A	1.88	0.53
3:F:224:HIS:HA	3:F:388:LEU:HD22	1.91	0.53
3:F:2032:GLN:O	3:F:2036:GLN:HG2	2.08	0.53
3:I:1208:VAL:HA	3:I:1211:LEU:HB2	1.90	0.53
3:I:1690:ASP:HB2	3:I:1693:GLN:HG3	1.90	0.53
3:I:2651:CYS:HB3	3:I:2654:TYR:HB3	1.89	0.53
3:C:3368:ARG:HH22	3:C:3400:VAL:HG13	1.73	0.53
3:F:2536:LEU:HD22	3:F:2547:ALA:HB2	1.90	0.53
3:F:4785:THR:HG22	7:F:5109:POV:H23	1.89	0.53
3:I:1561:VAL:HG12	3:I:1562:ILE:HG23	1.91	0.53
3:I:3730:ALA:O	3:I:3734:HIS:HB2	2.08	0.53
3:I:4818:MET:HB3	7:I:5111:POV:H14B	1.90	0.53
3:J:2032:GLN:O	3:J:2036:GLN:HG2	2.08	0.53
7:J:5112:POV:H24	7:F:5113:POV:H22A	1.88	0.53
3:C:2527:LEU:O	3:C:2531:ARG:HG2	2.09	0.53
3:F:127:MET:HE3	3:F:127:MET:H	1.73	0.53
3:F:1690:ASP:HB2	3:F:1693:GLN:HG3	1.90	0.53
3:F:2458:ARG:HG2	3:F:2510:TYR:CE1	2.44	0.53
3:I:4785:THR:HG22	7:I:5112:POV:H23	1.89	0.53
3:J:797:HIS:HD2	3:J:812:HIS:HB2	1.74	0.53
3:J:1561:VAL:HG12	3:J:1562:ILE:HG23	1.91	0.53
3:J:1690:ASP:HB2	3:J:1693:GLN:HG3	1.90	0.53
3:J:1738:LEU:HB2	3:J:2146:PRO:HD3	1.90	0.53
3:J:2527:LEU:O	3:J:2531:ARG:HG2	2.09	0.53
3:J:2710:LEU:HD12	3:J:2711:PRO:HD2	1.89	0.53
3:F:1444:GLU:HA	3:F:1508:ARG:HE	1.73	0.53
3:F:3202:PRO:HG2	3:F:3203:VAL:HG23	1.91	0.53
3:I:574:VAL:O	3:I:578:ILE:HG12	2.09	0.53
3:I:3368:ARG:HH22	3:I:3400:VAL:HG13	1.74	0.53
3:J:1694:LEU:HB3	3:J:1715:LEU:HD12	1.91	0.53
3:J:3277:LEU:HB3	3:J:3315:LEU:HD11	1.91	0.53
3:F:2355:ARG:O	3:F:2359:ARG:HG2	2.09	0.53
3:F:3368:ARG:HH22	3:F:3400:VAL:HG13	1.74	0.53
3:J:2875:ALA:HB2	3:J:2927:LEU:HD22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:574:VAL:O	3:C:578:ILE:HG12	2.09	0.53
3:C:2032:GLN:O	3:C:2036:GLN:HG2	2.08	0.53
2:E:17:LYS:HB2	2:E:20:GLN:HG3	1.90	0.53
3:F:1694:LEU:HB3	3:F:1715:LEU:HD12	1.91	0.53
3:F:3068:LEU:HG	3:F:3139:VAL:HG11	1.89	0.53
3:I:1694:LEU:HB3	3:I:1715:LEU:HD12	1.91	0.53
3:J:2823:ILE:HD13	3:J:2937:VAL:HG22	1.91	0.53
3:C:127:MET:HE3	3:C:127:MET:H	1.73	0.53
3:C:4634:GLU:HG2	3:C:4639:MET:HG3	1.91	0.53
3:F:844:ARG:HH11	3:F:1196:PRO:HB2	1.74	0.53
3:F:1561:VAL:HG12	3:F:1562:ILE:HG23	1.91	0.53
3:F:2381:GLU:HA	3:F:2384:ILE:HD12	1.90	0.53
3:F:3147:ILE:HG23	3:F:3152:PHE:HB2	1.90	0.53
3:I:2355:ARG:O	3:I:2359:ARG:HG2	2.09	0.53
3:J:404:ILE:HG21	3:J:481:GLU:HG2	1.91	0.53
3:J:418:LEU:HD13	3:J:493:ARG:HB3	1.91	0.53
3:J:1077:ALA:HB3	3:J:1189:LEU:HD22	1.91	0.53
3:J:1208:VAL:HA	3:J:1211:LEU:HB2	1.90	0.53
3:J:2195:PRO:HA	3:J:2198:MET:HB2	1.91	0.53
3:F:404:ILE:HG21	3:F:481:GLU:HG2	1.91	0.53
3:F:4231:MET:HA	3:F:4231:MET:HE3	1.90	0.53
3:I:844:ARG:HH11	3:I:1196:PRO:HB2	1.74	0.53
3:I:2381:GLU:HA	3:I:2384:ILE:HD12	1.90	0.53
3:I:2875:ALA:HB2	3:I:2927:LEU:HD22	1.91	0.53
1:K:8:GLY:HA3	1:K:20:LEU:HD23	1.89	0.53
3:J:574:VAL:O	3:J:578:ILE:HG12	2.09	0.53
3:J:689:THR:HG22	3:J:776:LEU:H	1.74	0.53
3:J:2648:TYR:HD2	3:J:2706:ILE:HA	1.74	0.53
3:J:3202:PRO:HG2	3:J:3203:VAL:HG23	1.90	0.53
3:J:4634:GLU:HG2	3:J:4639:MET:HG3	1.91	0.53
3:C:844:ARG:HH11	3:C:1196:PRO:HB2	1.74	0.53
3:C:1444:GLU:HA	3:C:1508:ARG:HE	1.73	0.53
3:C:1694:LEU:HB3	3:C:1715:LEU:HD12	1.91	0.53
3:C:2967:MET:HE2	3:C:3045:LYS:HB3	1.91	0.53
3:C:4222:VAL:HG11	3:C:4950:VAL:HA	1.91	0.53
3:F:2204:HIS:HB2	3:F:2250:MET:HE1	1.91	0.53
3:F:2527:LEU:O	3:F:2531:ARG:HG2	2.09	0.53
3:F:4222:VAL:HG11	3:F:4950:VAL:HA	1.91	0.53
2:H:17:LYS:HB2	2:H:20:GLN:HG3	1.90	0.53
3:I:205:ILE:HG23	3:I:271:GLY:HA3	1.91	0.53
3:I:2195:PRO:HA	3:I:2198:MET:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:2458:ARG:HG2	3:I:2510:TYR:CE1	2.44	0.53
3:I:4222:VAL:HG11	3:I:4950:VAL:HA	1.91	0.53
3:J:3068:LEU:HG	3:J:3139:VAL:HG11	1.89	0.52
3:J:3147:ILE:HG23	3:J:3152:PHE:HB2	1.90	0.52
3:C:797:HIS:HD2	3:C:812:HIS:HB2	1.74	0.52
3:C:1619:ARG:HA	3:C:1626:TRP:HA	1.92	0.52
3:C:1639:LEU:HB3	3:C:1648:MET:HG3	1.91	0.52
3:C:2644:LEU:HD13	3:C:2678:LEU:HD21	1.90	0.52
3:C:4017:LEU:HD22	3:C:4139:ILE:HG21	1.91	0.52
3:F:689:THR:HG22	3:F:776:LEU:H	1.74	0.52
3:F:2867:LEU:HD13	3:F:2928:LYS:HZ2	1.74	0.52
3:I:2823:ILE:HD13	3:I:2937:VAL:HG22	1.91	0.52
3:I:3277:LEU:HB3	3:I:3315:LEU:HD11	1.91	0.52
3:J:224:HIS:HA	3:J:388:LEU:HD22	1.91	0.52
3:J:2755:ILE:HG22	3:J:2810:LYS:HD3	1.90	0.52
3:J:4222:VAL:HG11	3:J:4950:VAL:HA	1.91	0.52
3:C:2204:HIS:HB2	3:C:2250:MET:HE1	1.91	0.52
3:C:2764:GLU:HG2	3:C:2855:TYR:HA	1.91	0.52
3:F:2195:PRO:HA	3:F:2198:MET:HB2	1.91	0.52
3:F:2967:MET:HE2	3:F:3045:LYS:HB3	1.91	0.52
3:I:1738:LEU:HB2	3:I:2146:PRO:HD3	1.90	0.52
3:J:2867:LEU:HD13	3:J:2928:LYS:HZ2	1.74	0.52
3:C:1970:GLN:HG2	3:C:3642:TYR:HA	1.92	0.52
3:C:4231:MET:HA	3:C:4231:MET:HE3	1.90	0.52
3:F:372:LEU:HD12	3:F:374:LYS:HG3	1.91	0.52
3:I:418:LEU:HD13	3:I:493:ARG:HB3	1.91	0.52
3:I:689:THR:HG22	3:I:776:LEU:H	1.74	0.52
3:I:3459:VAL:HA	3:I:3464:ILE:HB	1.91	0.52
3:J:882:TRP:CZ3	3:J:905:PRO:HA	2.44	0.52
3:J:1447:CYS:HB3	3:J:1555:LEU:HB3	1.92	0.52
3:J:1619:ARG:HA	3:J:1626:TRP:HA	1.92	0.52
2:B:29:MET:HA	2:B:35:LYS:HA	1.92	0.52
3:C:224:HIS:HA	3:C:388:LEU:HD22	1.91	0.52
3:C:404:ILE:HG21	3:C:481:GLU:HG2	1.91	0.52
3:C:1944:GLU:HB2	3:C:2123:LEU:HD21	1.92	0.52
3:C:3202:PRO:HG2	3:C:3203:VAL:HG23	1.91	0.52
3:C:4818:MET:HB3	7:C:5109:POV:H14B	1.90	0.52
3:F:574:VAL:O	3:F:578:ILE:HG12	2.09	0.52
3:F:2644:LEU:HD13	3:F:2678:LEU:HD21	1.90	0.52
3:I:404:ILE:HG21	3:I:481:GLU:HG2	1.91	0.52
3:J:372:LEU:HD12	3:J:374:LYS:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1944:GLU:HB2	3:J:2123:LEU:HD21	1.92	0.52
3:J:2644:LEU:HD13	3:J:2678:LEU:HD21	1.90	0.52
3:C:2755:ILE:HG22	3:C:2810:LYS:HD3	1.90	0.52
3:C:3459:VAL:HA	3:C:3464:ILE:HB	1.91	0.52
3:F:205:ILE:HG23	3:F:271:GLY:HA3	1.91	0.52
3:F:418:LEU:HD13	3:F:493:ARG:HB3	1.91	0.52
3:F:1639:LEU:HB3	3:F:1648:MET:HG3	1.91	0.52
3:F:1970:GLN:HG2	3:F:3642:TYR:HA	1.92	0.52
3:F:2764:GLU:HG2	3:F:2855:TYR:HA	1.91	0.52
3:I:234:SER:HB2	3:I:242:ARG:HA	1.92	0.52
3:I:1447:CYS:HB3	3:I:1555:LEU:HB3	1.92	0.52
1:K:38:ARG:HA	1:K:93:TYR:HA	1.92	0.52
2:L:17:LYS:HB2	2:L:20:GLN:HG3	1.90	0.52
3:J:205:ILE:HG23	3:J:271:GLY:HA3	1.91	0.52
3:J:234:SER:HB2	3:J:242:ARG:HA	1.92	0.52
3:C:418:LEU:HD13	3:C:493:ARG:HB3	1.91	0.52
3:C:1561:VAL:HG12	3:C:1562:ILE:HG23	1.90	0.52
3:F:234:SER:HB2	3:F:242:ARG:HA	1.92	0.52
3:F:1077:ALA:HB3	3:F:1189:LEU:HD22	1.91	0.52
3:F:3459:VAL:HA	3:F:3464:ILE:HB	1.91	0.52
1:G:38:ARG:HA	1:G:93:TYR:HA	1.92	0.52
3:I:797:HIS:HD2	3:I:812:HIS:HB2	1.74	0.52
3:I:1944:GLU:HB2	3:I:2123:LEU:HD21	1.92	0.52
3:J:5026:ASP:HA	3:J:5030:LYS:HD2	1.92	0.52
3:C:4785:THR:HG21	7:C:5111:POV:H2	1.91	0.52
3:C:5026:ASP:HA	3:C:5030:LYS:HD2	1.92	0.52
3:F:1944:GLU:HB2	3:F:2123:LEU:HD21	1.92	0.52
3:F:2875:ALA:HB2	3:F:2927:LEU:HD22	1.91	0.52
3:F:5026:ASP:HA	3:F:5030:LYS:HD2	1.92	0.52
3:I:1077:ALA:HB3	3:I:1189:LEU:HD22	1.91	0.52
3:I:2204:HIS:HB2	3:I:2250:MET:HE1	1.91	0.52
3:I:2648:TYR:HD2	3:I:2706:ILE:HA	1.74	0.52
3:I:3548:GLU:HG2	3:I:3552:PHE:CE2	2.45	0.52
3:J:844:ARG:HH11	3:J:1196:PRO:HB2	1.74	0.52
3:J:2458:ARG:HG2	3:J:2510:TYR:CE1	2.44	0.52
3:C:1077:ALA:HB3	3:C:1189:LEU:HD22	1.91	0.52
3:C:1738:LEU:HB2	3:C:2146:PRO:HD3	1.90	0.52
3:C:2195:PRO:HA	3:C:2198:MET:HB2	1.91	0.52
3:C:2648:TYR:HD2	3:C:2706:ILE:HA	1.74	0.52
3:C:2823:ILE:HD13	3:C:2937:VAL:HG22	1.91	0.52
3:C:3147:ILE:HG23	3:C:3152:PHE:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3529:ASP:HB3	3:C:3596:VAL:HG22	1.92	0.52
3:F:1619:ARG:HA	3:F:1626:TRP:HA	1.91	0.52
3:F:4658:ILE:HG13	3:F:4796:MET:HE3	1.92	0.52
3:I:3202:PRO:HG2	3:I:3203:VAL:HG23	1.90	0.52
3:I:4785:THR:HG21	7:I:5113:POV:H2	1.91	0.52
3:I:5026:ASP:HA	3:I:5030:LYS:HD2	1.92	0.52
3:J:2355:ARG:O	3:J:2359:ARG:HG2	2.09	0.52
3:J:4017:LEU:HD22	3:J:4139:ILE:HG21	1.91	0.52
3:C:1690:ASP:HB2	3:C:1693:GLN:HG3	1.90	0.52
7:C:5107:POV:H1	7:C:5108:POV:H13B	1.92	0.52
3:F:2823:ILE:HD13	3:F:2937:VAL:HG22	1.91	0.52
3:F:4017:LEU:HD22	3:F:4139:ILE:HG21	1.91	0.52
3:I:1475:THR:HA	3:I:1486:SER:HA	1.92	0.52
3:I:2967:MET:HE2	3:I:3045:LYS:HB3	1.91	0.52
3:J:127:MET:HE3	3:J:127:MET:H	1.73	0.52
3:J:3368:ARG:HH22	3:J:3400:VAL:HG13	1.73	0.52
3:J:3459:VAL:HA	3:J:3464:ILE:HB	1.91	0.52
3:C:2458:ARG:HG2	3:C:2510:TYR:CE1	2.44	0.52
7:C:5113:POV:H13B	7:F:5107:POV:H1	1.92	0.52
3:F:131:LEU:HD11	3:I:2460:LEU:HD23	1.92	0.52
3:F:1208:VAL:HA	3:F:1211:LEU:HB2	1.90	0.52
3:F:3277:LEU:HB3	3:F:3315:LEU:HD11	1.91	0.52
3:I:919:ASN:HA	3:I:922:LEU:HD13	1.92	0.52
3:I:2527:LEU:O	3:I:2531:ARG:HG2	2.09	0.52
3:I:4000:MET:HE1	3:I:4058:ILE:HG23	1.92	0.52
3:I:4017:LEU:HD22	3:I:4139:ILE:HG21	1.91	0.52
1:K:71:ARG:HB2	1:K:78:VAL:HG22	1.92	0.51
2:L:29:MET:HA	2:L:35:LYS:HA	1.92	0.51
3:J:1970:GLN:HG2	3:J:3642:TYR:HA	1.92	0.51
3:J:2204:HIS:HB2	3:J:2250:MET:HE1	1.91	0.51
3:J:2799:GLU:HA	3:J:2802:LYS:HB2	1.92	0.51
1:A:38:ARG:HA	1:A:93:TYR:HA	1.92	0.51
3:F:797:HIS:HD2	3:F:812:HIS:HB2	1.74	0.51
3:F:1804:LEU:HD12	3:F:1853:ILE:HG13	1.92	0.51
3:F:3262:ARG:HE	3:F:3329:ILE:HG13	1.75	0.51
3:F:3529:ASP:HB3	3:F:3596:VAL:HG22	1.92	0.51
1:G:71:ARG:HB2	1:G:78:VAL:HG22	1.92	0.51
2:H:29:MET:HA	2:H:35:LYS:HA	1.92	0.51
3:I:4634:GLU:HG2	3:I:4639:MET:HG3	1.91	0.51
3:J:131:LEU:HD11	3:C:2460:LEU:HD23	1.92	0.51
3:J:3262:ARG:HE	3:J:3329:ILE:HG13	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:3548:GLU:HG2	3:J:3552:PHE:CE2	2.45	0.51
3:J:4000:MET:HE1	3:J:4058:ILE:HG23	1.92	0.51
3:C:1102:VAL:HG11	3:C:1149:VAL:HG21	1.92	0.51
3:C:2355:ARG:O	3:C:2359:ARG:HG2	2.09	0.51
1:D:71:ARG:HB2	1:D:78:VAL:HG22	1.92	0.51
3:F:1102:VAL:HG11	3:F:1149:VAL:HG21	1.92	0.51
3:F:4000:MET:HE1	3:F:4058:ILE:HG23	1.92	0.51
3:I:1619:ARG:HA	3:I:1626:TRP:HA	1.92	0.51
3:I:1639:LEU:HB3	3:I:1648:MET:HG3	1.91	0.51
3:I:4567:LEU:HD13	3:I:4815:ASP:HB3	1.93	0.51
1:K:51:ILE:HG22	1:K:57:ILE:HA	1.93	0.51
3:J:1639:LEU:HB3	3:J:1648:MET:HG3	1.91	0.51
3:J:1804:LEU:HD12	3:J:1853:ILE:HG13	1.92	0.51
3:J:2764:GLU:HG2	3:J:2855:TYR:HA	1.91	0.51
3:J:3037:GLU:HB2	3:J:3088:VAL:HG11	1.93	0.51
3:J:4567:LEU:HD13	3:J:4815:ASP:HB3	1.93	0.51
3:J:4658:ILE:HG13	3:J:4796:MET:HE3	1.92	0.51
3:J:4785:THR:HG21	7:J:5108:POV:H2	1.91	0.51
1:A:65:GLY:H	1:A:67:PHE:HE1	1.59	0.51
3:C:205:ILE:HG22	3:C:207:SER:H	1.75	0.51
3:C:2875:ALA:HB2	3:C:2927:LEU:HD22	1.91	0.51
3:F:2799:GLU:HA	3:F:2802:LYS:HB2	1.92	0.51
3:F:4785:THR:HG21	7:F:5110:POV:H2	1.91	0.51
1:G:51:ILE:HG22	1:G:57:ILE:HA	1.93	0.51
3:I:372:LEU:HD12	3:I:374:LYS:HG3	1.91	0.51
3:I:3015:LEU:HG	3:I:3026:GLY:HA2	1.93	0.51
3:I:3320:LEU:HD23	3:I:3357:HIS:HB3	1.93	0.51
3:J:205:ILE:HG22	3:J:207:SER:H	1.76	0.51
3:J:670:GLU:HA	3:J:740:PRO:HB3	1.92	0.51
3:C:3548:GLU:HG2	3:C:3552:PHE:CE2	2.45	0.51
1:D:38:ARG:HA	1:D:93:TYR:HA	1.91	0.51
3:F:2755:ILE:HG22	3:F:2810:LYS:HD3	1.90	0.51
3:F:3548:GLU:HG2	3:F:3552:PHE:CE2	2.45	0.51
3:F:4567:LEU:HD13	3:F:4815:ASP:HB3	1.93	0.51
1:G:65:GLY:H	1:G:67:PHE:HE1	1.59	0.51
3:I:1970:GLN:HG2	3:I:3642:TYR:HA	1.92	0.51
3:I:2764:GLU:HG2	3:I:2855:TYR:HA	1.91	0.51
3:J:1286:MET:HE2	3:J:1464:PHE:HB3	1.92	0.51
1:A:111:ASN:HA	1:A:114:TYR:HB3	1.93	0.51
3:C:1804:LEU:HD12	3:C:1853:ILE:HG13	1.92	0.51
3:C:2604:GLU:HG2	3:C:2639:MET:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3277:LEU:HB3	3:C:3315:LEU:HD11	1.91	0.51
3:F:1475:THR:HA	3:F:1486:SER:HA	1.92	0.51
3:F:2648:TYR:HD2	3:F:2706:ILE:HA	1.74	0.51
3:F:3320:LEU:HD23	3:F:3357:HIS:HB3	1.93	0.51
1:A:71:ARG:HB2	1:A:78:VAL:HG22	1.93	0.51
1:A:82:MET:HA	1:A:82:MET:HE3	1.92	0.51
3:C:551:LEU:HB3	3:C:589:LEU:HD21	1.93	0.51
3:C:670:GLU:HA	3:C:740:PRO:HB3	1.92	0.51
3:C:1447:CYS:HB3	3:C:1555:LEU:HB3	1.92	0.51
1:D:65:GLY:H	1:D:67:PHE:HE1	1.59	0.51
3:I:3262:ARG:HE	3:I:3329:ILE:HG13	1.75	0.51
3:J:2967:MET:HE2	3:J:3045:LYS:HB3	1.91	0.51
1:A:51:ILE:HG22	1:A:57:ILE:HA	1.93	0.51
3:C:205:ILE:HG23	3:C:271:GLY:HA3	1.91	0.51
3:C:689:THR:HG22	3:C:776:LEU:H	1.74	0.51
3:C:3037:GLU:HB2	3:C:3088:VAL:HG11	1.93	0.51
3:C:4000:MET:HE1	3:C:4058:ILE:HG23	1.92	0.51
3:C:4567:LEU:HD13	3:C:4815:ASP:HB3	1.93	0.51
3:C:4658:ILE:HG13	3:C:4796:MET:HE3	1.92	0.51
3:F:551:LEU:HD11	3:F:564:LEU:HD22	1.93	0.51
3:F:551:LEU:HB3	3:F:589:LEU:HD21	1.93	0.51
3:F:1286:MET:HE2	3:F:1464:PHE:HB3	1.92	0.51
3:I:235:ALA:HB3	3:I:238:SER:HB2	1.93	0.51
3:I:1717:SER:HA	3:I:1721:GLU:HB2	1.93	0.51
3:J:1717:SER:HA	3:J:1721:GLU:HB2	1.93	0.51
1:A:107:TRP:CZ2	3:C:924:MET:SD	3.04	0.51
3:C:3198:ALA:HA	3:C:3201:MET:HE2	1.93	0.51
3:C:3263:TYR:HD2	3:C:3332:ALA:HA	1.74	0.51
3:F:1037:ASP:O	3:F:1041:GLN:HG2	2.11	0.51
3:F:3176:GLY:HA3	3:F:3268:HIS:CE1	2.46	0.51
7:F:5112:POV:H13B	7:I:5110:POV:H1	1.92	0.51
3:I:205:ILE:HG22	3:I:207:SER:H	1.76	0.51
3:I:667:MET:HB2	3:I:743:VAL:HA	1.93	0.51
3:C:551:LEU:HD11	3:C:564:LEU:HD22	1.92	0.51
3:C:1037:ASP:O	3:C:1041:GLN:HG2	2.11	0.51
3:C:1475:THR:HA	3:C:1486:SER:HA	1.92	0.51
3:C:3951:PHE:O	3:C:3955:MET:HB2	2.11	0.51
1:D:51:ILE:HG22	1:D:57:ILE:HA	1.93	0.51
1:G:69:ILE:HB	1:G:80:LEU:HD13	1.92	0.51
2:H:61:GLU:O	2:H:65:GLN:HB2	2.10	0.51
3:I:2660:GLY:HA2	3:I:2666:VAL:HG13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3951:PHE:O	3:I:3955:MET:HB2	2.11	0.51
3:J:907:LEU:H	3:J:960:MET:HE3	1.76	0.51
3:J:2821:TRP:HZ3	3:J:2878:LEU:HD13	1.77	0.51
3:J:3176:GLY:HA3	3:J:3268:HIS:CE1	2.46	0.51
2:B:61:GLU:O	2:B:65:GLN:HB2	2.11	0.51
3:C:234:SER:HB2	3:C:242:ARG:HA	1.92	0.51
3:C:1078:GLU:CD	3:C:1237:TRP:HE1	2.19	0.51
3:C:1119:GLU:HB3	3:C:1134:LEU:HD22	1.93	0.51
2:E:29:MET:HA	2:E:35:LYS:HA	1.92	0.51
3:F:1078:GLU:CD	3:F:1237:TRP:HE1	2.19	0.51
3:F:2660:GLY:HA2	3:F:2666:VAL:HG13	1.93	0.51
3:I:1078:GLU:CD	3:I:1237:TRP:HE1	2.19	0.51
3:I:2816:MET:HG3	3:I:2878:LEU:HD22	1.93	0.51
3:I:3176:GLY:HA3	3:I:3268:HIS:CE1	2.46	0.51
3:I:3263:TYR:HD2	3:I:3332:ALA:HA	1.75	0.51
3:J:3015:LEU:HG	3:J:3026:GLY:HA2	1.93	0.50
3:J:3263:TYR:HD2	3:J:3332:ALA:HA	1.75	0.50
3:J:3320:LEU:HD23	3:J:3357:HIS:HB3	1.93	0.50
3:J:3529:ASP:HB3	3:J:3596:VAL:HG22	1.92	0.50
3:C:575:LEU:HD22	3:C:606:LEU:HA	1.94	0.50
3:F:20:VAL:HG22	3:F:204:PRO:HB3	1.94	0.50
3:F:205:ILE:HG22	3:F:207:SER:H	1.75	0.50
3:F:2816:MET:HG3	3:F:2878:LEU:HD22	1.93	0.50
3:F:3590:GLU:O	3:F:3594:ARG:HG2	2.11	0.50
3:I:575:LEU:HD22	3:I:606:LEU:HA	1.94	0.50
3:I:1804:LEU:HD12	3:I:1853:ILE:HG13	1.92	0.50
1:K:111:ASN:HA	1:K:114:TYR:HB3	1.93	0.50
2:L:61:GLU:O	2:L:65:GLN:HB2	2.11	0.50
3:J:262:LEU:HD12	3:J:280:LEU:HD13	1.93	0.50
7:J:5105:POV:H1	7:I:5101:POV:H13B	1.92	0.50
7:J:5105:POV:H37	7:I:5101:POV:H37A	1.94	0.50
3:C:20:VAL:HG22	3:C:204:PRO:HB3	1.94	0.50
3:C:2799:GLU:HA	3:C:2802:LYS:HB2	1.92	0.50
3:F:2604:GLU:HG2	3:F:2639:MET:HG3	1.93	0.50
3:F:3263:TYR:HD2	3:F:3332:ALA:HA	1.74	0.50
3:I:3104:GLU:HA	3:I:3107:VAL:HG22	1.93	0.50
3:J:1119:GLU:HB3	3:J:1134:LEU:HD22	1.93	0.50
3:J:2460:LEU:HD23	3:I:131:LEU:HD11	1.93	0.50
1:A:69:ILE:HB	1:A:80:LEU:HD13	1.92	0.50
3:C:372:LEU:HD12	3:C:374:LYS:HG3	1.91	0.50
3:C:1286:MET:HE2	3:C:1464:PHE:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3104:GLU:HA	3:C:3107:VAL:HG22	1.93	0.50
7:C:5113:POV:H37A	7:F:5107:POV:H37	1.94	0.50
1:D:111:ASN:HA	1:D:114:TYR:HB3	1.93	0.50
2:E:66:MET:HE1	2:E:101:VAL:HB	1.93	0.50
3:F:235:ALA:HB3	3:F:238:SER:HB2	1.93	0.50
3:F:919:ASN:HA	3:F:922:LEU:HD13	1.92	0.50
3:F:1741:GLU:O	3:F:1745:ILE:HG12	2.12	0.50
3:F:1974:ARG:HH21	3:F:3642:TYR:HB2	1.76	0.50
3:I:341:TYR:CZ	3:I:392:ARG:HB2	2.47	0.50
3:I:551:LEU:HB3	3:I:589:LEU:HD21	1.93	0.50
3:I:1102:VAL:HG11	3:I:1149:VAL:HG21	1.92	0.50
2:L:40:ARG:CZ	3:J:674:PHE:HD2	2.25	0.50
3:J:551:LEU:HD11	3:J:564:LEU:HD22	1.92	0.50
3:J:1102:VAL:HG11	3:J:1149:VAL:HG21	1.92	0.50
3:J:3951:PHE:O	3:J:3955:MET:HB2	2.11	0.50
3:C:2867:LEU:HD13	3:C:2928:LYS:HZ2	1.76	0.50
3:C:3320:LEU:HD23	3:C:3357:HIS:HB3	1.93	0.50
3:F:882:TRP:CZ3	3:F:905:PRO:HA	2.44	0.50
3:F:1447:CYS:HB3	3:F:1555:LEU:HB3	1.92	0.50
3:F:3015:LEU:HG	3:F:3026:GLY:HA2	1.93	0.50
3:F:3198:ALA:HA	3:F:3201:MET:HE2	1.93	0.50
3:F:3368:ARG:O	3:F:3372:VAL:HG23	2.12	0.50
1:G:106:PRO:HB3	3:I:878:ILE:HG13	1.94	0.50
3:I:20:VAL:HG22	3:I:204:PRO:HB3	1.94	0.50
3:I:1694:LEU:HD11	3:I:1718:ILE:HD11	1.94	0.50
3:I:2867:LEU:HD13	3:I:2928:LYS:HZ2	1.77	0.50
3:I:4658:ILE:HG13	3:I:4796:MET:HE3	1.92	0.50
3:J:1078:GLU:CD	3:J:1237:TRP:HE1	2.19	0.50
3:J:2628:PHE:CZ	3:J:2735:PHE:HB2	2.47	0.50
3:J:3198:ALA:HA	3:J:3201:MET:HE2	1.93	0.50
3:J:3368:ARG:O	3:J:3372:VAL:HG23	2.12	0.50
3:C:919:ASN:HA	3:C:922:LEU:HD13	1.92	0.50
3:C:3262:ARG:HE	3:C:3329:ILE:HG13	1.75	0.50
3:C:3368:ARG:O	3:C:3372:VAL:HG23	2.12	0.50
3:F:262:LEU:HD12	3:F:280:LEU:HD13	1.93	0.50
3:F:1717:SER:HA	3:F:1721:GLU:HB2	1.93	0.50
1:G:82:MET:HA	1:G:82:MET:HE3	1.92	0.50
2:H:66:MET:HE1	2:H:101:VAL:HB	1.93	0.50
3:I:3368:ARG:O	3:I:3372:VAL:HG23	2.11	0.50
3:I:3590:GLU:O	3:I:3594:ARG:HG2	2.12	0.50
1:K:65:GLY:H	1:K:67:PHE:HE1	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:341:TYR:CZ	3:J:392:ARG:HB2	2.47	0.50
3:J:575:LEU:HD22	3:J:606:LEU:HA	1.94	0.50
3:J:3532:LEU:HD21	3:J:3560:GLN:HA	1.93	0.50
3:C:341:TYR:CZ	3:C:392:ARG:HB2	2.47	0.50
3:C:2010:LEU:HD22	3:C:3656:SER:HB2	1.94	0.50
1:D:82:MET:HA	1:D:82:MET:HE3	1.92	0.50
3:F:667:MET:HB2	3:F:743:VAL:HA	1.93	0.50
3:F:2230:THR:HA	3:F:2270:SER:HB2	1.93	0.50
3:F:3037:GLU:HB2	3:F:3088:VAL:HG11	1.93	0.50
7:F:5112:POV:H37A	7:I:5110:POV:H37	1.94	0.50
3:I:670:GLU:HG2	3:I:788:LYS:HB3	1.93	0.50
3:J:667:MET:HB2	3:J:743:VAL:HA	1.93	0.50
3:J:1694:LEU:HD11	3:J:1718:ILE:HD11	1.94	0.50
3:J:2816:MET:HG3	3:J:2878:LEU:HD22	1.93	0.50
3:J:3854:GLU:HG2	3:J:3867:ASN:HD21	1.77	0.50
3:C:1974:ARG:HH21	3:C:3642:TYR:HB2	1.76	0.50
3:C:2821:TRP:HZ3	3:C:2878:LEU:HD13	1.77	0.50
3:C:3532:LEU:HD21	3:C:3560:GLN:HA	1.93	0.50
2:E:49:ARG:HD2	2:E:52:LYS:HG3	1.94	0.50
3:F:1448:VAL:HG12	3:F:1554:VAL:HG23	1.93	0.50
3:F:3854:GLU:HG2	3:F:3867:ASN:HD21	1.77	0.50
3:I:1119:GLU:HB3	3:I:1134:LEU:HD22	1.93	0.50
3:I:2628:PHE:CZ	3:I:2735:PHE:HB2	2.47	0.50
3:I:4858:PHE:HZ	7:I:5101:POV:H37	1.77	0.50
2:L:7:ILE:HD11	2:L:73:LYS:HB2	1.94	0.50
3:J:1475:THR:HA	3:J:1486:SER:HA	1.92	0.50
3:J:2010:LEU:HD22	3:J:3656:SER:HB2	1.94	0.50
3:J:4858:PHE:HZ	7:C:5108:POV:H37	1.77	0.50
3:C:262:LEU:HD12	3:C:280:LEU:HD13	1.93	0.50
3:C:1815:LEU:HD22	3:C:1845:VAL:HG21	1.94	0.50
3:C:3176:GLY:HA3	3:C:3268:HIS:CE1	2.46	0.50
3:C:3854:GLU:HG2	3:C:3867:ASN:HD21	1.77	0.50
3:C:3965:LEU:HD23	3:C:3968:TYR:HD2	1.77	0.50
3:C:4858:PHE:HZ	7:C:5113:POV:H37	1.77	0.50
3:F:575:LEU:HD22	3:F:606:LEU:HA	1.94	0.50
3:F:1119:GLU:HB3	3:F:1134:LEU:HD22	1.93	0.50
3:F:4567:LEU:HD21	3:F:4816:ILE:HG22	1.94	0.50
3:F:4858:PHE:HZ	7:F:5112:POV:H37	1.77	0.50
3:I:670:GLU:HA	3:I:740:PRO:HB3	1.92	0.50
3:I:1286:MET:HE2	3:I:1464:PHE:HB3	1.92	0.50
3:I:3529:ASP:HB3	3:I:3596:VAL:HG22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3547:GLU:O	3:I:3551:GLU:HG2	2.12	0.50
3:J:3104:GLU:HA	3:J:3107:VAL:HG22	1.93	0.50
2:B:66:MET:HE1	2:B:101:VAL:HB	1.93	0.50
3:C:1448:VAL:HG12	3:C:1554:VAL:HG23	1.93	0.50
3:C:2628:PHE:CZ	3:C:2735:PHE:HB2	2.47	0.50
3:C:3015:LEU:HG	3:C:3026:GLY:HA2	1.93	0.50
1:D:69:ILE:HB	1:D:80:LEU:HD13	1.92	0.50
3:F:907:LEU:H	3:F:960:MET:HE3	1.77	0.50
3:F:974:HIS:CE1	3:F:976:ARG:HH22	2.30	0.50
2:H:49:ARG:HD2	2:H:52:LYS:HG3	1.94	0.50
3:I:262:LEU:HD12	3:I:280:LEU:HD13	1.93	0.50
1:K:69:ILE:HB	1:K:80:LEU:HD13	1.92	0.49
3:J:20:VAL:HG22	3:J:204:PRO:HB3	1.94	0.49
3:J:235:ALA:HB3	3:J:238:SER:HB2	1.93	0.49
3:J:1448:VAL:HG12	3:J:1554:VAL:HG23	1.93	0.49
3:J:2604:GLU:HG2	3:J:2639:MET:HG3	1.93	0.49
3:J:3590:GLU:O	3:J:3594:ARG:HG2	2.11	0.49
3:J:4242:ILE:HG12	3:J:4993:MET:HE2	1.94	0.49
3:J:4567:LEU:HD21	3:J:4816:ILE:HG22	1.94	0.49
3:C:907:LEU:H	3:C:960:MET:HE3	1.77	0.49
3:C:1717:SER:HA	3:C:1721:GLU:HB2	1.93	0.49
3:C:2816:MET:HG3	3:C:2878:LEU:HD22	1.93	0.49
7:C:5107:POV:H37	7:C:5108:POV:H37A	1.94	0.49
2:E:61:GLU:O	2:E:65:GLN:HB2	2.11	0.49
3:F:3219:TYR:HE2	3:F:3236:VAL:HG23	1.77	0.49
3:F:3951:PHE:O	3:F:3955:MET:HB2	2.11	0.49
3:I:551:LEU:HD11	3:I:564:LEU:HD22	1.93	0.49
3:I:2799:GLU:HA	3:I:2802:LYS:HB2	1.92	0.49
3:I:2821:TRP:HZ3	3:I:2878:LEU:HD13	1.76	0.49
3:I:3198:ALA:HA	3:I:3201:MET:HE2	1.93	0.49
3:I:3532:LEU:HD21	3:I:3560:GLN:HA	1.93	0.49
3:J:1815:LEU:HD22	3:J:1845:VAL:HG21	1.94	0.49
3:J:2230:THR:HA	3:J:2270:SER:HB2	1.93	0.49
3:J:2641:LEU:HD11	3:J:2698:MET:HG3	1.94	0.49
3:C:720:HIS:HB3	3:C:729:PRO:HA	1.94	0.49
3:C:3590:GLU:O	3:C:3594:ARG:HG2	2.11	0.49
3:C:4014:LYS:HG2	3:C:4135:PRO:HB3	1.95	0.49
3:C:4790:LEU:HD21	7:C:5110:POV:H23A	1.94	0.49
1:D:67:PHE:CD1	1:D:82:MET:HE1	2.47	0.49
1:G:111:ASN:HA	1:G:114:TYR:HB3	1.93	0.49
3:I:882:TRP:CZ3	3:I:905:PRO:HA	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1448:VAL:HG12	3:I:1554:VAL:HG23	1.93	0.49
3:I:1974:ARG:HH21	3:I:3642:TYR:HB2	1.76	0.49
3:I:2604:GLU:HG2	3:I:2639:MET:HG3	1.93	0.49
3:I:4242:ILE:HG12	3:I:4993:MET:HE2	1.94	0.49
1:K:82:MET:HA	1:K:82:MET:HE3	1.92	0.49
3:J:919:ASN:HA	3:J:922:LEU:HD13	1.92	0.49
3:J:1730:MET:HE3	3:J:1773:PRO:HG3	1.94	0.49
3:J:2660:GLY:HA2	3:J:2666:VAL:HG13	1.93	0.49
3:J:3107:VAL:HA	3:J:3175:LEU:HD21	1.95	0.49
3:J:3547:GLU:O	3:J:3551:GLU:HG2	2.12	0.49
3:C:131:LEU:HD11	3:F:2460:LEU:HD23	1.93	0.49
3:F:341:TYR:CZ	3:F:392:ARG:HB2	2.47	0.49
3:F:1815:LEU:HG	3:F:1865:MET:HE3	1.94	0.49
3:F:1819:VAL:HG22	3:F:1926:LEU:HD13	1.94	0.49
3:F:2628:PHE:CZ	3:F:2735:PHE:HB2	2.47	0.49
3:F:2821:TRP:HZ3	3:F:2878:LEU:HD13	1.77	0.49
3:F:4790:LEU:HD21	7:F:5109:POV:H23A	1.94	0.49
3:J:3965:LEU:HD23	3:J:3968:TYR:HD2	1.77	0.49
3:C:235:ALA:HB3	3:C:238:SER:HB2	1.93	0.49
3:C:667:MET:HB2	3:C:743:VAL:HA	1.93	0.49
3:C:974:HIS:CE1	3:C:976:ARG:HH22	2.30	0.49
3:C:1674:CYS:HB3	3:C:1685:LEU:HD12	1.95	0.49
3:C:2230:THR:HA	3:C:2270:SER:HB2	1.93	0.49
3:F:3547:GLU:O	3:F:3551:GLU:HG2	2.12	0.49
3:F:3965:LEU:HD23	3:F:3968:TYR:HD2	1.77	0.49
3:I:907:LEU:H	3:I:960:MET:HE3	1.76	0.49
3:I:1730:MET:HE3	3:I:1773:PRO:HG3	1.94	0.49
3:J:551:LEU:HB3	3:J:589:LEU:HD21	1.93	0.49
3:J:4014:LYS:HG2	3:J:4135:PRO:HB3	1.95	0.49
3:C:1730:MET:HE3	3:C:1773:PRO:HG3	1.94	0.49
3:C:3219:TYR:HE2	3:C:3236:VAL:HG23	1.77	0.49
3:F:670:GLU:HA	3:F:740:PRO:HB3	1.92	0.49
3:F:1674:CYS:HB3	3:F:1685:LEU:HD12	1.95	0.49
3:F:3104:GLU:HA	3:F:3107:VAL:HG22	1.93	0.49
3:I:4014:LYS:HG2	3:I:4135:PRO:HB3	1.95	0.49
2:L:42:ARG:HH22	3:J:1782:PHE:HE2	1.59	0.49
3:J:1037:ASP:O	3:J:1041:GLN:HG2	2.11	0.49
3:J:1974:ARG:HH21	3:J:3642:TYR:HB2	1.76	0.49
3:J:3226:GLU:HA	3:J:3229:ILE:HG12	1.94	0.49
2:B:49:ARG:HD2	2:B:52:LYS:HG3	1.94	0.49
3:C:670:GLU:HG2	3:C:788:LYS:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1815:LEU:HG	3:C:1865:MET:HE3	1.94	0.49
3:C:2660:GLY:HA2	3:C:2666:VAL:HG13	1.93	0.49
2:E:7:ILE:HD11	2:E:73:LYS:HB2	1.94	0.49
3:I:3037:GLU:HB2	3:I:3088:VAL:HG11	1.93	0.49
3:I:4567:LEU:HD21	3:I:4816:ILE:HG22	1.94	0.49
2:L:3:GLU:HB3	2:L:75:THR:HB	1.95	0.49
3:J:3219:TYR:HE2	3:J:3236:VAL:HG23	1.77	0.49
3:C:1741:GLU:O	3:C:1745:ILE:HG12	2.12	0.49
3:C:3107:VAL:HA	3:C:3175:LEU:HD21	1.95	0.49
3:F:1815:LEU:HD22	3:F:1845:VAL:HG21	1.94	0.49
3:F:2002:PRO:HD2	3:F:3863:GLY:HA2	1.95	0.49
3:I:1242:LEU:HD22	3:I:1243:PRO:HD2	1.95	0.49
3:I:1674:CYS:HB3	3:I:1685:LEU:HD12	1.95	0.49
3:I:2230:THR:HA	3:I:2270:SER:HB2	1.93	0.49
3:J:1674:CYS:HB3	3:J:1685:LEU:HD12	1.95	0.49
3:J:4790:LEU:HD21	7:J:5107:POV:H23A	1.94	0.49
3:C:1819:VAL:HG22	3:C:1926:LEU:HD13	1.94	0.49
3:C:2310:CYS:HB2	3:C:2324:ASN:HB3	1.95	0.49
3:C:2964:LEU:HD13	3:C:3038:MET:HE2	1.94	0.49
3:C:3547:GLU:O	3:C:3551:GLU:HG2	2.11	0.49
3:F:4014:LYS:HG2	3:F:4135:PRO:HB3	1.94	0.49
3:I:1037:ASP:O	3:I:1041:GLN:HG2	2.11	0.49
3:I:2233:CYS:HB3	3:I:2270:SER:HB3	1.95	0.49
3:I:3107:VAL:HA	3:I:3175:LEU:HD21	1.95	0.49
3:I:3989:VAL:HG13	3:I:4023:MET:HE2	1.95	0.49
3:I:4688:ILE:HG22	3:I:4689:THR:HG23	1.95	0.49
2:L:66:MET:HE1	2:L:101:VAL:HB	1.93	0.49
3:J:1115:LEU:HD21	3:J:1191:VAL:HG13	1.95	0.49
3:J:2002:PRO:HD2	3:J:3863:GLY:HA2	1.95	0.49
3:F:1179:PHE:HB2	3:F:1182:ILE:HD11	1.95	0.49
3:F:1730:MET:HE3	3:F:1773:PRO:HG3	1.94	0.49
3:F:2010:LEU:HD22	3:F:3656:SER:HB2	1.93	0.49
3:F:2641:LEU:HD11	3:F:2698:MET:HG3	1.94	0.49
3:F:3532:LEU:HD21	3:F:3560:GLN:HA	1.93	0.49
3:I:1115:LEU:HD21	3:I:1191:VAL:HG13	1.95	0.49
3:I:1815:LEU:HG	3:I:1865:MET:HE3	1.94	0.49
3:I:2871:LEU:HG	3:I:2927:LEU:HD21	1.95	0.49
3:I:3163:VAL:HG21	3:I:3232:LEU:HD21	1.95	0.49
1:K:67:PHE:CD1	1:K:82:MET:HE1	2.47	0.49
3:J:470:SER:HA	3:J:473:ASN:ND2	2.28	0.49
3:J:1741:GLU:O	3:J:1745:ILE:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:2927:LEU:HD12	3:J:2930:LEU:HD12	1.95	0.49
3:C:3226:GLU:HA	3:C:3229:ILE:HG12	1.94	0.49
3:F:720:HIS:HB3	3:F:729:PRO:HA	1.94	0.49
3:F:2871:LEU:HG	3:F:2927:LEU:HD21	1.95	0.49
3:F:3163:VAL:HG21	3:F:3232:LEU:HD21	1.95	0.49
3:F:3895:HIS:CE1	3:F:3970:GLN:HB3	2.48	0.49
1:G:67:PHE:CD1	1:G:82:MET:HE1	2.47	0.49
3:I:1819:VAL:HG22	3:I:1926:LEU:HD13	1.94	0.49
3:J:479:GLN:HE21	3:J:539:LEU:HD11	1.78	0.48
3:J:670:GLU:HG2	3:J:788:LYS:HB3	1.94	0.48
3:J:720:HIS:HB3	3:J:729:PRO:HA	1.94	0.48
3:J:974:HIS:CE1	3:J:976:ARG:HH22	2.30	0.48
3:J:2630:VAL:HG23	3:J:2637:ALA:HB1	1.95	0.48
3:J:3163:VAL:HG21	3:J:3232:LEU:HD21	1.95	0.48
2:B:3:GLU:HB3	2:B:75:THR:HB	1.95	0.48
3:C:479:GLN:HE21	3:C:539:LEU:HD11	1.78	0.48
3:C:1115:LEU:HD21	3:C:1191:VAL:HG13	1.95	0.48
3:F:1115:LEU:HD21	3:F:1191:VAL:HG13	1.95	0.48
3:F:2418:LEU:HD23	3:F:2418:LEU:H	1.78	0.48
3:F:4688:ILE:HG22	3:F:4689:THR:HG23	1.95	0.48
3:I:470:SER:HA	3:I:473:ASN:ND2	2.28	0.48
3:I:974:HIS:CE1	3:I:976:ARG:HH22	2.30	0.48
3:I:1741:GLU:O	3:I:1745:ILE:HG12	2.12	0.48
3:J:4744:ASP:HB3	3:J:4747:SER:HB3	1.96	0.48
2:B:7:ILE:HD11	2:B:73:LYS:HB2	1.94	0.48
3:C:1179:PHE:HB2	3:C:1182:ILE:HD11	1.95	0.48
3:C:2768:PHE:HB2	3:C:2857:PRO:HD2	1.95	0.48
3:C:4567:LEU:HD21	3:C:4816:ILE:HG22	1.94	0.48
3:F:670:GLU:HG2	3:F:788:LYS:HB3	1.94	0.48
3:F:1965:TYR:CE1	3:F:2031:LEU:HB2	2.48	0.48
3:F:2747:ILE:HG12	3:F:2755:ILE:HG13	1.95	0.48
3:F:3107:VAL:HA	3:F:3175:LEU:HD21	1.95	0.48
3:F:4104:THR:O	3:F:4108:ILE:HG12	2.14	0.48
3:F:4242:ILE:HG12	3:F:4993:MET:HE2	1.94	0.48
3:F:4701:TRP:CD2	7:F:5110:POV:H23	2.48	0.48
2:H:3:GLU:HB3	2:H:75:THR:HB	1.95	0.48
3:I:883:ALA:HB1	3:I:887:ILE:HD11	1.95	0.48
3:I:2010:LEU:HD22	3:I:3656:SER:HB2	1.94	0.48
3:I:2310:CYS:HB2	3:I:2324:ASN:HB3	1.95	0.48
3:I:2927:LEU:HD12	3:I:2930:LEU:HD12	1.95	0.48
3:I:3226:GLU:HA	3:I:3229:ILE:HG12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1819:VAL:HG22	3:J:1926:LEU:HD13	1.94	0.48
3:J:2768:PHE:HB2	3:J:2857:PRO:HD2	1.95	0.48
3:J:4701:TRP:CD2	7:J:5108:POV:H23	2.48	0.48
3:C:110:ARG:HD3	3:C:115:ARG:HH21	1.79	0.48
3:C:470:SER:HA	3:C:473:ASN:ND2	2.28	0.48
3:C:883:ALA:HB1	3:C:887:ILE:HD11	1.95	0.48
3:C:1965:TYR:CE1	3:C:2031:LEU:HB2	2.48	0.48
3:C:2927:LEU:HD12	3:C:2930:LEU:HD12	1.95	0.48
3:C:3163:VAL:HG21	3:C:3232:LEU:HD21	1.95	0.48
3:C:4096:ALA:O	3:C:4100:GLN:HG2	2.13	0.48
3:C:4242:ILE:HG12	3:C:4993:MET:HE2	1.94	0.48
3:F:883:ALA:HB1	3:F:887:ILE:HD11	1.95	0.48
3:F:2518:LEU:HD22	3:F:2568:LEU:HD23	1.96	0.48
3:I:1815:LEU:HD22	3:I:1845:VAL:HG21	1.94	0.48
3:I:4701:TRP:CD2	7:I:5113:POV:H23	2.48	0.48
2:L:49:ARG:HD2	2:L:52:LYS:HG3	1.94	0.48
3:J:2310:CYS:HB2	3:J:2324:ASN:HB3	1.95	0.48
3:J:2964:LEU:HD13	3:J:3038:MET:HE2	1.94	0.48
3:J:4096:ALA:O	3:J:4100:GLN:HG2	2.13	0.48
3:C:4648:LEU:HD12	3:C:4803:HIS:HE1	1.79	0.48
3:F:2310:CYS:HB2	3:F:2324:ASN:HB3	1.95	0.48
3:F:3989:VAL:HG13	3:F:4023:MET:HE2	1.95	0.48
3:I:1163:THR:HG22	3:I:1168:VAL:HA	1.96	0.48
3:I:2747:ILE:HG12	3:I:2755:ILE:HG13	1.95	0.48
3:I:3391:GLU:O	3:I:3395:ARG:HG3	2.13	0.48
3:J:1260:MET:HE1	3:J:1271:ARG:HB3	1.96	0.48
3:J:4104:THR:O	3:J:4108:ILE:HG12	2.14	0.48
3:C:2747:ILE:HG12	3:C:2755:ILE:HG13	1.96	0.48
3:C:4097:MET:HB3	3:C:4108:ILE:HD12	1.95	0.48
3:C:4744:ASP:HB3	3:C:4747:SER:HB3	1.95	0.48
3:C:4880:MET:HE2	3:C:4880:MET:HA	1.96	0.48
2:E:3:GLU:HB3	2:E:75:THR:HB	1.95	0.48
3:F:110:ARG:HD3	3:F:115:ARG:HH21	1.79	0.48
3:F:470:SER:HA	3:F:473:ASN:ND2	2.28	0.48
3:F:1694:LEU:HD11	3:F:1718:ILE:HD11	1.94	0.48
3:F:4097:MET:HB3	3:F:4108:ILE:HD12	1.95	0.48
3:F:4880:MET:HE2	3:F:4880:MET:HA	1.96	0.48
3:F:4880:MET:HE3	3:I:4578:LEU:HB3	1.95	0.48
3:I:1179:PHE:HB2	3:I:1182:ILE:HD11	1.95	0.48
3:I:2630:VAL:HG23	3:I:2637:ALA:HB1	1.95	0.48
3:I:3854:GLU:HG2	3:I:3867:ASN:HD21	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3895:HIS:CE1	3:I:3970:GLN:HB3	2.49	0.48
3:I:4744:ASP:HB3	3:I:4747:SER:HB3	1.96	0.48
3:J:1965:TYR:CE1	3:J:2031:LEU:HB2	2.48	0.48
3:J:2627:VAL:HA	3:J:2678:LEU:HD13	1.95	0.48
3:J:2816:MET:HE1	3:J:2930:LEU:HD11	1.96	0.48
3:J:3377:GLU:HA	3:J:3380:ARG:HG2	1.96	0.48
3:J:3895:HIS:CE1	3:J:3970:GLN:HB3	2.48	0.48
3:J:4679:ARG:HE	3:J:5017:ARG:NE	2.12	0.48
3:C:1694:LEU:HD11	3:C:1718:ILE:HD11	1.94	0.48
3:C:2871:LEU:HG	3:C:2927:LEU:HD21	1.95	0.48
3:F:4744:ASP:HB3	3:F:4747:SER:HB3	1.95	0.48
2:H:7:ILE:HD11	2:H:73:LYS:HB2	1.94	0.48
3:I:1260:MET:HE1	3:I:1271:ARG:HB3	1.96	0.48
3:I:2696:TYR:HE2	3:I:2997:PHE:HA	1.78	0.48
3:I:2964:LEU:HD13	3:I:3038:MET:HE2	1.94	0.48
3:I:3219:TYR:HE2	3:I:3236:VAL:HG23	1.77	0.48
3:I:4790:LEU:HD21	7:I:5112:POV:H23A	1.94	0.48
3:J:548:VAL:HG21	3:J:582:HIS:HD2	1.79	0.48
3:J:4880:MET:HE3	3:C:4578:LEU:HB3	1.96	0.48
1:A:67:PHE:CD1	1:A:82:MET:HE1	2.47	0.48
3:C:1079:LYS:HA	3:C:1189:LEU:HD11	1.96	0.48
3:C:4104:THR:O	3:C:4108:ILE:HG12	2.13	0.48
3:C:4701:TRP:CD2	7:C:5111:POV:H23	2.48	0.48
3:F:1689:VAL:HG21	3:F:1714:LEU:HD21	1.96	0.48
3:I:2166:LEU:HD11	3:I:2206:THR:HG23	1.96	0.48
3:J:883:ALA:HB1	3:J:887:ILE:HD11	1.95	0.48
3:J:2871:LEU:HG	3:J:2927:LEU:HD21	1.95	0.48
3:J:2960:LEU:HD21	3:J:3039:ILE:HD12	1.96	0.48
3:J:3538:THR:O	3:J:3542:LEU:HG	2.14	0.48
3:C:3895:HIS:CE1	3:C:3970:GLN:HB3	2.49	0.48
3:C:3989:VAL:HG13	3:C:4023:MET:HE2	1.95	0.48
3:F:2215:LEU:HD22	3:F:2265:LEU:HD11	1.96	0.48
3:I:3965:LEU:HD23	3:I:3968:TYR:HD2	1.77	0.48
3:J:1179:PHE:HB2	3:J:1182:ILE:HD11	1.95	0.48
3:J:1815:LEU:HG	3:J:1865:MET:HE3	1.94	0.48
3:J:2418:LEU:HD23	3:J:2418:LEU:H	1.78	0.48
3:J:2696:TYR:HE2	3:J:2997:PHE:HA	1.78	0.48
3:J:4688:ILE:HG22	3:J:4689:THR:HG23	1.95	0.48
7:J:5107:POV:H24A	7:J:5108:POV:H32	1.95	0.48
3:C:2233:CYS:HB3	3:C:2270:SER:HB3	1.95	0.48
3:C:2418:LEU:HD23	3:C:2418:LEU:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2518:LEU:HD22	3:C:2568:LEU:HD23	1.96	0.48
3:C:2641:LEU:HD11	3:C:2698:MET:HG3	1.94	0.48
3:C:2758:PHE:HE2	3:C:2926:LEU:HD12	1.79	0.48
3:F:233:ILE:HD11	3:F:301:VAL:HG21	1.96	0.48
3:F:1071:ARG:HD3	3:F:1071:ARG:HA	1.58	0.48
3:F:1079:LYS:HA	3:F:1189:LEU:HD11	1.96	0.48
3:F:1242:LEU:HD22	3:F:1243:PRO:HD2	1.95	0.48
3:I:110:ARG:HD3	3:I:115:ARG:HH21	1.79	0.48
3:I:233:ILE:HD11	3:I:301:VAL:HG21	1.96	0.48
3:I:720:HIS:HB3	3:I:729:PRO:HA	1.94	0.48
3:I:1437:VAL:HG11	3:I:1552:VAL:HG21	1.96	0.48
3:I:1530:THR:HG22	3:I:1535:GLU:HA	1.96	0.48
3:I:2758:PHE:HE2	3:I:2926:LEU:HD12	1.79	0.48
3:I:2816:MET:HE1	3:I:2930:LEU:HD11	1.96	0.48
3:I:3538:THR:O	3:I:3542:LEU:HG	2.14	0.48
3:I:3900:GLN:HB3	3:I:3976:ASN:HD21	1.79	0.48
3:I:4880:MET:HE2	3:I:4880:MET:HA	1.96	0.48
3:J:1163:THR:HG22	3:J:1168:VAL:HA	1.96	0.48
3:J:1242:LEU:HD22	3:J:1243:PRO:HD2	1.95	0.48
3:J:2747:ILE:HG12	3:J:2755:ILE:HG13	1.95	0.48
3:J:4880:MET:HA	3:J:4880:MET:HE2	1.96	0.48
3:C:745:SER:HB2	3:C:758:ARG:HB3	1.96	0.48
3:C:882:TRP:CZ3	3:C:905:PRO:HA	2.44	0.48
3:C:1689:VAL:HG21	3:C:1714:LEU:HD21	1.96	0.48
3:C:1839:VAL:HG23	3:C:1938:GLN:HG3	1.96	0.48
3:C:3900:GLN:HB3	3:C:3976:ASN:HD21	1.79	0.48
3:F:548:VAL:HG21	3:F:582:HIS:HD2	1.79	0.48
3:F:2927:LEU:HD12	3:F:2930:LEU:HD12	1.95	0.48
3:F:3226:GLU:HA	3:F:3229:ILE:HG12	1.94	0.48
3:F:4096:ALA:O	3:F:4100:GLN:HG2	2.13	0.48
3:I:479:GLN:HE21	3:I:539:LEU:HD11	1.78	0.48
3:I:2768:PHE:HB2	3:I:2857:PRO:HD2	1.95	0.48
3:I:4104:THR:O	3:I:4108:ILE:HG12	2.13	0.48
3:J:110:ARG:HD3	3:J:115:ARG:HH21	1.78	0.47
3:J:1530:THR:HG22	3:J:1535:GLU:HA	1.96	0.47
3:J:2518:LEU:HD22	3:J:2568:LEU:HD23	1.96	0.47
3:C:2960:LEU:HD21	3:C:3039:ILE:HD12	1.96	0.47
3:C:3377:GLU:HA	3:C:3380:ARG:HG2	1.96	0.47
7:C:5110:POV:H24A	7:C:5111:POV:H32	1.95	0.47
3:F:479:GLN:HE21	3:F:539:LEU:HD11	1.78	0.47
3:F:1462:MET:HA	3:F:1462:MET:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2166:LEU:HD11	3:F:2206:THR:HG23	1.96	0.47
3:F:2768:PHE:HB2	3:F:2857:PRO:HD2	1.95	0.47
3:F:2964:LEU:HD13	3:F:3038:MET:HE2	1.94	0.47
2:H:90:VAL:HG12	2:H:91:ILE:HG12	1.96	0.47
3:I:840:VAL:HG22	3:I:1199:VAL:HG22	1.96	0.47
3:I:2002:PRO:HD2	3:I:3863:GLY:HA2	1.95	0.47
3:I:2418:LEU:HD23	3:I:2418:LEU:H	1.78	0.47
3:I:2960:LEU:HD21	3:I:3039:ILE:HD12	1.96	0.47
3:I:3377:GLU:HA	3:I:3380:ARG:HG2	1.96	0.47
1:K:104:TYR:CD1	3:J:882:TRP:HZ2	2.32	0.47
3:J:840:VAL:HG22	3:J:1199:VAL:HG22	1.96	0.47
3:J:3900:GLN:HB3	3:J:3976:ASN:HD21	1.79	0.47
3:J:4097:MET:HB3	3:J:4108:ILE:HD12	1.95	0.47
3:J:4888:TYR:HA	3:I:4918:ILE:HD11	1.96	0.47
3:C:1242:LEU:HD22	3:C:1243:PRO:HD2	1.95	0.47
3:C:2215:LEU:HD22	3:C:2265:LEU:HD11	1.96	0.47
3:C:2630:VAL:HG23	3:C:2637:ALA:HB1	1.95	0.47
3:C:4177:TYR:HE1	3:C:4199:GLU:HB3	1.80	0.47
3:F:2630:VAL:HG23	3:F:2637:ALA:HB1	1.95	0.47
3:F:4679:ARG:HE	3:F:5017:ARG:NE	2.12	0.47
3:F:4918:ILE:HD11	3:I:4888:TYR:HA	1.96	0.47
3:I:1159:THR:HG22	3:I:1180:ARG:HA	1.96	0.47
3:I:4096:ALA:O	3:I:4100:GLN:HG2	2.13	0.47
7:I:5112:POV:H24A	7:I:5113:POV:H32	1.95	0.47
2:L:17:LYS:O	2:L:50:ILE:HB	2.14	0.47
3:J:365:LYS:HG3	3:J:368:ARG:HH21	1.79	0.47
3:J:924:MET:O	3:J:928:THR:HG23	2.15	0.47
3:J:1079:LYS:HA	3:J:1189:LEU:HD11	1.96	0.47
3:C:924:MET:O	3:C:928:THR:HG23	2.14	0.47
3:C:2563:THR:HG22	3:C:2606:CYS:HA	1.95	0.47
3:C:4918:ILE:HD11	3:F:4888:TYR:HA	1.96	0.47
3:F:1839:VAL:HG23	3:F:1938:GLN:HG3	1.96	0.47
3:F:2627:VAL:HA	3:F:2678:LEU:HD13	1.95	0.47
3:F:2696:TYR:HE2	3:F:2997:PHE:HA	1.78	0.47
3:F:2960:LEU:HD21	3:F:3039:ILE:HD12	1.96	0.47
3:F:3377:GLU:HA	3:F:3380:ARG:HG2	1.96	0.47
3:F:3538:THR:O	3:F:3542:LEU:HG	2.14	0.47
3:I:2563:THR:HG22	3:I:2606:CYS:HA	1.95	0.47
3:I:4097:MET:HB3	3:I:4108:ILE:HD12	1.95	0.47
3:I:4648:LEU:HD12	3:I:4803:HIS:HE1	1.79	0.47
3:J:1839:VAL:HG23	3:J:1938:GLN:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:3553:LEU:HD21	3:J:3596:VAL:HB	1.96	0.47
3:C:3391:GLU:O	3:C:3395:ARG:HG3	2.13	0.47
3:C:3875:MET:HA	3:C:3875:MET:HE2	1.95	0.47
3:C:4245:MET:SD	3:C:4993:MET:HE1	2.55	0.47
3:F:2827:ARG:HD2	3:F:2934:GLY:HA3	1.97	0.47
3:F:3391:GLU:O	3:F:3395:ARG:HG3	2.13	0.47
2:H:17:LYS:O	2:H:50:ILE:HB	2.14	0.47
3:I:2827:ARG:HD2	3:I:2934:GLY:HA3	1.97	0.47
3:I:4679:ARG:HE	3:I:5017:ARG:NE	2.12	0.47
3:J:131:LEU:HG	3:J:178:ARG:HH12	1.80	0.47
2:B:17:LYS:O	2:B:50:ILE:HB	2.14	0.47
3:C:1530:THR:HG22	3:C:1535:GLU:HA	1.96	0.47
3:C:2599:GLN:O	3:C:2603:ILE:HG13	2.15	0.47
3:C:2696:TYR:HE2	3:C:2997:PHE:HA	1.78	0.47
3:C:4679:ARG:HE	3:C:5017:ARG:NE	2.12	0.47
3:C:4688:ILE:HG22	3:C:4689:THR:HG23	1.95	0.47
3:F:144:GLU:HG3	3:F:175:SER:HB2	1.96	0.47
3:F:1159:THR:HG22	3:F:1180:ARG:HA	1.96	0.47
3:F:1163:THR:HG22	3:F:1168:VAL:HA	1.96	0.47
3:F:1808:ARG:HD2	3:F:1854:PHE:HA	1.97	0.47
3:F:2563:THR:HG22	3:F:2606:CYS:HA	1.95	0.47
3:I:548:VAL:HG21	3:I:582:HIS:HD2	1.79	0.47
3:I:924:MET:O	3:I:928:THR:HG23	2.15	0.47
3:I:1965:TYR:CE1	3:I:2031:LEU:HB2	2.48	0.47
3:I:2641:LEU:HD11	3:I:2698:MET:HG3	1.94	0.47
3:I:3553:LEU:HD21	3:I:3596:VAL:HB	1.96	0.47
3:J:1462:MET:HA	3:J:1462:MET:HE3	1.96	0.47
3:J:2599:GLN:O	3:J:2603:ILE:HG13	2.15	0.47
3:J:3989:VAL:HG13	3:J:4023:MET:HE2	1.95	0.47
3:J:4245:MET:SD	3:J:4993:MET:HE1	2.55	0.47
3:J:4944:ARG:HH22	3:I:4938:ASP:HB3	1.80	0.47
3:C:233:ILE:HD11	3:C:301:VAL:HG21	1.96	0.47
3:C:1260:MET:HE1	3:C:1271:ARG:HB3	1.96	0.47
3:C:2656:CYS:HA	3:C:2711:PRO:HG3	1.96	0.47
3:F:924:MET:O	3:F:928:THR:HG23	2.14	0.47
3:F:1437:VAL:HG11	3:F:1552:VAL:HG21	1.96	0.47
3:F:3336:LYS:O	3:F:3340:VAL:HG23	2.15	0.47
3:F:3996:PHE:O	3:F:4000:MET:HB2	2.15	0.47
3:F:4072:VAL:HG21	3:F:4129:ALA:HB2	1.97	0.47
3:I:3010:PHE:CE2	3:I:3074:SER:HB3	2.50	0.47
3:I:3875:MET:HE2	3:I:3875:MET:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:104:TYR:CD1	3:J:882:TRP:CZ2	3.03	0.47
3:J:2166:LEU:HD11	3:J:2206:THR:HG23	1.96	0.47
3:J:2215:LEU:HD22	3:J:2265:LEU:HD11	1.96	0.47
3:J:2233:CYS:HB3	3:J:2270:SER:HB3	1.95	0.47
3:J:2563:THR:HG22	3:J:2606:CYS:HA	1.95	0.47
3:J:2758:PHE:HE2	3:J:2926:LEU:HD12	1.79	0.47
3:J:3003:LEU:HB3	3:J:3004:PRO:HD3	1.97	0.47
3:J:3010:PHE:CE2	3:J:3074:SER:HB3	2.50	0.47
3:J:3391:GLU:O	3:J:3395:ARG:HG3	2.13	0.47
3:J:3875:MET:HE2	3:J:3875:MET:HA	1.95	0.47
3:J:4578:LEU:HB3	3:I:4880:MET:HE3	1.96	0.47
3:J:4918:ILE:HD11	3:C:4888:TYR:HA	1.97	0.47
3:C:131:LEU:HG	3:C:178:ARG:HH12	1.80	0.47
3:C:144:GLU:HG3	3:C:175:SER:HB2	1.96	0.47
3:C:365:LYS:HG3	3:C:368:ARG:HH21	1.79	0.47
3:C:2002:PRO:HD2	3:C:3863:GLY:HA2	1.95	0.47
3:C:3010:PHE:CE2	3:C:3074:SER:HB3	2.50	0.47
3:C:3538:THR:O	3:C:3542:LEU:HG	2.14	0.47
3:C:4692:PRO:HG2	3:C:4703:ARG:HH21	1.80	0.47
3:F:76:ARG:HH22	3:I:3936:TYR:HD1	1.62	0.47
3:F:2233:CYS:HB3	3:F:2270:SER:HB3	1.95	0.47
3:F:2233:CYS:SG	3:F:2270:SER:HB3	2.55	0.47
3:F:2816:MET:HE1	3:F:2930:LEU:HD11	1.96	0.47
3:F:3010:PHE:CE2	3:F:3074:SER:HB3	2.50	0.47
3:F:4648:LEU:HD12	3:F:4803:HIS:HE1	1.79	0.47
3:F:4692:PRO:HG2	3:F:4703:ARG:HH21	1.80	0.47
3:F:4897:ILE:HG13	3:F:4901:ILE:HG12	1.97	0.47
3:I:131:LEU:HG	3:I:178:ARG:HH12	1.80	0.47
3:I:745:SER:HB2	3:I:758:ARG:HB3	1.96	0.47
3:I:1079:LYS:HA	3:I:1189:LEU:HD11	1.96	0.47
3:I:2599:GLN:O	3:I:2603:ILE:HG13	2.15	0.47
3:I:2627:VAL:HA	3:I:2678:LEU:HD13	1.95	0.47
3:I:2656:CYS:HA	3:I:2711:PRO:HG3	1.96	0.47
3:I:2908:TYR:CZ	3:I:2916:LYS:HG3	2.50	0.47
3:I:3182:TYR:HA	3:I:3185:LYS:HE3	1.97	0.47
3:I:3996:PHE:O	3:I:4000:MET:HB2	2.15	0.47
3:I:4177:TYR:HE1	3:I:4199:GLU:HB3	1.80	0.47
3:J:144:GLU:HG3	3:J:175:SER:HB2	1.96	0.47
3:J:1094:ALA:HA	3:J:1100:MET:HE1	1.97	0.47
3:J:1208:VAL:HG13	3:J:1214:PHE:HD2	1.80	0.47
3:J:3103:ILE:HG21	3:J:3168:THR:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:3424:LEU:HD13	3:I:1216:ILE:HA	1.97	0.47
3:J:3936:TYR:HD1	3:I:76:ARG:HH22	1.62	0.47
1:A:6:GLU:HG3	1:A:121:THR:HG22	1.97	0.47
3:C:548:VAL:HG21	3:C:582:HIS:HD2	1.79	0.47
3:C:1163:THR:HG22	3:C:1168:VAL:HA	1.96	0.47
3:C:1437:VAL:HG11	3:C:1552:VAL:HG21	1.96	0.47
3:C:3553:LEU:HD21	3:C:3596:VAL:HB	1.96	0.47
3:C:3996:PHE:O	3:C:4000:MET:HB2	2.15	0.47
3:C:4072:VAL:HG21	3:C:4129:ALA:HB2	1.97	0.47
3:F:1260:MET:HE1	3:F:1271:ARG:HB3	1.96	0.47
3:F:1530:THR:HG22	3:F:1535:GLU:HA	1.96	0.47
7:F:5109:POV:H24A	7:F:5110:POV:H32	1.95	0.47
3:I:1527:MET:HG2	3:I:1540:PHE:HB2	1.97	0.47
3:I:1689:VAL:HG21	3:I:1714:LEU:HD21	1.96	0.47
3:I:2518:LEU:HD22	3:I:2568:LEU:HD23	1.96	0.47
3:I:3078:ARG:H	3:I:3152:PHE:HE1	1.63	0.47
3:I:3103:ILE:HG21	3:I:3168:THR:HG23	1.97	0.47
3:I:4118:ASP:HB3	3:I:4122:MET:HB2	1.97	0.47
1:K:6:GLU:HG3	1:K:121:THR:HG22	1.97	0.47
3:J:3788:GLY:HA3	3:J:3834:ALA:HB3	1.97	0.47
3:C:2233:CYS:SG	3:C:2270:SER:HB3	2.55	0.47
3:C:2627:VAL:HA	3:C:2678:LEU:HD13	1.95	0.47
2:E:17:LYS:O	2:E:50:ILE:HB	2.15	0.47
2:E:90:VAL:HG12	2:E:91:ILE:HG12	1.96	0.47
3:F:1527:MET:HG2	3:F:1540:PHE:HB2	1.97	0.47
3:I:365:LYS:HG3	3:I:368:ARG:HH21	1.79	0.47
3:I:1208:VAL:HG13	3:I:1214:PHE:HD2	1.80	0.47
3:I:1462:MET:HA	3:I:1462:MET:HE3	1.96	0.47
3:I:3336:LYS:O	3:I:3340:VAL:HG23	2.14	0.47
3:J:233:ILE:HD11	3:J:301:VAL:HG21	1.96	0.47
3:J:514:SER:O	3:J:518:ILE:HG13	2.15	0.47
3:J:2908:TYR:CZ	3:J:2916:LYS:HG3	2.50	0.47
3:J:4648:LEU:HD12	3:J:4803:HIS:HE1	1.79	0.47
3:J:4972:PRO:HG3	3:I:5024:ALA:HB3	1.97	0.47
1:A:111:ASN:HA	1:A:114:TYR:CB	2.45	0.47
3:C:76:ARG:HH22	3:F:3936:TYR:HD1	1.62	0.47
3:C:1159:THR:HG22	3:C:1180:ARG:HA	1.96	0.47
3:C:1462:MET:HE3	3:C:1462:MET:HA	1.96	0.47
3:C:1808:ARG:HD2	3:C:1854:PHE:HA	1.97	0.47
3:C:2908:TYR:CZ	3:C:2916:LYS:HG3	2.50	0.47
3:C:4897:ILE:HG13	3:C:4901:ILE:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:42:ARG:HH22	3:F:1782:PHE:HE2	1.62	0.47
3:F:365:LYS:HG3	3:F:368:ARG:HH21	1.79	0.47
3:F:818:ARG:HG2	3:F:1028:ASP:HA	1.97	0.47
3:F:840:VAL:HG22	3:F:1199:VAL:HG22	1.96	0.47
3:F:2794:TYR:HD1	3:F:2802:LYS:HE2	1.80	0.47
3:F:3003:LEU:HB3	3:F:3004:PRO:HD3	1.97	0.47
3:F:3078:ARG:H	3:F:3152:PHE:HE1	1.63	0.47
3:F:3900:GLN:HB3	3:F:3976:ASN:HD21	1.79	0.47
3:I:3788:GLY:HA3	3:I:3834:ALA:HB3	1.97	0.47
3:J:3805:LEU:HB3	3:J:3890:LEU:HB3	1.97	0.46
3:J:4072:VAL:HG21	3:J:4129:ALA:HB2	1.97	0.46
3:J:4897:ILE:HG13	3:J:4901:ILE:HG12	1.96	0.46
3:C:3788:GLY:HA3	3:C:3834:ALA:HB3	1.97	0.46
3:C:5024:ALA:HB3	3:F:4972:PRO:HG3	1.97	0.46
2:E:66:MET:HE2	2:E:72:ALA:HB3	1.97	0.46
3:F:745:SER:HB2	3:F:758:ARG:HB3	1.96	0.46
3:F:3081:MET:HG3	3:F:3156:VAL:HA	1.98	0.46
3:F:3592:ILE:HA	3:F:3595:ARG:HE	1.80	0.46
3:F:4118:ASP:HB3	3:F:4122:MET:HB2	1.97	0.46
3:I:2233:CYS:SG	3:I:2270:SER:HB3	2.55	0.46
3:I:2760:GLU:O	3:I:2764:GLU:HG3	2.16	0.46
3:I:2794:TYR:HD1	3:I:2802:LYS:HE2	1.80	0.46
3:I:3805:LEU:HB3	3:I:3890:LEU:HB3	1.98	0.46
2:L:66:MET:HE2	2:L:72:ALA:HB3	1.97	0.46
3:J:1689:VAL:HG21	3:J:1714:LEU:HD21	1.96	0.46
3:J:2238:TYR:O	3:J:2242:ILE:HG13	2.16	0.46
3:J:3182:TYR:HA	3:J:3185:LYS:HE3	1.97	0.46
3:C:2816:MET:HE1	3:C:2930:LEU:HD11	1.96	0.46
3:C:3003:LEU:HB3	3:C:3004:PRO:HD3	1.97	0.46
3:C:3182:TYR:HA	3:C:3185:LYS:HE3	1.97	0.46
3:C:3336:LYS:O	3:C:3340:VAL:HG23	2.15	0.46
3:C:4880:MET:HE3	3:F:4578:LEU:HB3	1.95	0.46
3:C:4897:ILE:O	3:C:4901:ILE:HG12	2.16	0.46
3:F:926:GLY:O	3:F:930:LYS:HG3	2.16	0.46
3:F:1216:ILE:HA	3:I:3424:LEU:HD13	1.97	0.46
3:F:2656:CYS:HA	3:F:2711:PRO:HG3	1.96	0.46
3:F:2758:PHE:HE2	3:F:2926:LEU:HD12	1.79	0.46
3:F:3553:LEU:HD21	3:F:3596:VAL:HB	1.97	0.46
3:F:4177:TYR:HE1	3:F:4199:GLU:HB3	1.80	0.46
3:I:514:SER:O	3:I:518:ILE:HG13	2.15	0.46
3:I:2215:LEU:HD22	3:I:2265:LEU:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3081:MET:HG3	3:I:3156:VAL:HA	1.97	0.46
1:K:68:THR:O	1:K:80:LEU:HA	2.15	0.46
3:J:2233:CYS:SG	3:J:2270:SER:HB3	2.55	0.46
3:J:3081:MET:HG3	3:J:3156:VAL:HA	1.97	0.46
3:J:4118:ASP:HB3	3:J:4122:MET:HB2	1.97	0.46
3:J:4692:PRO:HG2	3:J:4703:ARG:HH21	1.80	0.46
3:C:1527:MET:HG2	3:C:1540:PHE:HB2	1.97	0.46
3:C:3081:MET:HG3	3:C:3156:VAL:HA	1.98	0.46
3:F:2908:TYR:CZ	3:F:2916:LYS:HG3	2.50	0.46
3:F:3875:MET:HE2	3:F:3875:MET:HA	1.95	0.46
3:F:4897:ILE:O	3:F:4901:ILE:HG12	2.16	0.46
3:I:144:GLU:HG3	3:I:175:SER:HB2	1.96	0.46
3:I:586:ILE:HD12	3:I:606:LEU:HD11	1.98	0.46
3:I:2991:HIS:O	3:I:2995:ILE:HG13	2.15	0.46
3:I:3592:ILE:HA	3:I:3595:ARG:HE	1.80	0.46
2:L:90:VAL:HG12	2:L:91:ILE:HG12	1.96	0.46
3:J:1159:THR:HG22	3:J:1180:ARG:HA	1.96	0.46
3:J:1208:VAL:HB	3:C:3575:LEU:HD21	1.98	0.46
3:J:2760:GLU:O	3:J:2764:GLU:HG3	2.16	0.46
3:J:2827:ARG:HD2	3:J:2934:GLY:HA3	1.97	0.46
3:J:3592:ILE:HA	3:J:3595:ARG:HE	1.80	0.46
3:J:4897:ILE:O	3:J:4901:ILE:HG12	2.16	0.46
3:C:818:ARG:HG2	3:C:1028:ASP:HA	1.96	0.46
3:C:829:TYR:HB3	3:C:1073:ARG:HH12	1.81	0.46
3:C:2827:ARG:HD2	3:C:2934:GLY:HA3	1.97	0.46
3:C:3103:ILE:HG21	3:C:3168:THR:HG23	1.97	0.46
3:F:586:ILE:HD12	3:F:606:LEU:HD11	1.98	0.46
3:F:2991:HIS:O	3:F:2995:ILE:HG13	2.15	0.46
3:I:1839:VAL:HG23	3:I:1938:GLN:HG3	1.96	0.46
3:I:4692:PRO:HG2	3:I:4703:ARG:HH21	1.80	0.46
3:J:1808:ARG:HD2	3:J:1854:PHE:HA	1.97	0.46
3:J:2683:PHE:HD1	3:J:2703:LEU:HD21	1.80	0.46
2:B:66:MET:HE2	2:B:72:ALA:HB3	1.97	0.46
3:C:840:VAL:HG22	3:C:1199:VAL:HG22	1.96	0.46
1:D:6:GLU:HG3	1:D:121:THR:HG22	1.97	0.46
3:F:4245:MET:SD	3:F:4993:MET:HE1	2.55	0.46
3:I:3996:PHE:HZ	3:I:4019:LEU:HG	1.81	0.46
3:J:2656:CYS:HA	3:J:2711:PRO:HG3	1.96	0.46
3:J:2794:TYR:HD1	3:J:2802:LYS:HE2	1.80	0.46
3:J:3996:PHE:O	3:J:4000:MET:HB2	2.15	0.46
3:C:514:SER:O	3:C:518:ILE:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2637:ALA:C	3:C:2640:PRO:HD2	2.41	0.46
3:C:4118:ASP:HB3	3:C:4122:MET:HB2	1.97	0.46
3:F:541:SER:HB3	3:F:577:ILE:HD11	1.98	0.46
3:F:3182:TYR:HA	3:F:3185:LYS:HE3	1.97	0.46
3:I:483:MET:HE1	3:I:486:LEU:HD23	1.97	0.46
3:I:2748:PRO:HB2	3:I:2750:LYS:HG2	1.98	0.46
3:I:3003:LEU:HB3	3:I:3004:PRO:HD3	1.97	0.46
3:J:586:ILE:HD12	3:J:606:LEU:HD11	1.98	0.46
3:J:745:SER:HB2	3:J:758:ARG:HB3	1.96	0.46
3:J:1527:MET:HG2	3:J:1540:PHE:HB2	1.97	0.46
3:J:4938:ASP:HB3	3:C:4944:ARG:HH22	1.81	0.46
2:B:90:VAL:HG12	2:B:91:ILE:HG12	1.96	0.46
3:C:2760:GLU:O	3:C:2764:GLU:HG3	2.16	0.46
3:C:3550:ARG:HD3	3:C:3594:ARG:NH1	2.31	0.46
3:C:3592:ILE:HA	3:C:3595:ARG:HE	1.80	0.46
3:C:3996:PHE:HZ	3:C:4019:LEU:HG	1.81	0.46
1:D:98:ASP:HB3	1:D:115:ASP:HB3	1.98	0.46
3:F:131:LEU:HG	3:F:178:ARG:HH12	1.80	0.46
3:F:1074:ILE:O	3:F:1238:PHE:HA	2.16	0.46
3:F:1208:VAL:HG13	3:F:1214:PHE:HD2	1.80	0.46
3:F:2599:GLN:O	3:F:2603:ILE:HG13	2.15	0.46
3:F:2683:PHE:HD1	3:F:2703:LEU:HD21	1.80	0.46
3:F:3103:ILE:HG21	3:F:3168:THR:HG23	1.97	0.46
3:F:3996:PHE:HZ	3:F:4019:LEU:HG	1.81	0.46
1:G:6:GLU:HG3	1:G:121:THR:HG22	1.97	0.46
2:H:66:MET:HE2	2:H:72:ALA:HB3	1.97	0.46
3:I:829:TYR:HB3	3:I:1073:ARG:HH12	1.81	0.46
3:I:2238:TYR:O	3:I:2242:ILE:HG13	2.16	0.46
3:I:2683:PHE:HD1	3:I:2703:LEU:HD21	1.80	0.46
3:J:76:ARG:HH22	3:C:3936:TYR:HD1	1.62	0.46
3:J:2196:ASN:HD21	3:J:3862:ASP:HB3	1.81	0.46
3:J:3336:LYS:O	3:J:3340:VAL:HG23	2.15	0.46
3:J:3996:PHE:HZ	3:J:4019:LEU:HG	1.81	0.46
3:J:4177:TYR:HE1	3:J:4199:GLU:HB3	1.80	0.46
1:A:6:GLU:HA	1:A:22:CYS:HA	1.98	0.46
1:A:68:THR:O	1:A:80:LEU:HA	2.15	0.46
3:C:926:GLY:O	3:C:930:LYS:HG3	2.16	0.46
3:C:1094:ALA:HA	3:C:1100:MET:HE1	1.97	0.46
3:C:1208:VAL:HG13	3:C:1214:PHE:HD2	1.80	0.46
3:C:2166:LEU:HD11	3:C:2206:THR:HG23	1.96	0.46
3:C:3842:LEU:HB2	3:C:3929:SER:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:4938:ASP:HB3	3:F:4944:ARG:HH22	1.80	0.46
1:D:106:PRO:HB3	3:F:878:ILE:HG13	1.97	0.46
1:D:111:ASN:HA	1:D:114:TYR:CB	2.45	0.46
3:F:2196:ASN:HD21	3:F:3862:ASP:HB3	1.81	0.46
3:F:2637:ALA:C	3:F:2640:PRO:HD2	2.41	0.46
2:H:25:HIS:HB3	2:H:40:ARG:NE	2.31	0.46
3:I:2637:ALA:C	3:I:2640:PRO:HD2	2.41	0.46
3:I:4245:MET:SD	3:I:4993:MET:HE1	2.55	0.46
1:K:98:ASP:HB3	1:K:115:ASP:HB3	1.98	0.46
3:J:818:ARG:HG2	3:J:1028:ASP:HA	1.96	0.46
3:J:829:TYR:HB3	3:J:1073:ARG:HH12	1.81	0.46
3:J:2991:HIS:O	3:J:2995:ILE:HG13	2.15	0.46
3:J:3076:ASP:HA	3:J:3152:PHE:CZ	2.51	0.46
2:B:55:VAL:HA	3:C:1784:ALA:HA	1.98	0.46
3:C:3805:LEU:HB3	3:C:3890:LEU:HB3	1.97	0.46
3:F:3788:GLY:HA3	3:F:3834:ALA:HB3	1.97	0.46
3:F:3805:LEU:HB3	3:F:3890:LEU:HB3	1.97	0.46
3:F:5024:ALA:HB3	3:I:4972:PRO:HG3	1.97	0.46
7:F:5101:POV:H24A	7:F:5101:POV:H27A	1.67	0.46
1:G:68:THR:O	1:G:80:LEU:HA	2.15	0.46
1:G:98:ASP:HB3	1:G:115:ASP:HB3	1.98	0.46
1:G:111:ASN:HA	1:G:114:TYR:CB	2.46	0.46
3:I:863:LEU:HD21	3:I:930:LYS:HG2	1.98	0.46
3:I:1247:PRO:HA	3:I:1598:GLN:HG2	1.98	0.46
3:I:2196:ASN:HD21	3:I:3862:ASP:HB3	1.81	0.46
3:I:2454:ARG:HH21	3:I:2458:ARG:NH2	2.14	0.46
3:I:4072:VAL:HG21	3:I:4129:ALA:HB2	1.97	0.46
2:L:25:HIS:HB3	2:L:40:ARG:NE	2.31	0.46
3:J:1074:ILE:O	3:J:1238:PHE:HA	2.16	0.46
3:J:1437:VAL:HG11	3:J:1552:VAL:HG21	1.96	0.46
3:J:2596:THR:O	3:J:2600:ARG:HG3	2.16	0.46
3:J:3378:GLN:O	3:J:3382:GLU:HG2	2.16	0.46
3:J:3575:LEU:HD21	3:I:1208:VAL:HB	1.97	0.46
3:J:3842:LEU:HB2	3:J:3929:SER:HB2	1.98	0.46
3:C:1216:ILE:HA	3:F:3424:LEU:HD13	1.97	0.46
3:C:2196:ASN:HD21	3:C:3862:ASP:HB3	1.81	0.46
3:C:2596:THR:O	3:C:2600:ARG:HG3	2.16	0.46
3:C:3281:LEU:HD23	3:C:3315:LEU:HD13	1.98	0.46
3:F:829:TYR:HB3	3:F:1073:ARG:HH12	1.81	0.46
3:F:2238:TYR:O	3:F:2242:ILE:HG13	2.16	0.46
3:I:926:GLY:O	3:I:930:LYS:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1808:ARG:HD2	3:I:1854:PHE:HA	1.97	0.46
3:I:1925:GLY:O	3:I:1929:MET:HG2	2.16	0.46
3:I:2924:GLN:O	3:I:2928:LYS:HG2	2.16	0.46
3:J:926:GLY:O	3:J:930:LYS:HG3	2.16	0.45
3:J:1101:ARG:HH12	3:J:1114:GLU:HB3	1.81	0.45
3:J:1524:THR:HG23	3:J:1526:LEU:HB3	1.99	0.45
3:J:2512:ILE:HG21	3:J:2518:LEU:HD13	1.98	0.45
3:C:1074:ILE:O	3:C:1238:PHE:HA	2.16	0.45
3:C:2794:TYR:HD1	3:C:2802:LYS:HE2	1.80	0.45
3:F:945:LYS:HB3	3:F:947:GLU:HG2	1.98	0.45
3:F:1094:ALA:HA	3:F:1100:MET:HE1	1.97	0.45
3:F:2512:ILE:HG21	3:F:2518:LEU:HD13	1.98	0.45
3:F:2924:GLN:O	3:F:2928:LYS:HG2	2.16	0.45
3:I:3076:ASP:HA	3:I:3152:PHE:CZ	2.51	0.45
3:J:3770:LEU:HB2	3:J:3804:ILE:HD11	1.98	0.45
1:A:98:ASP:HB3	1:A:115:ASP:HB3	1.98	0.45
3:C:586:ILE:HD12	3:C:606:LEU:HD11	1.98	0.45
3:C:2238:TYR:O	3:C:2242:ILE:HG13	2.16	0.45
3:C:3078:ARG:H	3:C:3152:PHE:HE1	1.63	0.45
2:E:77:THR:HG22	2:E:79:ASP:H	1.81	0.45
3:F:514:SER:O	3:F:518:ILE:HG13	2.15	0.45
3:F:544:LEU:HD21	3:F:574:VAL:HB	1.99	0.45
3:F:1208:VAL:HB	3:I:3575:LEU:HD21	1.97	0.45
3:F:3719:ASP:O	3:F:3723:MET:HG2	2.17	0.45
3:I:541:SER:HB3	3:I:577:ILE:HD11	1.98	0.45
3:I:3036:LYS:HE3	3:I:3036:LYS:HB2	1.68	0.45
3:I:3842:LEU:HB2	3:I:3929:SER:HB2	1.98	0.45
3:J:1216:ILE:HA	3:C:3424:LEU:HD13	1.97	0.45
3:J:2454:ARG:HH21	3:J:2458:ARG:NH2	2.13	0.45
3:J:2748:PRO:HB2	3:J:2750:LYS:HG2	1.98	0.45
3:J:2924:GLN:O	3:J:2928:LYS:HG2	2.16	0.45
3:J:4018:ASP:HA	3:J:4021:LYS:HE2	1.99	0.45
2:B:56:ILE:HG12	3:C:1783:VAL:O	2.16	0.45
3:C:248:GLU:HG3	3:C:371:VAL:HG21	1.99	0.45
3:C:483:MET:HE1	3:C:486:LEU:HD23	1.97	0.45
3:C:2512:ILE:HG21	3:C:2518:LEU:HD13	1.98	0.45
3:C:2683:PHE:HD1	3:C:2703:LEU:HD21	1.80	0.45
3:F:20:VAL:HA	3:F:204:PRO:HA	1.98	0.45
3:F:349:GLN:HE21	3:F:354:GLY:HA2	1.81	0.45
3:F:863:LEU:HD21	3:F:930:LYS:HG2	1.98	0.45
3:F:1958:LEU:HD23	3:F:2138:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2751:LEU:O	3:F:2755:ILE:HG12	2.16	0.45
3:F:2760:GLU:O	3:F:2764:GLU:HG3	2.16	0.45
3:F:3105:LYS:HE3	3:F:3128:ASN:HD22	1.81	0.45
2:H:77:THR:HG22	2:H:79:ASP:H	1.81	0.45
3:I:1074:ILE:O	3:I:1238:PHE:HA	2.16	0.45
3:I:1524:THR:HG23	3:I:1526:LEU:HB3	1.99	0.45
3:I:1958:LEU:HD23	3:I:2138:LEU:HD21	1.98	0.45
3:I:4897:ILE:HG13	3:I:4901:ILE:HG12	1.96	0.45
2:L:40:ARG:HB3	3:J:677:ALA:HB1	1.98	0.45
3:J:248:GLU:HG3	3:J:371:VAL:HG21	1.99	0.45
3:J:3099:ALA:O	3:J:3103:ILE:HG12	2.17	0.45
3:C:1042:ALA:O	3:C:1046:LEU:HG	2.17	0.45
3:C:1101:ARG:HH12	3:C:1114:GLU:HB3	1.81	0.45
3:C:2924:GLN:O	3:C:2928:LYS:HG2	2.16	0.45
1:D:6:GLU:HA	1:D:22:CYS:HA	1.98	0.45
1:D:68:THR:O	1:D:80:LEU:HA	2.15	0.45
3:F:1039:LEU:H	3:F:1039:LEU:HD12	1.82	0.45
3:F:1524:THR:HG23	3:F:1526:LEU:HB3	1.99	0.45
3:F:3144:PHE:HB3	3:F:3200:ALA:HB3	1.98	0.45
3:F:3842:LEU:HB2	3:F:3929:SER:HB2	1.98	0.45
3:I:573:GLU:O	3:I:577:ILE:HG12	2.17	0.45
3:I:1042:ALA:O	3:I:1046:LEU:HG	2.17	0.45
3:I:1094:ALA:HA	3:I:1100:MET:HE1	1.97	0.45
3:I:2751:LEU:O	3:I:2755:ILE:HG12	2.16	0.45
3:I:2973:PHE:CD1	3:I:2995:ILE:HG12	2.52	0.45
3:I:3719:ASP:O	3:I:3723:MET:HG2	2.17	0.45
1:K:111:ASN:HA	1:K:114:TYR:CB	2.45	0.45
2:L:77:THR:HG22	2:L:79:ASP:H	1.81	0.45
3:J:902:ARG:HH12	3:J:904:HIS:CE1	2.35	0.45
3:J:1000:ARG:HD2	3:J:1005:TRP:CD1	2.52	0.45
3:J:2637:ALA:C	3:J:2640:PRO:HD2	2.41	0.45
3:J:3550:ARG:HD3	3:J:3594:ARG:NH1	2.31	0.45
3:J:3719:ASP:O	3:J:3723:MET:HG2	2.17	0.45
3:J:5024:ALA:HB3	3:C:4972:PRO:HG3	1.97	0.45
3:C:932:LEU:HB3	3:C:937:CYS:HB2	1.99	0.45
3:C:3076:ASP:HA	3:C:3152:PHE:CZ	2.51	0.45
3:C:3099:ALA:O	3:C:3103:ILE:HG12	2.17	0.45
3:C:3144:PHE:HB3	3:C:3200:ALA:HB3	1.98	0.45
3:C:4018:ASP:HA	3:C:4021:LYS:HE2	1.99	0.45
2:E:8:SER:HB2	2:E:71:ARG:HB3	1.99	0.45
3:F:902:ARG:HH12	3:F:904:HIS:CE1	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1101:ARG:HH12	3:F:1114:GLU:HB3	1.81	0.45
3:F:2454:ARG:HH21	3:F:2458:ARG:NH2	2.13	0.45
3:I:275:ARG:HH11	3:I:338:GLU:HG3	1.81	0.45
3:I:818:ARG:HG2	3:I:1028:ASP:HA	1.96	0.45
3:I:2512:ILE:HG21	3:I:2518:LEU:HD13	1.98	0.45
3:I:3770:LEU:HB2	3:I:3804:ILE:HD11	1.98	0.45
3:J:20:VAL:HA	3:J:204:PRO:HA	1.98	0.45
3:J:483:MET:HE1	3:J:486:LEU:HD23	1.97	0.45
3:J:499:THR:HG23	3:J:502:HIS:H	1.82	0.45
3:J:3144:PHE:HB3	3:J:3200:ALA:HB3	1.98	0.45
2:B:8:SER:HB2	2:B:71:ARG:HB3	1.99	0.45
3:C:541:SER:HB3	3:C:577:ILE:HD11	1.98	0.45
3:C:1090:PHE:O	3:C:1151:CYS:HB2	2.17	0.45
3:C:1208:VAL:HB	3:F:3575:LEU:HD21	1.97	0.45
3:F:1000:ARG:HD2	3:F:1005:TRP:CD1	2.52	0.45
3:F:3281:LEU:HD23	3:F:3315:LEU:HD13	1.99	0.45
3:F:4018:ASP:HA	3:F:4021:LYS:HE2	1.99	0.45
3:F:4202:ARG:O	3:F:4206:GLU:HG2	2.17	0.45
3:I:902:ARG:HH12	3:I:904:HIS:CE1	2.35	0.45
3:I:932:LEU:HD23	3:I:988:LEU:HD11	1.99	0.45
3:I:4897:ILE:O	3:I:4901:ILE:HG12	2.15	0.45
3:J:2751:LEU:O	3:J:2755:ILE:HG12	2.16	0.45
2:B:77:THR:HG22	2:B:79:ASP:H	1.80	0.45
3:C:2454:ARG:HH21	3:C:2458:ARG:NH2	2.14	0.45
3:C:2977:LEU:O	3:C:2981:VAL:HG22	2.17	0.45
3:C:2991:HIS:O	3:C:2995:ILE:HG13	2.15	0.45
3:C:3793:MET:HE3	3:C:3793:MET:HB3	1.83	0.45
7:C:5101:POV:H27A	7:C:5101:POV:H24A	1.67	0.45
3:F:483:MET:HE1	3:F:486:LEU:HD23	1.97	0.45
3:F:3770:LEU:HB2	3:F:3804:ILE:HD11	1.98	0.45
1:K:99:ARG:HG2	3:J:920:TYR:CE1	2.52	0.45
3:J:544:LEU:HD21	3:J:574:VAL:HB	1.99	0.45
3:J:1090:PHE:O	3:J:1151:CYS:HB2	2.17	0.45
3:J:1925:GLY:O	3:J:1929:MET:HG2	2.16	0.45
3:J:3078:ARG:H	3:J:3152:PHE:HE1	1.63	0.45
3:C:573:GLU:O	3:C:577:ILE:HG12	2.16	0.45
3:C:1000:ARG:HD2	3:C:1005:TRP:CD1	2.52	0.45
3:C:2559:LEU:O	3:C:2563:THR:HG23	2.17	0.45
3:C:2748:PRO:HB2	3:C:2750:LYS:HG2	1.98	0.45
3:C:3105:LYS:HE3	3:C:3128:ASN:HD22	1.81	0.45
3:C:3281:LEU:HD21	3:C:3312:LEU:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3683:GLN:O	3:C:3687:GLU:HB2	2.17	0.45
3:F:1680:ARG:HH21	3:F:1681:VAL:HG22	1.82	0.45
3:F:2596:THR:O	3:F:2600:ARG:HG3	2.16	0.45
3:F:3550:ARG:HD3	3:F:3594:ARG:NH1	2.31	0.45
3:I:2758:PHE:HD2	3:I:2813:LEU:HD11	1.82	0.45
3:I:3099:ALA:O	3:I:3103:ILE:HG12	2.17	0.45
3:I:3281:LEU:HD21	3:I:3312:LEU:HA	1.99	0.45
3:I:3281:LEU:HD23	3:I:3315:LEU:HD13	1.99	0.45
3:J:893:TYR:HA	3:J:903:LEU:HB3	1.99	0.45
3:J:932:LEU:HB3	3:J:937:CYS:HB2	1.99	0.45
3:J:2973:PHE:CD1	3:J:2995:ILE:HG12	2.52	0.45
3:J:3036:LYS:HE3	3:J:3036:LYS:HB2	1.68	0.45
3:C:215:THR:HG22	3:C:273:HIS:HA	1.99	0.45
3:C:544:LEU:HD21	3:C:574:VAL:HB	1.99	0.45
3:C:1290:ARG:HH22	3:C:1644:GLU:HG3	1.82	0.45
3:C:3378:GLN:O	3:C:3382:GLU:HG2	2.16	0.45
3:F:248:GLU:HG3	3:F:371:VAL:HG21	1.99	0.45
3:F:932:LEU:HD23	3:F:988:LEU:HD11	1.99	0.45
3:F:1042:ALA:O	3:F:1046:LEU:HG	2.17	0.45
3:F:1925:GLY:O	3:F:1929:MET:HG2	2.16	0.45
3:F:2575:ARG:HB3	3:F:2578:MET:SD	2.57	0.45
3:F:2677:LYS:HD3	3:F:2909:ASP:HB2	1.99	0.45
3:F:3076:ASP:HA	3:F:3152:PHE:CZ	2.51	0.45
3:I:349:GLN:HE21	3:I:354:GLY:HA2	1.81	0.45
3:I:1079:LYS:HD3	3:I:1655:GLU:HG2	1.99	0.45
3:I:1101:ARG:HH12	3:I:1114:GLU:HB3	1.81	0.45
3:I:2575:ARG:HB3	3:I:2578:MET:SD	2.57	0.45
3:I:2677:LYS:HD3	3:I:2909:ASP:HB2	1.98	0.45
3:I:3105:LYS:HE3	3:I:3128:ASN:HD22	1.81	0.45
3:J:1960:ALA:HB1	3:J:1964:ARG:HH12	1.82	0.45
3:J:3281:LEU:HD23	3:J:3315:LEU:HD13	1.98	0.45
3:C:863:LEU:HD21	3:C:930:LYS:HG2	1.98	0.45
3:C:902:ARG:HH12	3:C:904:HIS:CE1	2.35	0.45
3:C:2575:ARG:HB3	3:C:2578:MET:SD	2.57	0.45
3:F:1079:LYS:HD3	3:F:1655:GLU:HG2	1.99	0.45
3:F:2748:PRO:HB2	3:F:2750:LYS:HG2	1.98	0.45
3:F:3378:GLN:O	3:F:3382:GLU:HG2	2.16	0.45
3:F:3860:ASN:HB2	3:F:3865:VAL:HG12	1.99	0.45
2:H:55:VAL:HA	3:I:1784:ALA:HA	1.98	0.45
3:I:215:THR:HG22	3:I:273:HIS:HA	1.99	0.45
3:I:603:LEU:HA	3:I:606:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1290:ARG:HH22	3:I:1644:GLU:HG3	1.82	0.45
3:I:3144:PHE:HB3	3:I:3200:ALA:HB3	1.98	0.45
3:I:3683:GLN:O	3:I:3687:GLU:HB2	2.17	0.45
1:K:6:GLU:HA	1:K:22:CYS:HA	1.98	0.44
3:J:349:GLN:HE21	3:J:354:GLY:HA2	1.81	0.44
3:J:541:SER:HB3	3:J:577:ILE:HD11	1.98	0.44
3:J:1039:LEU:H	3:J:1039:LEU:HD12	1.82	0.44
3:J:1079:LYS:HD3	3:J:1655:GLU:HG2	1.99	0.44
3:J:2575:ARG:HB3	3:J:2578:MET:SD	2.57	0.44
3:J:3105:LYS:HE3	3:J:3128:ASN:HD22	1.81	0.44
3:J:3683:GLN:O	3:J:3687:GLU:HB2	2.17	0.44
3:J:3966:THR:HG22	3:J:4026:MET:HA	1.98	0.44
3:C:275:ARG:HH11	3:C:338:GLU:HG3	1.81	0.44
3:C:349:GLN:HE21	3:C:354:GLY:HA2	1.81	0.44
3:C:1524:THR:HG23	3:C:1526:LEU:HB3	1.98	0.44
3:C:2677:LYS:HD3	3:C:2909:ASP:HB2	1.98	0.44
3:C:2821:TRP:HZ2	3:C:2877:GLN:HB3	1.82	0.44
3:F:1090:PHE:O	3:F:1151:CYS:HB2	2.17	0.44
3:F:2001:PRO:O	3:F:2005:GLN:HG2	2.18	0.44
3:F:2758:PHE:HD2	3:F:2813:LEU:HD11	1.82	0.44
3:F:3099:ALA:O	3:F:3103:ILE:HG12	2.17	0.44
3:F:3203:VAL:HG13	3:F:3214:ASN:HD22	1.82	0.44
3:F:3281:LEU:HD21	3:F:3312:LEU:HA	1.99	0.44
3:I:20:VAL:HA	3:I:204:PRO:HA	1.98	0.44
3:I:893:TYR:HA	3:I:903:LEU:HB3	1.99	0.44
3:I:945:LYS:HB3	3:I:947:GLU:HG2	1.98	0.44
3:I:1000:ARG:HD2	3:I:1005:TRP:CD1	2.52	0.44
3:I:3378:GLN:O	3:I:3382:GLU:HG2	2.16	0.44
3:J:863:LEU:HD21	3:J:930:LYS:HG2	1.98	0.44
3:J:2268:GLN:HA	3:J:2330:ARG:HH22	1.82	0.44
3:J:3281:LEU:HD21	3:J:3312:LEU:HA	1.99	0.44
2:B:42:ARG:HH22	3:C:1782:PHE:HE2	1.65	0.44
3:C:945:LYS:HB3	3:C:947:GLU:HG2	1.98	0.44
3:C:1680:ARG:HH21	3:C:1681:VAL:HG22	1.82	0.44
3:C:1925:GLY:O	3:C:1929:MET:HG2	2.16	0.44
3:C:2268:GLN:HA	3:C:2330:ARG:HH22	1.82	0.44
3:F:275:ARG:HH11	3:F:338:GLU:HG3	1.81	0.44
3:F:739:ALA:HB1	3:F:740:PRO:HD2	1.99	0.44
3:F:1247:PRO:HA	3:F:1598:GLN:HG2	1.98	0.44
3:F:1290:ARG:HH22	3:F:1644:GLU:HG3	1.82	0.44
3:F:2113:SER:O	3:F:2117:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2973:PHE:CD1	3:F:2995:ILE:HG12	2.52	0.44
3:F:3068:LEU:HD23	3:F:3139:VAL:HG21	1.99	0.44
3:F:3966:THR:HG22	3:F:4026:MET:HA	1.98	0.44
2:H:8:SER:HB2	2:H:71:ARG:HB3	1.99	0.44
2:H:56:ILE:HG12	3:I:1783:VAL:O	2.17	0.44
3:I:1680:ARG:HH21	3:I:1681:VAL:HG22	1.82	0.44
3:I:1960:ALA:HB1	3:I:1964:ARG:HH12	1.82	0.44
3:I:2698:MET:HE3	3:I:2698:MET:HB2	1.90	0.44
3:I:2737:PRO:HB2	3:I:2884:ASN:HA	1.99	0.44
3:I:3068:LEU:HD23	3:I:3139:VAL:HG21	1.99	0.44
3:J:603:LEU:HA	3:J:606:LEU:HD12	1.99	0.44
3:J:932:LEU:HD23	3:J:988:LEU:HD11	1.99	0.44
3:J:1858:ASP:O	3:J:1862:ILE:HG13	2.18	0.44
3:J:2677:LYS:HD3	3:J:2909:ASP:HB2	1.98	0.44
3:J:2821:TRP:HZ2	3:J:2877:GLN:HB3	1.82	0.44
3:J:4569:LEU:HD21	3:J:4649:LEU:HG	2.00	0.44
2:B:25:HIS:HB3	2:B:40:ARG:NE	2.31	0.44
3:C:20:VAL:HA	3:C:204:PRO:HA	1.98	0.44
3:C:1247:PRO:HA	3:C:1598:GLN:HG2	1.98	0.44
3:C:2751:LEU:O	3:C:2755:ILE:HG12	2.16	0.44
1:D:13:GLN:HA	1:D:126:SER:HB2	2.00	0.44
3:F:932:LEU:HB3	3:F:937:CYS:HB2	1.99	0.44
3:F:1858:ASP:O	3:F:1862:ILE:HG13	2.18	0.44
3:F:2257:LEU:HD13	3:F:2275:VAL:HG13	1.99	0.44
3:F:4856:PHE:CD2	3:F:4879:MET:HE1	2.53	0.44
1:G:6:GLU:HA	1:G:22:CYS:HA	1.98	0.44
3:I:932:LEU:HB3	3:I:937:CYS:HB2	1.99	0.44
3:I:1100:MET:SD	3:I:1198:GLN:HB3	2.58	0.44
3:I:3550:ARG:HD3	3:I:3594:ARG:NH1	2.31	0.44
3:I:3860:ASN:HB2	3:I:3865:VAL:HG12	2.00	0.44
3:I:3966:THR:HG22	3:I:4026:MET:HA	1.98	0.44
3:I:4018:ASP:HA	3:I:4021:LYS:HE2	1.98	0.44
3:I:4202:ARG:O	3:I:4206:GLU:HG2	2.17	0.44
3:I:4723:LYS:O	3:I:4727:LYS:HG2	2.18	0.44
1:K:94:TYR:CE2	1:K:119:GLN:HA	2.52	0.44
3:J:215:THR:HG22	3:J:273:HIS:HA	1.99	0.44
3:J:1042:ALA:O	3:J:1046:LEU:HG	2.17	0.44
3:J:1958:LEU:HD23	3:J:2138:LEU:HD21	1.98	0.44
3:J:2758:PHE:HD2	3:J:2813:LEU:HD11	1.82	0.44
1:A:94:TYR:CE2	1:A:119:GLN:HA	2.52	0.44
3:C:826:ILE:HG22	3:C:827:LYS:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2737:PRO:HB2	3:C:2884:ASN:HA	1.99	0.44
3:C:2758:PHE:HD2	3:C:2813:LEU:HD11	1.82	0.44
2:E:25:HIS:HB3	2:E:40:ARG:NE	2.31	0.44
3:F:421:PHE:HE2	3:F:436:LEU:HD21	1.82	0.44
3:F:551:LEU:HD13	3:F:589:LEU:HD11	2.00	0.44
3:F:893:TYR:HA	3:F:903:LEU:HB3	1.99	0.44
3:F:1130:GLN:HG2	3:F:1138:PRO:HA	2.00	0.44
3:F:3758:MET:O	3:F:3762:ARG:HG3	2.18	0.44
3:F:4723:LYS:O	3:F:4727:LYS:HG2	2.18	0.44
3:I:248:GLU:HG3	3:I:371:VAL:HG21	1.99	0.44
3:I:2596:THR:O	3:I:2600:ARG:HG3	2.16	0.44
3:I:4816:ILE:HD12	7:I:5105:POV:H21H	1.99	0.44
2:L:55:VAL:HA	3:J:1784:ALA:HA	2.00	0.44
3:J:275:ARG:HH11	3:J:338:GLU:HG3	1.81	0.44
3:J:1290:ARG:HH22	3:J:1644:GLU:HG3	1.82	0.44
3:J:2490:MET:HE3	3:J:2490:MET:HA	2.00	0.44
3:J:2737:PRO:HB2	3:J:2884:ASN:HA	1.99	0.44
3:J:4202:ARG:O	3:J:4206:GLU:HG2	2.17	0.44
3:J:4241:THR:O	3:J:4245:MET:HE3	2.18	0.44
3:J:4943:LEU:O	3:J:4947:GLN:HG2	2.17	0.44
7:J:5112:POV:H27A	7:J:5112:POV:H24A	1.67	0.44
3:C:551:LEU:HD13	3:C:589:LEU:HD11	1.99	0.44
3:C:4241:THR:O	3:C:4245:MET:HE3	2.18	0.44
3:F:2737:PRO:HB2	3:F:2884:ASN:HA	1.99	0.44
3:F:2747:ILE:HB	3:F:2814:LYS:HG2	1.99	0.44
3:F:3683:GLN:O	3:F:3687:GLU:HB2	2.17	0.44
1:G:13:GLN:HA	1:G:126:SER:HB2	2.00	0.44
1:G:94:TYR:CE2	1:G:119:GLN:HA	2.52	0.44
3:I:568:LEU:HD12	3:I:602:VAL:HG13	2.00	0.44
3:I:826:ILE:HG22	3:I:827:LYS:HG2	2.00	0.44
3:I:1758:ARG:HH12	3:I:2037:ASP:HA	1.83	0.44
3:I:1858:ASP:O	3:I:1862:ILE:HG13	2.18	0.44
3:I:2113:SER:O	3:I:2117:VAL:HG23	2.17	0.44
3:I:4090:LYS:HG3	3:I:4112:LEU:HD22	1.99	0.44
1:K:66:ARG:C	1:K:66:ARG:HE	2.26	0.44
3:J:1758:ARG:HH12	3:J:2037:ASP:HA	1.83	0.44
3:C:196:MET:N	3:C:196:MET:HE3	2.33	0.44
3:C:1079:LYS:HD3	3:C:1655:GLU:HG2	1.99	0.44
3:C:3770:LEU:HB2	3:C:3804:ILE:HD11	1.98	0.44
3:C:4090:LYS:HG3	3:C:4112:LEU:HD22	1.99	0.44
3:C:4202:ARG:O	3:C:4206:GLU:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1248:VAL:HG22	3:F:1599:MET:HB3	2.00	0.44
3:F:2490:MET:HA	3:F:2490:MET:HE3	2.00	0.44
3:F:2821:TRP:HZ2	3:F:2877:GLN:HB3	1.83	0.44
3:F:3107:VAL:HG11	3:F:3171:SER:HB2	2.00	0.44
3:F:4765:LEU:HA	3:F:4768:LEU:HD12	2.00	0.44
3:F:4938:ASP:HB3	3:I:4944:ARG:HH22	1.81	0.44
3:F:4943:LEU:O	3:F:4947:GLN:HG2	2.17	0.44
3:I:1090:PHE:O	3:I:1151:CYS:HB2	2.17	0.44
3:I:1130:GLN:HG2	3:I:1138:PRO:HA	2.00	0.44
3:J:568:LEU:HD12	3:J:602:VAL:HG13	2.00	0.44
3:J:573:GLU:O	3:J:577:ILE:HG12	2.16	0.44
3:J:826:ILE:HG22	3:J:827:LYS:HG2	2.00	0.44
3:J:945:LYS:HB3	3:J:947:GLU:HG2	1.98	0.44
3:J:2559:LEU:O	3:J:2563:THR:HG23	2.17	0.44
3:J:2914:LYS:HD2	3:J:2915:GLU:HG2	2.00	0.44
3:J:4668:LEU:O	3:J:4672:LYS:HG3	2.18	0.44
3:C:603:LEU:HA	3:C:606:LEU:HD12	1.99	0.44
3:C:893:TYR:HA	3:C:903:LEU:HB3	1.99	0.44
3:C:1039:LEU:H	3:C:1039:LEU:HD12	1.82	0.44
3:C:1958:LEU:HD23	3:C:2138:LEU:HD21	1.98	0.44
3:C:2158:CYS:O	3:C:2162:ILE:HG13	2.18	0.44
3:C:3719:ASP:O	3:C:3723:MET:HG2	2.17	0.44
3:C:4569:LEU:HD21	3:C:4649:LEU:HG	2.00	0.44
3:C:4668:LEU:O	3:C:4672:LYS:HG3	2.18	0.44
3:C:4943:LEU:O	3:C:4947:GLN:HG2	2.17	0.44
1:D:94:TYR:CE2	1:D:119:GLN:HA	2.52	0.44
3:F:826:ILE:HG22	3:F:827:LYS:HG2	2.00	0.44
3:F:1100:MET:SD	3:F:1198:GLN:HB3	2.58	0.44
3:F:2158:CYS:O	3:F:2162:ILE:HG13	2.18	0.44
3:F:2559:LEU:O	3:F:2563:THR:HG23	2.17	0.44
1:G:18:LEU:HD23	1:G:18:LEU:HA	1.88	0.44
1:G:66:ARG:HE	1:G:66:ARG:C	2.26	0.44
3:I:1248:VAL:HG22	3:I:1599:MET:HB3	2.00	0.44
3:I:2257:LEU:HD13	3:I:2275:VAL:HG13	1.99	0.44
3:I:2490:MET:HA	3:I:2490:MET:HE3	2.00	0.44
3:I:2821:TRP:HZ2	3:I:2877:GLN:HB3	1.82	0.44
3:I:2914:LYS:HD2	3:I:2915:GLU:HG2	2.00	0.44
3:I:4241:THR:O	3:I:4245:MET:HE3	2.18	0.44
3:J:1006:SER:C	3:J:1021:LEU:HD21	2.43	0.44
3:J:1247:PRO:HA	3:J:1598:GLN:HG2	1.98	0.44
3:J:1680:ARG:HH21	3:J:1681:VAL:HG22	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:2257:LEU:HD13	3:J:2275:VAL:HG13	1.99	0.44
3:J:2369:ARG:HG3	3:J:2372:GLY:H	1.83	0.44
3:J:2608:MET:HA	3:J:2608:MET:HE3	1.99	0.44
3:J:3107:VAL:HG11	3:J:3171:SER:HB2	2.00	0.44
3:J:4245:MET:HE2	3:J:4245:MET:HB3	1.89	0.44
3:J:4723:LYS:O	3:J:4727:LYS:HG2	2.18	0.44
3:J:4816:ILE:HD12	7:J:5113:POV:H21H	2.00	0.44
7:J:5104:POV:H11	7:J:5105:POV:H14A	2.00	0.44
3:C:499:THR:HG23	3:C:502:HIS:H	1.82	0.44
3:C:689:THR:HA	3:C:778:PHE:HE2	1.83	0.44
3:C:2001:PRO:O	3:C:2005:GLN:HG2	2.18	0.44
3:C:2113:SER:O	3:C:2117:VAL:HG23	2.17	0.44
3:C:3758:MET:O	3:C:3762:ARG:HG3	2.18	0.44
3:C:3860:ASN:HB2	3:C:3865:VAL:HG12	1.99	0.44
3:F:689:THR:HA	3:F:778:PHE:HE2	1.83	0.44
3:F:1006:SER:C	3:F:1021:LEU:HD21	2.43	0.44
3:F:2514:ASN:OD1	3:F:2517:PHE:HB3	2.18	0.44
3:F:2977:LEU:O	3:F:2981:VAL:HG22	2.17	0.44
3:F:3969:ILE:HG23	3:F:3980:LEU:HD12	2.00	0.44
3:F:4241:THR:O	3:F:4245:MET:HE3	2.18	0.44
2:H:42:ARG:HH22	3:I:1782:PHE:HE2	1.64	0.44
3:I:499:THR:HG23	3:I:502:HIS:H	1.82	0.44
3:I:544:LEU:HD21	3:I:574:VAL:HB	1.99	0.44
3:I:1046:LEU:HB3	3:I:1051:TYR:HD2	1.83	0.44
3:I:2559:LEU:O	3:I:2563:THR:HG23	2.17	0.44
3:I:2608:MET:HA	3:I:2608:MET:HE3	1.99	0.44
3:J:551:LEU:HD13	3:J:589:LEU:HD11	1.99	0.44
3:J:689:THR:HA	3:J:778:PHE:HE2	1.83	0.44
3:J:739:ALA:HB1	3:J:740:PRO:HD2	1.99	0.44
3:J:1248:VAL:HG22	3:J:1599:MET:HB3	2.00	0.44
3:J:1269:CYS:SG	3:J:1563:GLN:HB2	2.58	0.44
3:J:1435:TYR:CZ	3:J:1550:PRO:HB3	2.53	0.44
3:J:2001:PRO:O	3:J:2005:GLN:HG2	2.18	0.44
3:J:2977:LEU:O	3:J:2981:VAL:HG22	2.17	0.44
3:J:3201:MET:HE2	3:J:3201:MET:HB3	1.90	0.44
3:C:62:LEU:HB2	3:C:261:ARG:HH21	1.83	0.44
3:C:153:ALA:HB1	3:C:199:LEU:HD22	2.00	0.44
3:C:1130:GLN:HG2	3:C:1138:PRO:HA	2.00	0.44
3:C:1248:VAL:HG22	3:C:1599:MET:HB3	2.00	0.44
3:C:2490:MET:HA	3:C:2490:MET:HE3	2.00	0.44
3:C:2608:MET:HA	3:C:2608:MET:HE3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2914:LYS:HD2	3:C:2915:GLU:HG2	2.00	0.44
3:C:3203:VAL:HG13	3:C:3214:ASN:HD22	1.82	0.44
3:F:499:THR:HG23	3:F:502:HIS:H	1.82	0.44
3:F:573:GLU:O	3:F:577:ILE:HG12	2.16	0.44
3:F:3793:MET:HE3	3:F:3793:MET:HB3	1.83	0.44
3:I:733:PRO:HG2	3:I:762:CYS:HB3	2.00	0.44
3:I:817:PRO:HG2	3:I:1022:VAL:HG21	2.00	0.44
3:I:1269:CYS:SG	3:I:1563:GLN:HB2	2.58	0.44
3:I:1435:TYR:CZ	3:I:1550:PRO:HB3	2.53	0.44
3:I:2747:ILE:HB	3:I:2814:LYS:HG2	1.99	0.44
3:I:2977:LEU:O	3:I:2981:VAL:HG22	2.17	0.44
3:I:3203:VAL:HG13	3:I:3214:ASN:HD22	1.82	0.44
3:I:3916:ILE:HG22	3:I:3980:LEU:HD21	2.00	0.44
3:J:62:LEU:HB2	3:J:261:ARG:HH21	1.83	0.43
3:J:153:ALA:HB1	3:J:199:LEU:HD22	2.00	0.43
3:J:733:PRO:HG2	3:J:762:CYS:HB3	2.00	0.43
3:J:1100:MET:SD	3:J:1198:GLN:HB3	2.58	0.43
3:J:1130:GLN:HG2	3:J:1138:PRO:HA	2.00	0.43
3:J:2113:SER:O	3:J:2117:VAL:HG23	2.17	0.43
3:J:2158:CYS:O	3:J:2162:ILE:HG13	2.18	0.43
3:J:2514:ASN:OD1	3:J:2517:PHE:HB3	2.18	0.43
3:J:3916:ILE:HG22	3:J:3980:LEU:HD21	2.00	0.43
3:J:3969:ILE:HG23	3:J:3980:LEU:HD12	2.00	0.43
3:J:4765:LEU:HA	3:J:4768:LEU:HD12	2.00	0.43
3:J:4856:PHE:CD2	3:J:4879:MET:HE1	2.53	0.43
3:C:739:ALA:HB1	3:C:740:PRO:HD2	1.99	0.43
3:C:932:LEU:HD23	3:C:988:LEU:HD11	1.99	0.43
3:C:1220:GLN:HG2	3:F:3523:ASN:CG	2.43	0.43
3:C:2514:ASN:OD1	3:C:2517:PHE:HB3	2.18	0.43
3:C:3068:LEU:HD23	3:C:3139:VAL:HG21	1.99	0.43
3:C:3107:VAL:HG11	3:C:3171:SER:HB2	2.00	0.43
3:C:3969:ILE:HG23	3:C:3980:LEU:HD12	2.00	0.43
7:C:5106:POV:H11	7:C:5107:POV:H14A	2.00	0.43
3:F:215:THR:HG22	3:F:273:HIS:HA	1.99	0.43
3:F:364:PRO:O	3:F:368:ARG:HG3	2.18	0.43
3:F:2325:PRO:HB2	3:F:2421:ALA:HB1	2.00	0.43
3:F:3316:LEU:HD13	3:F:3345:ILE:HG23	2.00	0.43
1:G:36:TRP:HE3	1:G:93:TYR:HD2	1.66	0.43
3:I:421:PHE:HE2	3:I:436:LEU:HD21	1.82	0.43
3:I:551:LEU:HD13	3:I:589:LEU:HD11	2.00	0.43
3:I:689:THR:HA	3:I:778:PHE:HE2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:222:LEU:HB3	3:J:388:LEU:HD13	2.00	0.43
3:J:2142:TYR:CZ	3:J:2197:LEU:HB2	2.53	0.43
3:J:3127:GLN:HG2	3:J:3129:LEU:H	1.84	0.43
3:J:3860:ASN:HB2	3:J:3865:VAL:HG12	2.00	0.43
1:A:13:GLN:HA	1:A:126:SER:HB2	2.00	0.43
3:C:421:PHE:HE2	3:C:436:LEU:HD21	1.82	0.43
3:C:981:GLN:HG3	3:C:1047:LEU:HD11	2.01	0.43
3:C:1006:SER:C	3:C:1021:LEU:HD21	2.43	0.43
3:C:3966:THR:HG22	3:C:4026:MET:HA	1.98	0.43
3:F:1046:LEU:HB3	3:F:1051:TYR:HD2	1.83	0.43
3:F:2268:GLN:HA	3:F:2330:ARG:HH22	1.82	0.43
3:F:2580:ASP:HA	3:F:2583:LEU:HD12	2.00	0.43
3:F:4090:LYS:HG3	3:F:4112:LEU:HD22	1.99	0.43
1:G:4:LEU:HB3	1:G:95:CYS:SG	2.59	0.43
3:I:196:MET:HE3	3:I:196:MET:N	2.33	0.43
3:I:983:THR:O	3:I:987:ARG:HG2	2.19	0.43
3:I:1286:MET:HE3	3:I:1286:MET:HB3	1.88	0.43
3:I:2268:GLN:HA	3:I:2330:ARG:HH22	1.82	0.43
3:I:2580:ASP:HA	3:I:2583:LEU:HD12	2.00	0.43
3:I:4928:LEU:HD23	3:I:4931:ILE:HD12	2.00	0.43
3:J:252:VAL:HA	3:J:255:HIS:ND1	2.33	0.43
3:J:421:PHE:HE2	3:J:436:LEU:HD21	1.82	0.43
3:J:1087:ARG:HB3	3:J:1223:PHE:CD2	2.54	0.43
3:J:2747:ILE:HB	3:J:2814:LYS:HG2	1.99	0.43
1:A:4:LEU:HB3	1:A:95:CYS:SG	2.59	0.43
3:C:1269:CYS:SG	3:C:1563:GLN:HB2	2.59	0.43
3:C:1435:TYR:CZ	3:C:1550:PRO:HB3	2.53	0.43
3:C:1960:ALA:HB1	3:C:1964:ARG:HH12	1.82	0.43
3:C:2747:ILE:HB	3:C:2814:LYS:HG2	1.99	0.43
3:C:2765:LYS:HE3	3:C:2861:ASP:HB2	1.99	0.43
3:C:2926:LEU:O	3:C:2930:LEU:HG	2.18	0.43
3:C:4856:PHE:CD2	3:C:4879:MET:HE1	2.53	0.43
1:D:4:LEU:HB3	1:D:95:CYS:SG	2.59	0.43
1:D:36:TRP:HE3	1:D:93:TYR:HD2	1.66	0.43
3:F:462:GLU:HB2	3:F:3710:LEU:HD13	2.01	0.43
3:F:1939:MET:HE3	3:F:1939:MET:HB2	1.50	0.43
3:F:2142:TYR:CZ	3:F:2197:LEU:HB2	2.53	0.43
3:F:3036:LYS:HB2	3:F:3036:LYS:HE3	1.68	0.43
3:F:3201:MET:HE2	3:F:3201:MET:HB3	1.90	0.43
3:I:364:PRO:O	3:I:368:ARG:HG3	2.18	0.43
3:I:946:ALA:HB1	3:I:972:LEU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1617:THR:HB	3:I:1628:VAL:HG22	2.00	0.43
3:I:2001:PRO:O	3:I:2005:GLN:HG2	2.17	0.43
3:I:2142:TYR:CZ	3:I:2197:LEU:HB2	2.53	0.43
3:I:2325:PRO:HB2	3:I:2421:ALA:HB1	2.00	0.43
3:I:2926:LEU:O	3:I:2930:LEU:HG	2.18	0.43
3:I:3127:GLN:HG2	3:I:3129:LEU:H	1.84	0.43
3:I:4569:LEU:HD21	3:I:4649:LEU:HG	2.00	0.43
2:L:8:SER:HB2	2:L:71:ARG:HB3	1.99	0.43
2:L:14:THR:OG1	2:L:106:LEU:HD23	2.19	0.43
3:J:462:GLU:HB2	3:J:3710:LEU:HD13	2.01	0.43
3:J:3316:LEU:HD13	3:J:3345:ILE:HG23	2.00	0.43
1:A:37:TYR:CE2	1:A:47:LEU:HD13	2.54	0.43
3:C:223:PHE:HB2	3:C:389:PHE:O	2.19	0.43
3:C:568:LEU:HD12	3:C:602:VAL:HG13	2.00	0.43
3:C:1100:MET:SD	3:C:1198:GLN:HB3	2.58	0.43
3:C:2013:LYS:HB2	3:C:3661:TRP:CE2	2.54	0.43
3:C:2973:PHE:CD1	3:C:2995:ILE:HG12	2.52	0.43
3:C:3066:ASN:O	3:C:3070:ILE:HG12	2.18	0.43
3:C:4844:LEU:HD11	3:C:4924:VAL:HG13	2.01	0.43
7:C:5106:POV:H25A	7:C:5106:POV:H22	1.90	0.43
3:F:222:LEU:HB3	3:F:388:LEU:HD13	2.00	0.43
3:F:2926:LEU:O	3:F:2930:LEU:HG	2.18	0.43
7:F:5106:POV:H11	7:F:5107:POV:H14A	2.00	0.43
3:I:153:ALA:HB1	3:I:199:LEU:HD22	2.00	0.43
3:I:224:HIS:CE1	3:I:386:ASP:HA	2.53	0.43
3:I:462:GLU:HB2	3:I:3710:LEU:HD13	2.01	0.43
3:I:981:GLN:HG3	3:I:1047:LEU:HD11	2.01	0.43
3:I:2514:ASN:OD1	3:I:2517:PHE:HB3	2.18	0.43
3:I:3210:LEU:HD22	3:I:3213:TYR:HE2	1.84	0.43
3:J:195:PHE:HB3	3:C:2361:PRO:HG3	2.01	0.43
3:J:4581:LYS:HD2	7:J:5112:POV:H15	2.00	0.43
3:J:4844:LEU:HD11	3:J:4924:VAL:HG13	2.01	0.43
3:C:2012:PHE:CZ	3:C:2031:LEU:HD23	2.53	0.43
3:C:2913:ALA:HA	3:C:2916:LYS:HB3	2.00	0.43
3:C:4928:LEU:HD23	3:C:4931:ILE:HD12	2.00	0.43
2:E:55:VAL:HA	3:F:1784:ALA:HA	1.99	0.43
3:F:946:ALA:HB1	3:F:972:LEU:HB3	2.00	0.43
3:F:1220:GLN:HG2	3:I:3523:ASN:CG	2.43	0.43
3:F:2131:LEU:HD23	3:F:2131:LEU:HA	1.90	0.43
3:F:2608:MET:HE3	3:F:2608:MET:HA	1.99	0.43
3:F:2914:LYS:HD2	3:F:2915:GLU:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:3066:ASN:O	3:F:3070:ILE:HG12	2.19	0.43
3:F:4687:TYR:CE1	3:F:4703:ARG:HG2	2.54	0.43
3:I:252:VAL:HA	3:I:255:HIS:ND1	2.33	0.43
3:I:1006:SER:C	3:I:1021:LEU:HD21	2.43	0.43
3:I:2013:LYS:HB2	3:I:3661:TRP:CE2	2.54	0.43
3:I:2765:LYS:HE3	3:I:2861:ASP:HB2	1.99	0.43
3:I:3758:MET:O	3:I:3762:ARG:HG3	2.18	0.43
3:I:3969:ILE:HG23	3:I:3980:LEU:HD12	2.00	0.43
3:I:4765:LEU:HA	3:I:4768:LEU:HD12	2.00	0.43
1:K:13:GLN:HA	1:K:126:SER:HB2	2.00	0.43
3:J:224:HIS:CE1	3:J:386:ASP:HA	2.54	0.43
3:J:2012:PHE:CZ	3:J:2031:LEU:HD23	2.53	0.43
3:J:3068:LEU:HD23	3:J:3139:VAL:HG21	1.99	0.43
3:J:4823:LEU:HD23	3:J:4823:LEU:HA	1.83	0.43
1:A:66:ARG:HE	1:A:66:ARG:C	2.26	0.43
3:C:1617:THR:HB	3:C:1628:VAL:HG22	2.00	0.43
3:C:3210:LEU:HD22	3:C:3213:TYR:HE2	1.84	0.43
3:C:3316:LEU:HD13	3:C:3345:ILE:HG23	2.00	0.43
1:D:37:TYR:CE2	1:D:47:LEU:HD13	2.54	0.43
2:E:14:THR:OG1	2:E:106:LEU:HD23	2.19	0.43
3:F:981:GLN:HG3	3:F:1047:LEU:HD11	2.00	0.43
3:F:1269:CYS:SG	3:F:1563:GLN:HB2	2.58	0.43
3:F:1435:TYR:CZ	3:F:1550:PRO:HB3	2.53	0.43
3:F:1960:ALA:HB1	3:F:1964:ARG:HH12	1.82	0.43
3:F:3210:LEU:HD22	3:F:3213:TYR:HE2	1.84	0.43
3:F:4569:LEU:HD21	3:F:4649:LEU:HG	2.00	0.43
3:F:4787:ASN:HA	3:F:4790:LEU:HD12	2.00	0.43
3:F:4823:LEU:HD23	3:F:4823:LEU:HA	1.84	0.43
2:H:14:THR:OG1	2:H:106:LEU:HD23	2.19	0.43
3:I:223:PHE:HB2	3:I:389:PHE:O	2.19	0.43
3:I:2158:CYS:O	3:I:2162:ILE:HG13	2.18	0.43
3:I:3066:ASN:O	3:I:3070:ILE:HG12	2.19	0.43
3:I:3316:LEU:HD13	3:I:3345:ILE:HG23	2.00	0.43
3:I:4581:LYS:HD2	7:I:5104:POV:H15	2.00	0.43
3:I:4943:LEU:O	3:I:4947:GLN:HG2	2.17	0.43
1:K:36:TRP:HE3	1:K:93:TYR:HD2	1.66	0.43
2:L:50:ILE:HG21	2:L:64:ALA:HB2	2.01	0.43
2:L:74:LEU:O	2:L:98:ILE:HA	2.19	0.43
3:J:196:MET:N	3:J:196:MET:HE3	2.33	0.43
3:J:2765:LYS:HE3	3:J:2861:ASP:HB2	1.99	0.43
3:J:4787:ASN:HA	3:J:4790:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:4928:LEU:HD23	3:J:4931:ILE:HD12	2.00	0.43
2:B:14:THR:OG1	2:B:106:LEU:HD23	2.19	0.43
3:C:64:ILE:HA	3:C:111:HIS:CE1	2.54	0.43
3:C:289:ARG:HD2	3:C:301:VAL:HG23	2.00	0.43
3:C:1087:ARG:HB3	3:C:1223:PHE:CD2	2.54	0.43
3:C:1858:ASP:O	3:C:1862:ILE:HG13	2.18	0.43
3:C:2142:TYR:CZ	3:C:2197:LEU:HB2	2.53	0.43
3:C:2671:GLU:O	3:C:2675:THR:HG22	2.19	0.43
3:C:4687:TYR:CE1	3:C:4703:ARG:HG2	2.54	0.43
1:D:66:ARG:HE	1:D:66:ARG:C	2.26	0.43
2:E:56:ILE:HG12	3:F:1783:VAL:O	2.18	0.43
3:F:195:PHE:HB3	3:I:2361:PRO:HG3	2.01	0.43
3:F:196:MET:N	3:F:196:MET:HE3	2.33	0.43
3:F:252:VAL:HA	3:F:255:HIS:ND1	2.33	0.43
3:F:3010:PHE:HE2	3:F:3074:SER:HB3	1.84	0.43
3:F:4668:LEU:O	3:F:4672:LYS:HG3	2.18	0.43
3:I:739:ALA:HB1	3:I:740:PRO:HD2	1.99	0.43
3:I:1039:LEU:HD12	3:I:1039:LEU:H	1.82	0.43
3:I:1087:ARG:HB3	3:I:1223:PHE:CD2	2.54	0.43
3:I:2012:PHE:CZ	3:I:2031:LEU:HD23	2.53	0.43
7:I:5109:POV:H11	7:I:5110:POV:H14A	2.00	0.43
1:K:4:LEU:HB3	1:K:95:CYS:SG	2.58	0.43
1:K:37:TYR:CE2	1:K:47:LEU:HD13	2.54	0.43
2:L:49:ARG:HD2	2:L:52:LYS:HE3	2.01	0.43
3:J:981:GLN:HG3	3:J:1047:LEU:HD11	2.00	0.43
3:J:2671:GLU:O	3:J:2675:THR:HG22	2.19	0.43
3:J:3244:PRO:HG2	3:J:3249:LEU:HD12	2.01	0.43
3:J:3758:MET:O	3:J:3762:ARG:HG3	2.18	0.43
2:B:74:LEU:O	2:B:98:ILE:HA	2.19	0.43
3:C:195:PHE:HB3	3:F:2361:PRO:HG3	2.01	0.43
3:C:1046:LEU:HB3	3:C:1051:TYR:HD2	1.83	0.43
3:C:2257:LEU:HD13	3:C:2275:VAL:HG13	1.99	0.43
3:C:2670:GLU:HG3	3:C:2913:ALA:H	1.84	0.43
3:C:3127:GLN:HG2	3:C:3129:LEU:H	1.83	0.43
3:C:4723:LYS:O	3:C:4727:LYS:HG2	2.18	0.43
2:E:50:ILE:HG21	2:E:64:ALA:HB2	2.01	0.43
3:F:64:ILE:HA	3:F:111:HIS:CE1	2.54	0.43
3:F:153:ALA:HB1	3:F:199:LEU:HD22	2.00	0.43
3:F:1758:ARG:HH12	3:F:2037:ASP:HA	1.83	0.43
3:F:2013:LYS:HB2	3:F:3661:TRP:CE2	2.54	0.43
3:F:4161:ARG:HD3	3:F:4164:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:289:ARG:HD2	3:I:301:VAL:HG23	2.00	0.43
3:J:289:ARG:HD2	3:J:301:VAL:HG23	2.00	0.43
3:J:1046:LEU:HB3	3:J:1051:TYR:HD2	1.83	0.43
3:J:2142:TYR:CE1	3:J:2197:LEU:HB2	2.54	0.43
3:J:2615:ARG:HB3	3:J:2618:MET:SD	2.59	0.43
3:J:2926:LEU:O	3:J:2930:LEU:HG	2.18	0.43
3:J:3955:MET:HG2	3:J:4019:LEU:HD22	2.01	0.43
3:J:4090:LYS:HG3	3:J:4112:LEU:HD22	1.99	0.43
2:B:50:ILE:HG21	2:B:64:ALA:HB2	2.01	0.43
3:C:1483:VAL:HG21	3:C:1486:SER:HB2	2.01	0.43
3:C:2325:PRO:HB2	3:C:2421:ALA:HB1	2.00	0.43
3:C:2467:VAL:HG23	3:C:2521:VAL:HG12	2.01	0.43
3:C:2470:ILE:HG22	3:C:2525:GLY:HA3	2.00	0.43
3:C:3036:LYS:HE3	3:C:3036:LYS:HB2	1.68	0.43
3:C:4161:ARG:HD3	3:C:4164:LEU:HD12	2.01	0.43
3:F:289:ARG:HD2	3:F:301:VAL:HG23	2.00	0.43
3:F:533:ASN:HB2	3:F:536:ASN:HB2	2.00	0.43
3:F:568:LEU:HD12	3:F:602:VAL:HG13	2.00	0.43
3:F:603:LEU:HA	3:F:606:LEU:HD12	1.99	0.43
3:F:2369:ARG:HG3	3:F:2372:GLY:H	1.83	0.43
3:F:2765:LYS:HE3	3:F:2861:ASP:HB2	1.99	0.43
1:G:37:TYR:CE2	1:G:47:LEU:HD13	2.54	0.43
2:H:4:ILE:HD12	2:H:4:ILE:HA	1.91	0.43
2:H:49:ARG:HD2	2:H:52:LYS:HE3	2.01	0.43
3:I:1071:ARG:HA	3:I:1071:ARG:HD3	1.58	0.43
3:I:1483:VAL:HG21	3:I:1486:SER:HB2	2.01	0.43
3:I:1939:MET:HB2	3:I:1939:MET:HE3	1.50	0.43
3:I:2615:ARG:HB3	3:I:2618:MET:SD	2.59	0.43
3:I:3817:LEU:HD11	3:I:3821:LYS:HE3	2.01	0.43
3:I:4668:LEU:O	3:I:4672:LYS:HG3	2.18	0.43
3:I:4787:ASN:HA	3:I:4790:LEU:HD12	2.00	0.43
3:I:4994:TYR:CZ	3:I:4998:LYS:HD2	2.54	0.43
3:J:533:ASN:HB2	3:J:536:ASN:HB2	2.00	0.43
3:J:817:PRO:HG2	3:J:1022:VAL:HG21	2.00	0.43
3:J:983:THR:O	3:J:987:ARG:HG2	2.19	0.43
3:J:1220:GLN:HG2	3:C:3523:ASN:CG	2.43	0.43
3:J:2361:PRO:HG3	3:I:195:PHE:HB3	2.01	0.43
3:J:2580:ASP:HA	3:J:2583:LEU:HD12	2.00	0.43
3:J:2670:GLU:HG3	3:J:2913:ALA:H	1.84	0.43
3:J:3523:ASN:CG	3:I:1220:GLN:HG2	2.43	0.43
3:C:462:GLU:HB2	3:C:3710:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:983:THR:O	3:C:987:ARG:HG2	2.19	0.43
3:C:1758:ARG:HH12	3:C:2037:ASP:HA	1.83	0.43
3:C:2142:TYR:CE1	3:C:2197:LEU:HB2	2.54	0.43
3:C:2765:LYS:HZ1	3:C:2860:PRO:HA	1.83	0.43
3:C:3244:PRO:HG2	3:C:3249:LEU:HD12	2.01	0.43
3:C:3955:MET:HG2	3:C:4019:LEU:HD22	2.01	0.43
2:E:4:ILE:HD12	2:E:4:ILE:HA	1.91	0.43
3:F:436:LEU:HB2	3:F:438:ILE:HG13	2.01	0.43
3:F:2470:ILE:HG22	3:F:2525:GLY:HA3	2.00	0.43
1:G:37:TYR:O	1:G:94:TYR:HB2	2.19	0.43
3:I:372:LEU:HD23	3:I:372:LEU:H	1.84	0.43
3:I:665:GLU:HB2	3:I:792:LEU:HB2	2.01	0.43
3:I:2369:ARG:HG3	3:I:2372:GLY:H	1.83	0.43
3:I:2670:GLU:HG3	3:I:2913:ALA:H	1.84	0.43
3:I:4068:LEU:HD23	3:I:4111:LEU:HD13	2.01	0.43
3:J:3339:ALA:O	3:J:3343:GLN:HG2	2.19	0.42
3:J:4068:LEU:HD23	3:J:4111:LEU:HD13	2.01	0.42
3:C:665:GLU:HB2	3:C:792:LEU:HB2	2.01	0.42
3:C:868:GLU:O	3:C:872:GLU:HG2	2.19	0.42
3:C:1211:LEU:HD23	3:C:1211:LEU:HA	1.85	0.42
3:C:2332:LEU:HD22	3:C:2429:LEU:HA	2.01	0.42
3:C:2580:ASP:HA	3:C:2583:LEU:HD12	2.00	0.42
3:C:3264:THR:HA	3:C:3267:PRO:HG3	2.01	0.42
3:C:4994:TYR:CZ	3:C:4998:LYS:HD2	2.54	0.42
3:F:733:PRO:HG2	3:F:762:CYS:HB3	2.00	0.42
3:F:817:PRO:HG2	3:F:1022:VAL:HG21	2.00	0.42
3:F:1243:PRO:HB2	3:F:1600:LEU:HD11	2.01	0.42
3:F:2346:VAL:HG13	3:F:2349:ASN:HB2	2.01	0.42
3:F:2671:GLU:O	3:F:2675:THR:HG22	2.19	0.42
3:F:4105:GLY:O	3:F:4109:GLN:HG2	2.19	0.42
3:F:4581:LYS:HD2	7:F:5101:POV:H15	2.00	0.42
2:H:50:ILE:HG21	2:H:64:ALA:HB2	2.01	0.42
3:I:868:GLU:O	3:I:872:GLU:HG2	2.19	0.42
3:I:2913:ALA:HA	3:I:2916:LYS:HB3	2.00	0.42
3:I:3107:VAL:HG11	3:I:3171:SER:HB2	2.00	0.42
3:I:3339:ALA:O	3:I:3343:GLN:HG2	2.19	0.42
3:I:4844:LEU:HD11	3:I:4924:VAL:HG13	2.01	0.42
3:I:4856:PHE:CD2	3:I:4879:MET:HE1	2.53	0.42
3:J:875:ALA:HA	3:J:878:ILE:HG22	2.01	0.42
3:J:1617:THR:HB	3:J:1628:VAL:HG22	2.00	0.42
3:J:1856:ASP:O	3:J:1860:LYS:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:2470:ILE:HG22	3:J:2525:GLY:HA3	2.00	0.42
3:J:3203:VAL:HG13	3:J:3214:ASN:HD22	1.82	0.42
3:J:3885:PHE:HE1	3:J:3919:THR:HG23	1.84	0.42
3:J:4994:TYR:CZ	3:J:4998:LYS:HD2	2.54	0.42
3:C:1243:PRO:HB2	3:C:1600:LEU:HD11	2.01	0.42
3:C:2248:ARG:NH1	3:C:2248:ARG:HB2	2.35	0.42
3:C:4581:LYS:HD2	7:C:5101:POV:H15	2.00	0.42
2:E:49:ARG:HD2	2:E:52:LYS:HE3	2.01	0.42
3:F:62:LEU:HB2	3:F:261:ARG:HH21	1.83	0.42
3:F:223:PHE:HB2	3:F:389:PHE:O	2.19	0.42
3:F:2012:PHE:CZ	3:F:2031:LEU:HD23	2.53	0.42
3:F:2670:GLU:HG3	3:F:2913:ALA:H	1.84	0.42
3:F:3667:HIS:HD2	3:F:3669:PHE:HD1	1.66	0.42
3:F:4666:VAL:O	3:F:4670:ILE:HG12	2.20	0.42
3:F:4725:LEU:HD11	3:F:4734:ARG:HG3	2.01	0.42
3:F:4844:LEU:HD11	3:F:4924:VAL:HG13	2.01	0.42
3:I:62:LEU:HB2	3:I:261:ARG:HH21	1.83	0.42
3:I:2332:LEU:HD22	3:I:2429:LEU:HA	2.01	0.42
3:I:2671:GLU:O	3:I:2675:THR:HG22	2.19	0.42
3:I:3793:MET:HE3	3:I:3793:MET:HB3	1.83	0.42
3:I:4687:TYR:CE1	3:I:4703:ARG:HG2	2.54	0.42
2:L:57:LYS:HE3	2:L:57:LYS:HB3	1.75	0.42
3:J:2346:VAL:HG13	3:J:2349:ASN:HB2	2.01	0.42
3:J:2913:ALA:HA	3:J:2916:LYS:HB3	2.00	0.42
3:J:3066:ASN:O	3:J:3070:ILE:HG12	2.19	0.42
3:J:3264:THR:HA	3:J:3267:PRO:HG3	2.01	0.42
1:A:36:TRP:HE3	1:A:93:TYR:HD2	1.66	0.42
2:B:49:ARG:HD2	2:B:52:LYS:HE3	2.01	0.42
3:C:224:HIS:CE1	3:C:386:ASP:HA	2.54	0.42
3:C:372:LEU:H	3:C:372:LEU:HD23	1.84	0.42
3:C:3010:PHE:HE2	3:C:3074:SER:HB3	1.84	0.42
3:C:3263:TYR:HE1	3:C:3270:ILE:HB	1.85	0.42
3:C:3667:HIS:HD2	3:C:3669:PHE:HD1	1.66	0.42
3:F:875:ALA:HA	3:F:878:ILE:HG22	2.01	0.42
3:F:1087:ARG:HB3	3:F:1223:PHE:CD2	2.54	0.42
3:F:1617:THR:HB	3:F:1628:VAL:HG22	2.00	0.42
3:F:2142:TYR:CE1	3:F:2197:LEU:HB2	2.54	0.42
3:F:2193:GLN:HG2	3:F:2194:HIS:CD2	2.54	0.42
3:F:2615:ARG:HB3	3:F:2618:MET:SD	2.59	0.42
3:F:4698:LYS:HE3	3:F:4698:LYS:HB2	1.87	0.42
3:F:4816:ILE:HD12	7:F:5102:POV:H21H	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:2346:VAL:HG13	3:I:2349:ASN:HB2	2.01	0.42
3:I:2863:SER:HB2	3:I:2924:GLN:HB2	2.01	0.42
3:I:4161:ARG:HD3	3:I:4164:LEU:HD12	2.01	0.42
1:K:37:TYR:O	1:K:94:TYR:HB2	2.19	0.42
3:J:946:ALA:HB1	3:J:972:LEU:HB3	2.00	0.42
3:J:1078:GLU:HB2	3:J:1081:TYR:CD2	2.55	0.42
3:J:1483:VAL:HG21	3:J:1486:SER:HB2	2.01	0.42
3:J:2248:ARG:HB2	3:J:2248:ARG:NH1	2.35	0.42
3:J:2770:LYS:HA	3:J:2770:LYS:HD3	1.88	0.42
3:J:3667:HIS:HD2	3:J:3669:PHE:HD1	1.67	0.42
3:J:4161:ARG:HD3	3:J:4164:LEU:HD12	2.01	0.42
3:J:4725:LEU:HD11	3:J:4734:ARG:HG3	2.01	0.42
3:C:252:VAL:HA	3:C:255:HIS:ND1	2.33	0.42
3:C:733:PRO:HG2	3:C:762:CYS:HB3	2.00	0.42
3:C:3339:ALA:O	3:C:3343:GLN:HG2	2.19	0.42
3:C:4105:GLY:O	3:C:4109:GLN:HG2	2.19	0.42
3:C:4666:VAL:O	3:C:4670:ILE:HG12	2.20	0.42
3:C:4765:LEU:HA	3:C:4768:LEU:HD12	2.00	0.42
3:C:4787:ASN:HA	3:C:4790:LEU:HD12	2.00	0.42
3:C:4823:LEU:HD23	3:C:4823:LEU:HA	1.84	0.42
3:F:541:SER:HA	3:F:574:VAL:HG12	2.01	0.42
3:F:2355:ARG:HH21	3:F:2453:ILE:HD11	1.84	0.42
3:F:2467:VAL:HG23	3:F:2521:VAL:HG12	2.01	0.42
3:I:222:LEU:HB3	3:I:388:LEU:HD13	2.00	0.42
3:I:2142:TYR:CE1	3:I:2197:LEU:HB2	2.54	0.42
2:L:89:GLY:HA2	3:J:627:PRO:HG3	2.01	0.42
3:J:223:PHE:HB2	3:J:389:PHE:O	2.19	0.42
3:J:541:SER:HA	3:J:574:VAL:HG12	2.01	0.42
3:J:2013:LYS:HB2	3:J:3661:TRP:CE2	2.54	0.42
3:J:2193:GLN:HG2	3:J:2194:HIS:CD2	2.54	0.42
3:J:2962:GLN:HG3	3:J:2965:ARG:HH21	1.84	0.42
3:J:3269:VAL:HG12	3:J:3274:LEU:HG	2.02	0.42
3:J:4998:LYS:HD3	3:J:5003:HIS:HD2	1.85	0.42
1:A:99:ARG:HG2	3:C:920:TYR:CE1	2.55	0.42
1:A:101:PRO:HB2	1:A:104:TYR:HB3	2.02	0.42
3:C:50:GLU:HA	3:C:51:PRO:HD3	1.92	0.42
3:C:714:TYR:HE1	3:C:777:PHE:HE2	1.68	0.42
3:C:2369:ARG:HG3	3:C:2372:GLY:H	1.83	0.42
3:C:3269:VAL:HG12	3:C:3274:LEU:HG	2.02	0.42
3:C:4816:ILE:HD12	7:C:5102:POV:H21H	2.00	0.42
3:F:291:LEU:HD11	3:F:299:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2332:LEU:HD22	3:F:2429:LEU:HA	2.01	0.42
3:F:2863:SER:HB2	3:F:2924:GLN:HB2	2.01	0.42
3:F:3339:ALA:O	3:F:3343:GLN:HG2	2.19	0.42
3:F:3916:ILE:HG22	3:F:3980:LEU:HD21	2.00	0.42
1:G:101:PRO:HD3	3:I:920:TYR:CE2	2.54	0.42
2:H:48:PHE:HB2	2:H:54:GLU:OE2	2.20	0.42
3:I:533:ASN:HB2	3:I:536:ASN:HB2	2.00	0.42
3:I:829:TYR:HB3	3:I:1073:ARG:NH1	2.35	0.42
3:I:1243:PRO:HB2	3:I:1600:LEU:HD11	2.01	0.42
3:I:1514:LEU:H	3:I:1514:LEU:HD23	1.85	0.42
3:I:1856:ASP:O	3:I:1860:LYS:HG3	2.19	0.42
3:J:364:PRO:O	3:J:368:ARG:HG3	2.18	0.42
3:J:412:ASN:O	3:J:416:LYS:HG2	2.20	0.42
3:J:2638:LYS:HG3	3:J:2698:MET:SD	2.60	0.42
3:J:3210:LEU:HD22	3:J:3213:TYR:HE2	1.84	0.42
3:C:291:LEU:HD11	3:C:299:LEU:HD12	2.01	0.42
3:C:364:PRO:O	3:C:368:ARG:HG3	2.18	0.42
3:C:1033:ARG:HA	3:C:1036:ARG:HG2	2.02	0.42
3:C:1856:ASP:O	3:C:1860:LYS:HG3	2.19	0.42
3:C:2638:LYS:HG3	3:C:2698:MET:SD	2.60	0.42
3:C:3284:TRP:HA	3:C:3287:ARG:HD3	2.02	0.42
3:C:3916:ILE:HG22	3:C:3980:LEU:HD21	2.00	0.42
3:F:224:HIS:CE1	3:F:386:ASP:HA	2.54	0.42
3:F:1483:VAL:HG21	3:F:1486:SER:HB2	2.01	0.42
3:F:1514:LEU:HD23	3:F:1514:LEU:H	1.85	0.42
3:F:2248:ARG:NH1	3:F:2248:ARG:HB2	2.34	0.42
3:F:2913:ALA:HA	3:F:2916:LYS:HB3	2.00	0.42
3:F:3127:GLN:HG2	3:F:3129:LEU:H	1.83	0.42
3:F:3263:TYR:HE1	3:F:3270:ILE:HB	1.85	0.42
3:F:3284:TRP:HA	3:F:3287:ARG:HD3	2.02	0.42
3:F:3955:MET:HG2	3:F:4019:LEU:HD22	2.01	0.42
3:F:4922:PHE:O	3:F:4927:ILE:HG12	2.20	0.42
3:F:4928:LEU:HD23	3:F:4931:ILE:HD12	2.00	0.42
3:I:64:ILE:HA	3:I:111:HIS:CE1	2.54	0.42
3:I:1033:ARG:HA	3:I:1036:ARG:HG2	2.02	0.42
3:I:2470:ILE:HG22	3:I:2525:GLY:HA3	2.00	0.42
1:K:101:PRO:HB2	1:K:104:TYR:HB3	2.02	0.42
3:J:2325:PRO:HB2	3:J:2421:ALA:HB1	2.00	0.42
3:C:222:LEU:HB3	3:C:388:LEU:HD13	2.00	0.42
3:C:1078:GLU:HB2	3:C:1081:TYR:CD2	2.55	0.42
3:C:2193:GLN:HG2	3:C:2194:HIS:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2615:ARG:HB3	3:C:2618:MET:SD	2.59	0.42
3:C:3169:LEU:HA	3:C:3172:ILE:HG12	2.01	0.42
1:D:37:TYR:O	1:D:94:TYR:HB2	2.19	0.42
1:D:101:PRO:HB2	1:D:104:TYR:HB3	2.02	0.42
3:F:868:GLU:O	3:F:872:GLU:HG2	2.19	0.42
3:F:1033:ARG:HA	3:F:1036:ARG:HG2	2.02	0.42
3:F:2968:ASP:O	3:F:2971:GLN:HG2	2.20	0.42
3:F:3817:LEU:HD11	3:F:3821:LYS:HE3	2.01	0.42
1:G:101:PRO:HB2	1:G:104:TYR:HB3	2.02	0.42
3:I:2548:LEU:HD12	3:I:2548:LEU:HA	1.94	0.42
3:I:3885:PHE:HB2	3:I:3960:GLN:HG3	2.01	0.42
2:L:4:ILE:HD12	2:L:4:ILE:HA	1.91	0.42
3:J:372:LEU:HD23	3:J:372:LEU:H	1.84	0.42
3:J:483:MET:HA	3:J:483:MET:HE3	2.01	0.42
3:J:684:VAL:HG22	3:J:781:VAL:HG12	2.02	0.42
3:J:868:GLU:O	3:J:872:GLU:HG2	2.19	0.42
3:J:2467:VAL:HG23	3:J:2521:VAL:HG12	2.01	0.42
3:J:3180:ASN:HD21	3:J:3183:VAL:HG13	1.85	0.42
3:J:4698:LYS:HB2	3:J:4698:LYS:HE3	1.87	0.42
3:C:436:LEU:HB2	3:C:438:ILE:HG13	2.01	0.42
3:C:537:CYS:SG	3:C:570:GLU:HB2	2.60	0.42
3:C:946:ALA:HB1	3:C:972:LEU:HB3	2.00	0.42
3:C:2128:TYR:HE1	3:C:3672:ARG:HD2	1.85	0.42
3:C:2355:ARG:HH21	3:C:2453:ILE:HD11	1.85	0.42
3:C:2962:GLN:HG3	3:C:2965:ARG:HH21	1.84	0.42
3:C:3946:GLN:H	3:C:3946:GLN:HG2	1.71	0.42
3:C:3965:LEU:O	3:C:3969:ILE:HG12	2.19	0.42
3:F:120:CYS:HA	3:F:135:VAL:HG12	2.02	0.42
3:F:537:CYS:SG	3:F:570:GLU:HB2	2.60	0.42
3:F:665:GLU:HB2	3:F:792:LEU:HB2	2.01	0.42
3:F:714:TYR:HE1	3:F:777:PHE:HE2	1.68	0.42
3:F:3250:MET:HA	3:F:3253:ILE:HG22	2.01	0.42
3:F:4998:LYS:HD3	3:F:5003:HIS:HD2	1.85	0.42
3:I:3667:HIS:HD2	3:I:3669:PHE:HD1	1.67	0.42
3:I:3965:LEU:O	3:I:3969:ILE:HG12	2.19	0.42
3:I:4998:LYS:HD3	3:I:5003:HIS:HD2	1.85	0.42
2:L:48:PHE:HB2	2:L:54:GLU:OE2	2.20	0.42
3:J:436:LEU:HB2	3:J:438:ILE:HG13	2.01	0.42
3:J:938:HIS:H	3:J:1053:ILE:HG21	1.84	0.42
3:J:1243:PRO:HB2	3:J:1600:LEU:HD11	2.01	0.42
3:J:2797:PHE:HB3	3:J:2802:LYS:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:3965:LEU:O	3:J:3969:ILE:HG12	2.19	0.42
3:J:4105:GLY:O	3:J:4109:GLN:HG2	2.19	0.42
3:J:4790:LEU:HB3	7:J:5106:POV:H32A	2.01	0.42
3:J:4859:PHE:HB3	3:J:4913:ARG:HD3	2.02	0.42
1:A:37:TYR:O	1:A:94:TYR:HB2	2.19	0.42
3:C:1032:LYS:HB3	3:C:1036:ARG:NH2	2.35	0.42
3:C:1071:ARG:HD3	3:C:1071:ARG:HA	1.58	0.42
3:C:1514:LEU:H	3:C:1514:LEU:HD23	1.85	0.42
3:C:2863:SER:HB2	3:C:2924:GLN:HB2	2.01	0.42
3:C:3725:TYR:O	3:C:3729:MET:HG3	2.20	0.42
3:C:3885:PHE:HE1	3:C:3919:THR:HG23	1.84	0.42
3:C:4998:LYS:HD3	3:C:5003:HIS:HD2	1.85	0.42
3:F:3725:TYR:O	3:F:3729:MET:HG3	2.20	0.42
3:F:3965:LEU:O	3:F:3969:ILE:HG12	2.19	0.42
3:F:4994:TYR:CZ	3:F:4998:LYS:HD2	2.54	0.42
3:I:1802:ILE:O	3:I:1804:LEU:HD22	2.20	0.42
3:I:2393:ASP:HA	3:I:2418:LEU:HD21	2.02	0.42
3:I:2968:ASP:O	3:I:2971:GLN:HG2	2.20	0.42
3:I:4105:GLY:O	3:I:4109:GLN:HG2	2.19	0.42
3:I:4725:LEU:HD11	3:I:4734:ARG:HG3	2.01	0.42
1:K:104:TYR:HD1	3:J:882:TRP:CZ2	2.38	0.42
3:J:829:TYR:HB3	3:J:1073:ARG:NH1	2.35	0.42
3:J:1505:GLN:HE22	3:J:1508:ARG:HG3	1.85	0.42
3:J:2968:ASP:O	3:J:2971:GLN:HG2	2.20	0.42
3:J:3100:SER:O	3:J:3104:GLU:HG2	2.20	0.42
3:J:3263:TYR:HE1	3:J:3270:ILE:HB	1.85	0.42
3:J:3885:PHE:HB2	3:J:3960:GLN:HG3	2.02	0.42
2:B:48:PHE:HB2	2:B:54:GLU:OE2	2.20	0.42
3:C:120:CYS:HA	3:C:135:VAL:HG12	2.02	0.42
3:C:483:MET:HA	3:C:483:MET:HE3	2.01	0.42
3:C:533:ASN:HB2	3:C:536:ASN:HB2	2.00	0.42
3:C:567:VAL:HG12	3:C:574:VAL:HG21	2.02	0.42
3:C:938:HIS:H	3:C:1053:ILE:HG21	1.84	0.42
3:C:2097:LEU:O	3:C:2101:MET:HB2	2.20	0.42
3:C:4725:LEU:HD11	3:C:4734:ARG:HG3	2.01	0.42
3:C:4765:LEU:HD23	3:C:4768:LEU:HD12	2.02	0.42
2:E:48:PHE:HB2	2:E:54:GLU:OE2	2.20	0.42
3:F:1802:ILE:O	3:F:1804:LEU:HD22	2.20	0.42
3:F:1934:SER:O	3:F:1938:GLN:HG2	2.20	0.42
3:F:2101:MET:HG2	3:F:2104:ARG:HH21	1.85	0.42
3:F:2166:LEU:HD23	3:F:2166:LEU:HA	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2765:LYS:HD3	3:F:2765:LYS:HA	1.84	0.42
3:F:4068:LEU:HD23	3:F:4111:LEU:HD13	2.01	0.42
3:F:4839:MET:HE2	3:F:4839:MET:HB2	1.91	0.42
3:I:537:CYS:SG	3:I:570:GLU:HB2	2.60	0.42
3:I:684:VAL:HG22	3:I:781:VAL:HG12	2.02	0.42
3:I:908:VAL:HG11	3:I:912:SER:HB3	2.02	0.42
3:I:1730:MET:HE2	3:I:1730:MET:HB2	1.95	0.42
3:I:2097:LEU:O	3:I:2101:MET:HB2	2.20	0.42
3:I:2638:LYS:HG3	3:I:2698:MET:SD	2.60	0.42
3:I:4666:VAL:O	3:I:4670:ILE:HG12	2.20	0.42
3:J:291:LEU:HD11	3:J:299:LEU:HD12	2.01	0.41
3:J:2607:LEU:HD12	3:J:2607:LEU:HA	1.88	0.41
3:J:3284:TRP:HA	3:J:3287:ARG:HD3	2.02	0.41
3:J:3817:LEU:HD11	3:J:3821:LYS:HE3	2.01	0.41
1:A:2:VAL:HG22	1:A:27:SER:H	1.85	0.41
3:C:817:PRO:HG2	3:C:1022:VAL:HG21	2.00	0.41
3:C:2101:MET:HG2	3:C:2104:ARG:HH21	1.85	0.41
2:E:74:LEU:O	2:E:98:ILE:HA	2.19	0.41
3:F:871:ARG:HG3	3:F:925:SER:OG	2.20	0.41
3:F:983:THR:O	3:F:987:ARG:HG2	2.19	0.41
3:F:1286:MET:HE3	3:F:1286:MET:HB3	1.88	0.41
3:I:877:ASN:HB3	3:I:970:LEU:HB2	2.02	0.41
3:I:977:LEU:HD23	3:I:982:THR:HG22	2.01	0.41
3:I:2193:GLN:HG2	3:I:2194:HIS:CD2	2.54	0.41
3:I:2962:GLN:HG3	3:I:2965:ARG:HH21	1.84	0.41
3:I:3105:LYS:HE3	3:I:3128:ASN:ND2	2.35	0.41
3:I:3955:MET:HG2	3:I:4019:LEU:HD22	2.01	0.41
3:J:64:ILE:HA	3:J:111:HIS:CE1	2.54	0.41
3:J:665:GLU:HB2	3:J:792:LEU:HB2	2.01	0.41
3:J:978:THR:O	3:J:982:THR:HG23	2.20	0.41
3:J:1032:LYS:HB3	3:J:1036:ARG:NH2	2.35	0.41
3:J:1211:LEU:HD23	3:J:1211:LEU:HA	1.85	0.41
3:J:2332:LEU:HD22	3:J:2429:LEU:HA	2.01	0.41
3:J:3183:VAL:O	3:J:3187:ARG:HG3	2.20	0.41
3:J:4687:TYR:CE1	3:J:4703:ARG:HG2	2.54	0.41
3:J:4765:LEU:HD23	3:J:4768:LEU:HD12	2.02	0.41
3:J:4866:SER:HB2	3:J:4873:ASP:HB2	2.02	0.41
3:C:541:SER:HA	3:C:574:VAL:HG12	2.01	0.41
3:C:978:THR:O	3:C:982:THR:HG23	2.21	0.41
3:C:3100:SER:O	3:C:3104:GLU:HG2	2.20	0.41
3:C:3250:MET:HA	3:C:3253:ILE:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:4090:LYS:HE3	3:C:4090:LYS:HB2	1.90	0.41
7:C:5107:POV:H25A	7:C:5107:POV:H22	1.81	0.41
1:D:2:VAL:HG22	1:D:27:SER:H	1.85	0.41
3:F:908:VAL:HG11	3:F:912:SER:HB3	2.02	0.41
3:F:1078:GLU:HB2	3:F:1081:TYR:CD2	2.55	0.41
3:F:1078:GLU:HB2	3:F:1081:TYR:CE2	2.56	0.41
3:F:2638:LYS:HG3	3:F:2698:MET:SD	2.60	0.41
3:F:2886:TRP:CZ3	3:F:2904:LEU:HB3	2.56	0.41
3:F:3180:ASN:HD21	3:F:3183:VAL:HG13	1.85	0.41
3:F:3244:PRO:HG2	3:F:3249:LEU:HD12	2.01	0.41
3:F:3264:THR:HA	3:F:3267:PRO:HG3	2.01	0.41
3:F:3342:ALA:O	3:F:3345:ILE:HG22	2.20	0.41
7:F:5113:POV:H3	7:F:5113:POV:H12A	2.03	0.41
3:I:235:ALA:HA	3:I:257:ARG:NH1	2.36	0.41
3:I:1934:SER:O	3:I:1938:GLN:HG2	2.20	0.41
3:I:3100:SER:O	3:I:3104:GLU:HG2	2.20	0.41
3:I:3244:PRO:HG2	3:I:3249:LEU:HD12	2.01	0.41
3:I:3263:TYR:HE1	3:I:3270:ILE:HB	1.85	0.41
1:K:18:LEU:HD23	1:K:18:LEU:HA	1.88	0.41
3:J:615:ARG:HD3	3:J:615:ARG:HA	1.84	0.41
3:J:1638:ALA:HB1	3:J:1647:CYS:HB2	2.03	0.41
3:J:1802:ILE:O	3:J:1804:LEU:HD22	2.20	0.41
3:J:2182:ILE:HG23	3:J:2235:PHE:HB2	2.02	0.41
3:J:2355:ARG:HH21	3:J:2453:ILE:HD11	1.85	0.41
3:J:2960:LEU:HD12	3:J:3035:GLU:HB2	2.03	0.41
3:J:3270:ILE:HG23	3:J:3274:LEU:HD12	2.02	0.41
3:C:412:ASN:O	3:C:416:LYS:HG2	2.20	0.41
3:C:582:HIS:O	3:C:586:ILE:HG13	2.20	0.41
3:C:871:ARG:HG3	3:C:925:SER:OG	2.20	0.41
3:C:977:LEU:HD23	3:C:982:THR:HG22	2.01	0.41
3:C:2698:MET:HE3	3:C:2698:MET:HB2	1.90	0.41
3:C:4866:SER:HB2	3:C:4873:ASP:HB2	2.02	0.41
3:F:372:LEU:HD23	3:F:372:LEU:H	1.84	0.41
3:F:615:ARG:HD3	3:F:615:ARG:HA	1.84	0.41
3:F:2097:LEU:O	3:F:2101:MET:HB2	2.20	0.41
3:F:2821:TRP:CZ2	3:F:2877:GLN:HB3	2.55	0.41
3:F:3169:LEU:HA	3:F:3172:ILE:HG12	2.01	0.41
3:F:4248:ALA:HA	3:F:4251:ILE:HG12	2.02	0.41
3:I:2355:ARG:HH21	3:I:2453:ILE:HD11	1.85	0.41
7:I:5102:POV:H3	7:I:5102:POV:H12A	2.03	0.41
3:J:461:HIS:CE1	3:J:465:GLN:HE22	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:470:SER:HA	3:J:473:ASN:HD21	1.85	0.41
3:J:714:TYR:HE1	3:J:777:PHE:HE2	1.68	0.41
3:J:2526:PHE:HZ	3:J:2561:LEU:HD23	1.86	0.41
3:J:2863:SER:HB2	3:J:2924:GLN:HB2	2.01	0.41
3:J:4081:VAL:HG22	3:J:4088:ILE:HB	2.03	0.41
3:J:4248:ALA:HA	3:J:4251:ILE:HG12	2.03	0.41
3:C:908:VAL:HG11	3:C:912:SER:HB3	2.02	0.41
3:C:1003:GLN:HB3	3:C:1016:ARG:HH21	1.86	0.41
3:C:2526:PHE:HZ	3:C:2561:LEU:HD23	1.86	0.41
3:C:4790:LEU:HB3	7:C:5109:POV:H32A	2.01	0.41
3:F:684:VAL:HG22	3:F:781:VAL:HG12	2.02	0.41
3:F:829:TYR:HB3	3:F:1073:ARG:NH1	2.35	0.41
3:F:2128:TYR:HE1	3:F:3672:ARG:HD2	1.85	0.41
3:F:3105:LYS:HE3	3:F:3128:ASN:ND2	2.35	0.41
3:F:4859:PHE:HB3	3:F:4913:ARG:HD3	2.02	0.41
7:F:5107:POV:H22	7:F:5107:POV:H25A	1.81	0.41
1:G:2:VAL:HG22	1:G:27:SER:H	1.86	0.41
3:I:120:CYS:HA	3:I:135:VAL:HG12	2.02	0.41
3:I:1285:GLU:HB3	3:I:1462:MET:HE2	2.03	0.41
3:I:2960:LEU:HD12	3:I:3035:GLU:HB2	2.03	0.41
3:I:3270:ILE:HG23	3:I:3274:LEU:HD12	2.02	0.41
3:I:3428:ASN:O	3:I:3432:GLU:HG2	2.21	0.41
3:I:3725:TYR:O	3:I:3729:MET:HG3	2.20	0.41
3:I:4765:LEU:HD23	3:I:4768:LEU:HD12	2.02	0.41
3:I:4992:LEU:HD12	3:I:4992:LEU:HA	1.83	0.41
3:J:316:PHE:HB3	3:J:346:CYS:HB3	2.02	0.41
3:J:977:LEU:HD23	3:J:982:THR:HG22	2.01	0.41
3:J:1269:CYS:HA	3:J:1564:PHE:O	2.20	0.41
3:J:1285:GLU:HB3	3:J:1462:MET:HE2	2.03	0.41
3:J:3105:LYS:HE3	3:J:3128:ASN:ND2	2.35	0.41
3:J:3169:LEU:HA	3:J:3172:ILE:HG12	2.01	0.41
3:J:4922:PHE:O	3:J:4927:ILE:HG12	2.20	0.41
7:J:5111:POV:H25A	7:J:5111:POV:H28	1.92	0.41
3:C:684:VAL:HG22	3:C:781:VAL:HG12	2.02	0.41
3:C:875:ALA:HA	3:C:878:ILE:HG22	2.01	0.41
3:C:1285:GLU:HB3	3:C:1462:MET:HE2	2.03	0.41
3:C:1638:ALA:HB1	3:C:1647:CYS:HB2	2.03	0.41
3:C:2182:ILE:HG23	3:C:2235:PHE:HB2	2.02	0.41
3:C:2346:VAL:HG13	3:C:2349:ASN:HB2	2.01	0.41
3:C:2393:ASP:HA	3:C:2418:LEU:HD21	2.02	0.41
3:C:2522:LEU:HD22	3:C:2569:PHE:HZ	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2624:ARG:HG3	3:C:2910:THR:O	2.21	0.41
3:C:2968:ASP:O	3:C:2971:GLN:HG2	2.20	0.41
3:C:4068:LEU:HD23	3:C:4111:LEU:HD13	2.01	0.41
3:F:468:LEU:HD22	3:F:472:ARG:HH21	1.85	0.41
3:F:3270:ILE:HG23	3:F:3274:LEU:HD12	2.02	0.41
3:F:3885:PHE:HE1	3:F:3919:THR:HG23	1.84	0.41
2:H:74:LEU:O	2:H:98:ILE:HA	2.19	0.41
3:I:291:LEU:HD11	3:I:299:LEU:HD12	2.01	0.41
3:I:714:TYR:HE1	3:I:777:PHE:HE2	1.68	0.41
3:I:871:ARG:HG3	3:I:925:SER:OG	2.20	0.41
3:I:1078:GLU:HB2	3:I:1081:TYR:CD2	2.55	0.41
3:I:2467:VAL:HG23	3:I:2521:VAL:HG12	2.01	0.41
3:I:2821:TRP:CZ2	3:I:2877:GLN:HB3	2.55	0.41
3:I:3342:ALA:O	3:I:3345:ILE:HG22	2.20	0.41
3:I:4859:PHE:HB3	3:I:4913:ARG:HD3	2.02	0.41
3:J:235:ALA:HA	3:J:257:ARG:NH1	2.36	0.41
3:J:567:VAL:HG12	3:J:574:VAL:HG21	2.02	0.41
3:J:1033:ARG:HA	3:J:1036:ARG:HG2	2.02	0.41
3:J:2522:LEU:HD22	3:J:2569:PHE:HZ	1.86	0.41
3:J:4989:MET:HG2	3:J:4993:MET:HE3	2.02	0.41
3:C:1286:MET:HE3	3:C:1286:MET:HB3	1.88	0.41
3:C:1287:LEU:HG	3:C:1289:LEU:HG	2.03	0.41
3:C:3390:GLY:O	3:C:3394:VAL:HG13	2.21	0.41
1:D:51:ILE:HD13	1:D:69:ILE:HG12	2.03	0.41
3:F:483:MET:HE3	3:F:483:MET:HA	2.01	0.41
3:F:978:THR:O	3:F:982:THR:HG23	2.20	0.41
3:F:1269:CYS:HA	3:F:1564:PHE:O	2.20	0.41
3:F:1505:GLN:HE22	3:F:1508:ARG:HG3	1.85	0.41
3:F:1856:ASP:O	3:F:1860:LYS:HG3	2.19	0.41
3:F:3428:ASN:O	3:F:3432:GLU:HG2	2.21	0.41
7:F:5114:POV:H28	7:F:5114:POV:H25A	1.92	0.41
3:I:284:HIS:CE1	3:I:286:THR:HB	2.56	0.41
3:I:316:PHE:HB3	3:I:346:CYS:HB3	2.02	0.41
3:I:412:ASN:O	3:I:416:LYS:HG2	2.20	0.41
3:I:436:LEU:HB2	3:I:438:ILE:HG13	2.01	0.41
3:I:1575:LEU:HD23	3:I:1575:LEU:HA	1.93	0.41
3:I:2797:PHE:HB3	3:I:2802:LYS:HD3	2.02	0.41
3:I:3183:VAL:O	3:I:3187:ARG:HG3	2.20	0.41
3:I:3269:VAL:HG12	3:I:3274:LEU:HG	2.02	0.41
3:I:3284:TRP:HA	3:I:3287:ARG:HD3	2.02	0.41
3:I:3683:GLN:HB2	3:I:3694:LYS:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3885:PHE:HE1	3:I:3919:THR:HG23	1.84	0.41
3:I:4922:PHE:O	3:I:4927:ILE:HG12	2.20	0.41
3:J:120:CYS:HA	3:J:135:VAL:HG12	2.02	0.41
3:J:908:VAL:HG11	3:J:912:SER:HB3	2.02	0.41
3:J:2101:MET:HG2	3:J:2104:ARG:HH21	1.85	0.41
3:J:2128:TYR:HE1	3:J:3672:ARG:HD2	1.85	0.41
3:J:3324:VAL:HB	3:J:3361:THR:HG22	2.03	0.41
3:J:3683:GLN:HB2	3:J:3694:LYS:HE3	2.03	0.41
3:J:4666:VAL:O	3:J:4670:ILE:HG12	2.20	0.41
7:J:5110:POV:H3	7:J:5110:POV:H12A	2.03	0.41
3:C:316:PHE:HB3	3:C:346:CYS:HB3	2.02	0.41
3:C:1227:ALA:HB1	3:C:1230:MET:HB2	2.03	0.41
3:C:3183:VAL:O	3:C:3187:ARG:HG3	2.20	0.41
3:C:3342:ALA:O	3:C:3345:ILE:HG22	2.20	0.41
3:C:4197:ILE:HG12	3:C:4990:PHE:HB3	2.03	0.41
7:C:5114:POV:H12A	7:C:5114:POV:H3	2.03	0.41
3:F:412:ASN:O	3:F:416:LYS:HG2	2.20	0.41
3:F:1227:ALA:HB1	3:F:1230:MET:HB2	2.03	0.41
3:F:1638:ALA:HB1	3:F:1647:CYS:HB2	2.03	0.41
3:F:2962:GLN:HG3	3:F:2965:ARG:HH21	1.84	0.41
3:F:4790:LEU:HB3	7:F:5108:POV:H32A	2.02	0.41
3:I:541:SER:HA	3:I:574:VAL:HG12	2.01	0.41
3:I:938:HIS:H	3:I:1053:ILE:HG21	1.85	0.41
3:I:2182:ILE:HG23	3:I:2235:PHE:HB2	2.02	0.41
3:I:2419:GLY:O	3:I:2423:MET:HG3	2.20	0.41
3:I:4989:MET:HG2	3:I:4993:MET:HE3	2.02	0.41
3:J:537:CYS:SG	3:J:570:GLU:HB2	2.60	0.41
3:J:871:ARG:HG3	3:J:925:SER:OG	2.20	0.41
3:J:877:ASN:HB3	3:J:970:LEU:HB2	2.02	0.41
3:J:1286:MET:HE3	3:J:1286:MET:HB3	1.88	0.41
3:J:1514:LEU:HD23	3:J:1514:LEU:H	1.85	0.41
3:J:1934:SER:O	3:J:1938:GLN:HG2	2.20	0.41
3:J:2131:LEU:HD23	3:J:2131:LEU:HA	1.90	0.41
3:J:2624:ARG:HG3	3:J:2910:THR:O	2.21	0.41
3:J:3725:TYR:O	3:J:3729:MET:HG3	2.20	0.41
3:C:1000:ARG:HH12	3:C:1018:ASN:ND2	2.19	0.41
3:C:1023:PRO:HB3	3:C:1025:ARG:NH2	2.35	0.41
3:C:1505:GLN:HE22	3:C:1508:ARG:HG3	1.85	0.41
3:C:3203:VAL:HG13	3:C:3214:ASN:ND2	2.36	0.41
3:C:3817:LEU:HD11	3:C:3821:LYS:HE3	2.01	0.41
3:C:3885:PHE:HB2	3:C:3960:GLN:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:4248:ALA:HA	3:C:4251:ILE:HG12	2.02	0.41
3:C:4543:GLU:HA	3:C:4546:VAL:HG12	2.02	0.41
3:F:582:HIS:O	3:F:586:ILE:HG13	2.20	0.41
3:F:2419:GLY:O	3:F:2423:MET:HG3	2.20	0.41
3:F:2743:LEU:HD21	3:F:2811:GLU:HG2	2.03	0.41
3:F:3100:SER:O	3:F:3104:GLU:HG2	2.20	0.41
3:F:3324:VAL:HB	3:F:3361:THR:HG22	2.03	0.41
3:F:3390:GLY:O	3:F:3394:VAL:HG13	2.21	0.41
3:F:3885:PHE:HB2	3:F:3960:GLN:HG3	2.02	0.41
3:F:4765:LEU:HD23	3:F:4768:LEU:HD12	2.02	0.41
1:G:51:ILE:HD13	1:G:69:ILE:HG12	2.03	0.41
3:I:470:SER:HA	3:I:473:ASN:HD21	1.85	0.41
3:I:582:HIS:O	3:I:586:ILE:HG13	2.20	0.41
3:I:1032:LYS:HB3	3:I:1036:ARG:NH2	2.35	0.41
3:I:1638:ALA:HB1	3:I:1647:CYS:HB2	2.03	0.41
3:I:2101:MET:HG2	3:I:2104:ARG:HH21	1.85	0.41
3:I:3010:PHE:HE2	3:I:3074:SER:HB3	1.84	0.41
3:I:4045:VAL:O	3:I:4049:VAL:HG13	2.21	0.41
7:I:5109:POV:H25A	7:I:5109:POV:H22	1.90	0.41
1:K:2:VAL:HG22	1:K:27:SER:H	1.85	0.41
1:K:51:ILE:HD13	1:K:69:ILE:HG12	2.03	0.41
2:L:31:GLN:NE2	3:J:1299:GLN:HB3	2.36	0.41
3:J:284:HIS:CE1	3:J:286:THR:HB	2.56	0.41
3:J:1003:GLN:HB3	3:J:1016:ARG:HH21	1.86	0.41
3:J:1023:PRO:HB3	3:J:1025:ARG:NH2	2.35	0.41
3:J:1071:ARG:HD3	3:J:1071:ARG:HA	1.58	0.41
3:J:1227:ALA:HB1	3:J:1230:MET:HB2	2.03	0.41
3:J:1601:MET:HA	3:J:1602:PRO:HD3	1.95	0.41
3:J:2419:GLY:O	3:J:2423:MET:HG3	2.20	0.41
3:J:3075:LEU:HD23	3:J:3075:LEU:HA	1.95	0.41
3:J:3203:VAL:HG13	3:J:3214:ASN:ND2	2.36	0.41
3:J:3250:MET:HA	3:J:3253:ILE:HG22	2.01	0.41
3:J:3428:ASN:O	3:J:3432:GLU:HG2	2.21	0.41
3:J:3946:GLN:H	3:J:3946:GLN:HG2	1.71	0.41
3:J:4045:VAL:O	3:J:4049:VAL:HG13	2.21	0.41
3:J:4122:MET:HE3	3:J:4122:MET:HA	2.03	0.41
3:J:4543:GLU:HA	3:J:4546:VAL:HG12	2.02	0.41
2:B:24:VAL:HG23	2:B:26:TYR:HD2	1.86	0.41
3:C:235:ALA:HA	3:C:257:ARG:NH1	2.36	0.41
3:C:461:HIS:CE1	3:C:465:GLN:HE22	2.39	0.41
3:C:1078:GLU:HB2	3:C:1081:TYR:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1802:ILE:O	3:C:1804:LEU:HD22	2.20	0.41
3:C:2797:PHE:HB3	3:C:2802:LYS:HD3	2.02	0.41
3:C:3180:ASN:HD21	3:C:3183:VAL:HG13	1.85	0.41
3:C:4081:VAL:HG22	3:C:4088:ILE:HB	2.03	0.41
3:C:4247:ILE:HD11	3:C:4667:PRO:HB2	2.03	0.41
3:C:4922:PHE:O	3:C:4927:ILE:HG12	2.20	0.41
3:C:4989:MET:HG2	3:C:4993:MET:HE3	2.02	0.41
3:F:235:ALA:HA	3:F:257:ARG:NH1	2.36	0.41
3:F:461:HIS:CE1	3:F:465:GLN:HE22	2.39	0.41
3:F:567:VAL:HG12	3:F:574:VAL:HG21	2.02	0.41
3:F:1000:ARG:HH12	3:F:1018:ASN:ND2	2.19	0.41
3:F:1023:PRO:HB3	3:F:1025:ARG:NH2	2.36	0.41
3:F:1287:LEU:HG	3:F:1289:LEU:HG	2.03	0.41
3:F:1459:GLN:NE2	3:F:1470:ARG:HG2	2.36	0.41
3:F:1747:LEU:HD12	3:F:2037:ASP:HB3	2.03	0.41
3:F:2393:ASP:HA	3:F:2418:LEU:HD21	2.02	0.41
3:F:2522:LEU:HD22	3:F:2569:PHE:HZ	1.86	0.41
3:F:2939:ARG:HD2	3:F:2946:LEU:HD13	2.02	0.41
3:F:2989:SER:HB2	3:F:2992:GLU:HB3	2.03	0.41
3:F:3269:VAL:HG12	3:F:3274:LEU:HG	2.02	0.41
3:F:4767:TRP:O	3:F:4771:ILE:HG23	2.21	0.41
3:F:4989:MET:HG2	3:F:4993:MET:HE3	2.02	0.41
3:I:50:GLU:HA	3:I:51:PRO:HD3	1.92	0.41
3:I:483:MET:HA	3:I:483:MET:HE3	2.01	0.41
3:I:714:TYR:HE2	3:I:1472:VAL:HG21	1.86	0.41
3:I:875:ALA:HA	3:I:878:ILE:HG22	2.01	0.41
3:I:978:THR:O	3:I:982:THR:HG23	2.20	0.41
3:I:1078:GLU:HB2	3:I:1081:TYR:CE2	2.56	0.41
3:I:1269:CYS:HA	3:I:1564:PHE:O	2.20	0.41
3:I:1505:GLN:HE22	3:I:1508:ARG:HG3	1.85	0.41
3:I:2211:MET:HE3	3:I:2232:CYS:HB2	2.03	0.41
3:I:2989:SER:HB2	3:I:2992:GLU:HB3	2.03	0.41
3:I:3203:VAL:HG21	3:I:3217:SER:HA	2.03	0.41
3:I:3264:THR:HA	3:I:3267:PRO:HG3	2.01	0.41
3:I:4790:LEU:HB3	7:I:5111:POV:H32A	2.01	0.41
3:I:4866:SER:HB2	3:I:4873:ASP:HB2	2.02	0.41
2:L:24:VAL:HG23	2:L:26:TYR:HD2	1.86	0.41
3:J:664:PHE:HB3	3:J:811:CYS:SG	2.61	0.41
3:J:1000:ARG:HH12	3:J:1018:ASN:ND2	2.19	0.41
3:J:1735:ILE:HG13	3:J:1771:LEU:HB2	2.03	0.41
3:J:2178:MET:HB3	3:J:2228:MET:CE	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:2939:ARG:HD2	3:J:2946:LEU:HD13	2.02	0.41
3:C:877:ASN:HB3	3:C:970:LEU:HB2	2.02	0.41
3:C:1613:LEU:HD23	3:C:1634:LEU:HD13	2.03	0.41
3:C:1934:SER:O	3:C:1938:GLN:HG2	2.20	0.41
3:C:2952:GLU:HA	3:C:2957:PHE:HD2	1.86	0.41
3:C:2960:LEU:HD12	3:C:3035:GLU:HB2	2.03	0.41
3:C:3201:MET:HE2	3:C:3201:MET:HB3	1.89	0.41
3:C:3203:VAL:HG21	3:C:3217:SER:HA	2.03	0.41
3:F:664:PHE:HB3	3:F:811:CYS:SG	2.61	0.41
3:F:1032:LYS:HB3	3:F:1036:ARG:NH2	2.35	0.41
3:F:2526:PHE:HZ	3:F:2561:LEU:HD23	1.86	0.41
3:F:3683:GLN:HB2	3:F:3694:LYS:HE3	2.03	0.41
3:F:4197:ILE:HG12	3:F:4990:PHE:HB3	2.03	0.41
3:F:4866:SER:HB2	3:F:4873:ASP:HB2	2.02	0.41
3:I:664:PHE:HB3	3:I:811:CYS:SG	2.61	0.41
3:I:1023:PRO:HB3	3:I:1025:ARG:NH2	2.35	0.41
3:I:1931:LEU:HD22	3:I:1935:VAL:HG11	2.03	0.41
3:I:2128:TYR:HE1	3:I:3672:ARG:HD2	1.85	0.41
3:I:2131:LEU:HD23	3:I:2131:LEU:HA	1.90	0.41
3:I:2939:ARG:HD2	3:I:2946:LEU:HD13	2.02	0.41
3:I:2996:LYS:HA	3:I:2996:LYS:HD3	1.96	0.41
3:I:3250:MET:HA	3:I:3253:ILE:HG22	2.01	0.41
7:I:5110:POV:H22	7:I:5110:POV:H25A	1.81	0.41
3:J:2393:ASP:HA	3:J:2418:LEU:HD21	2.02	0.40
3:J:3107:VAL:HG12	3:J:3175:LEU:HG	2.03	0.40
3:J:3342:ALA:O	3:J:3345:ILE:HG22	2.20	0.40
3:J:3930:ILE:HG22	3:J:3995:VAL:HG11	2.03	0.40
3:C:470:SER:HA	3:C:473:ASN:HD21	1.85	0.40
3:C:664:PHE:HB3	3:C:811:CYS:SG	2.61	0.40
3:C:1093:GLU:HB3	3:C:1201:HIS:HB3	2.03	0.40
3:C:2743:LEU:HD21	3:C:2811:GLU:HG2	2.03	0.40
3:C:3316:LEU:HD22	3:C:3346:VAL:HA	2.03	0.40
3:C:3683:GLN:HB2	3:C:3694:LYS:HE3	2.03	0.40
3:C:4767:TRP:O	3:C:4771:ILE:HG23	2.21	0.40
3:C:4859:PHE:HB3	3:C:4913:ARG:HD3	2.02	0.40
3:C:4865:LYS:HE3	3:C:4885:PHE:CZ	2.56	0.40
3:F:284:HIS:CE1	3:F:286:THR:HB	2.56	0.40
3:F:938:HIS:H	3:F:1053:ILE:HG21	1.85	0.40
3:F:977:LEU:HD23	3:F:982:THR:HG22	2.01	0.40
3:F:1285:GLU:HB3	3:F:1462:MET:HE2	2.03	0.40
3:F:1613:LEU:HD23	3:F:1634:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:3183:VAL:O	3:F:3187:ARG:HG3	2.20	0.40
3:I:468:LEU:HD22	3:I:472:ARG:HH21	1.85	0.40
3:I:1227:ALA:HB1	3:I:1230:MET:HB2	2.03	0.40
3:I:2248:ARG:NH1	3:I:2248:ARG:HB2	2.34	0.40
3:I:2522:LEU:HD22	3:I:2569:PHE:HZ	1.86	0.40
3:I:2526:PHE:HZ	3:I:2561:LEU:HD23	1.86	0.40
3:I:2630:VAL:N	3:I:2631:PRO:HD2	2.36	0.40
3:I:3169:LEU:HA	3:I:3172:ILE:HG12	2.01	0.40
3:I:3180:ASN:HD21	3:I:3183:VAL:HG13	1.85	0.40
3:I:4248:ALA:HA	3:I:4251:ILE:HG12	2.02	0.40
3:I:4586:PRO:HA	3:I:4587:PRO:HD3	1.99	0.40
3:I:4767:TRP:O	3:I:4771:ILE:HG23	2.21	0.40
3:I:4865:LYS:HE3	3:I:4885:PHE:CZ	2.56	0.40
3:J:551:LEU:HD22	3:J:589:LEU:HD11	2.04	0.40
3:J:582:HIS:O	3:J:586:ILE:HG13	2.20	0.40
3:J:1297:PHE:CE1	3:J:1548:LEU:HD23	2.57	0.40
3:J:2097:LEU:O	3:J:2101:MET:HB2	2.20	0.40
3:J:2465:ASP:O	3:J:2469:ILE:HG22	2.22	0.40
3:J:3158:LEU:HD23	3:J:3158:LEU:HA	1.96	0.40
1:A:36:TRP:CE3	1:A:93:TYR:HD2	2.39	0.40
3:C:714:TYR:HE2	3:C:1472:VAL:HG21	1.86	0.40
3:C:1931:LEU:HD22	3:C:1935:VAL:HG11	2.03	0.40
3:C:2460:LEU:HD23	3:C:2460:LEU:HA	1.93	0.40
3:C:3018:LEU:HD13	3:C:3074:SER:HA	2.03	0.40
3:C:3105:LYS:HE3	3:C:3128:ASN:ND2	2.35	0.40
3:C:3250:MET:HE2	3:C:3311:HIS:CE1	2.57	0.40
3:F:316:PHE:HB3	3:F:346:CYS:HB3	2.02	0.40
3:F:877:ASN:HB3	3:F:970:LEU:HB2	2.02	0.40
3:F:2190:VAL:HA	3:F:2193:GLN:HB3	2.04	0.40
3:F:2211:MET:HE3	3:F:2232:CYS:HB2	2.03	0.40
3:F:2236:LEU:HD23	3:F:2236:LEU:HA	1.94	0.40
3:F:4579:PHE:CD1	3:F:4639:MET:HE1	2.57	0.40
3:I:461:HIS:CE1	3:I:465:GLN:HE22	2.39	0.40
3:I:772:ASN:HD22	3:I:1470:ARG:NH2	2.19	0.40
3:I:1459:GLN:NE2	3:I:1470:ARG:HG2	2.36	0.40
3:I:1494:MET:HB2	3:I:1494:MET:HE2	1.83	0.40
3:I:3203:VAL:HG13	3:I:3214:ASN:ND2	2.36	0.40
3:I:3604:TYR:O	3:I:3607:GLU:HG3	2.22	0.40
3:I:4081:VAL:HG22	3:I:4088:ILE:HB	2.03	0.40
3:I:4245:MET:HE2	3:I:4245:MET:HB3	1.89	0.40
3:I:4778:TRP:O	3:I:4782:VAL:HG12	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:714:TYR:HE2	3:J:1472:VAL:HG21	1.86	0.40
3:J:1093:GLU:HB3	3:J:1201:HIS:HB3	2.03	0.40
3:J:2431:ASP:HB2	3:J:2501:SER:HB2	2.04	0.40
3:J:3650:CYS:O	3:J:3654:LEU:HG	2.21	0.40
3:J:3729:MET:HB3	3:J:3770:LEU:HD21	2.04	0.40
3:J:4197:ILE:HG12	3:J:4990:PHE:HB3	2.03	0.40
3:J:4778:TRP:O	3:J:4782:VAL:HG12	2.22	0.40
3:J:4865:LYS:HE3	3:J:4885:PHE:CZ	2.56	0.40
2:B:57:LYS:HB3	2:B:57:LYS:HE3	1.75	0.40
3:C:829:TYR:HB3	3:C:1073:ARG:NH1	2.35	0.40
3:C:2166:LEU:HD23	3:C:2166:LEU:HA	1.91	0.40
3:C:2190:VAL:HA	3:C:2193:GLN:HB3	2.04	0.40
3:C:2419:GLY:O	3:C:2423:MET:HG3	2.20	0.40
3:C:2886:TRP:CZ3	3:C:2904:LEU:HB3	2.56	0.40
3:C:2939:ARG:HD2	3:C:2946:LEU:HD13	2.02	0.40
3:C:4778:TRP:O	3:C:4782:VAL:HG12	2.22	0.40
7:C:5115:POV:H28	7:C:5115:POV:H25A	1.92	0.40
1:D:23:THR:HA	1:D:77:THR:HG22	2.04	0.40
3:F:663:TYR:CE1	3:F:745:SER:HB3	2.57	0.40
3:F:772:ASN:HD22	3:F:1470:ARG:NH2	2.19	0.40
3:F:2431:ASP:HB2	3:F:2501:SER:HB2	2.04	0.40
3:F:2611:CYS:HB3	3:F:2643:LEU:HD11	2.04	0.40
3:F:2630:VAL:N	3:F:2631:PRO:HD2	2.36	0.40
3:F:3650:CYS:O	3:F:3654:LEU:HG	2.21	0.40
3:F:4779:LYS:O	3:F:4783:ILE:HG23	2.21	0.40
3:I:1000:ARG:HH12	3:I:1018:ASN:ND2	2.19	0.40
3:I:1735:ILE:HG13	3:I:1771:LEU:HB2	2.03	0.40
3:I:4888:TYR:CD2	3:I:4889:VAL:HG23	2.56	0.40
3:J:2765:LYS:HD3	3:J:2765:LYS:HA	1.84	0.40
3:J:3010:PHE:HE2	3:J:3074:SER:HB3	1.84	0.40
3:J:4848:VAL:HG13	3:J:4886:HIS:HB3	2.03	0.40
1:A:23:THR:HA	1:A:77:THR:HG22	2.04	0.40
3:C:551:LEU:HD22	3:C:589:LEU:HD11	2.04	0.40
3:C:1111:PRO:HG3	3:C:1605:TRP:CD1	2.57	0.40
3:C:1459:GLN:NE2	3:C:1470:ARG:HG2	2.36	0.40
3:C:1747:LEU:HD12	3:C:2037:ASP:HB3	2.03	0.40
3:C:1939:MET:HB2	3:C:1939:MET:HE3	1.50	0.40
3:C:3107:VAL:HG12	3:C:3175:LEU:HG	2.03	0.40
3:C:4555:LEU:HD22	3:C:4562:LEU:HD11	2.04	0.40
3:C:4779:LYS:O	3:C:4783:ILE:HG23	2.21	0.40
3:F:1003:GLN:HB3	3:F:1016:ARG:HH21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1131:ARG:HB2	3:F:1179:PHE:CZ	2.57	0.40
3:F:1506:GLN:HA	3:F:1508:ARG:NH1	2.37	0.40
3:F:2182:ILE:HG23	3:F:2235:PHE:HB2	2.02	0.40
3:F:2952:GLU:HA	3:F:2957:PHE:HD2	1.86	0.40
3:F:3316:LEU:HD22	3:F:3346:VAL:HA	2.03	0.40
3:F:4247:ILE:HD11	3:F:4667:PRO:HB2	2.03	0.40
3:F:4848:VAL:HG13	3:F:4886:HIS:HB3	2.03	0.40
3:I:526:LEU:HD21	3:I:540:PHE:CZ	2.57	0.40
3:I:3674:ILE:HD13	3:I:3674:ILE:HA	1.89	0.40
3:I:4247:ILE:HD11	3:I:4667:PRO:HB2	2.03	0.40
3:I:4555:LEU:HD22	3:I:4562:LEU:HD11	2.04	0.40
3:J:345:LEU:HD21	3:J:389:PHE:CZ	2.57	0.40
3:J:1078:GLU:HB2	3:J:1081:TYR:CE2	2.56	0.40
3:J:2698:MET:HE3	3:J:2698:MET:HB2	1.90	0.40
3:J:2886:TRP:CZ3	3:J:2904:LEU:HB3	2.56	0.40
3:J:3203:VAL:HG21	3:J:3217:SER:HA	2.03	0.40
3:J:4021:LYS:HE2	3:J:4021:LYS:HB3	1.91	0.40
3:C:284:HIS:CE1	3:C:286:THR:HB	2.56	0.40
3:C:468:LEU:HD22	3:C:472:ARG:HH21	1.85	0.40
3:C:526:LEU:HD21	3:C:540:PHE:CZ	2.57	0.40
3:C:1076:ARG:HB3	3:C:1191:VAL:HG23	2.03	0.40
3:C:1131:ARG:HB2	3:C:1179:PHE:CZ	2.57	0.40
3:C:1506:GLN:HA	3:C:1508:ARG:NH1	2.37	0.40
3:C:2285:GLU:HB3	3:C:3858:MET:HE2	2.04	0.40
3:C:2431:ASP:HB2	3:C:2501:SER:HB2	2.04	0.40
3:C:3270:ILE:HG23	3:C:3274:LEU:HD12	2.02	0.40
3:C:3428:ASN:O	3:C:3432:GLU:HG2	2.21	0.40
3:C:3604:TYR:O	3:C:3607:GLU:HG3	2.22	0.40
3:C:3650:CYS:O	3:C:3654:LEU:HG	2.21	0.40
3:C:3930:ILE:HG22	3:C:3995:VAL:HG11	2.03	0.40
3:F:1297:PHE:CE1	3:F:1548:LEU:HD23	2.57	0.40
3:F:1931:LEU:HD22	3:F:1935:VAL:HG11	2.03	0.40
3:F:2809:ILE:H	3:F:2809:ILE:HD12	1.86	0.40
3:F:2960:LEU:HD12	3:F:3035:GLU:HB2	2.03	0.40
3:F:3107:VAL:HG12	3:F:3175:LEU:HG	2.04	0.40
3:F:3203:VAL:HG13	3:F:3214:ASN:ND2	2.36	0.40
3:F:3392:LEU:HD23	3:F:3395:ARG:HD2	2.04	0.40
2:H:57:LYS:HB3	2:H:57:LYS:HE3	1.75	0.40
3:I:551:LEU:HD22	3:I:589:LEU:HD11	2.04	0.40
3:I:567:VAL:HG12	3:I:574:VAL:HG21	2.02	0.40
3:I:1297:PHE:CE1	3:I:1548:LEU:HD23	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:2624:ARG:HG3	3:I:2910:THR:O	2.21	0.40
3:I:2743:LEU:HD21	3:I:2811:GLU:HG2	2.03	0.40
3:I:2754:PHE:HB3	3:I:2825:LYS:HE2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	124/126 (98%)	111 (90%)	11 (9%)	2 (2%)	7	31
1	D	124/126 (98%)	111 (90%)	11 (9%)	2 (2%)	7	31
1	G	124/126 (98%)	111 (90%)	11 (9%)	2 (2%)	7	31
1	K	124/126 (98%)	111 (90%)	11 (9%)	2 (2%)	7	31
2	B	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
2	E	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
2	H	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
2	L	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
3	C	4287/5027 (85%)	4191 (98%)	96 (2%)	0	100	100
3	F	4287/5027 (85%)	4190 (98%)	97 (2%)	0	100	100
3	I	4287/5027 (85%)	4190 (98%)	97 (2%)	0	100	100
3	J	4287/5027 (85%)	4190 (98%)	97 (2%)	0	100	100
All	All	18064/21040 (86%)	17605 (98%)	451 (2%)	8 (0%)	100	100

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	49	ALA

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Mol	Chain	Res	Type
1	A	49	ALA
1	D	49	ALA
1	G	49	ALA
1	K	44	GLN
1	A	44	GLN
1	D	44	GLN
1	G	44	GLN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	104/104 (100%)	103 (99%)	1 (1%)	68	76
1	D	104/104 (100%)	102 (98%)	2 (2%)	50	68
1	G	104/104 (100%)	103 (99%)	1 (1%)	68	76
1	K	104/104 (100%)	102 (98%)	2 (2%)	50	68
2	B	88/88 (100%)	86 (98%)	2 (2%)	44	66
2	E	88/88 (100%)	86 (98%)	2 (2%)	44	66
2	H	88/88 (100%)	86 (98%)	2 (2%)	44	66
2	L	88/88 (100%)	86 (98%)	2 (2%)	44	66
3	C	3690/4270 (86%)	3670 (100%)	20 (0%)	81	83
3	F	3690/4270 (86%)	3671 (100%)	19 (0%)	81	83
3	I	3690/4270 (86%)	3672 (100%)	18 (0%)	81	83
3	J	3690/4270 (86%)	3671 (100%)	19 (0%)	81	83
All	All	15528/17848 (87%)	15438 (99%)	90 (1%)	76	81

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	38	ARG
1	K	61	ASP
2	L	14	THR

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Mol	Chain	Res	Type
2	L	80	VAL
3	J	341	TYR
3	J	702	TRP
3	J	988	LEU
3	J	1022	VAL
3	J	1152	MET
3	J	1617	THR
3	J	1736	VAL
3	J	2211	MET
3	J	2565	CYS
3	J	2577	ILE
3	J	2579	VAL
3	J	2797	PHE
3	J	2906	VAL
3	J	3020	THR
3	J	3520	ILE
3	J	3734	HIS
3	J	4580	TYR
3	J	4720	VAL
3	J	5014	TYR
1	A	38	ARG
2	B	14	THR
2	B	80	VAL
3	C	341	TYR
3	C	672	VAL
3	C	702	TRP
3	C	988	LEU
3	C	1022	VAL
3	C	1152	MET
3	C	1617	THR
3	C	1736	VAL
3	C	2211	MET
3	C	2565	CYS
3	C	2577	ILE
3	C	2579	VAL
3	C	2797	PHE
3	C	2906	VAL
3	C	3020	THR
3	C	3520	ILE
3	C	3734	HIS
3	C	4580	TYR
3	C	4720	VAL

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Mol	Chain	Res	Type
3	C	5014	TYR
1	D	38	ARG
1	D	61	ASP
2	E	14	THR
2	E	80	VAL
3	F	341	TYR
3	F	702	TRP
3	F	988	LEU
3	F	1022	VAL
3	F	1152	MET
3	F	1617	THR
3	F	1736	VAL
3	F	2211	MET
3	F	2565	CYS
3	F	2577	ILE
3	F	2579	VAL
3	F	2797	PHE
3	F	2906	VAL
3	F	3020	THR
3	F	3520	ILE
3	F	3734	HIS
3	F	4580	TYR
3	F	4720	VAL
3	F	5014	TYR
1	G	38	ARG
2	H	14	THR
2	H	80	VAL
3	I	341	TYR
3	I	702	TRP
3	I	988	LEU
3	I	1022	VAL
3	I	1152	MET
3	I	1617	THR
3	I	1736	VAL
3	I	2211	MET
3	I	2577	ILE
3	I	2579	VAL
3	I	2797	PHE
3	I	2906	VAL
3	I	3020	THR
3	I	3520	ILE
3	I	3734	HIS

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Mol	Chain	Res	Type
3	I	4580	TYR
3	I	4720	VAL
3	I	5014	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (151) such sidechains are listed below:

Mol	Chain	Res	Type
3	J	44	ASN
3	J	138	GLN
3	J	151	HIS
3	J	461	HIS
3	J	479	GLN
3	J	495	ASN
3	J	639	ASN
3	J	681	HIS
3	J	705	ASN
3	J	921	ASN
3	J	923	GLN
3	J	994	ASN
3	J	1133	HIS
3	J	1198	GLN
3	J	1201	HIS
3	J	1244	GLN
3	J	1505	GLN
3	J	1590	GLN
3	J	1614	GLN
3	J	1663	HIS
3	J	2169	GLN
3	J	2196	ASN
3	J	2487	GLN
3	J	2584	HIS
3	J	3030	HIS
3	J	3146	HIS
3	J	3378	GLN
3	J	3761	GLN
3	J	3867	ASN
3	J	3869	GLN
3	J	3927	GLN
3	J	4020	GLN
3	J	4034	ASN
3	J	4714	ASN
3	J	4864	ASN

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Mol	Chain	Res	Type
3	J	5031	GLN
3	C	44	ASN
3	C	151	HIS
3	C	461	HIS
3	C	479	GLN
3	C	495	ASN
3	C	593	HIS
3	C	639	ASN
3	C	681	HIS
3	C	705	ASN
3	C	923	GLN
3	C	994	ASN
3	C	1133	HIS
3	C	1198	GLN
3	C	1201	HIS
3	C	1244	GLN
3	C	1459	GLN
3	C	1505	GLN
3	C	1590	GLN
3	C	1614	GLN
3	C	1663	HIS
3	C	2127	GLN
3	C	2169	GLN
3	C	2196	ASN
3	C	2260	ASN
3	C	2487	GLN
3	C	2584	HIS
3	C	3030	HIS
3	C	3146	HIS
3	C	3378	GLN
3	C	3761	GLN
3	C	3867	ASN
3	C	3869	GLN
3	C	3927	GLN
3	C	4034	ASN
3	C	4714	ASN
3	C	4864	ASN
3	C	5003	HIS
3	C	5031	GLN
3	F	138	GLN
3	F	151	HIS
3	F	461	HIS

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Mol	Chain	Res	Type
3	F	479	GLN
3	F	495	ASN
3	F	639	ASN
3	F	681	HIS
3	F	705	ASN
3	F	923	GLN
3	F	994	ASN
3	F	1133	HIS
3	F	1198	GLN
3	F	1201	HIS
3	F	1244	GLN
3	F	1505	GLN
3	F	1590	GLN
3	F	1614	GLN
3	F	1663	HIS
3	F	2127	GLN
3	F	2169	GLN
3	F	2196	ASN
3	F	2260	ASN
3	F	2487	GLN
3	F	2584	HIS
3	F	2883	HIS
3	F	3030	HIS
3	F	3146	HIS
3	F	3378	GLN
3	F	3761	GLN
3	F	3867	ASN
3	F	3869	GLN
3	F	3927	GLN
3	F	4020	GLN
3	F	4034	ASN
3	F	4650	HIS
3	F	4714	ASN
3	F	4812	HIS
3	F	4864	ASN
3	F	5003	HIS
3	F	5031	GLN
3	I	44	ASN
3	I	138	GLN
3	I	151	HIS
3	I	461	HIS
3	I	479	GLN

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Mol	Chain	Res	Type
3	I	495	ASN
3	I	639	ASN
3	I	681	HIS
3	I	705	ASN
3	I	994	ASN
3	I	1133	HIS
3	I	1198	GLN
3	I	1201	HIS
3	I	1244	GLN
3	I	1480	GLN
3	I	1505	GLN
3	I	1590	GLN
3	I	1614	GLN
3	I	1663	HIS
3	I	2127	GLN
3	I	2169	GLN
3	I	2196	ASN
3	I	2487	GLN
3	I	2584	HIS
3	I	3030	HIS
3	I	3146	HIS
3	I	3378	GLN
3	I	3867	ASN
3	I	3869	GLN
3	I	3927	GLN
3	I	4020	GLN
3	I	4034	ASN
3	I	4650	HIS
3	I	4714	ASN
3	I	4812	HIS
3	I	4864	ASN
3	I	5031	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 56 ligands modelled in this entry, 8 are monoatomic - leaving 48 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
7	POV	C	5109	-	25,25,51	0.80	1 (4%)	29,32,59	0.66	0
7	POV	C	5106	-	34,34,51	0.58	0	40,42,59	0.61	0
7	POV	F	5108	-	25,25,51	0.80	1 (4%)	29,32,59	0.66	0
7	POV	F	5114	-	31,31,51	0.62	0	37,39,59	0.57	0
7	POV	F	5101	-	35,35,51	0.59	0	41,43,59	0.51	0
7	POV	J	5111	-	31,31,51	0.62	0	37,39,59	0.57	0
7	POV	I	5103	-	31,31,51	0.62	0	37,39,59	0.57	0
5	CFF	J	5102	-	15,15,15	0.51	0	23,23,23	0.72	1 (4%)
4	ATP	F	5103	-	32,33,33	0.28	0	48,52,52	0.39	0
7	POV	F	5109	-	23,23,51	0.66	0	28,30,59	0.65	0
7	POV	I	5102	-	44,44,51	0.53	0	50,52,59	0.50	0
7	POV	C	5111	-	33,33,51	0.60	0	39,41,59	0.53	0
7	POV	C	5115	-	31,31,51	0.62	0	37,39,59	0.57	0
7	POV	I	5105	-	12,12,51	0.23	0	11,11,59	0.25	0
7	POV	J	5106	-	25,25,51	0.80	1 (4%)	29,32,59	0.66	0
7	POV	I	5110	-	43,43,51	0.54	0	49,51,59	0.50	0
7	POV	C	5107	-	43,43,51	0.54	0	49,51,59	0.50	0
7	POV	C	5113	-	47,47,51	0.52	0	53,55,59	0.49	0
5	CFF	I	5107	-	15,15,15	0.51	0	23,23,23	0.72	1 (4%)
7	POV	C	5114	-	44,44,51	0.53	0	50,52,59	0.50	0
7	POV	J	5110	-	44,44,51	0.53	0	50,52,59	0.50	0
7	POV	J	5108	-	33,33,51	0.60	0	39,41,59	0.53	0
7	POV	I	5109	-	34,34,51	0.58	0	40,42,59	0.61	0
7	POV	C	5110	-	23,23,51	0.66	0	28,30,59	0.65	0
5	CFF	C	5104	-	15,15,15	0.51	0	23,23,23	0.72	1 (4%)
7	POV	C	5108	-	47,47,51	0.52	0	53,55,59	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	POV	I	5111	-	25,25,51	0.80	1 (4%)	29,32,59	0.66	0
7	POV	F	5102	-	12,12,51	0.23	0	11,11,59	0.25	0
4	ATP	I	5106	-	32,33,33	0.28	0	48,52,52	0.39	0
7	POV	F	5106	-	34,34,51	0.58	0	40,42,59	0.61	0
7	POV	F	5107	-	43,43,51	0.54	0	49,51,59	0.50	0
7	POV	C	5102	-	12,12,51	0.23	0	11,11,59	0.25	0
7	POV	J	5105	-	43,43,51	0.54	0	49,51,59	0.50	0
7	POV	I	5112	-	23,23,51	0.66	0	28,30,59	0.65	0
7	POV	J	5112	-	35,35,51	0.59	0	41,43,59	0.51	0
7	POV	I	5101	-	47,47,51	0.52	0	53,55,59	0.49	0
7	POV	J	5113	-	12,12,51	0.23	0	11,11,59	0.25	0
7	POV	J	5107	-	23,23,51	0.66	0	28,30,59	0.65	0
5	CFF	F	5104	-	15,15,15	0.51	0	23,23,23	0.72	1 (4%)
7	POV	C	5101	-	35,35,51	0.59	0	41,43,59	0.51	0
4	ATP	C	5103	-	32,33,33	0.28	0	48,52,52	0.39	0
7	POV	J	5104	-	34,34,51	0.58	0	40,42,59	0.61	0
7	POV	F	5110	-	33,33,51	0.60	0	39,41,59	0.54	0
7	POV	F	5112	-	47,47,51	0.52	0	53,55,59	0.49	0
7	POV	I	5113	-	33,33,51	0.60	0	39,41,59	0.54	0
4	ATP	J	5101	-	32,33,33	0.28	0	48,52,52	0.39	0
7	POV	I	5104	-	35,35,51	0.59	0	41,43,59	0.51	0
7	POV	F	5113	-	44,44,51	0.53	0	50,52,59	0.50	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
7	POV	C	5109	-	-	10/28/28/55	-
7	POV	C	5106	-	-	10/38/38/55	-
7	POV	F	5108	-	-	10/28/28/55	-
7	POV	F	5114	-	-	9/35/35/55	-
7	POV	F	5101	-	-	13/39/39/55	-
7	POV	J	5111	-	-	9/35/35/55	-
7	POV	I	5103	-	-	9/35/35/55	-
4	ATP	F	5103	-	-	2/22/38/38	0/3/3/3
5	CFF	J	5102	-	-	-	0/2/2/2
7	POV	F	5109	-	-	2/26/26/55	-
7	POV	I	5102	-	-	11/48/48/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	POV	C	5111	-	-	8/37/37/55	-
7	POV	C	5115	-	-	9/35/35/55	-
7	POV	I	5105	-	-	0/10/10/55	-
7	POV	J	5106	-	-	10/28/28/55	-
7	POV	I	5110	-	-	12/47/47/55	-
7	POV	C	5107	-	-	12/47/47/55	-
7	POV	C	5113	-	-	13/51/51/55	-
5	CFF	I	5107	-	-	-	0/2/2/2
7	POV	C	5114	-	-	11/48/48/55	-
7	POV	J	5110	-	-	11/48/48/55	-
7	POV	J	5108	-	-	8/37/37/55	-
7	POV	I	5109	-	-	10/38/38/55	-
7	POV	C	5110	-	-	2/26/26/55	-
7	POV	I	5111	-	-	10/28/28/55	-
7	POV	C	5108	-	-	13/51/51/55	-
5	CFF	C	5104	-	-	-	0/2/2/2
7	POV	F	5102	-	-	0/10/10/55	-
4	ATP	I	5106	-	-	2/22/38/38	0/3/3/3
7	POV	F	5106	-	-	10/38/38/55	-
7	POV	F	5107	-	-	12/47/47/55	-
7	POV	C	5102	-	-	0/10/10/55	-
7	POV	J	5105	-	-	12/47/47/55	-
7	POV	I	5112	-	-	2/26/26/55	-
7	POV	J	5112	-	-	13/39/39/55	-
7	POV	I	5101	-	-	13/51/51/55	-
7	POV	J	5113	-	-	0/10/10/55	-
7	POV	J	5107	-	-	2/26/26/55	-
7	POV	C	5101	-	-	13/39/39/55	-
5	CFF	F	5104	-	-	-	0/2/2/2
4	ATP	C	5103	-	-	2/22/38/38	0/3/3/3
7	POV	J	5104	-	-	10/38/38/55	-
7	POV	F	5110	-	-	8/37/37/55	-
7	POV	F	5112	-	-	13/51/51/55	-
7	POV	I	5113	-	-	8/37/37/55	-
4	ATP	J	5101	-	-	2/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	POV	I	5104	-	-	13/39/39/55	-
7	POV	F	5113	-	-	11/48/48/55	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	5109	POV	O21-C2	-2.55	1.43	1.46
7	J	5106	POV	O21-C2	-2.54	1.43	1.46
7	F	5108	POV	O21-C2	-2.54	1.43	1.46
7	I	5111	POV	O21-C2	-2.54	1.43	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	5102	CFF	C12-N3-C2	2.25	121.25	117.33
5	C	5104	CFF	C12-N3-C2	2.25	121.25	117.33
5	I	5107	CFF	C12-N3-C2	2.25	121.25	117.33
5	F	5104	CFF	C12-N3-C2	2.25	121.25	117.33

There are no chirality outliers.

All (360) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	J	5104	POV	C11-O12-P-O11
7	J	5104	POV	C11-O12-P-O13
7	J	5104	POV	C11-O12-P-O14
7	J	5104	POV	O12-C11-C12-N
7	J	5105	POV	C1-O11-P-O14
7	J	5106	POV	C1-O11-P-O12
7	J	5106	POV	C1-O11-P-O13
7	J	5106	POV	C1-O11-P-O14
7	J	5106	POV	C11-O12-P-O11
7	J	5106	POV	C11-O12-P-O13
7	J	5106	POV	C11-O12-P-O14
7	J	5106	POV	O12-C11-C12-N
7	J	5106	POV	O22-C21-O21-C2
7	J	5108	POV	O22-C21-O21-C2
7	J	5110	POV	C1-O11-P-O12
7	J	5110	POV	C1-O11-P-O13
7	J	5110	POV	C1-O11-P-O14
7	J	5111	POV	C11-O12-P-O11

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Mol	Chain	Res	Type	Atoms
7	J	5111	POV	C11-O12-P-O14
7	J	5111	POV	O12-C11-C12-N
7	J	5111	POV	C12-C11-O12-P
7	J	5112	POV	C11-O12-P-O14
7	C	5101	POV	C11-O12-P-O14
7	C	5106	POV	C11-O12-P-O11
7	C	5106	POV	C11-O12-P-O13
7	C	5106	POV	C11-O12-P-O14
7	C	5106	POV	O12-C11-C12-N
7	C	5107	POV	C1-O11-P-O14
7	C	5108	POV	C1-O11-P-O12
7	C	5108	POV	C2-C1-O11-P
7	C	5109	POV	C1-O11-P-O12
7	C	5109	POV	C1-O11-P-O13
7	C	5109	POV	C1-O11-P-O14
7	C	5109	POV	C11-O12-P-O11
7	C	5109	POV	C11-O12-P-O13
7	C	5109	POV	C11-O12-P-O14
7	C	5109	POV	O12-C11-C12-N
7	C	5109	POV	O22-C21-O21-C2
7	C	5111	POV	O22-C21-O21-C2
7	C	5113	POV	C1-O11-P-O12
7	C	5113	POV	C2-C1-O11-P
7	C	5114	POV	C1-O11-P-O12
7	C	5114	POV	C1-O11-P-O13
7	C	5114	POV	C1-O11-P-O14
7	C	5115	POV	C11-O12-P-O11
7	C	5115	POV	C11-O12-P-O14
7	C	5115	POV	O12-C11-C12-N
7	C	5115	POV	C12-C11-O12-P
7	F	5101	POV	C11-O12-P-O14
7	F	5106	POV	C11-O12-P-O11
7	F	5106	POV	C11-O12-P-O13
7	F	5106	POV	C11-O12-P-O14
7	F	5106	POV	O12-C11-C12-N
7	F	5107	POV	C1-O11-P-O14
7	F	5108	POV	C1-O11-P-O12
7	F	5108	POV	C1-O11-P-O13
7	F	5108	POV	C1-O11-P-O14
7	F	5108	POV	C11-O12-P-O11
7	F	5108	POV	C11-O12-P-O13
7	F	5108	POV	C11-O12-P-O14

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Mol	Chain	Res	Type	Atoms
7	F	5108	POV	O12-C11-C12-N
7	F	5108	POV	O22-C21-O21-C2
7	F	5110	POV	O22-C21-O21-C2
7	F	5112	POV	C1-O11-P-O12
7	F	5112	POV	C2-C1-O11-P
7	F	5113	POV	C1-O11-P-O12
7	F	5113	POV	C1-O11-P-O13
7	F	5113	POV	C1-O11-P-O14
7	F	5114	POV	C11-O12-P-O11
7	F	5114	POV	C11-O12-P-O14
7	F	5114	POV	O12-C11-C12-N
7	F	5114	POV	C12-C11-O12-P
7	I	5101	POV	C1-O11-P-O12
7	I	5101	POV	C2-C1-O11-P
7	I	5102	POV	C1-O11-P-O12
7	I	5102	POV	C1-O11-P-O13
7	I	5102	POV	C1-O11-P-O14
7	I	5103	POV	C11-O12-P-O11
7	I	5103	POV	C11-O12-P-O14
7	I	5103	POV	O12-C11-C12-N
7	I	5103	POV	C12-C11-O12-P
7	I	5104	POV	C11-O12-P-O14
7	I	5109	POV	C11-O12-P-O11
7	I	5109	POV	C11-O12-P-O13
7	I	5109	POV	C11-O12-P-O14
7	I	5109	POV	O12-C11-C12-N
7	I	5110	POV	C1-O11-P-O14
7	I	5111	POV	C1-O11-P-O12
7	I	5111	POV	C1-O11-P-O13
7	I	5111	POV	C1-O11-P-O14
7	I	5111	POV	C11-O12-P-O11
7	I	5111	POV	C11-O12-P-O13
7	I	5111	POV	C11-O12-P-O14
7	I	5111	POV	O12-C11-C12-N
7	I	5111	POV	O22-C21-O21-C2
7	I	5113	POV	O22-C21-O21-C2
7	J	5104	POV	O22-C21-O21-C2
7	C	5106	POV	O22-C21-O21-C2
7	F	5106	POV	O22-C21-O21-C2
7	I	5109	POV	O22-C21-O21-C2
7	J	5104	POV	C22-C21-O21-C2
7	J	5108	POV	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
7	C	5106	POV	C22-C21-O21-C2
7	C	5111	POV	C22-C21-O21-C2
7	F	5106	POV	C22-C21-O21-C2
7	F	5110	POV	C22-C21-O21-C2
7	I	5109	POV	C22-C21-O21-C2
7	I	5113	POV	C22-C21-O21-C2
7	J	5112	POV	C21-C22-C23-C24
7	C	5101	POV	C21-C22-C23-C24
7	F	5101	POV	C21-C22-C23-C24
7	I	5104	POV	C21-C22-C23-C24
7	J	5111	POV	C23-C24-C25-C26
7	C	5115	POV	C23-C24-C25-C26
7	F	5114	POV	C23-C24-C25-C26
7	I	5103	POV	C23-C24-C25-C26
7	J	5110	POV	C22-C23-C24-C25
7	C	5114	POV	C22-C23-C24-C25
7	F	5113	POV	C22-C23-C24-C25
7	I	5102	POV	C22-C23-C24-C25
7	C	5108	POV	C36-C37-C38-C39
7	C	5113	POV	C36-C37-C38-C39
7	F	5112	POV	C36-C37-C38-C39
7	I	5101	POV	C36-C37-C38-C39
7	C	5108	POV	C26-C27-C28-C29
7	C	5113	POV	C26-C27-C28-C29
7	F	5112	POV	C26-C27-C28-C29
7	I	5101	POV	C26-C27-C28-C29
7	J	5108	POV	C25-C26-C27-C28
7	C	5111	POV	C25-C26-C27-C28
7	F	5110	POV	C25-C26-C27-C28
7	I	5113	POV	C25-C26-C27-C28
7	J	5112	POV	O11-C1-C2-O21
7	C	5101	POV	O11-C1-C2-O21
7	F	5101	POV	O11-C1-C2-O21
7	I	5104	POV	O11-C1-C2-O21
7	J	5105	POV	C21-C22-C23-C24
7	C	5107	POV	C21-C22-C23-C24
7	F	5107	POV	C21-C22-C23-C24
7	I	5110	POV	C21-C22-C23-C24
7	J	5104	POV	C32-C31-O31-C3
7	C	5106	POV	C32-C31-O31-C3
7	F	5106	POV	C32-C31-O31-C3
7	I	5109	POV	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
7	J	5112	POV	C23-C24-C25-C26
7	C	5101	POV	C23-C24-C25-C26
7	F	5101	POV	C23-C24-C25-C26
7	I	5104	POV	C23-C24-C25-C26
7	J	5104	POV	C2-C1-O11-P
7	C	5106	POV	C2-C1-O11-P
7	F	5106	POV	C2-C1-O11-P
7	I	5109	POV	C2-C1-O11-P
7	J	5112	POV	C24-C25-C26-C27
7	C	5101	POV	C24-C25-C26-C27
7	F	5101	POV	C24-C25-C26-C27
7	I	5104	POV	C24-C25-C26-C27
7	J	5104	POV	O32-C31-O31-C3
7	C	5106	POV	O32-C31-O31-C3
7	F	5106	POV	O32-C31-O31-C3
7	I	5109	POV	O32-C31-O31-C3
7	J	5104	POV	C1-C2-O21-C21
7	C	5106	POV	C1-C2-O21-C21
7	F	5106	POV	C1-C2-O21-C21
7	I	5109	POV	C1-C2-O21-C21
7	J	5106	POV	O11-C1-C2-O21
7	C	5109	POV	O11-C1-C2-O21
7	F	5108	POV	O11-C1-C2-O21
7	I	5111	POV	O11-C1-C2-O21
7	J	5105	POV	C32-C33-C34-C35
7	C	5107	POV	C32-C33-C34-C35
7	F	5107	POV	C32-C33-C34-C35
7	I	5110	POV	C32-C33-C34-C35
7	J	5107	POV	O11-C1-C2-C3
7	J	5112	POV	O11-C1-C2-C3
7	C	5101	POV	O11-C1-C2-C3
7	C	5108	POV	O11-C1-C2-C3
7	C	5110	POV	O11-C1-C2-C3
7	C	5113	POV	O11-C1-C2-C3
7	F	5101	POV	O11-C1-C2-C3
7	F	5109	POV	O11-C1-C2-C3
7	F	5112	POV	O11-C1-C2-C3
7	I	5101	POV	O11-C1-C2-C3
7	I	5104	POV	O11-C1-C2-C3
7	I	5112	POV	O11-C1-C2-C3
7	J	5107	POV	O11-C1-C2-O21
7	C	5110	POV	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
7	F	5109	POV	O11-C1-C2-O21
7	I	5112	POV	O11-C1-C2-O21
7	J	5111	POV	C2-C1-O11-P
7	C	5115	POV	C2-C1-O11-P
7	F	5114	POV	C2-C1-O11-P
7	I	5103	POV	C2-C1-O11-P
7	C	5108	POV	C24-C25-C26-C27
7	C	5113	POV	C24-C25-C26-C27
7	F	5112	POV	C24-C25-C26-C27
7	I	5101	POV	C24-C25-C26-C27
7	J	5110	POV	C22-C21-O21-C2
7	C	5114	POV	C22-C21-O21-C2
7	F	5113	POV	C22-C21-O21-C2
7	I	5102	POV	C22-C21-O21-C2
7	C	5108	POV	C211-C212-C213-C214
7	C	5113	POV	C211-C212-C213-C214
7	F	5112	POV	C211-C212-C213-C214
7	I	5101	POV	C211-C212-C213-C214
7	J	5106	POV	O11-C1-C2-C3
7	C	5109	POV	O11-C1-C2-C3
7	F	5108	POV	O11-C1-C2-C3
7	I	5111	POV	O11-C1-C2-C3
7	J	5112	POV	C12-C11-O12-P
7	C	5101	POV	C12-C11-O12-P
7	F	5101	POV	C12-C11-O12-P
7	I	5104	POV	C12-C11-O12-P
7	J	5112	POV	O12-C11-C12-N
7	C	5101	POV	O12-C11-C12-N
7	F	5101	POV	O12-C11-C12-N
7	I	5104	POV	O12-C11-C12-N
7	J	5110	POV	O22-C21-O21-C2
7	C	5114	POV	O22-C21-O21-C2
7	F	5113	POV	O22-C21-O21-C2
7	I	5102	POV	O22-C21-O21-C2
7	I	5104	POV	C22-C23-C24-C25
7	J	5112	POV	C22-C23-C24-C25
7	C	5101	POV	C22-C23-C24-C25
7	F	5101	POV	C22-C23-C24-C25
7	J	5110	POV	O11-C1-C2-C3
7	C	5114	POV	O11-C1-C2-C3
7	F	5113	POV	O11-C1-C2-C3
7	I	5102	POV	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
7	J	5110	POV	O11-C1-C2-O21
7	C	5108	POV	O11-C1-C2-O21
7	C	5113	POV	O11-C1-C2-O21
7	C	5114	POV	O11-C1-C2-O21
7	F	5112	POV	O11-C1-C2-O21
7	F	5113	POV	O11-C1-C2-O21
7	I	5101	POV	O11-C1-C2-O21
7	I	5102	POV	O11-C1-C2-O21
7	C	5108	POV	C33-C34-C35-C36
7	C	5113	POV	C33-C34-C35-C36
7	F	5112	POV	C33-C34-C35-C36
7	I	5101	POV	C33-C34-C35-C36
7	J	5105	POV	C1-C2-C3-O31
7	C	5107	POV	C1-C2-C3-O31
7	F	5107	POV	C1-C2-C3-O31
7	I	5110	POV	C1-C2-C3-O31
7	J	5105	POV	C1-O11-P-O12
7	J	5105	POV	C11-O12-P-O14
7	J	5111	POV	C1-O11-P-O14
7	C	5107	POV	C1-O11-P-O12
7	C	5107	POV	C11-O12-P-O14
7	C	5108	POV	C1-O11-P-O14
7	C	5113	POV	C1-O11-P-O14
7	C	5115	POV	C1-O11-P-O14
7	F	5107	POV	C1-O11-P-O12
7	F	5107	POV	C11-O12-P-O14
7	F	5112	POV	C1-O11-P-O14
7	F	5114	POV	C1-O11-P-O14
7	I	5101	POV	C1-O11-P-O14
7	I	5103	POV	C1-O11-P-O14
7	I	5110	POV	C1-O11-P-O12
7	I	5110	POV	C11-O12-P-O14
7	J	5108	POV	C24-C25-C26-C27
7	C	5111	POV	C24-C25-C26-C27
7	F	5110	POV	C24-C25-C26-C27
7	I	5113	POV	C24-C25-C26-C27
7	J	5105	POV	C26-C27-C28-C29
7	C	5107	POV	C26-C27-C28-C29
7	F	5107	POV	C26-C27-C28-C29
7	I	5110	POV	C26-C27-C28-C29
7	J	5112	POV	C25-C26-C27-C28
7	C	5101	POV	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
7	F	5101	POV	C25-C26-C27-C28
7	I	5104	POV	C25-C26-C27-C28
4	J	5101	ATP	O4'-C1'-N9-C8
4	C	5103	ATP	O4'-C1'-N9-C8
4	F	5103	ATP	O4'-C1'-N9-C8
4	I	5106	ATP	O4'-C1'-N9-C8
4	J	5101	ATP	O4'-C1'-N9-C4
4	C	5103	ATP	O4'-C1'-N9-C4
4	F	5103	ATP	O4'-C1'-N9-C4
4	I	5106	ATP	O4'-C1'-N9-C4
7	C	5108	POV	C37-C38-C39-C310
7	C	5113	POV	C37-C38-C39-C310
7	F	5112	POV	C37-C38-C39-C310
7	I	5101	POV	C37-C38-C39-C310
7	J	5112	POV	C2-C1-O11-P
7	C	5101	POV	C2-C1-O11-P
7	F	5101	POV	C2-C1-O11-P
7	I	5104	POV	C2-C1-O11-P
7	J	5105	POV	O22-C21-O21-C2
7	C	5107	POV	O22-C21-O21-C2
7	F	5107	POV	O22-C21-O21-C2
7	I	5110	POV	O22-C21-O21-C2
7	J	5110	POV	C23-C24-C25-C26
7	C	5114	POV	C23-C24-C25-C26
7	F	5113	POV	C23-C24-C25-C26
7	I	5102	POV	C23-C24-C25-C26
7	J	5111	POV	O31-C31-C32-C33
7	C	5115	POV	O31-C31-C32-C33
7	F	5114	POV	O31-C31-C32-C33
7	I	5103	POV	O31-C31-C32-C33
7	J	5105	POV	C34-C35-C36-C37
7	C	5107	POV	C34-C35-C36-C37
7	F	5107	POV	C34-C35-C36-C37
7	I	5110	POV	C34-C35-C36-C37
7	J	5111	POV	C24-C25-C26-C27
7	C	5115	POV	C24-C25-C26-C27
7	F	5114	POV	C24-C25-C26-C27
7	I	5103	POV	C24-C25-C26-C27
7	C	5108	POV	O31-C31-C32-C33
7	C	5113	POV	O31-C31-C32-C33
7	F	5112	POV	O31-C31-C32-C33
7	I	5101	POV	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
7	J	5105	POV	C33-C34-C35-C36
7	C	5107	POV	C33-C34-C35-C36
7	I	5110	POV	C33-C34-C35-C36
7	F	5107	POV	C33-C34-C35-C36
7	J	5108	POV	C12-C11-O12-P
7	C	5111	POV	C12-C11-O12-P
7	F	5110	POV	C12-C11-O12-P
7	I	5113	POV	C12-C11-O12-P
7	J	5112	POV	O21-C21-C22-C23
7	C	5101	POV	O21-C21-C22-C23
7	F	5101	POV	O21-C21-C22-C23
7	I	5104	POV	O21-C21-C22-C23
7	J	5110	POV	C27-C28-C29-C210
7	C	5114	POV	C27-C28-C29-C210
7	F	5113	POV	C27-C28-C29-C210
7	I	5102	POV	C27-C28-C29-C210
7	J	5105	POV	C22-C21-O21-C2
7	C	5107	POV	C22-C21-O21-C2
7	F	5107	POV	C22-C21-O21-C2
7	I	5110	POV	C22-C21-O21-C2
7	J	5108	POV	C11-C12-N-C14
7	J	5108	POV	C11-C12-N-C15
7	C	5111	POV	C11-C12-N-C14
7	C	5111	POV	C11-C12-N-C15
7	F	5110	POV	C11-C12-N-C14
7	F	5110	POV	C11-C12-N-C15
7	I	5113	POV	C11-C12-N-C14
7	I	5113	POV	C11-C12-N-C15
7	J	5108	POV	C11-C12-N-C13
7	C	5111	POV	C11-C12-N-C13
7	F	5110	POV	C11-C12-N-C13
7	I	5113	POV	C11-C12-N-C13
7	J	5112	POV	O22-C21-C22-C23
7	C	5101	POV	O22-C21-C22-C23
7	F	5101	POV	O22-C21-C22-C23
7	I	5104	POV	O22-C21-C22-C23
7	J	5105	POV	O31-C31-C32-C33
7	C	5107	POV	O31-C31-C32-C33
7	C	5108	POV	O21-C21-C22-C23
7	C	5113	POV	O21-C21-C22-C23
7	F	5107	POV	O31-C31-C32-C33
7	F	5112	POV	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
7	I	5101	POV	O21-C21-C22-C23
7	I	5110	POV	O31-C31-C32-C33
7	J	5110	POV	C29-C210-C211-C212
7	C	5114	POV	C29-C210-C211-C212
7	F	5113	POV	C29-C210-C211-C212
7	I	5102	POV	C29-C210-C211-C212

There are no ring outliers.

39 monomers are involved in 75 short contacts:

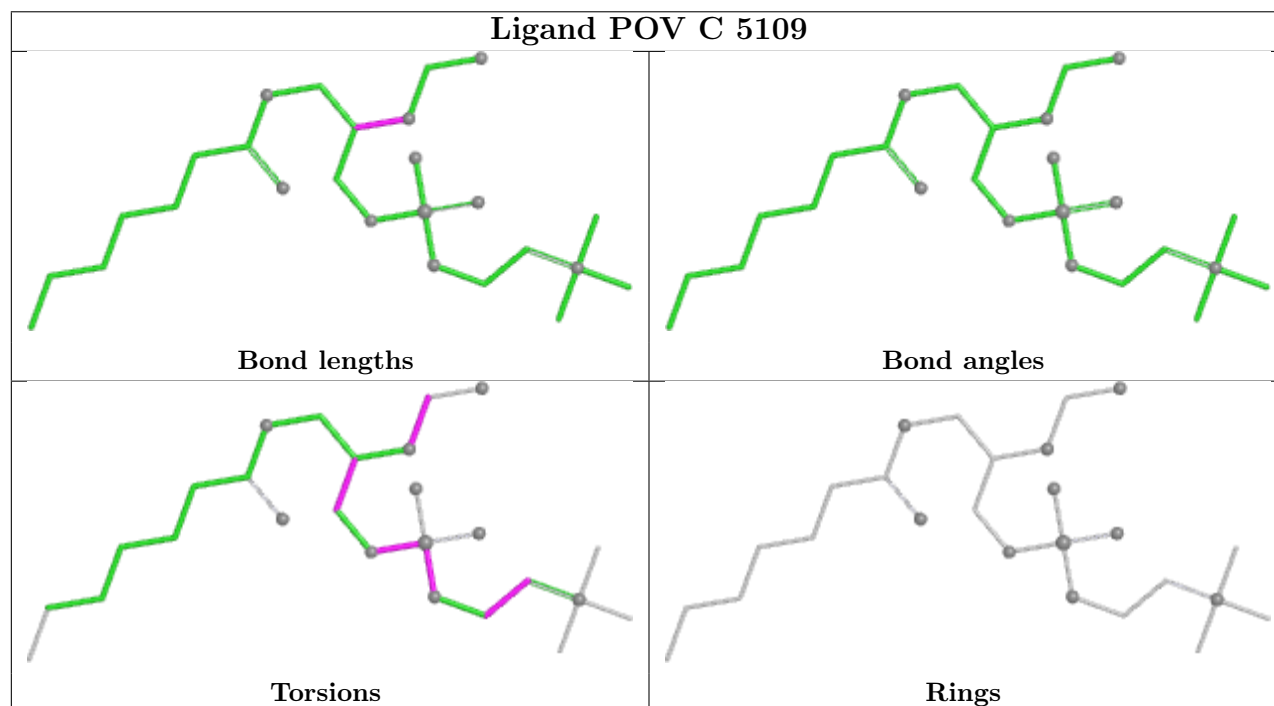
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	5109	POV	2	0
7	C	5106	POV	2	0
7	F	5108	POV	2	0
7	F	5114	POV	1	0
7	F	5101	POV	3	0
7	J	5111	POV	1	0
7	F	5109	POV	3	0
7	I	5102	POV	2	0
7	C	5111	POV	4	0
7	C	5115	POV	1	0
7	I	5105	POV	1	0
7	J	5106	POV	2	0
7	I	5110	POV	4	0
7	C	5107	POV	4	0
7	C	5113	POV	3	0
7	C	5114	POV	2	0
7	J	5110	POV	2	0
7	J	5108	POV	4	0
7	I	5109	POV	2	0
7	C	5110	POV	3	0
7	C	5108	POV	3	0
7	I	5111	POV	2	0
7	F	5102	POV	1	0
7	F	5106	POV	1	0
7	F	5107	POV	4	0
7	C	5102	POV	1	0
7	J	5105	POV	3	0
7	I	5112	POV	3	0
7	J	5112	POV	3	0
7	I	5101	POV	3	0
7	J	5113	POV	1	0

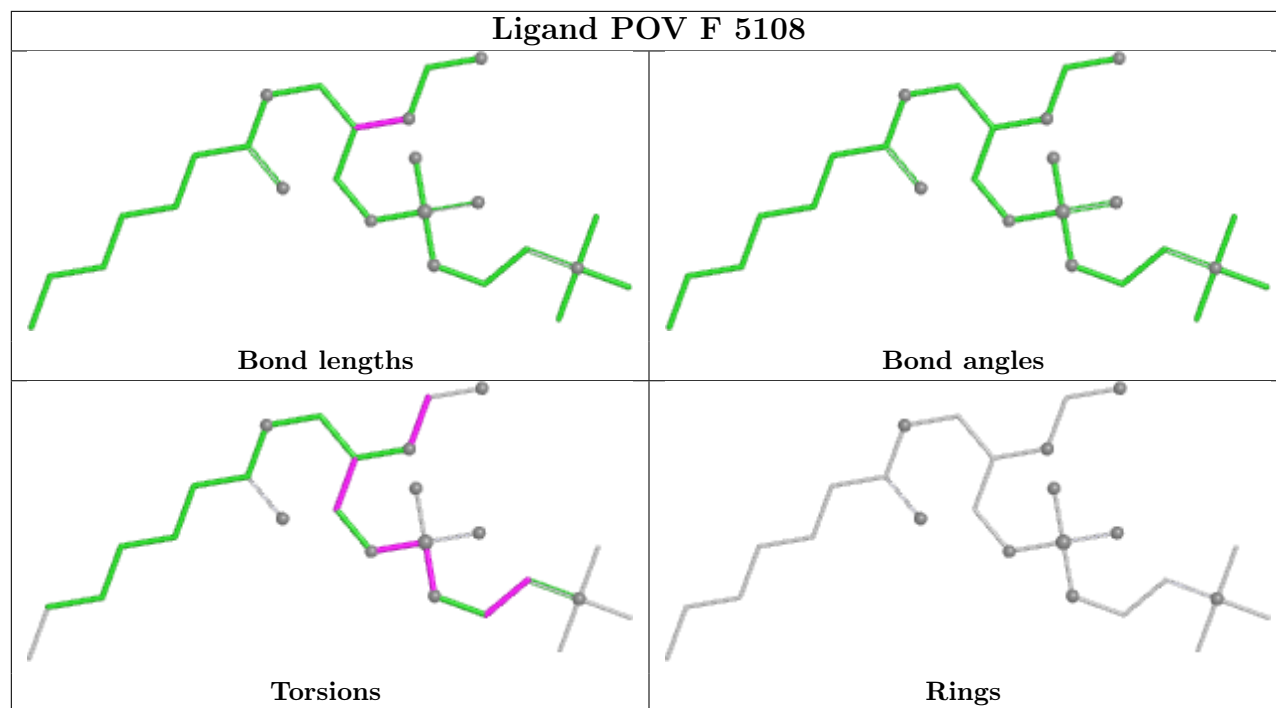
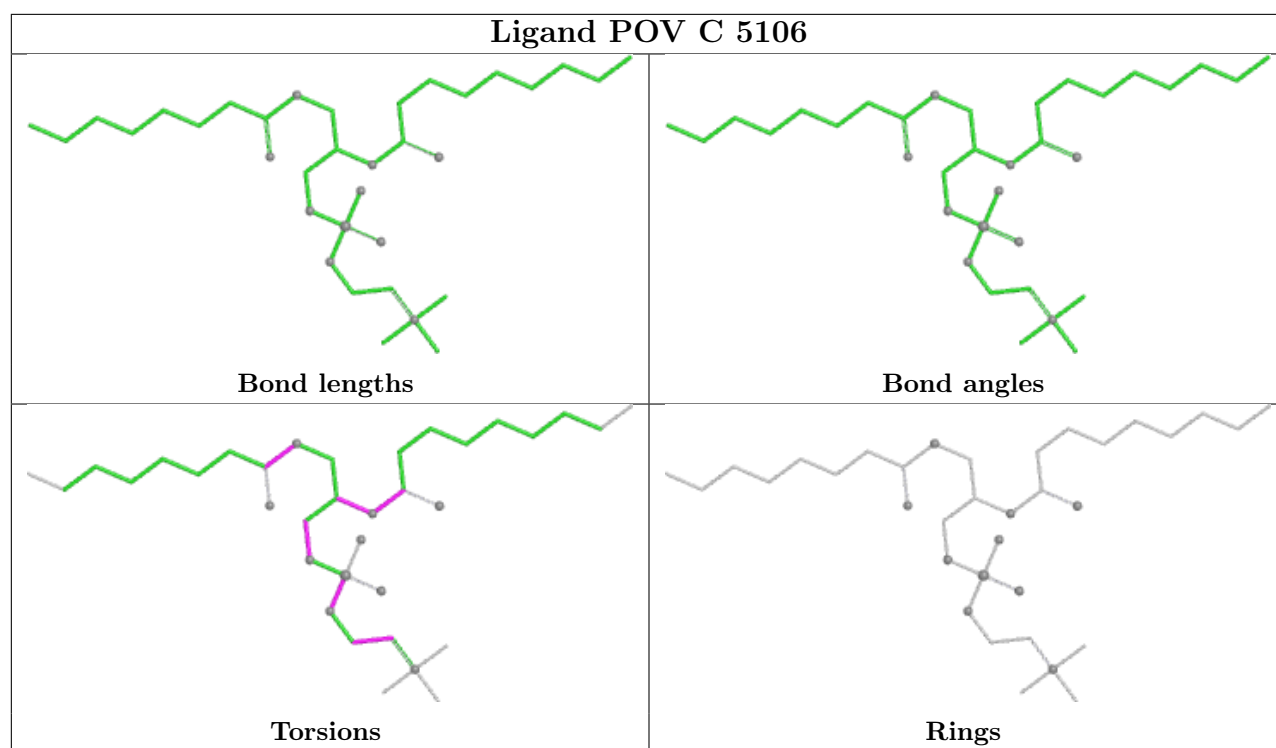
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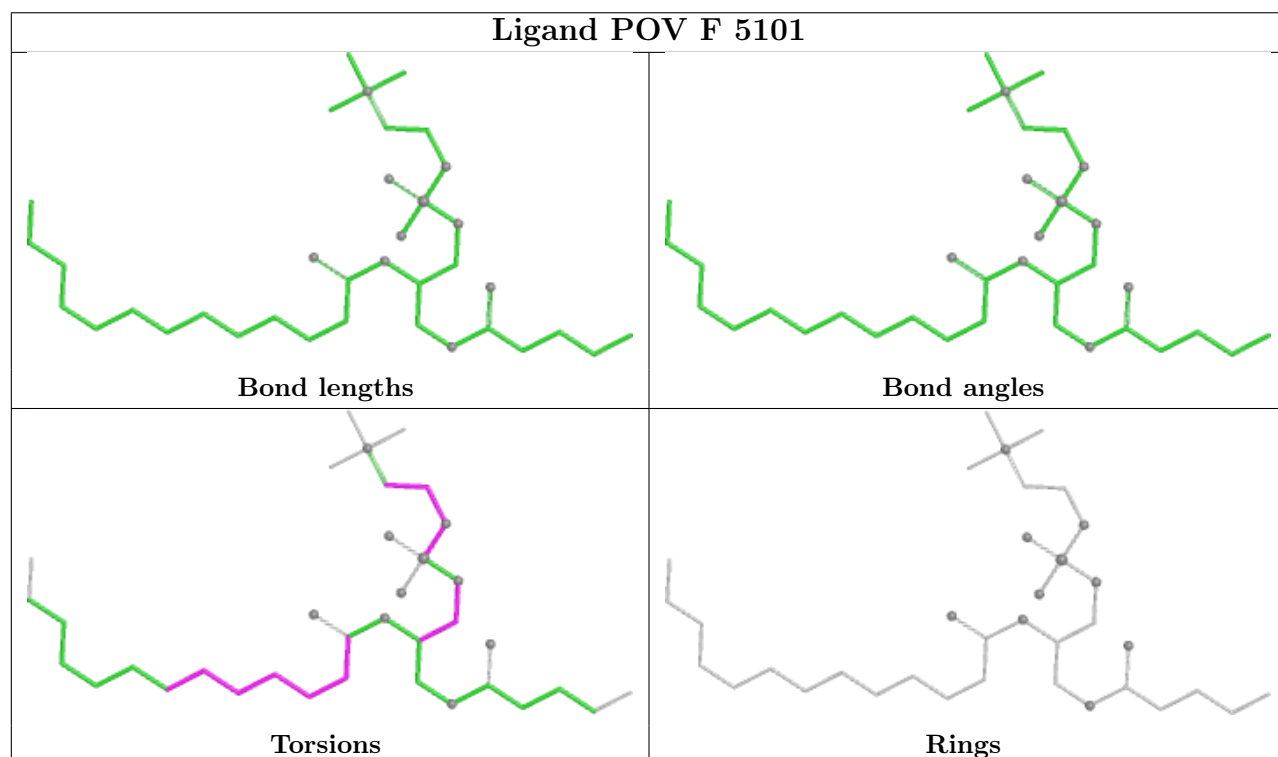
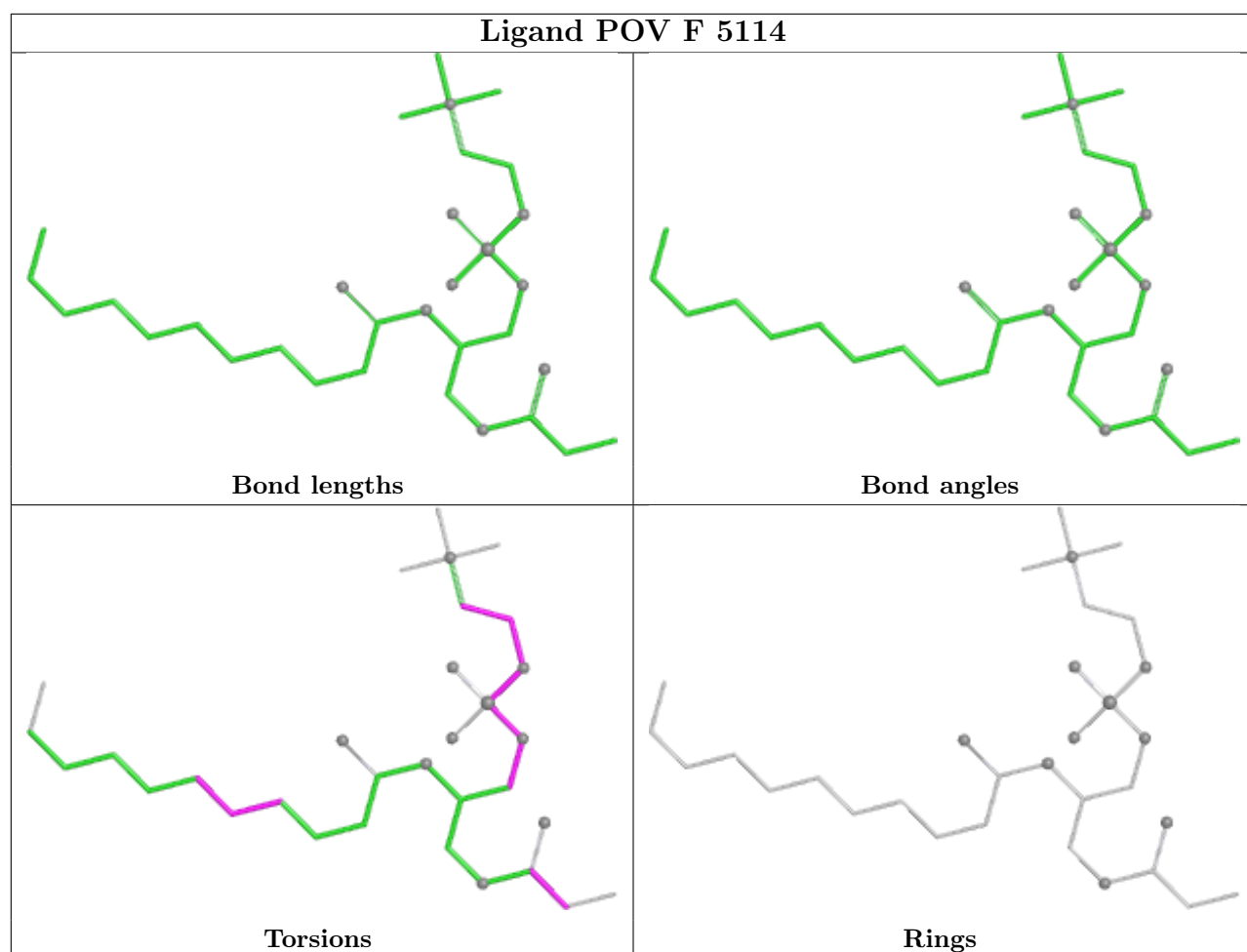
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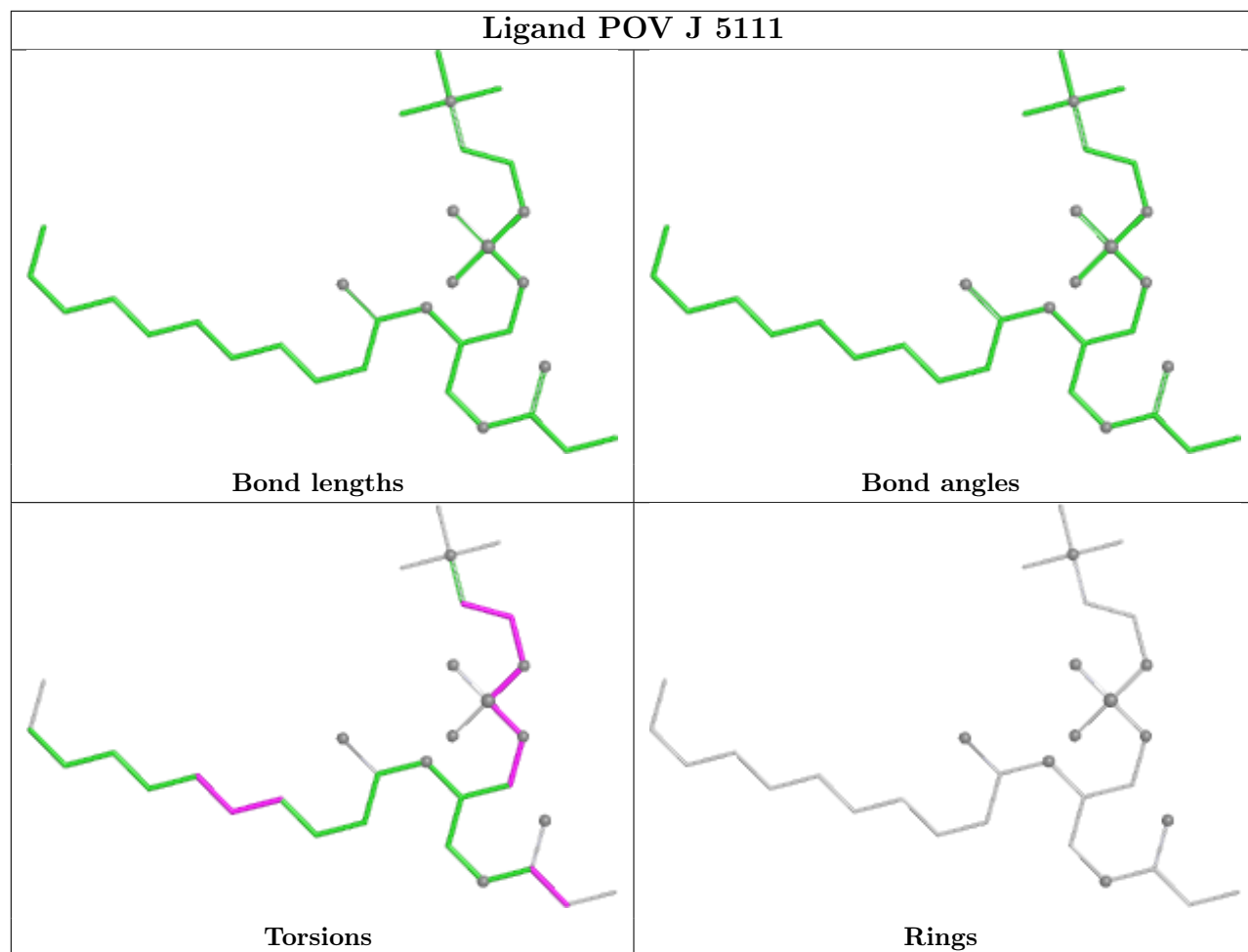
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	J	5107	POV	3	0
7	C	5101	POV	3	0
7	J	5104	POV	1	0
7	F	5110	POV	4	0
7	F	5112	POV	3	0
7	I	5113	POV	4	0
7	I	5104	POV	2	0
7	F	5113	POV	2	0

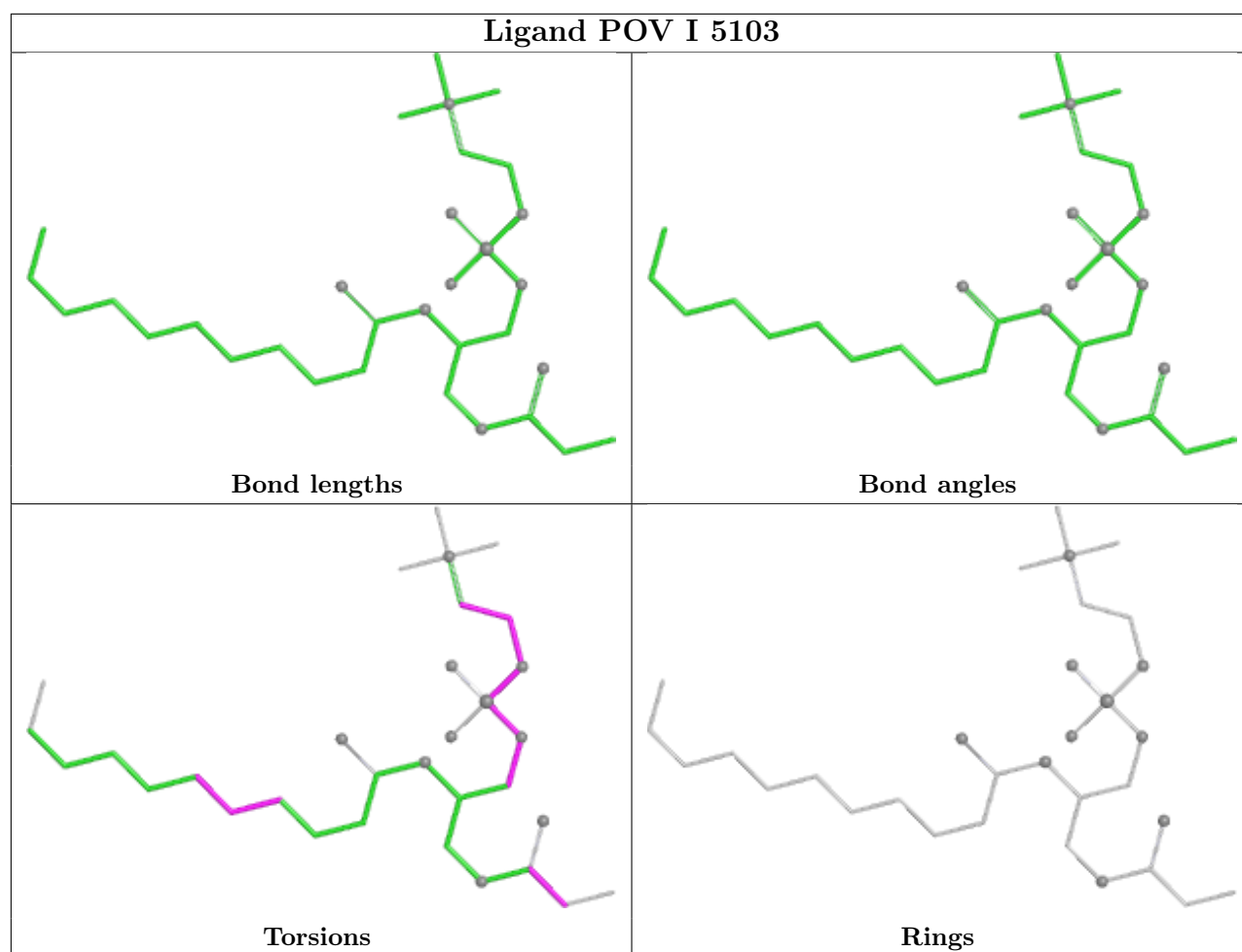
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

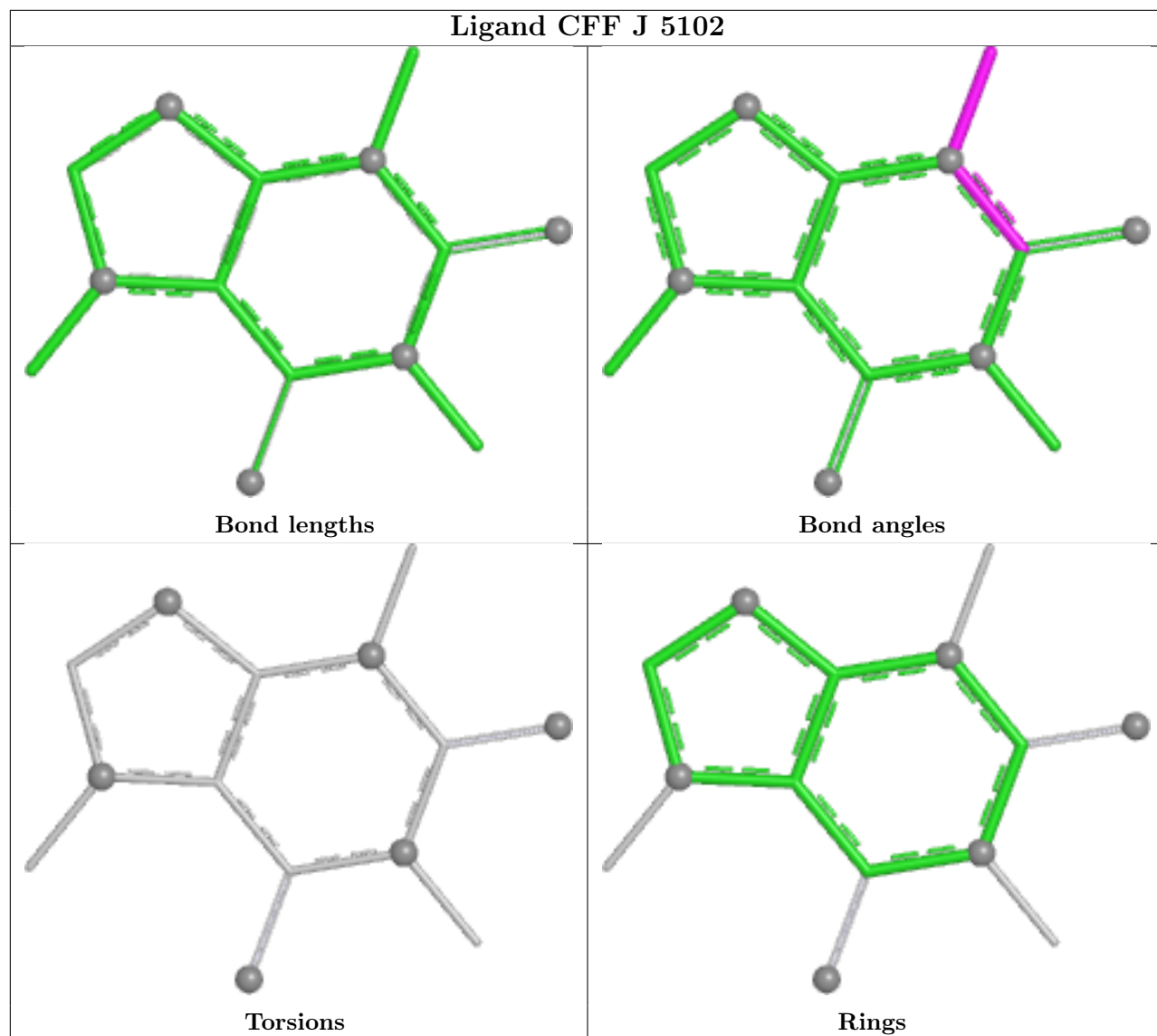


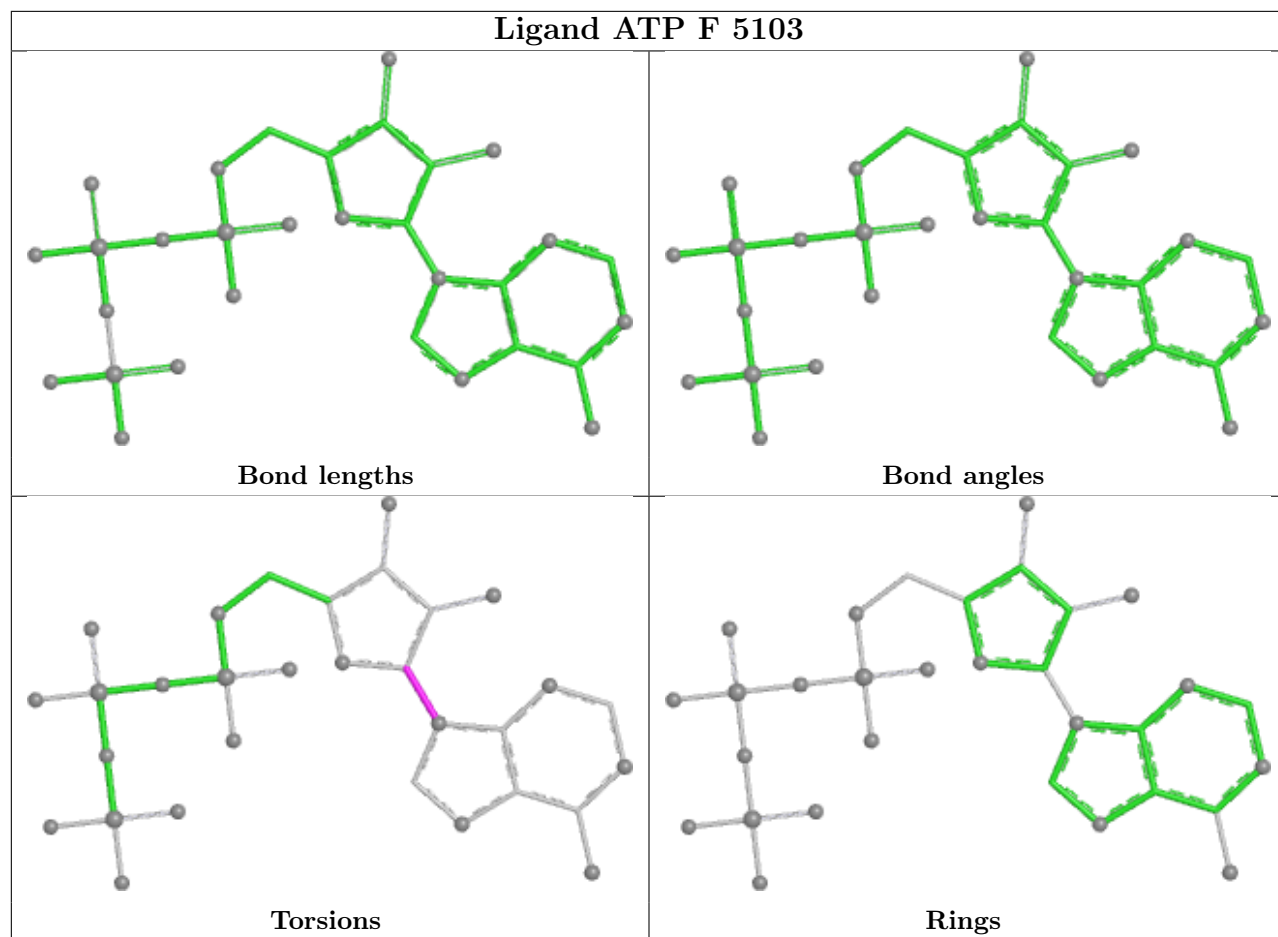


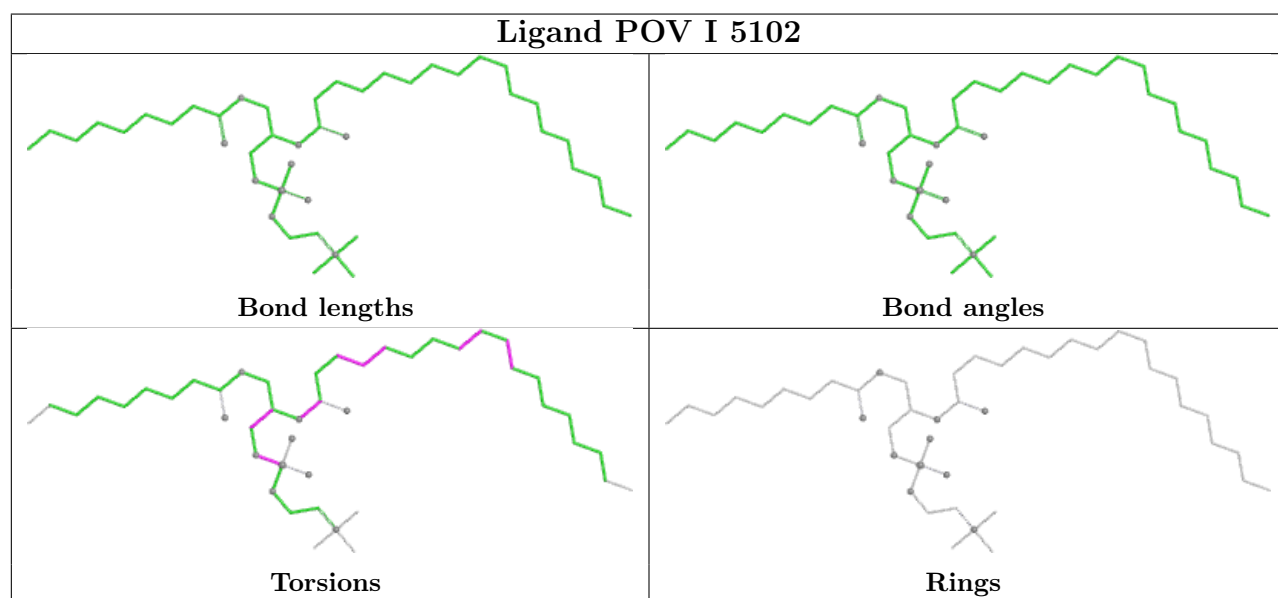
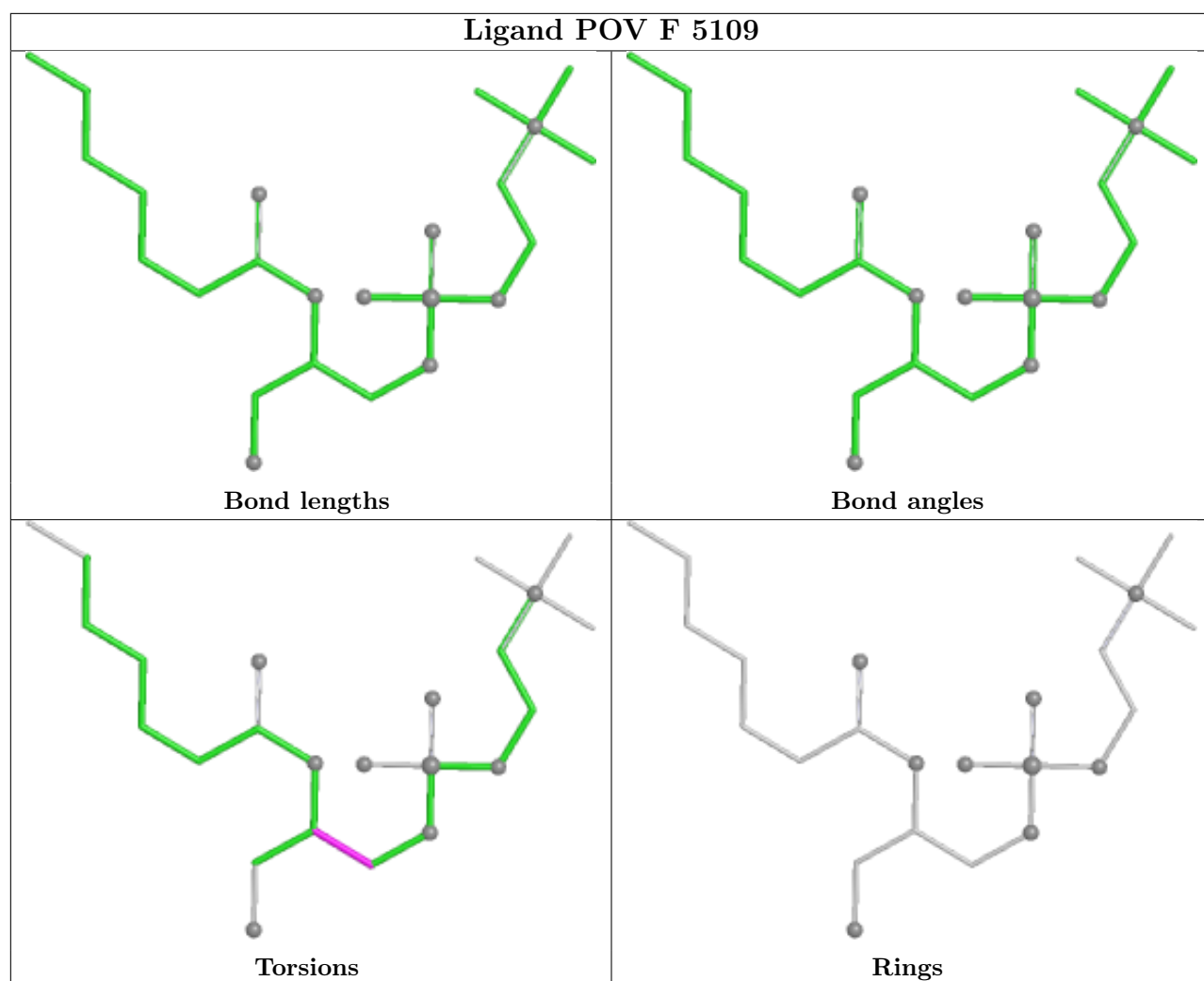


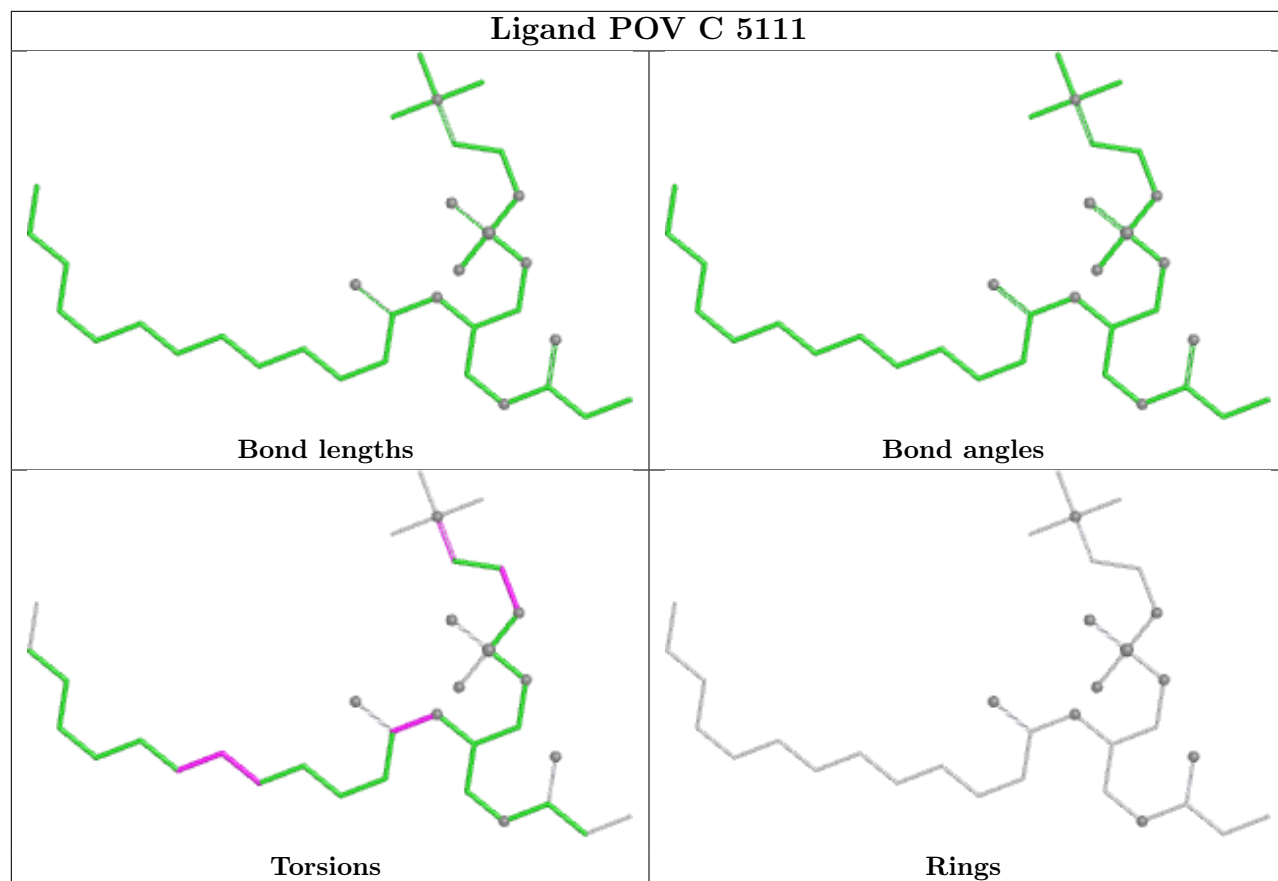


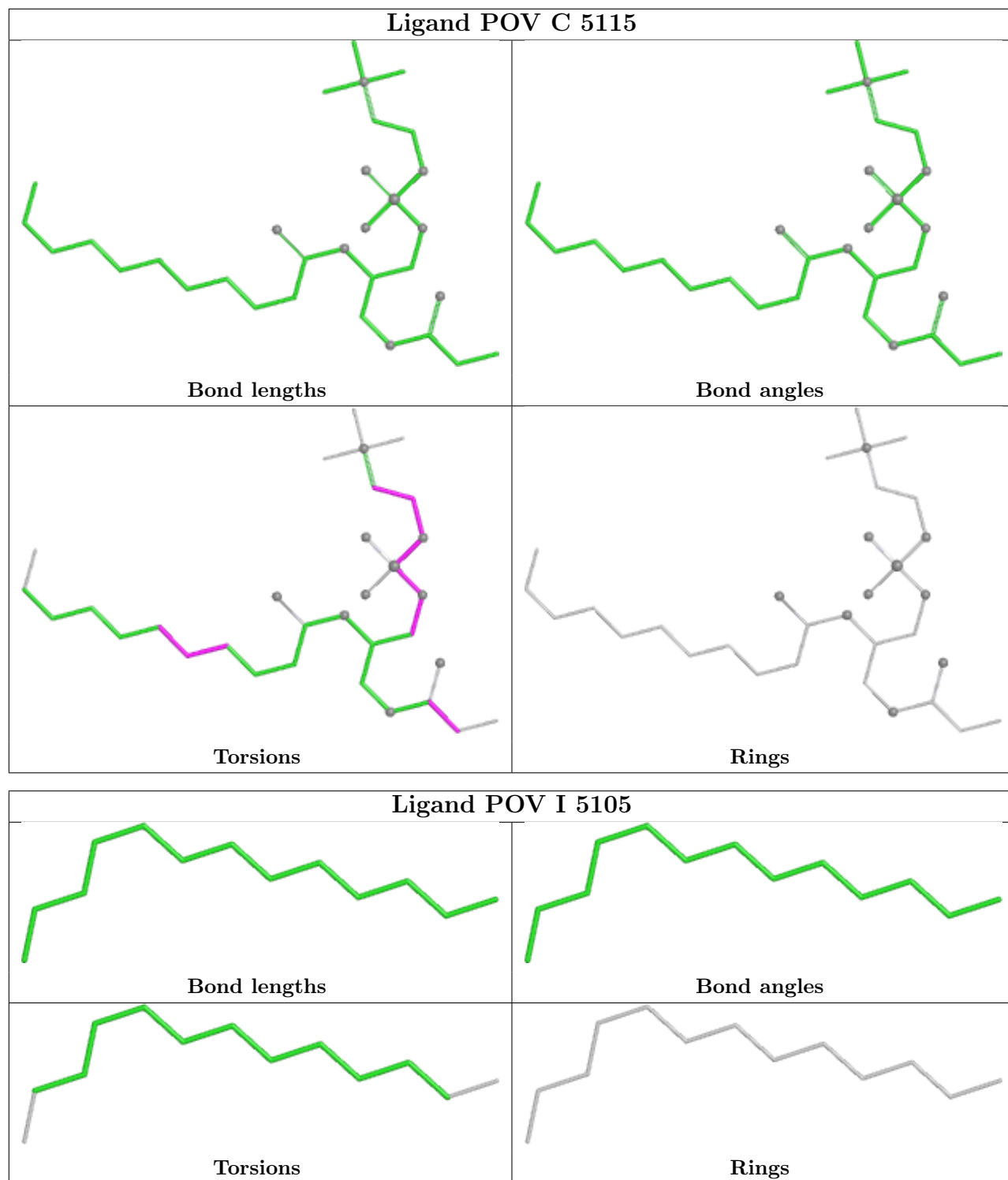


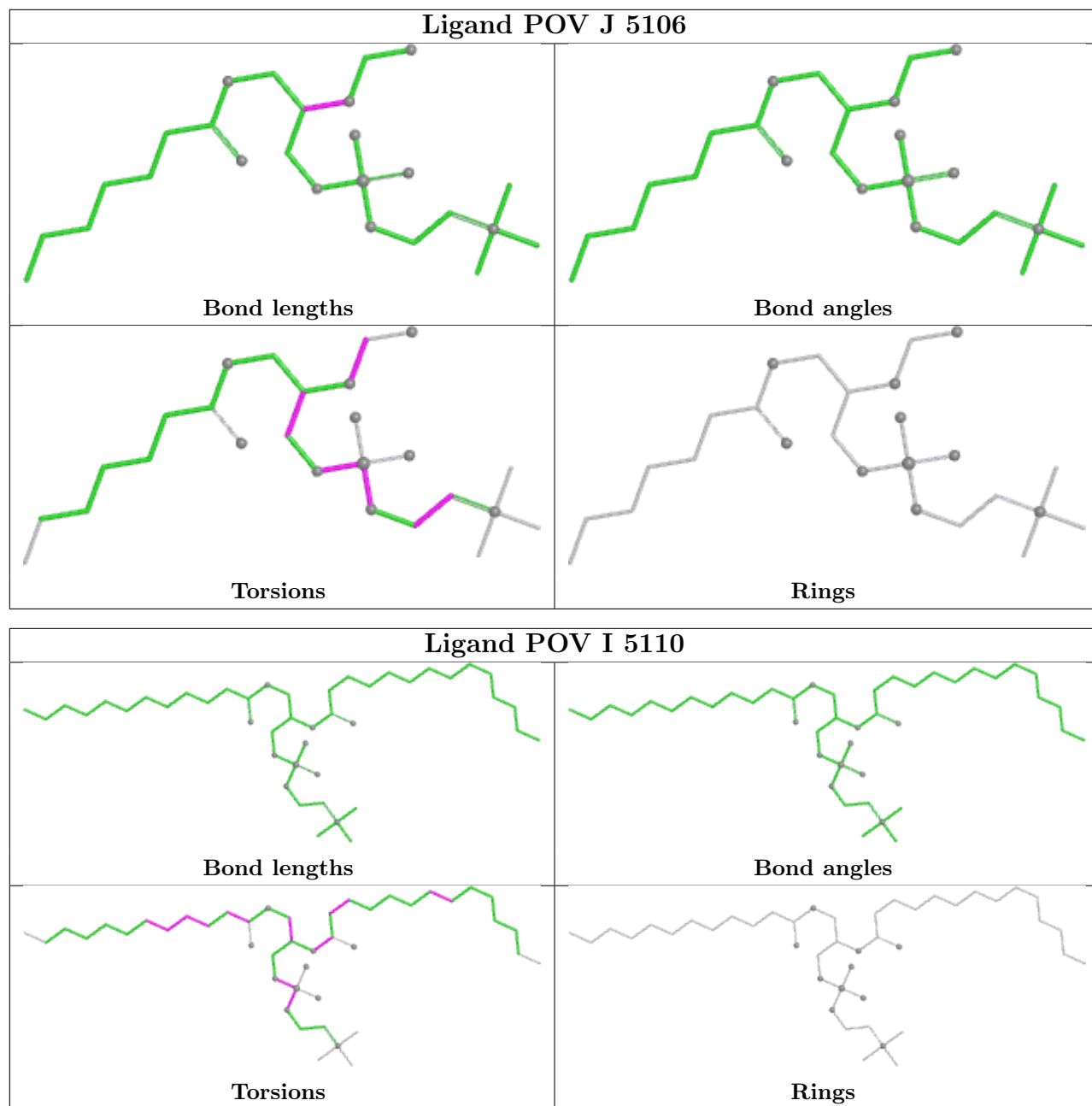


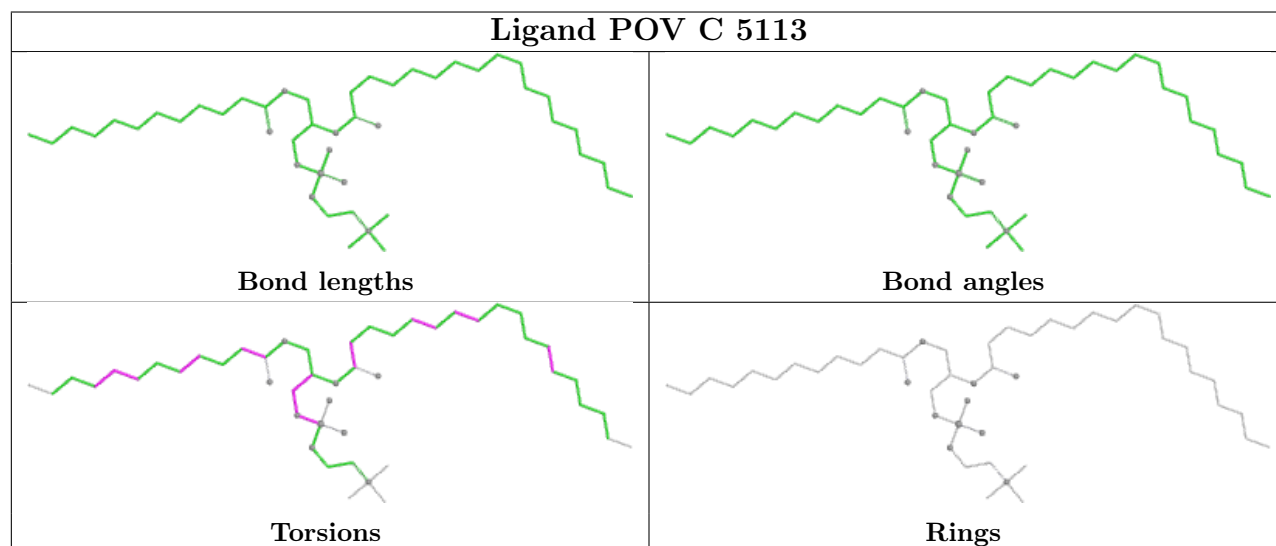
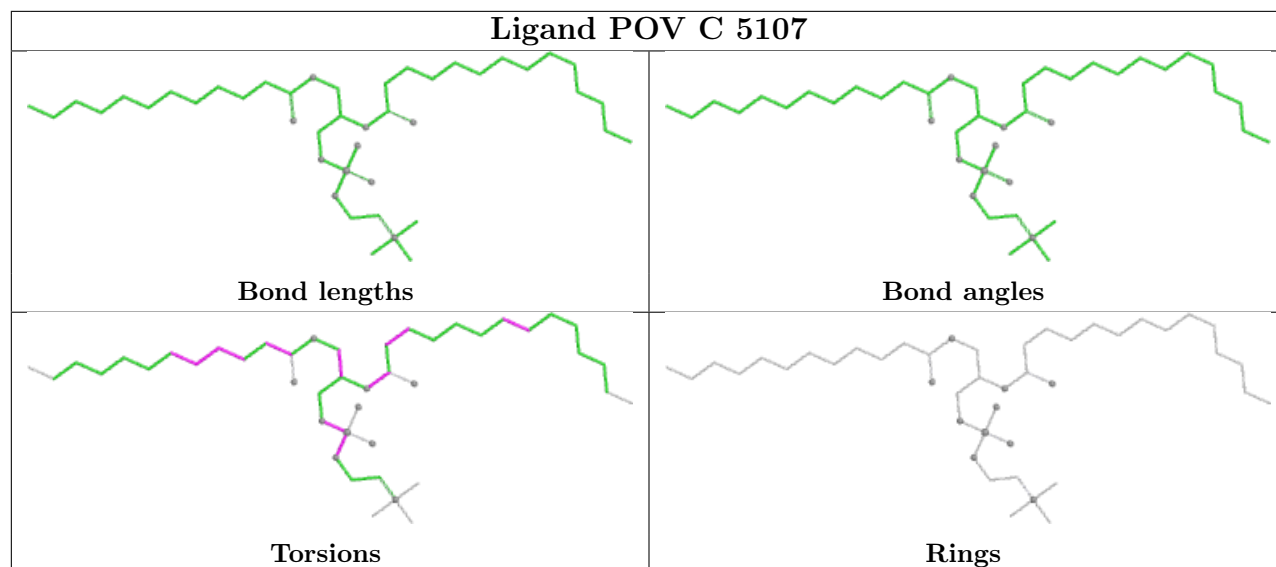




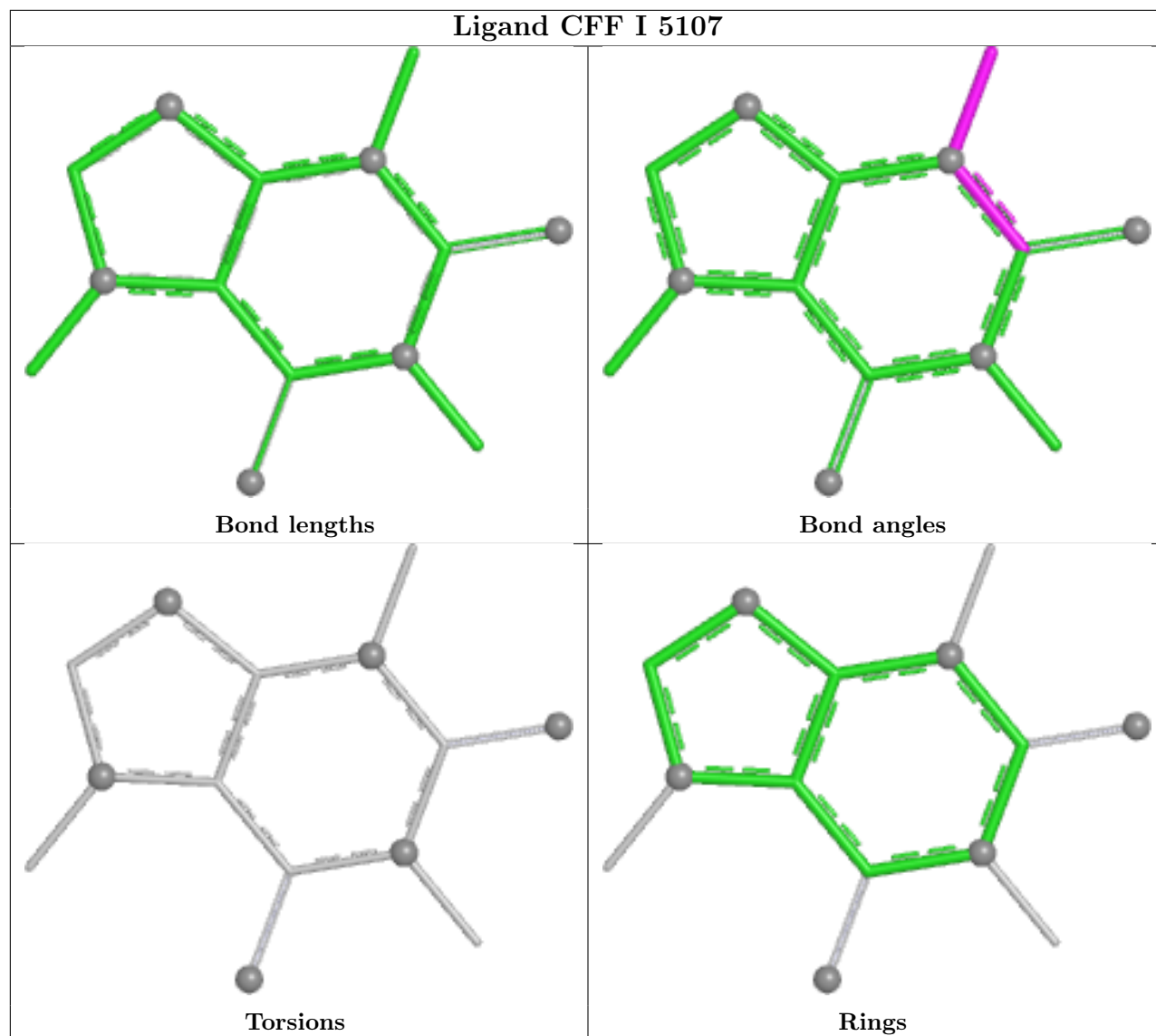




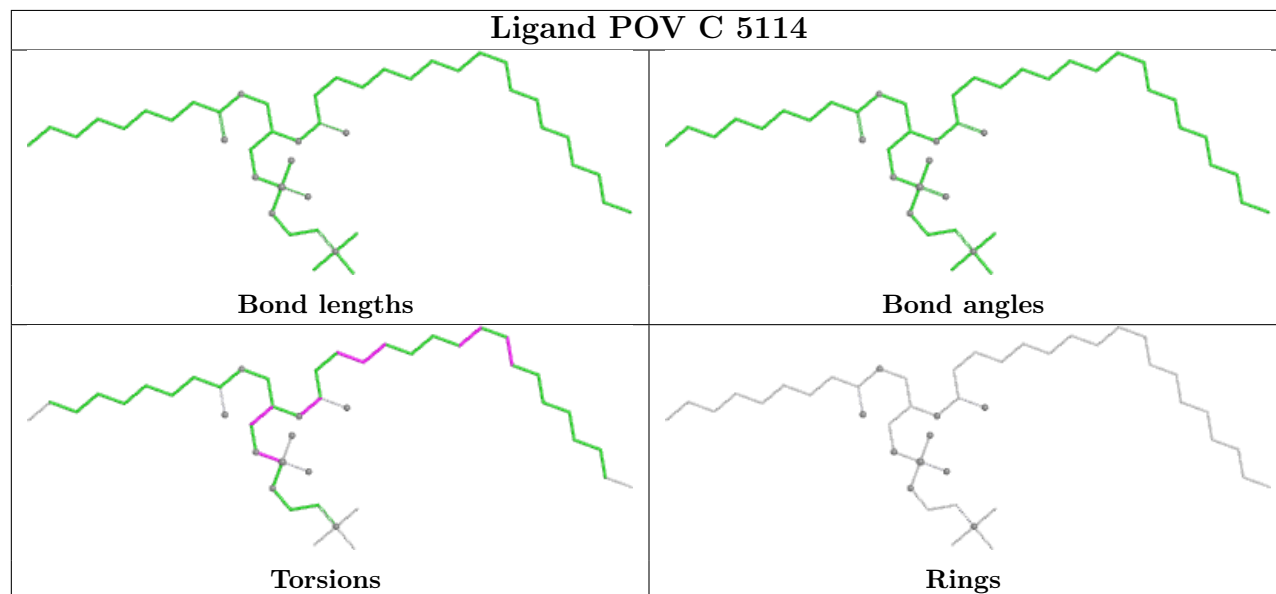


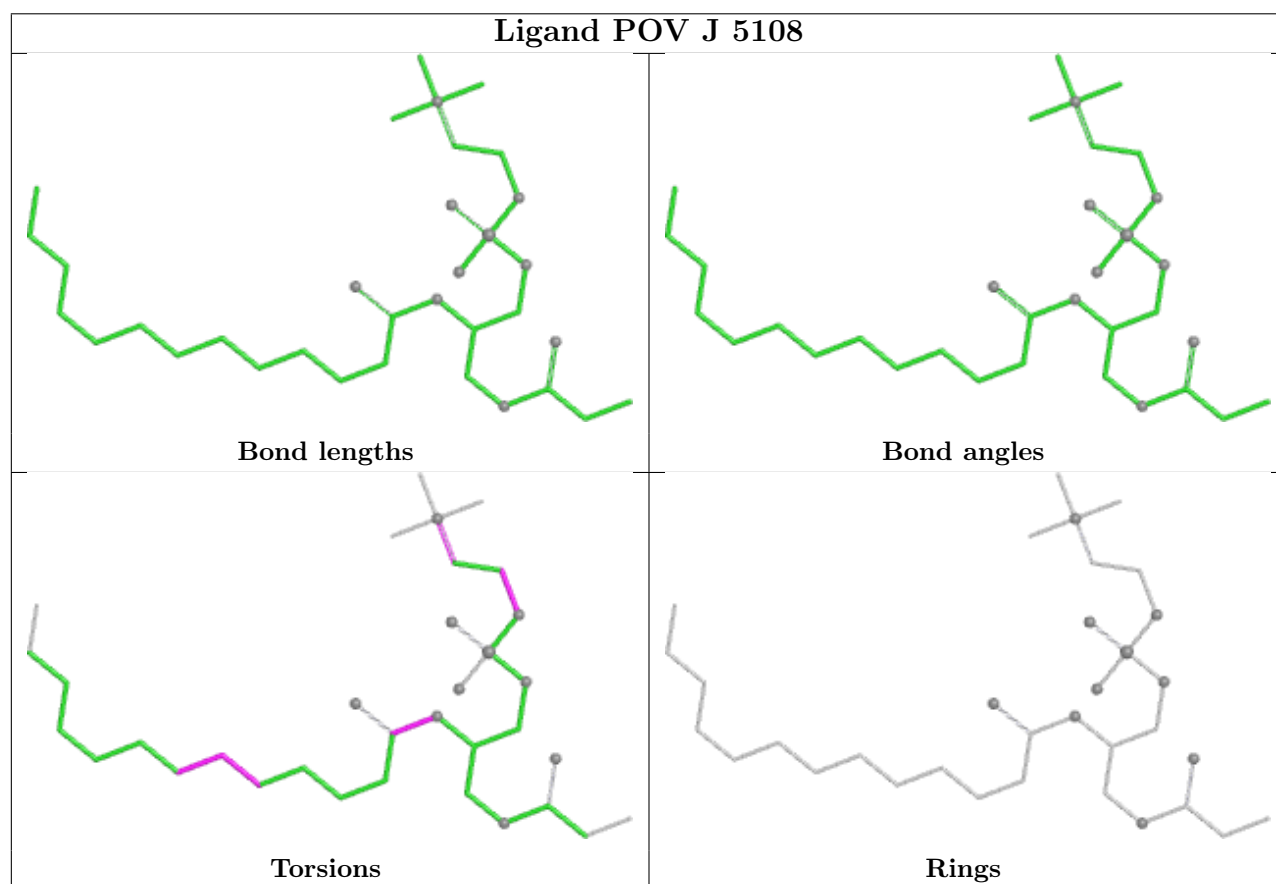
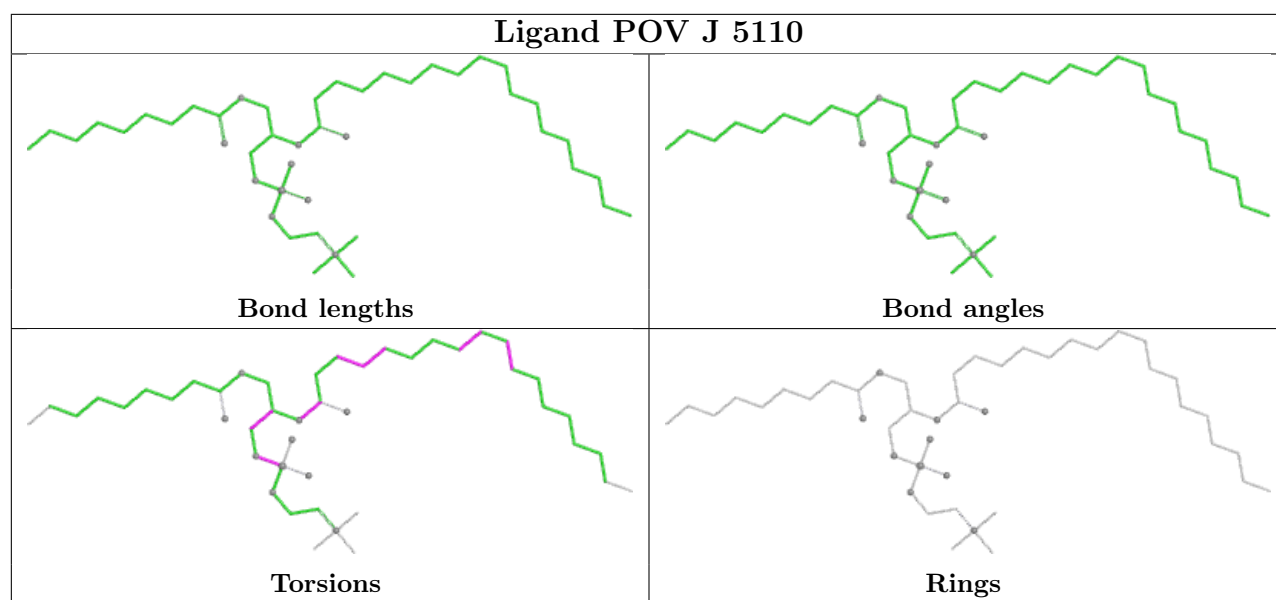


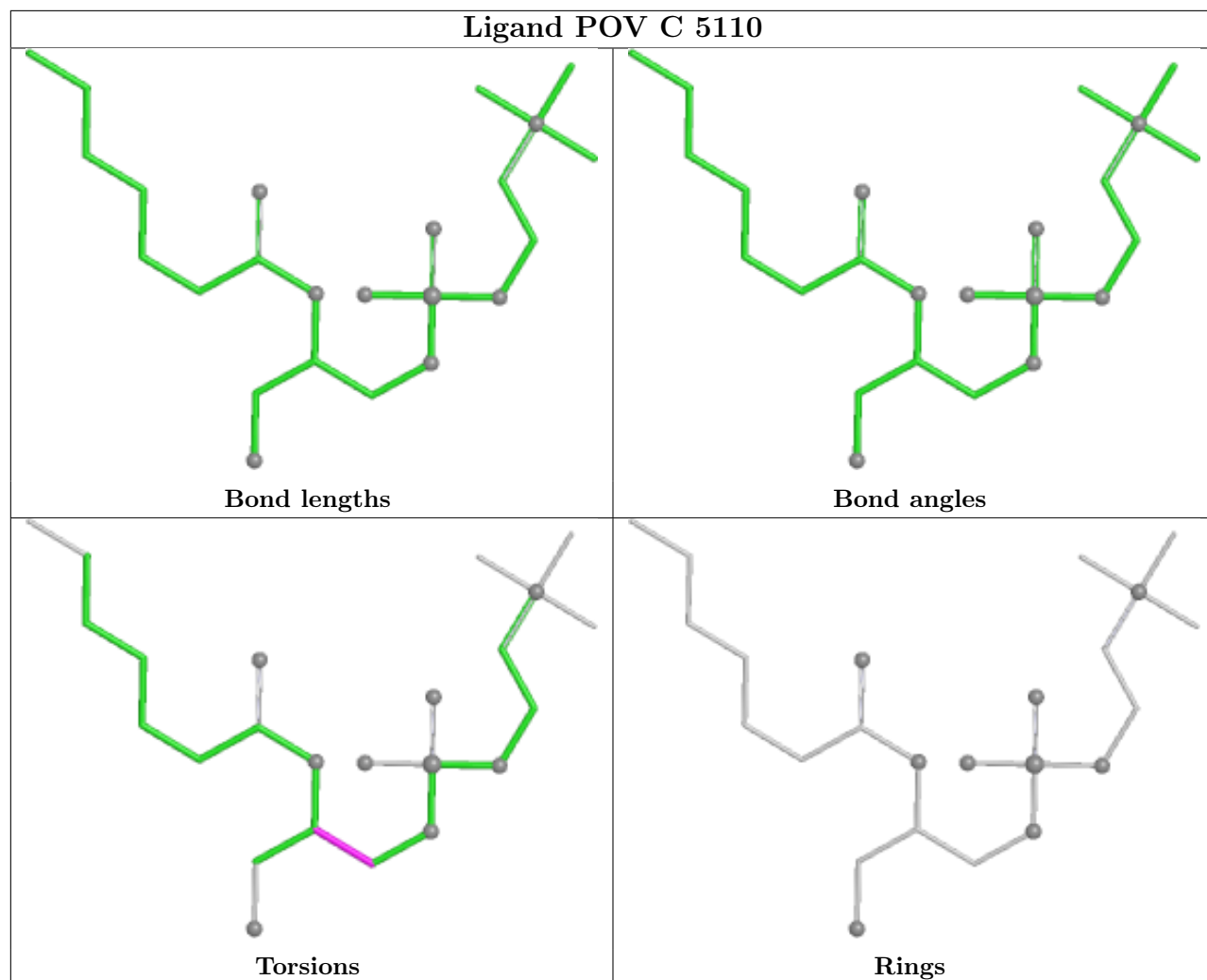
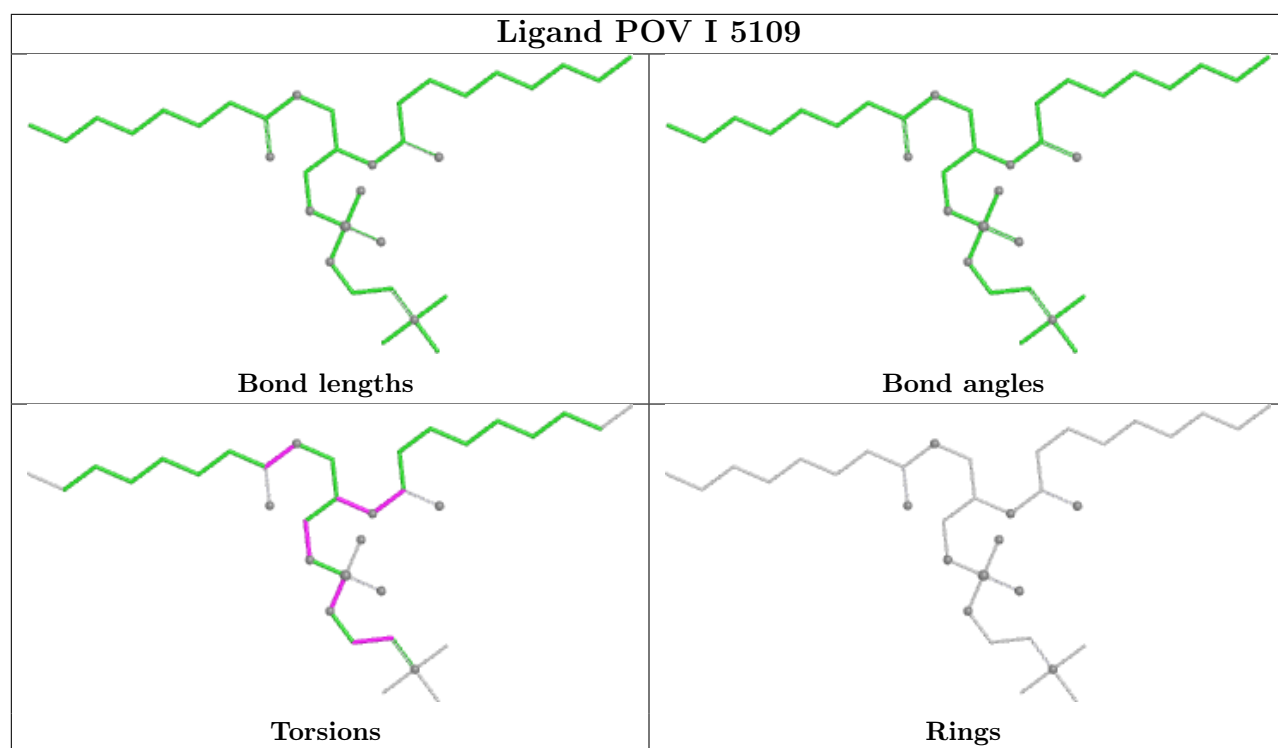
Ligand CFF I 5107

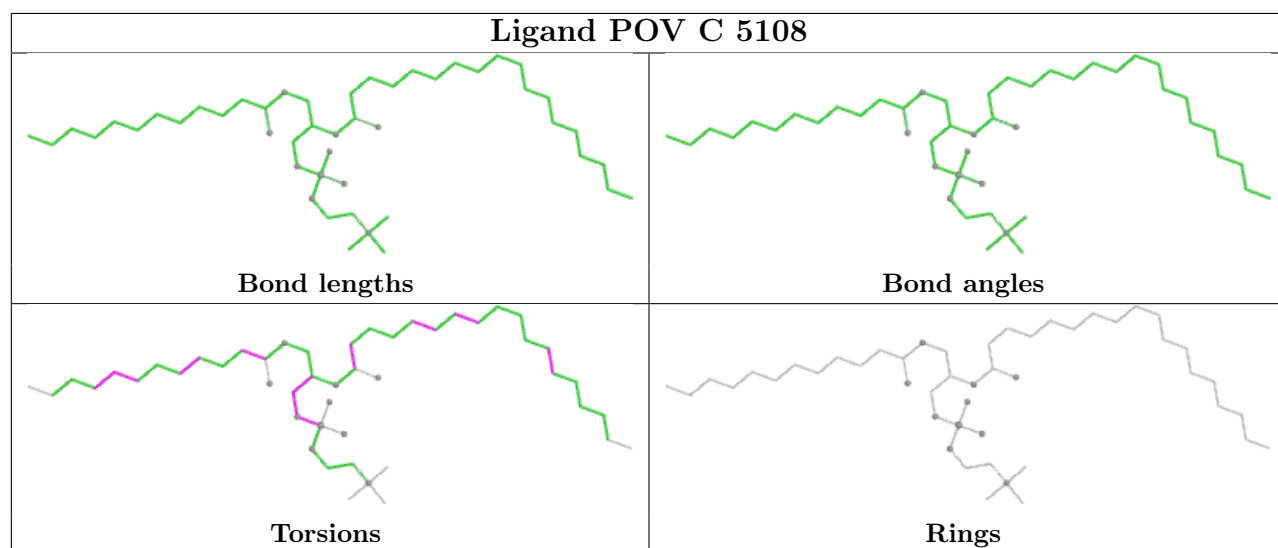
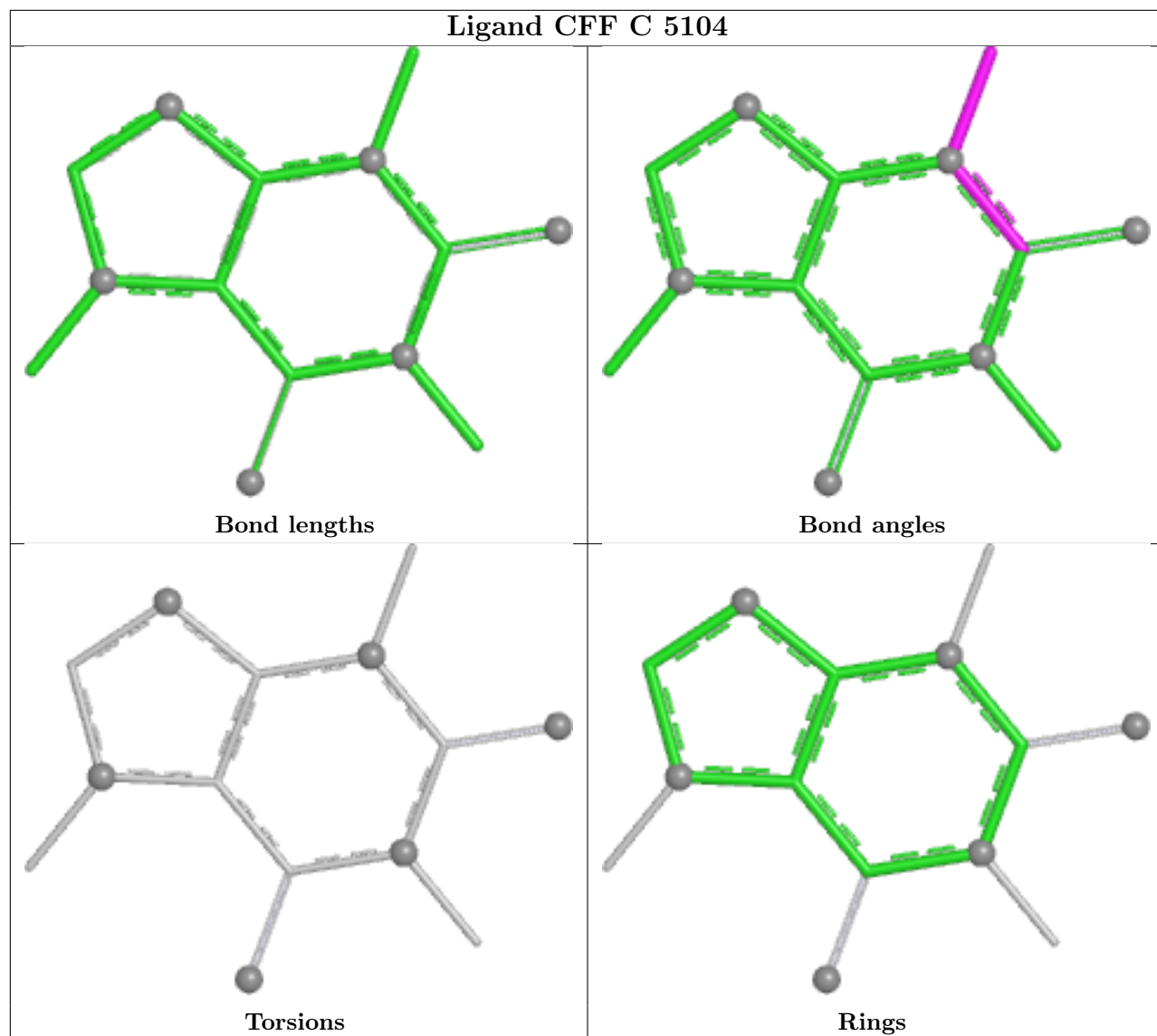


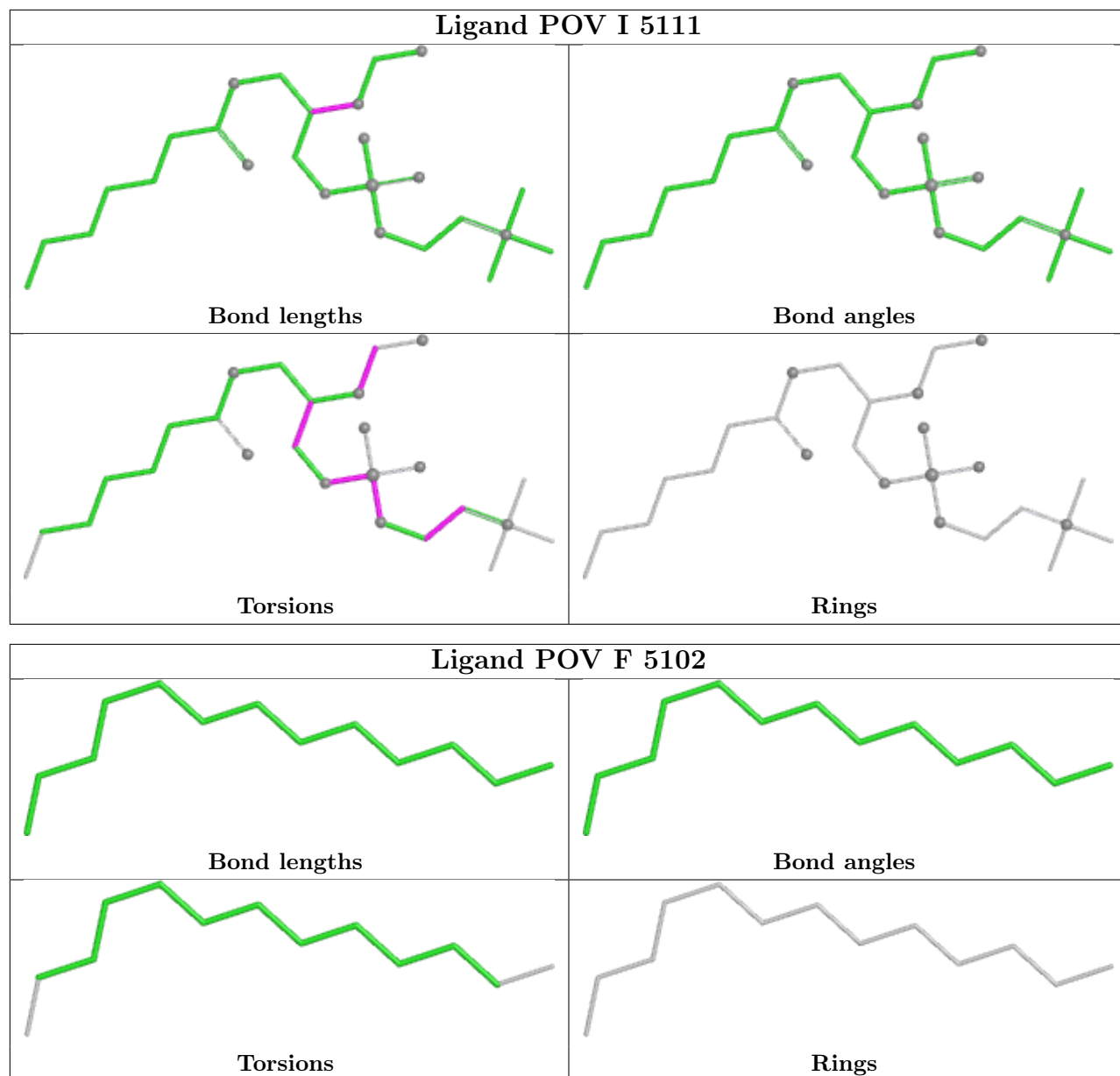
Ligand POV C 5114

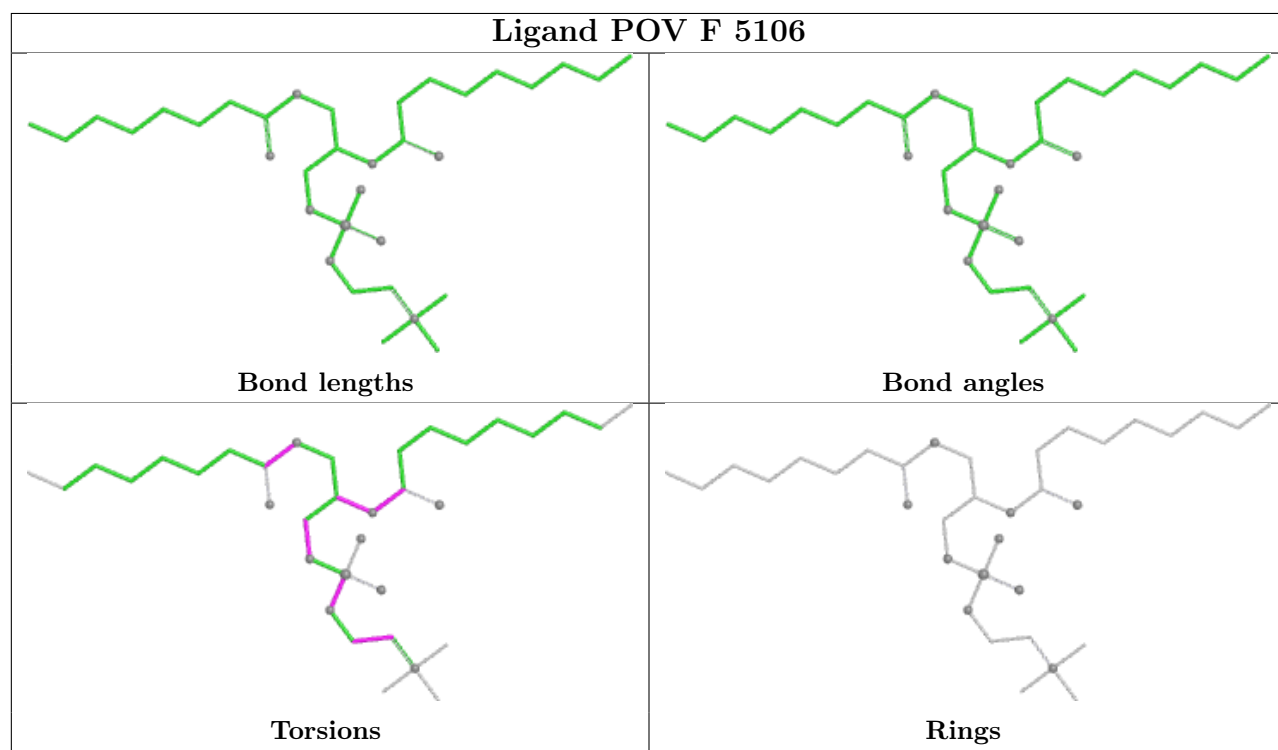
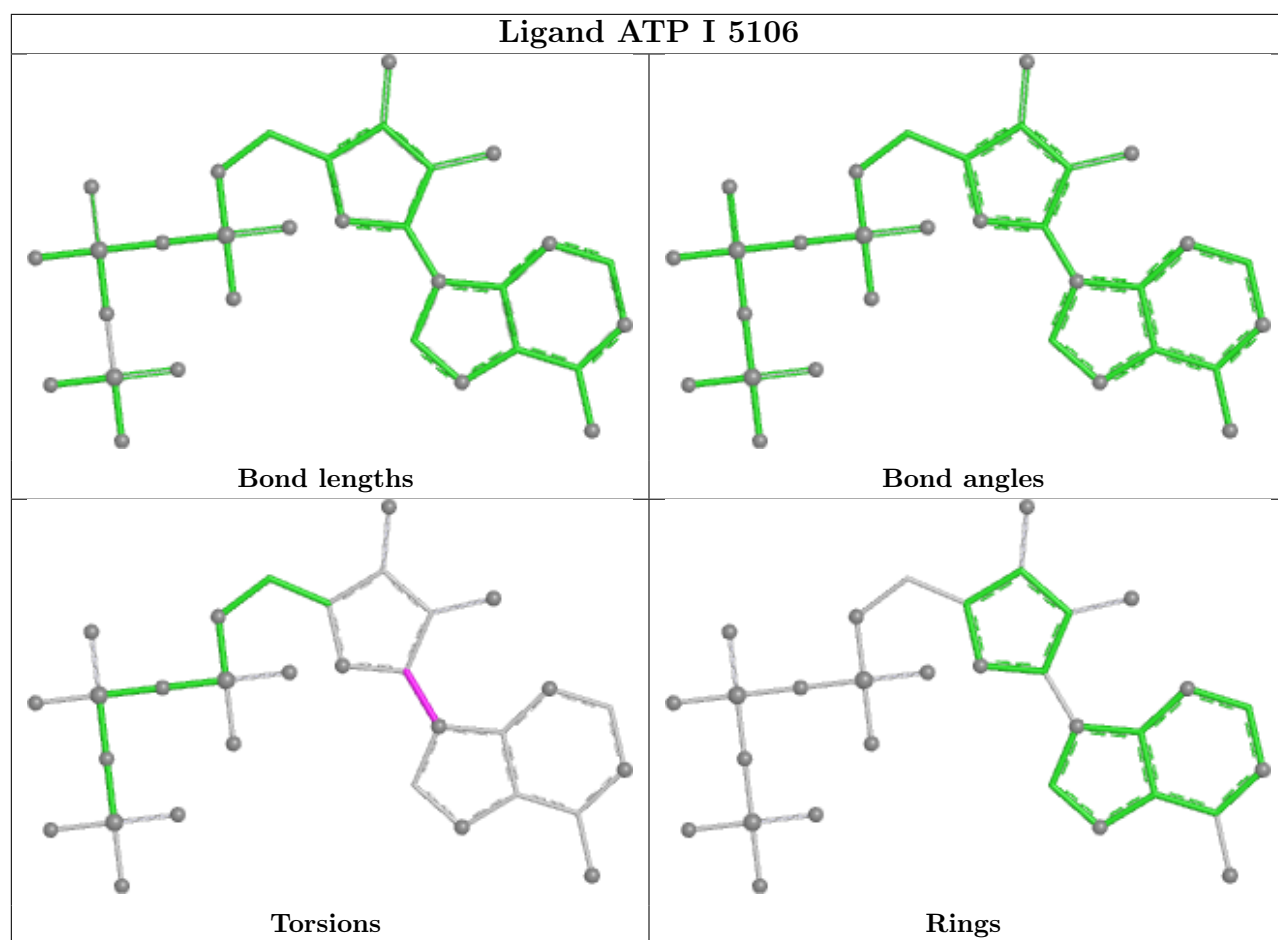


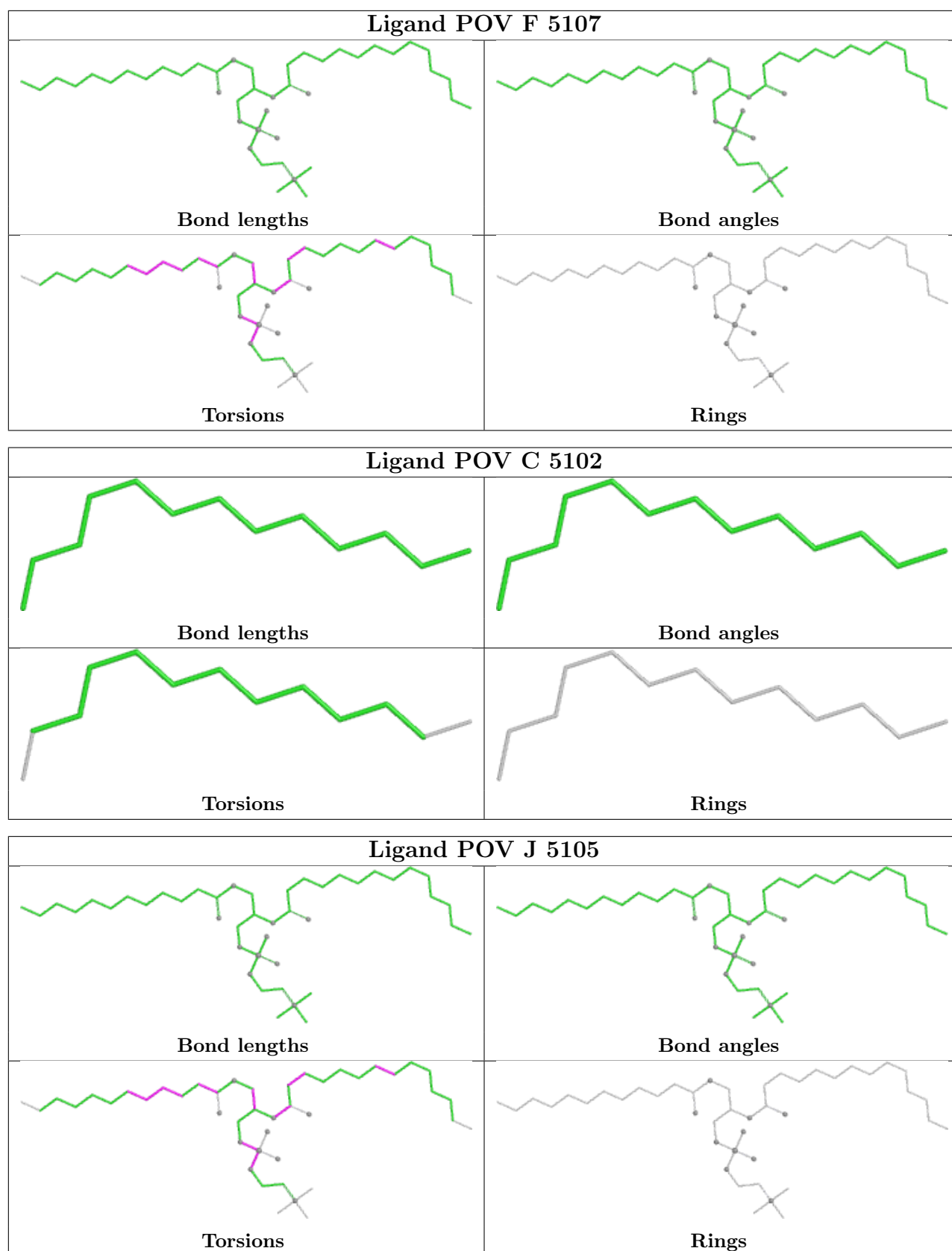


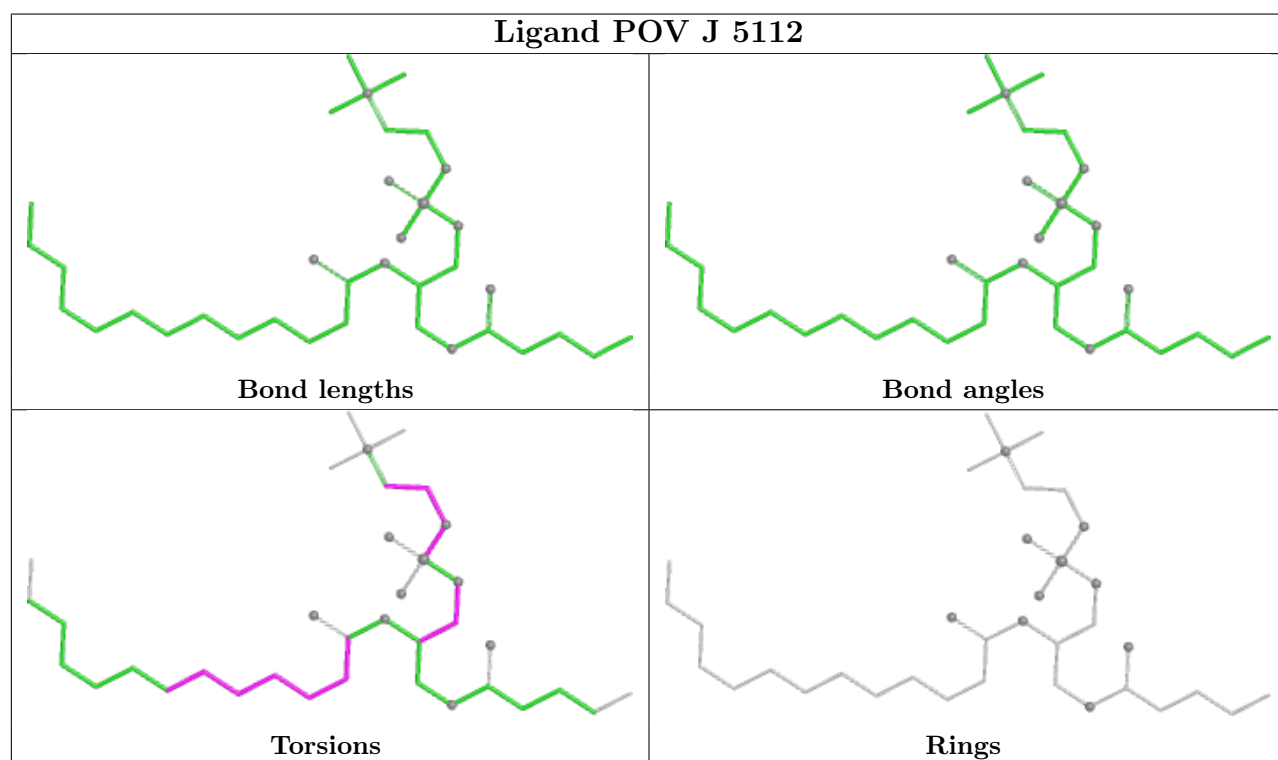
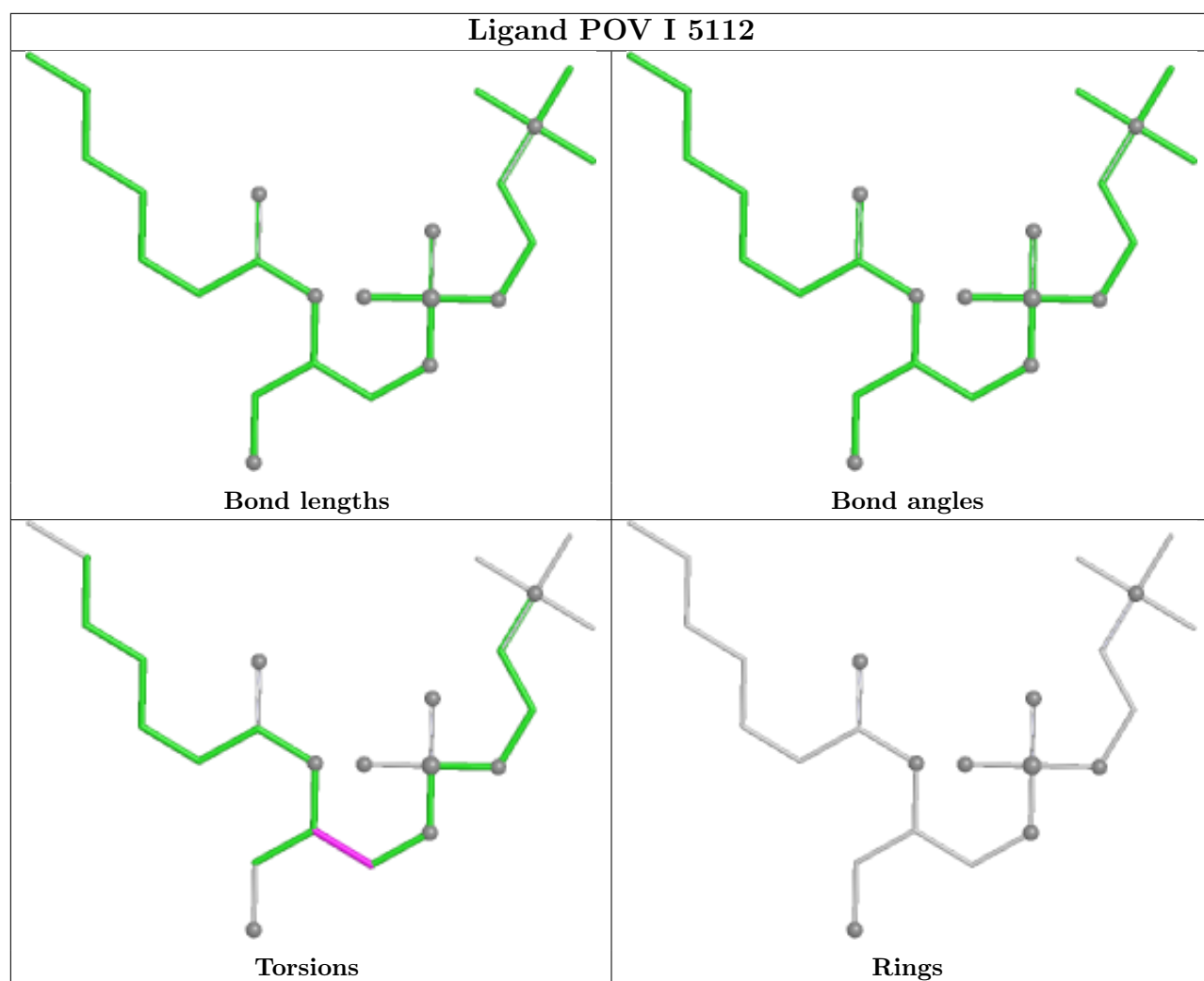


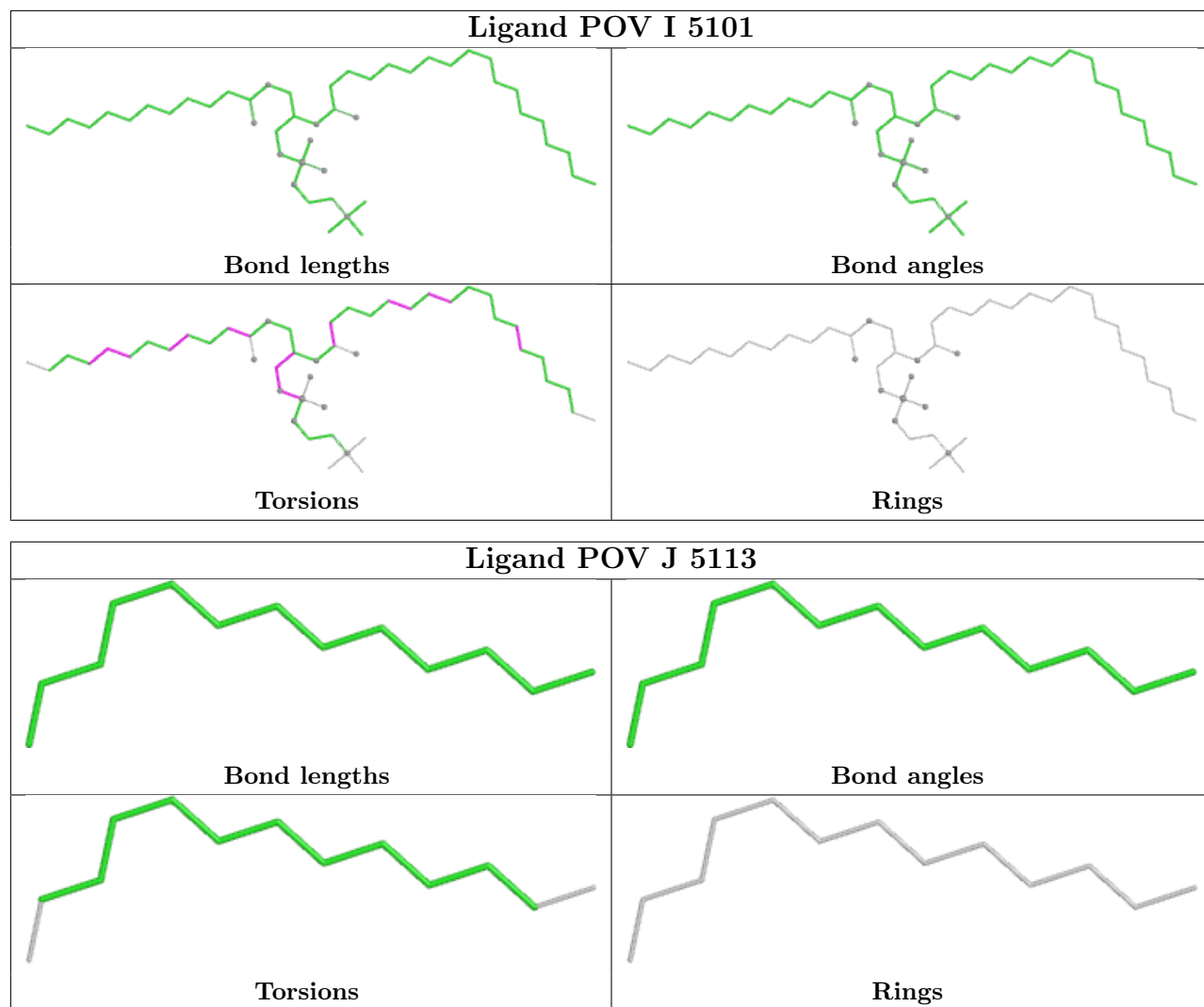


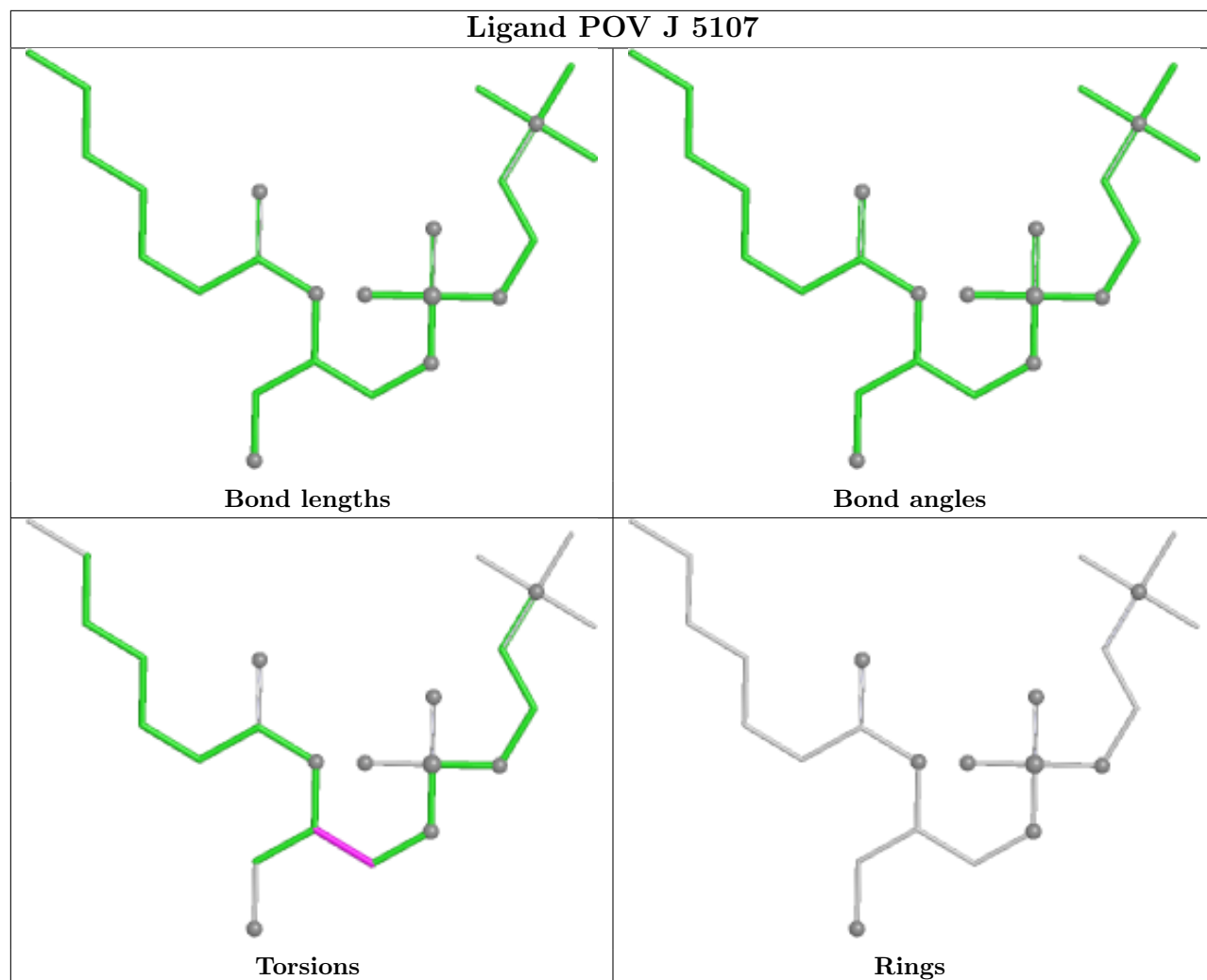


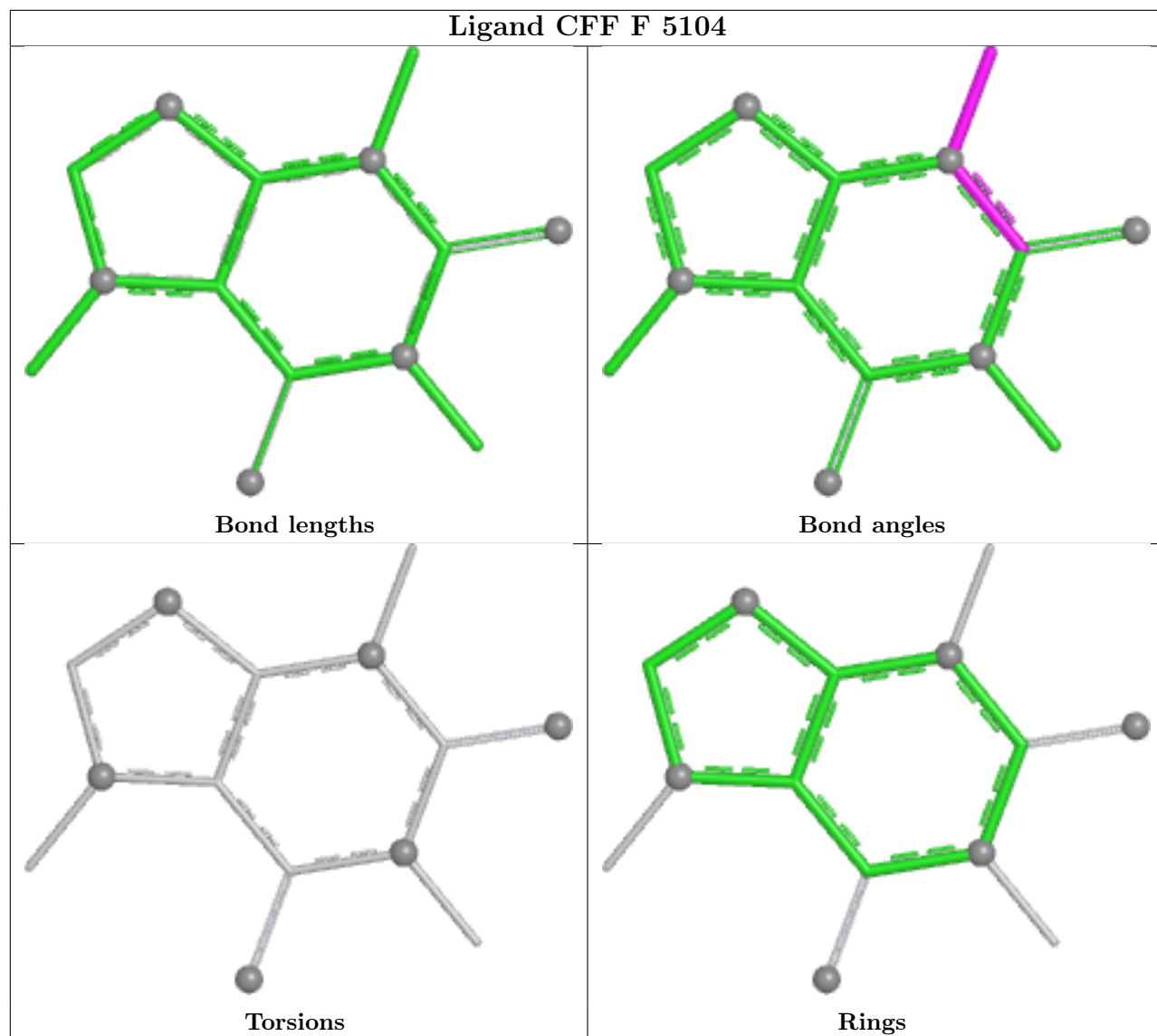


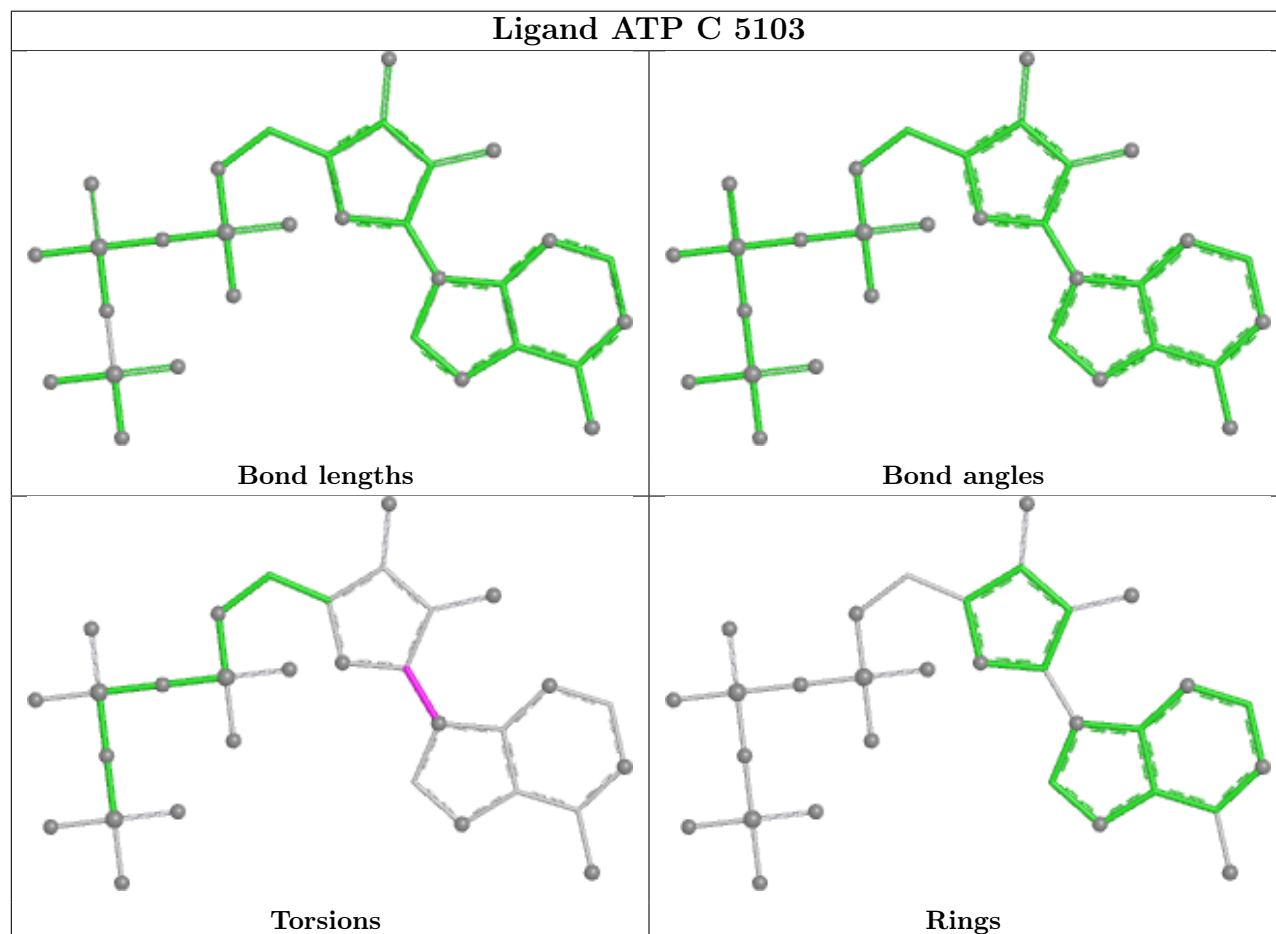
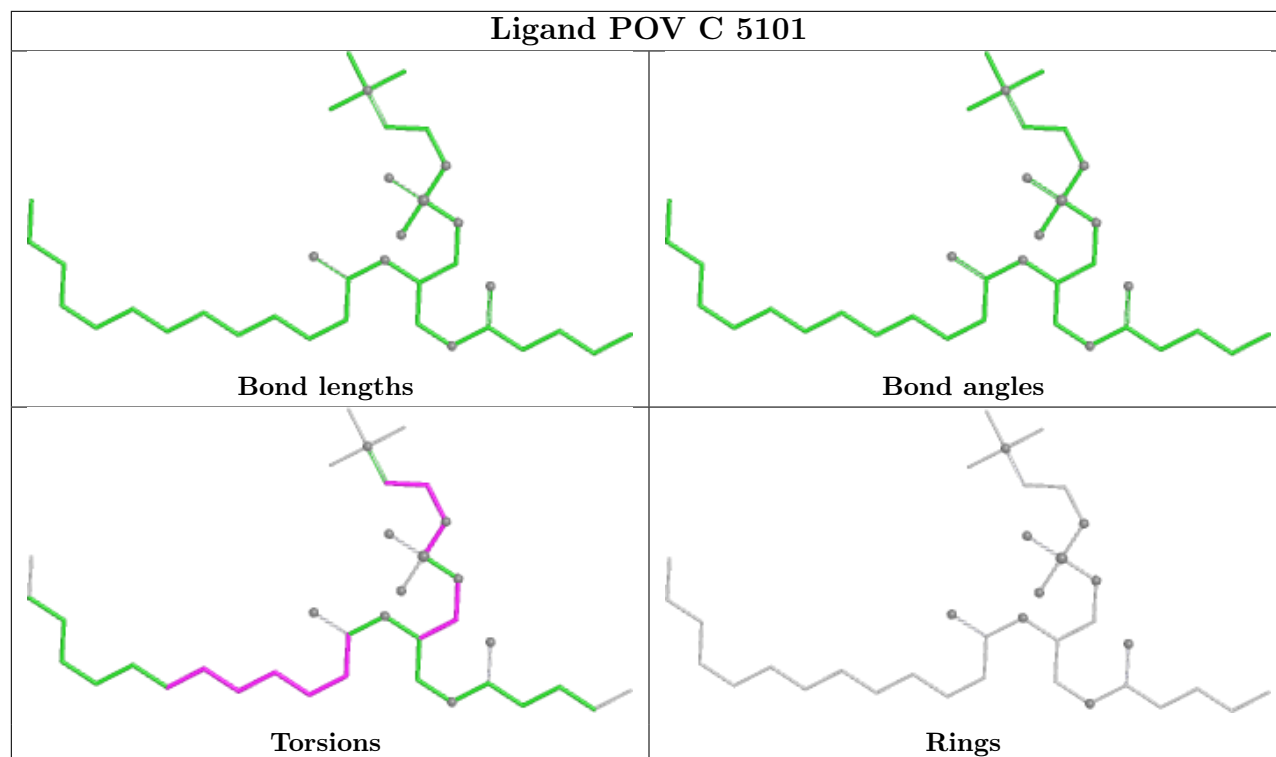


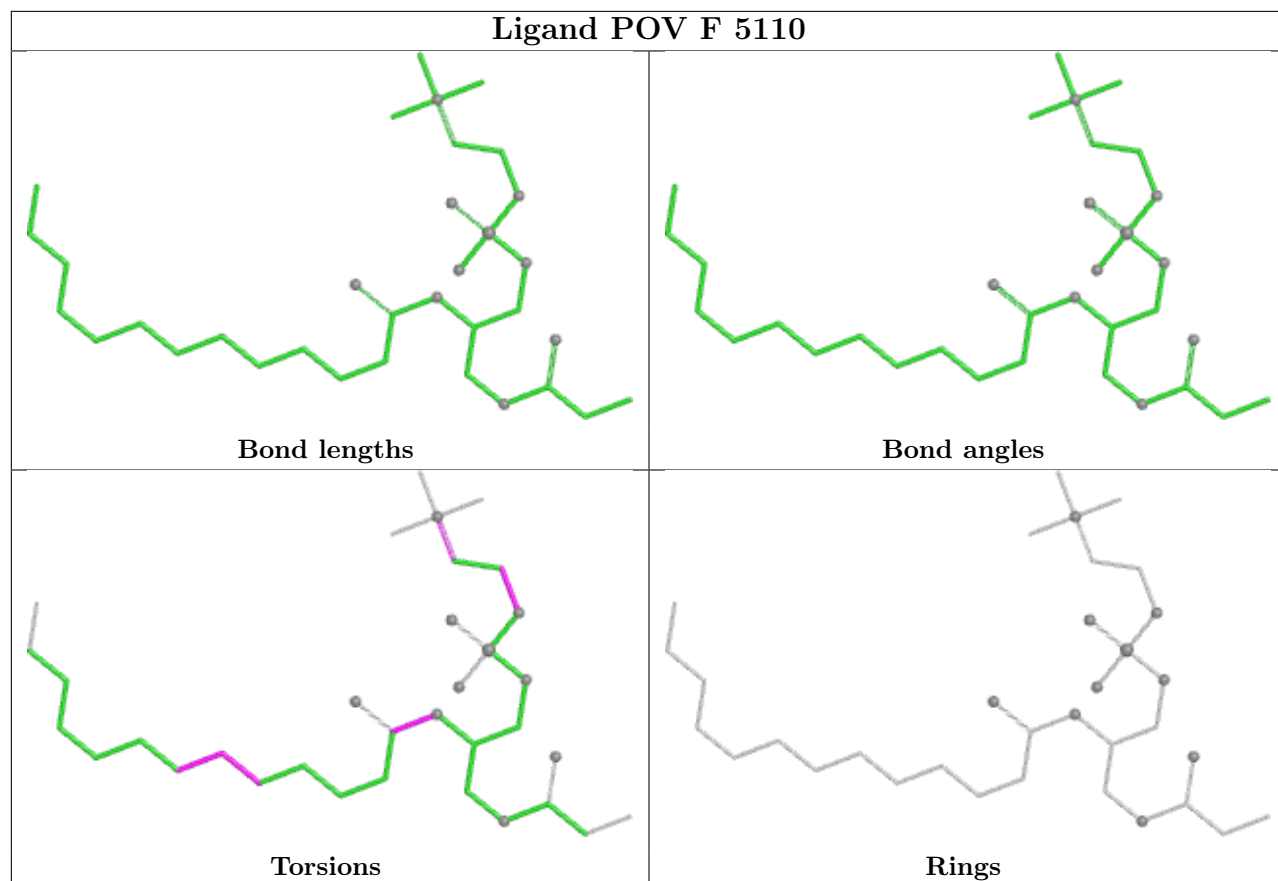
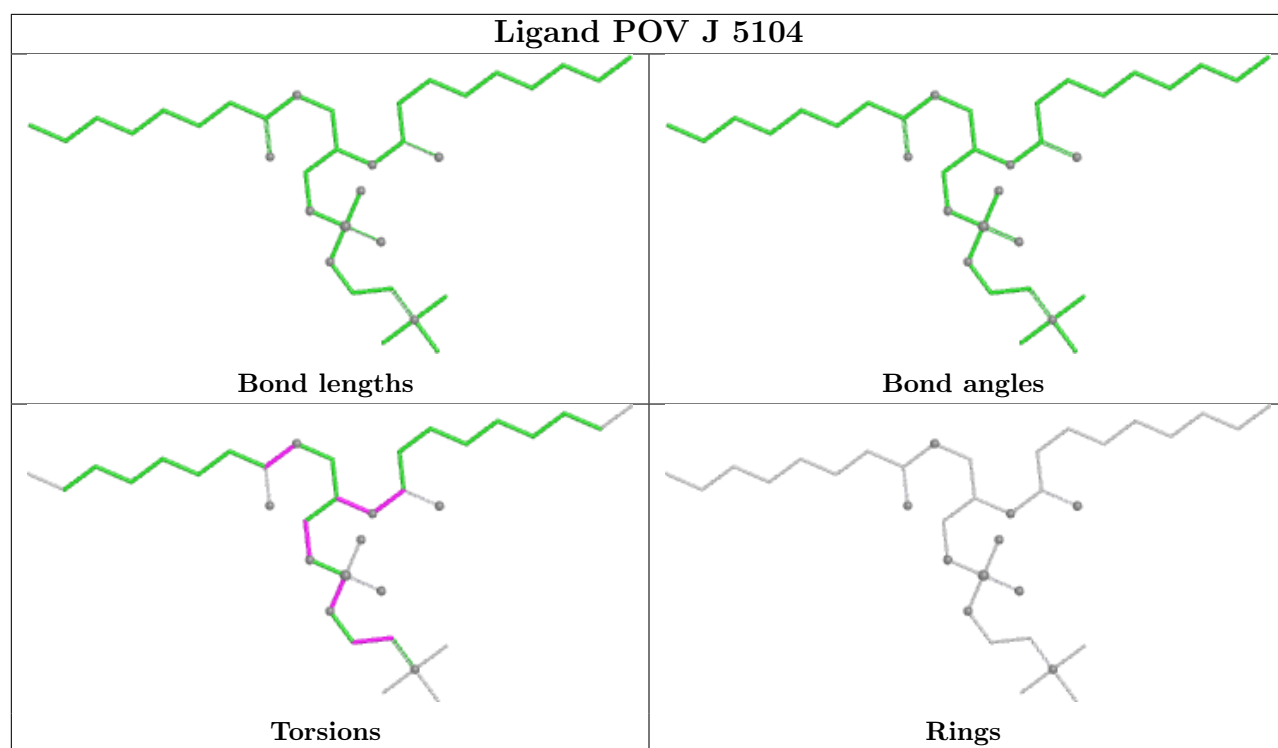


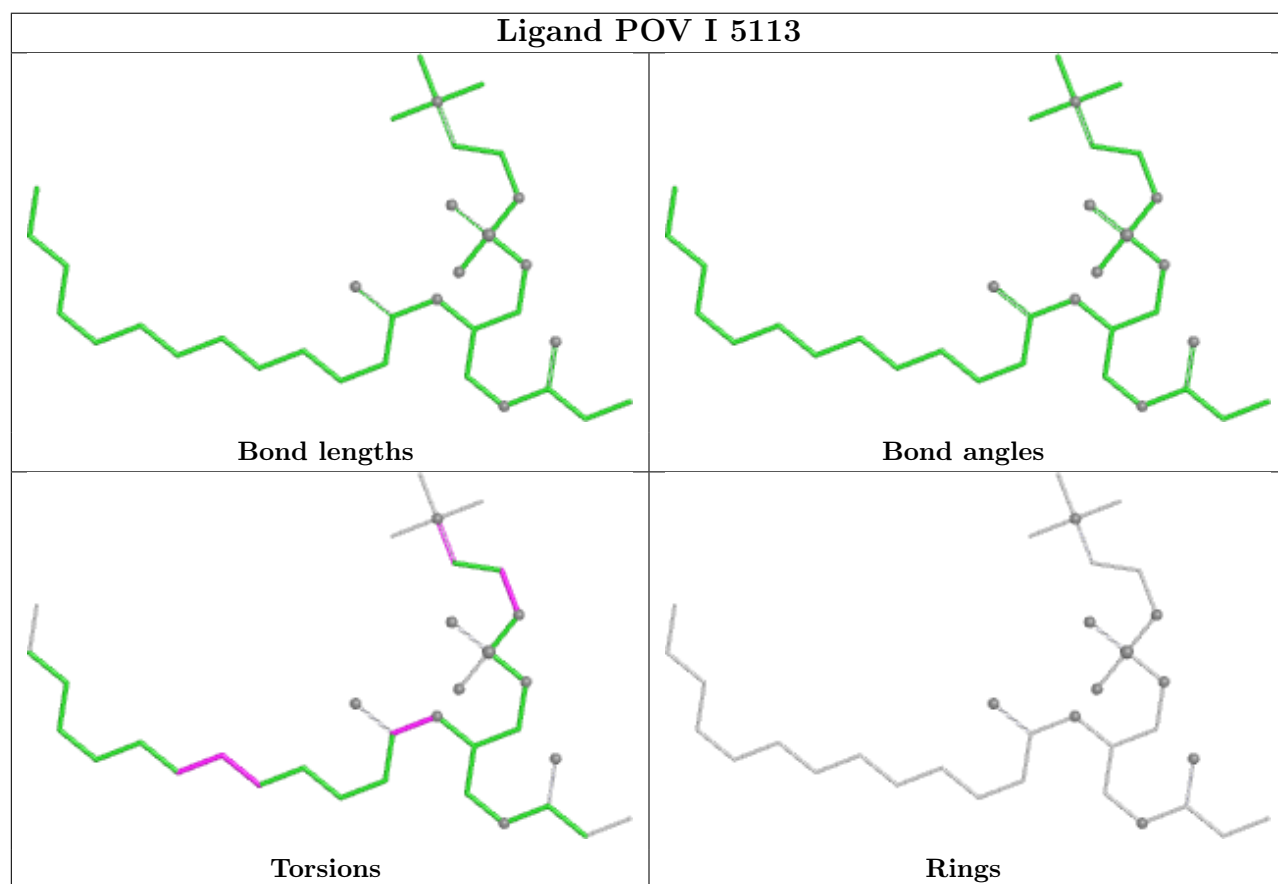
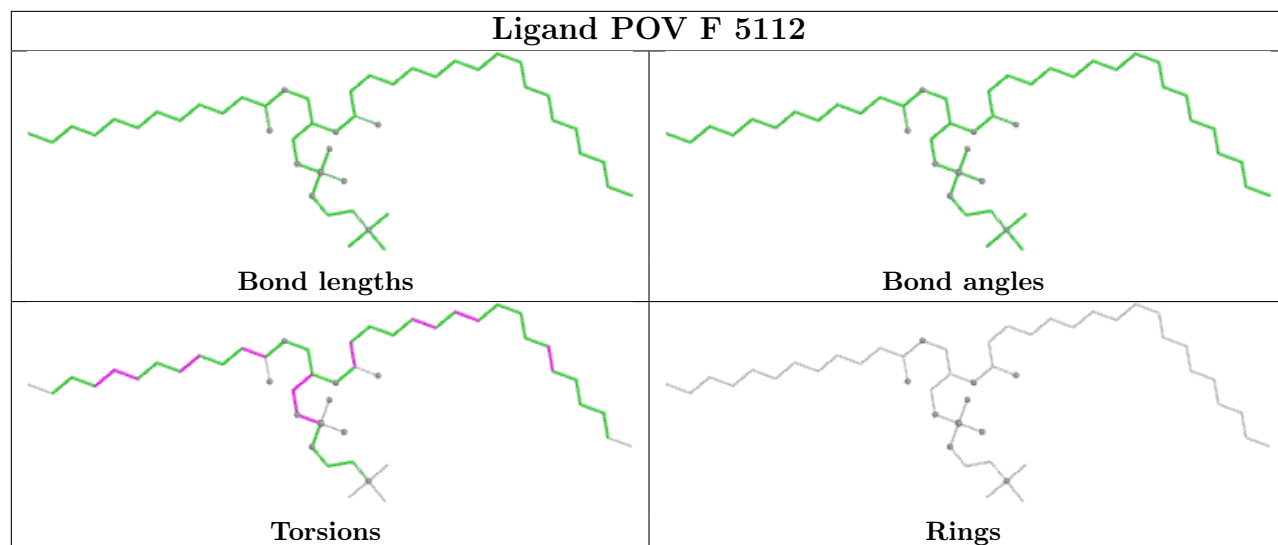


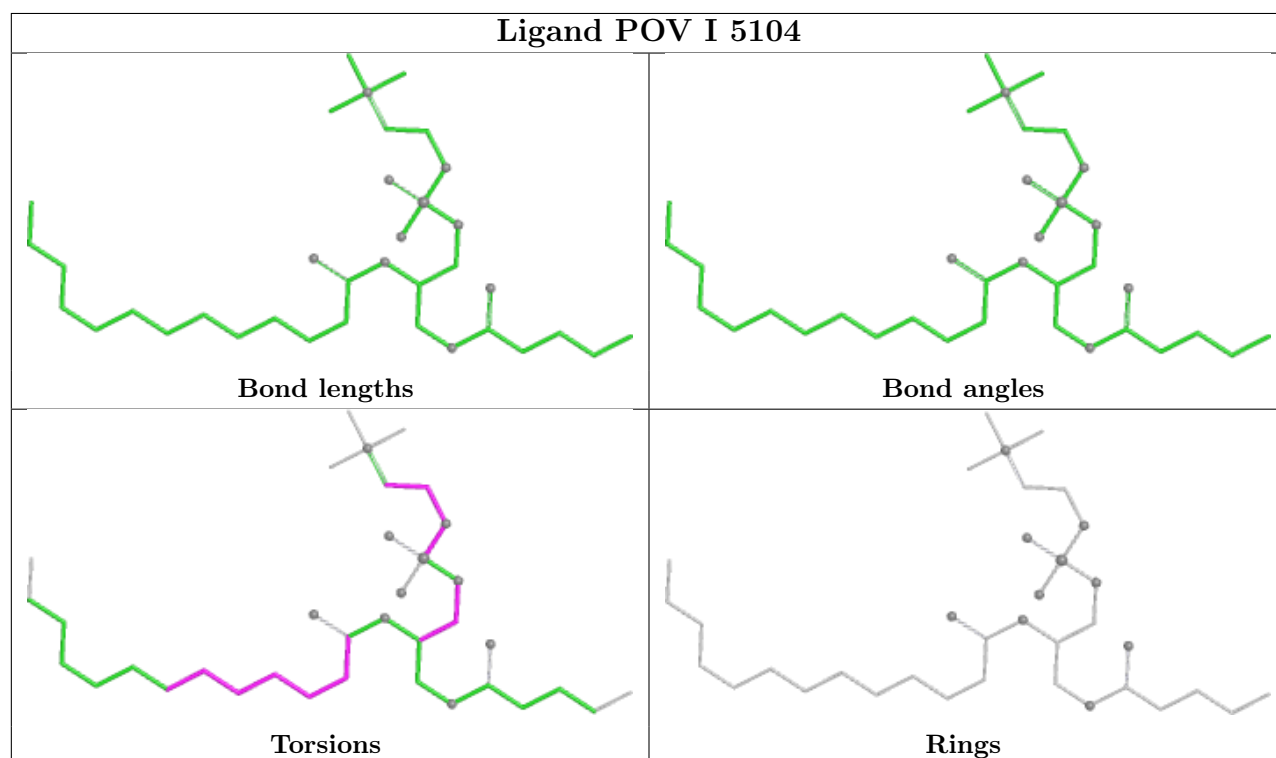
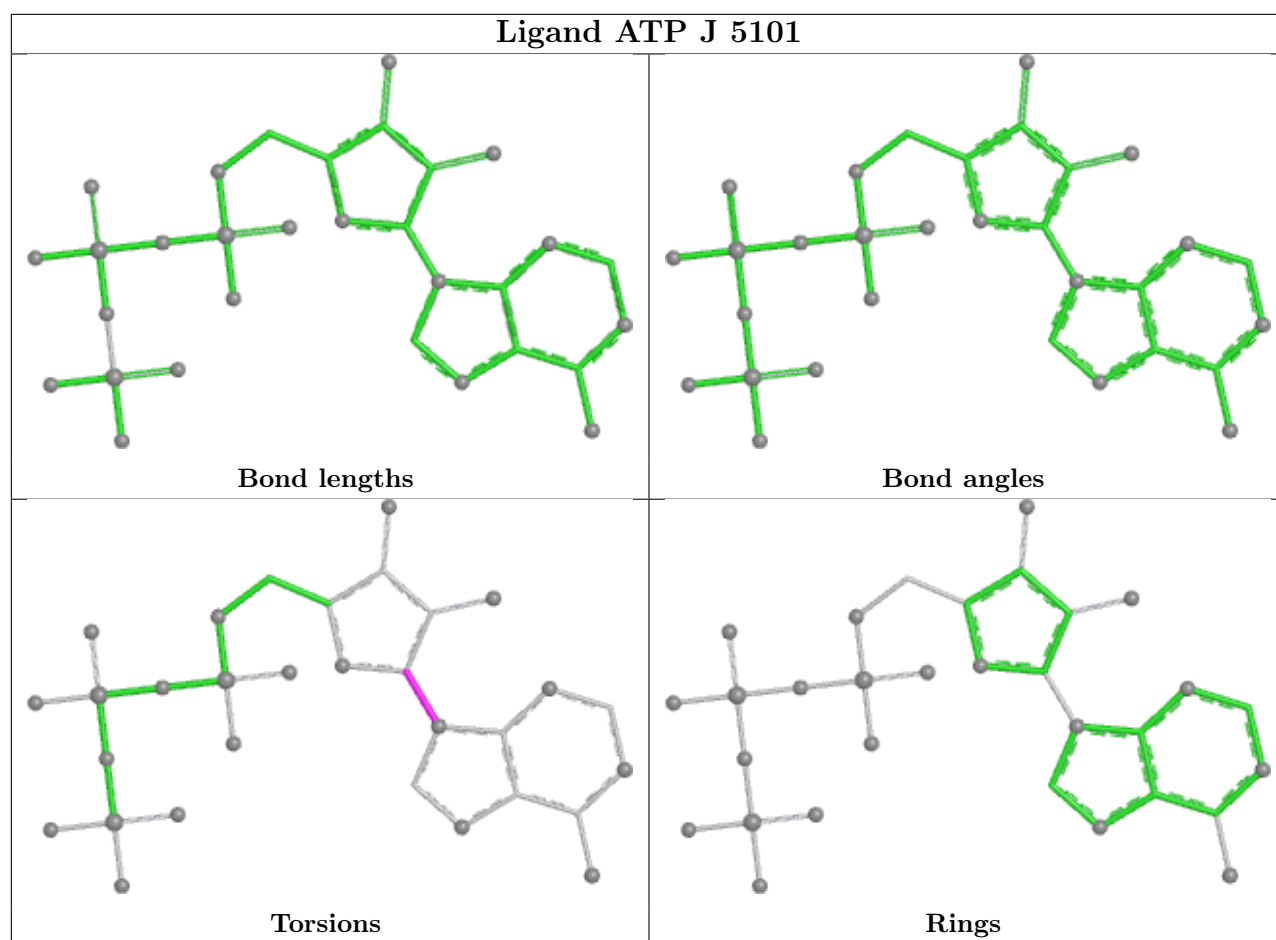


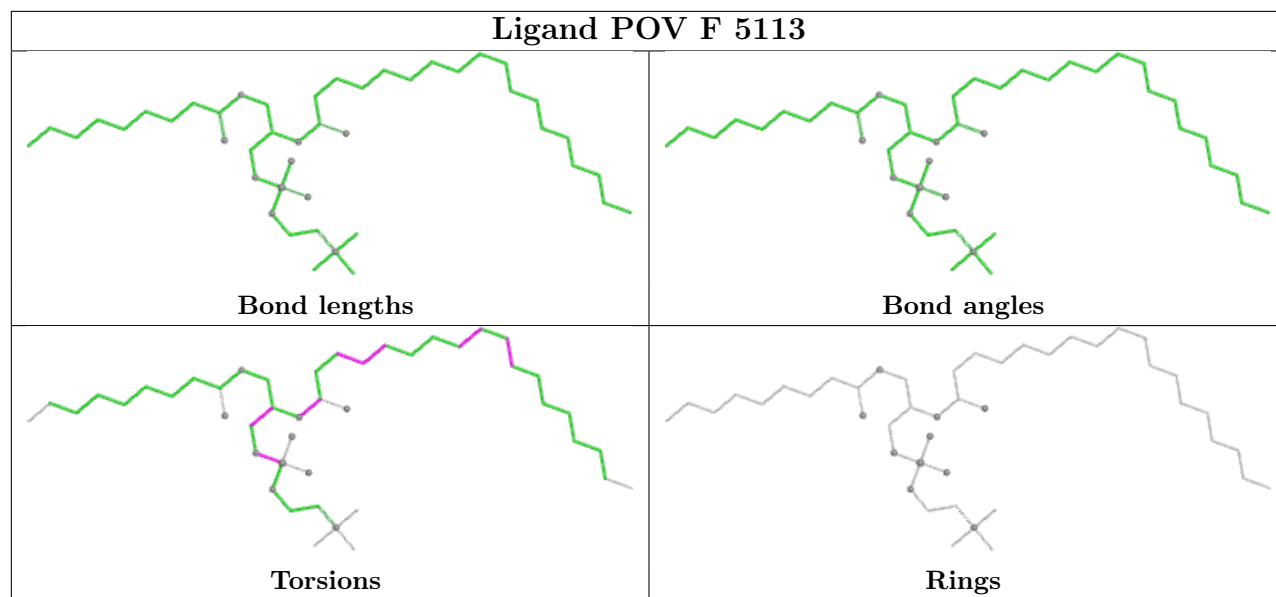












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

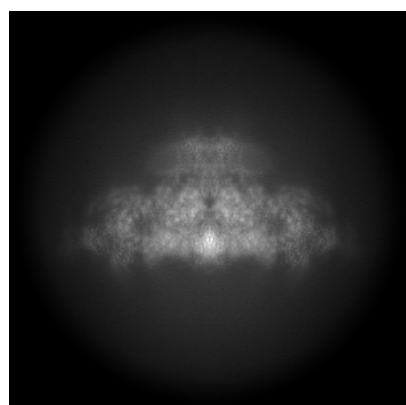
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53834. These allow visual inspection of the internal detail of the map and identification of artifacts.

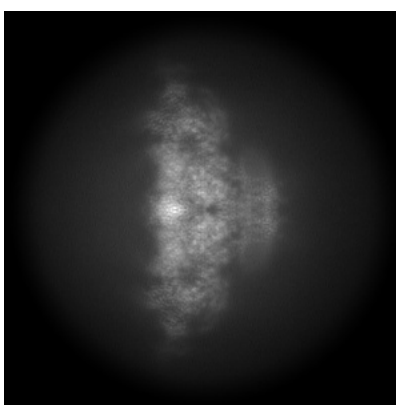
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

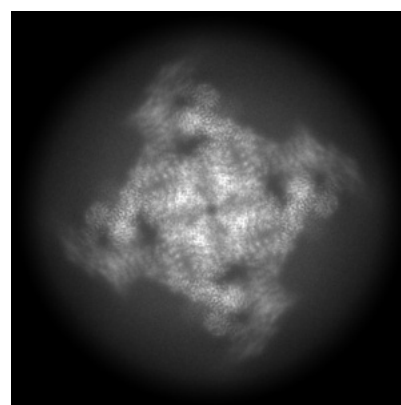
6.1.1 Primary map



X



Y

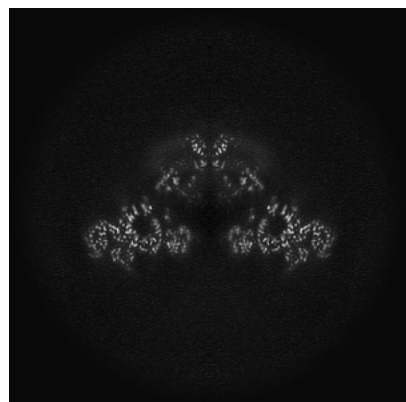


Z

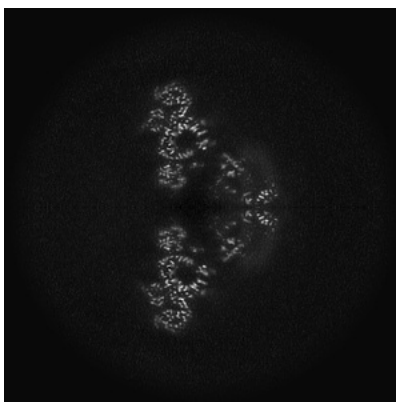
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

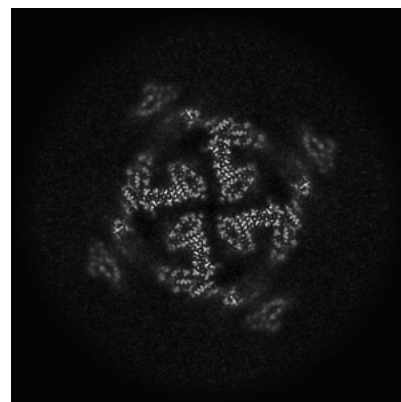
6.2.1 Primary map



X Index: 168



Y Index: 168

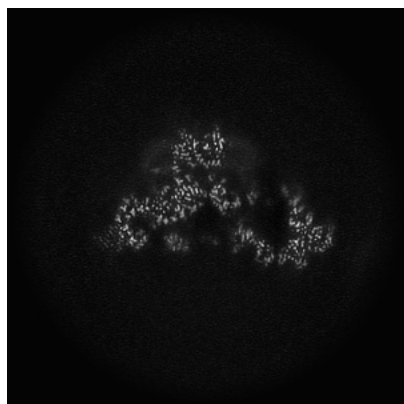


Z Index: 168

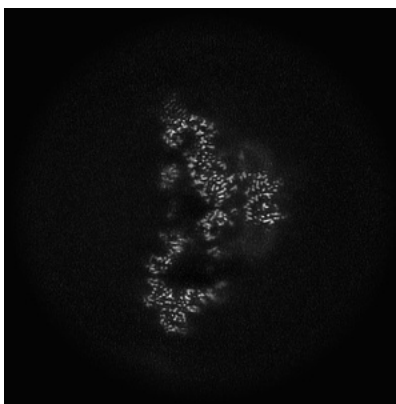
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

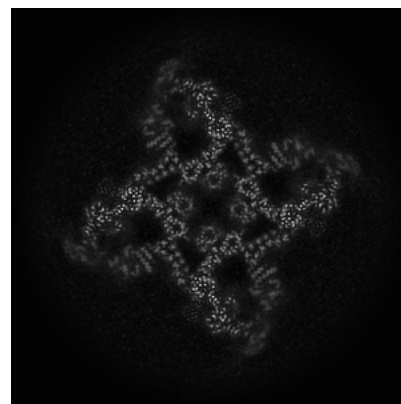
6.3.1 Primary map



X Index: 157



Y Index: 157

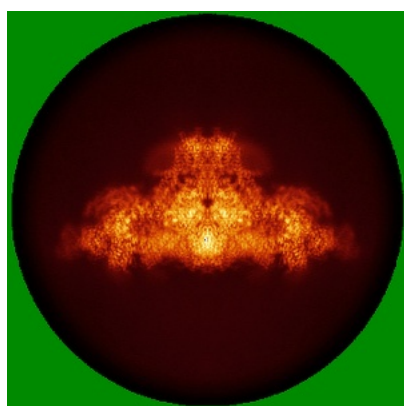


Z Index: 144

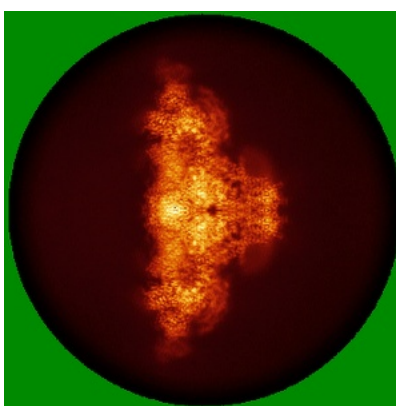
The images above show the largest variance slices of the map in three orthogonal directions.

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

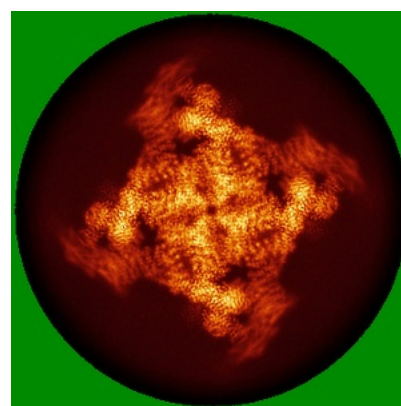
6.4.1 Primary map



X



Y

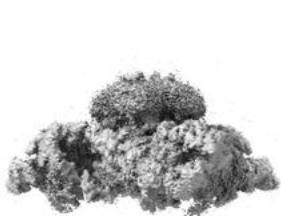


Z

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

6.5 Orthogonal surface views [i](#)

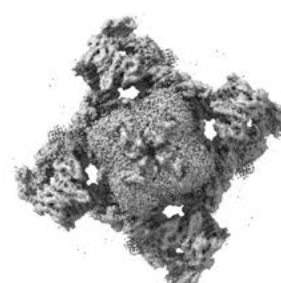
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

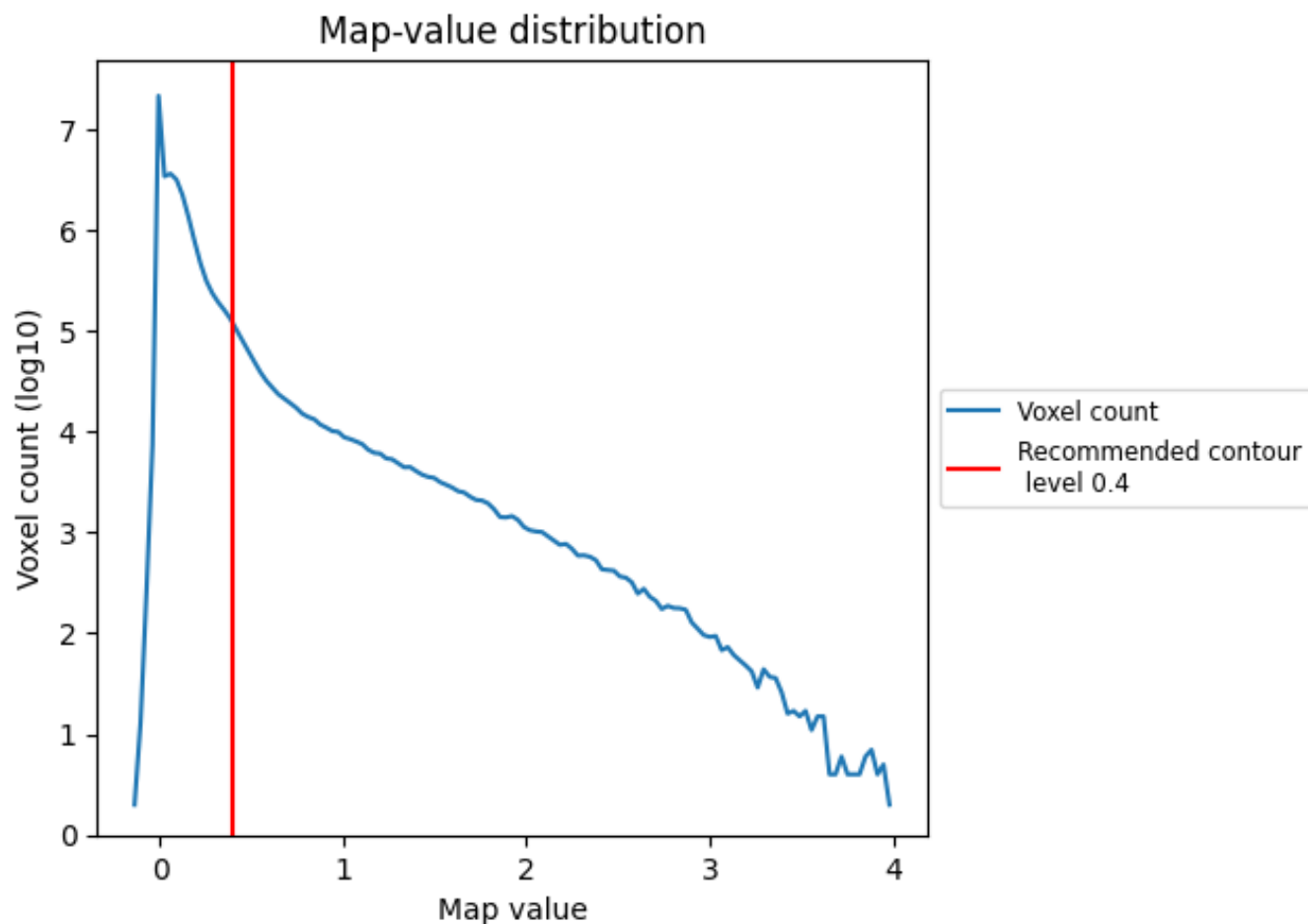
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

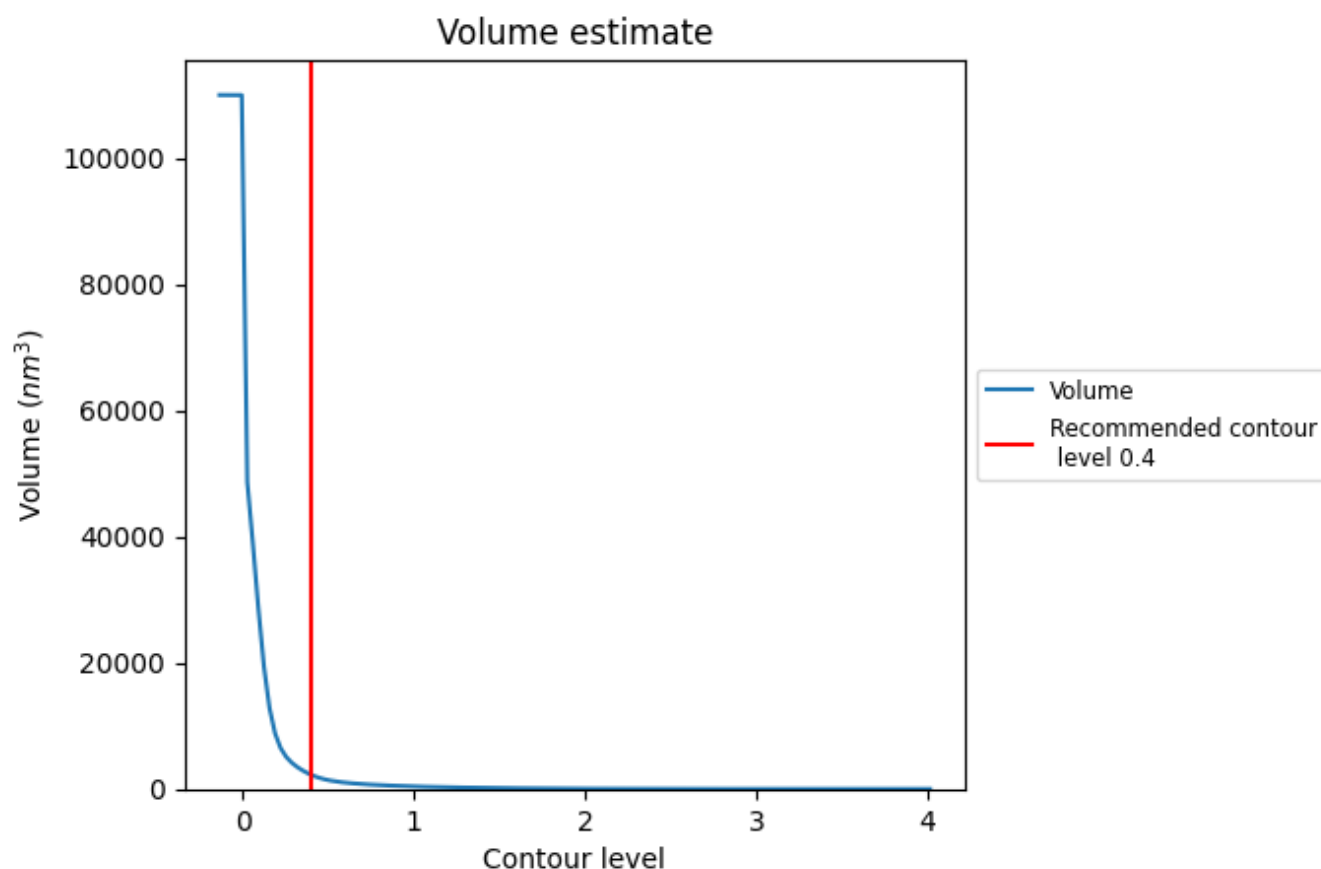
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

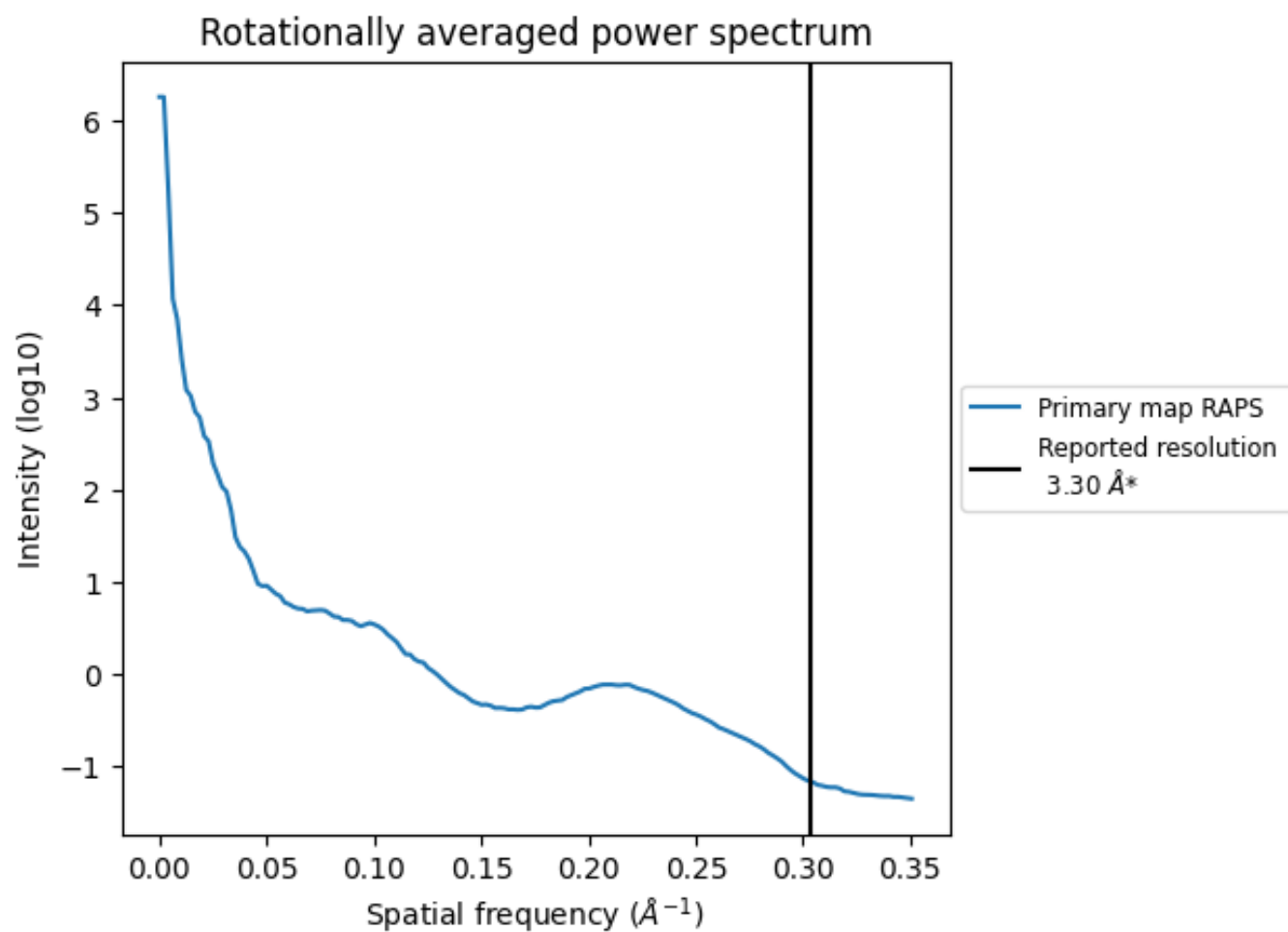
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2246 nm^3 ; this corresponds to an approximate mass of 2029 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 0.303 Å⁻¹

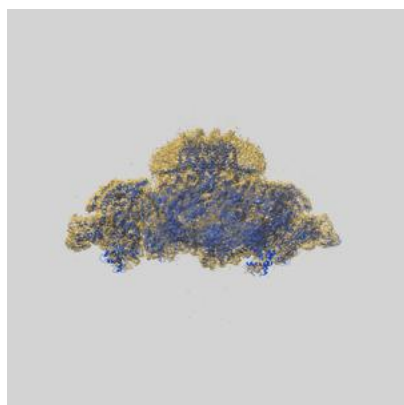
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

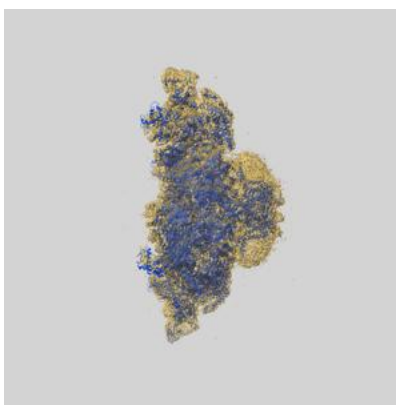
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53834 and PDB model 9R8O. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

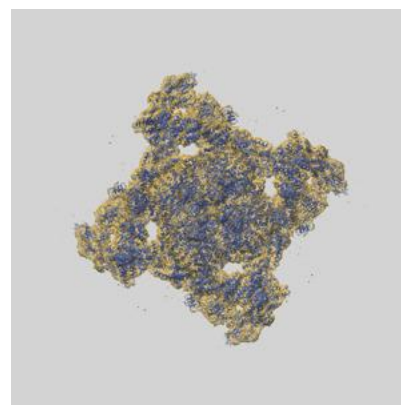
9.1 Map-model overlay [i](#)



X



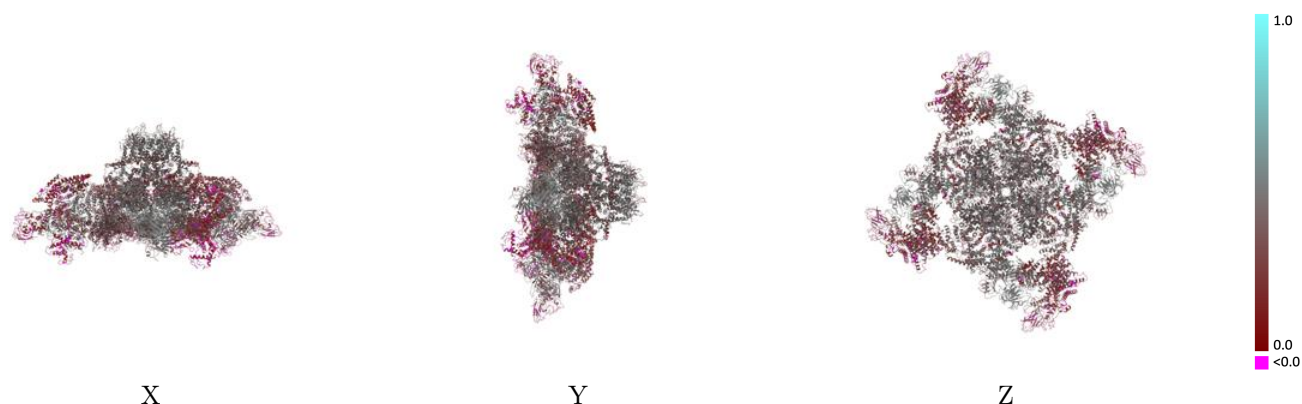
Y



Z

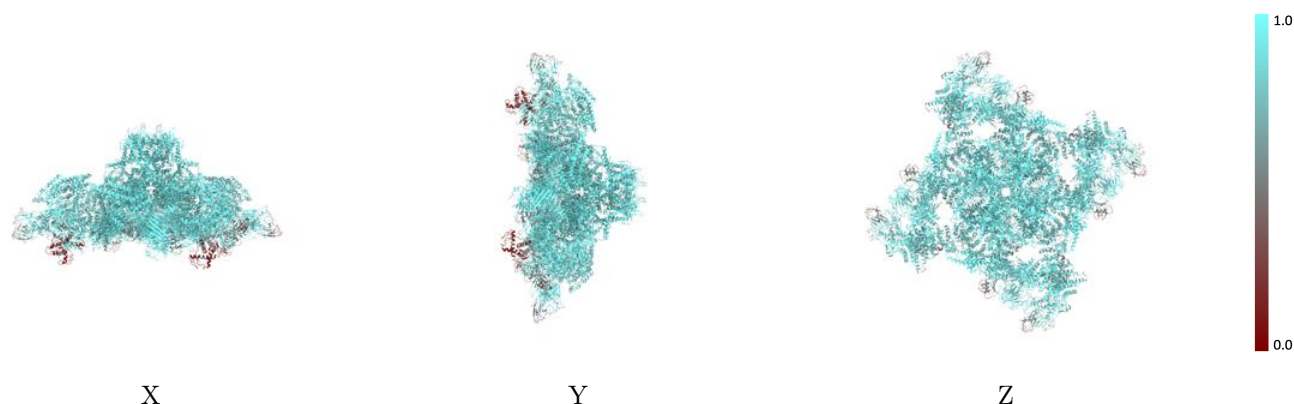
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



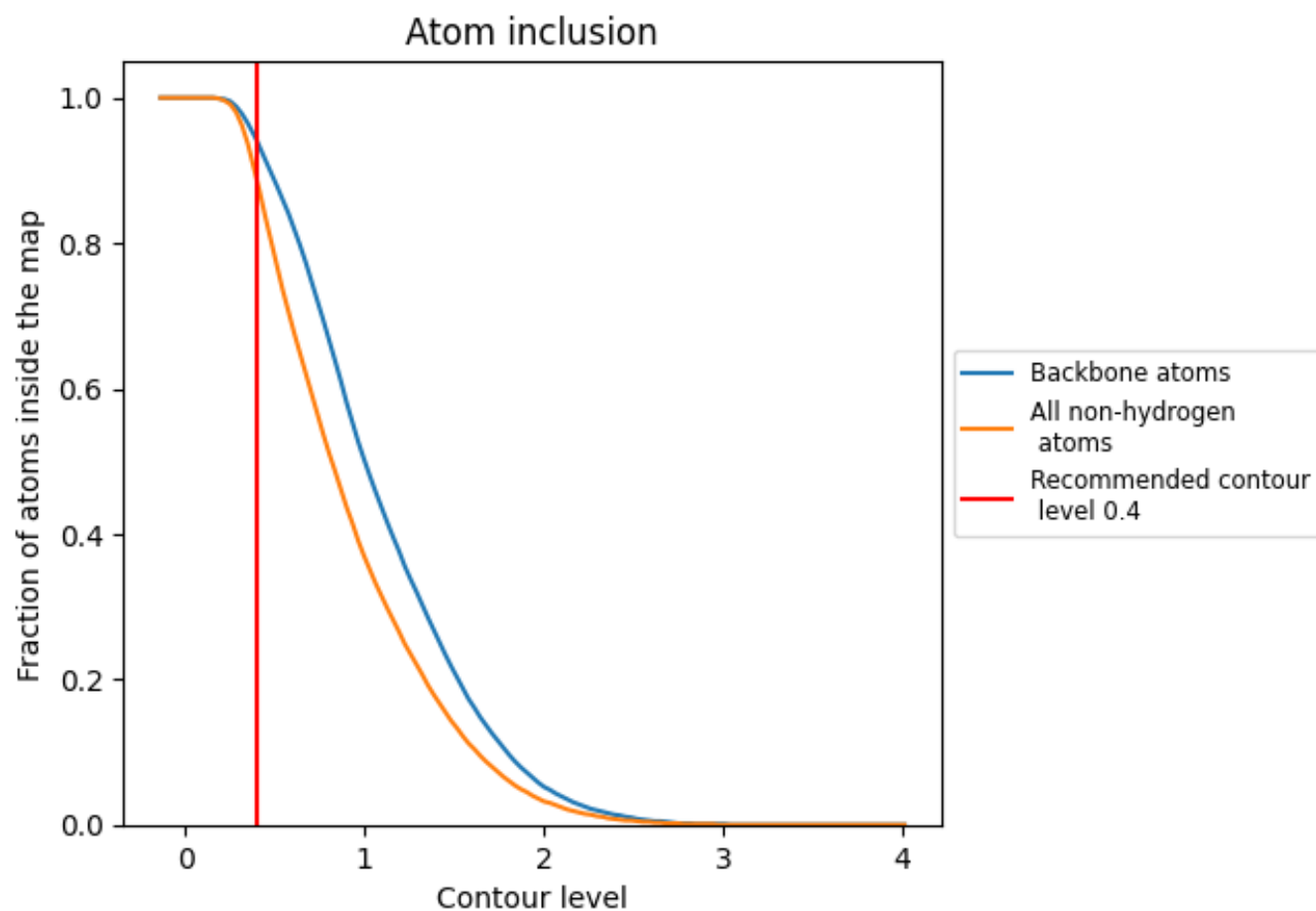
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 89% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8890	0.3420
A	0.6020	0.1580
B	0.5360	0.3510
C	0.9060	0.3460
D	0.5960	0.1580
E	0.5270	0.3530
F	0.9050	0.3470
G	0.5950	0.1570
H	0.5360	0.3530
I	0.9050	0.3470
J	0.9050	0.3460
K	0.6020	0.1640
L	0.5240	0.3530

