



Full wwPDB EM Validation Report ⓘ

Apr 10, 2026 – 01:33 PM UTC

PDB ID : 9HEQ / pdb_00009heq
EMDB ID : EMD-52091
Title : Open-state RyR1 in 0.01% POPC micelles, in complex with a nanobody and FKBP12
Authors : Li, C.; Efremov, R.G.
Deposited on : 2024-11-14
Resolution : 3.60 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:

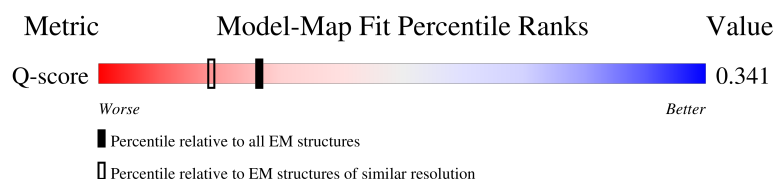
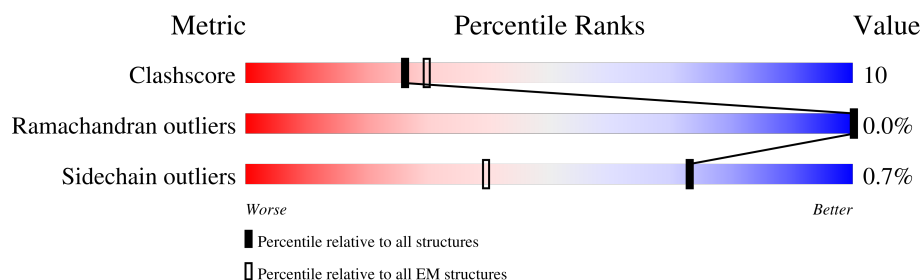
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.60 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	12797 (3.10 - 4.10)

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	5027	 5% 66% 20% 14%
1	C	5027	 5% 65% 20% 14%
1	G	5027	 5% 65% 20% 14%
1	J	5027	 5% 66% 20% 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	126	<div> <div>53%</div> <div>73%</div> <div>27%</div> </div>
2	D	126	<div> <div>53%</div> <div>71%</div> <div>29%</div> </div>
2	H	126	<div> <div>53%</div> <div>73%</div> <div>27%</div> </div>
2	K	126	<div> <div>53%</div> <div>73%</div> <div>27%</div> </div>
3	E	107	<div> <div>55%</div> <div>67%</div> <div>31%</div> <div>•</div> </div>
3	F	107	<div> <div>54%</div> <div>72%</div> <div>26%</div> <div>•</div> </div>
3	I	107	<div> <div>53%</div> <div>71%</div> <div>27%</div> <div>•</div> </div>
3	L	107	<div> <div>54%</div> <div>73%</div> <div>25%</div> <div>•</div> </div>

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 145440 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4319	Total	C	N	O	S	0	0
			34138	21741	5891	6279	227		
1	C	4319	Total	C	N	O	S	0	0
			34154	21753	5891	6283	227		
1	G	4319	Total	C	N	O	S	0	0
			34138	21741	5891	6279	227		
1	J	4319	Total	C	N	O	S	0	0
			34138	21741	5891	6279	227		

- Molecule 2 is a protein called Nanobody 9657.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	126	Total	C	N	O	S	0	0
			967	597	170	195	5		
2	D	126	Total	C	N	O	S	0	0
			967	597	170	195	5		
2	H	126	Total	C	N	O	S	0	0
			967	597	170	195	5		
2	K	126	Total	C	N	O	S	0	0
			967	597	170	195	5		

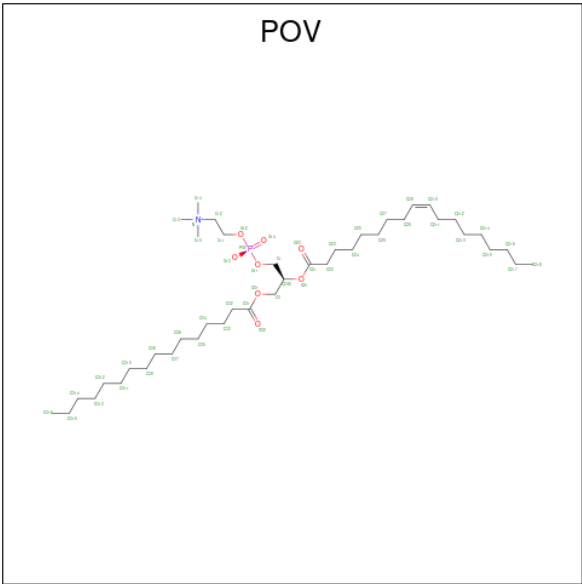
- Molecule 3 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
3	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
3	I	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
3	L	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
E	100	ASP	GLY	conflict	UNP Q8HYX6
F	100	ASP	GLY	conflict	UNP Q8HYX6
I	100	ASP	GLY	conflict	UNP Q8HYX6
L	100	ASP	GLY	conflict	UNP Q8HYX6

- Molecule 4 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
4	A	1	Total	C				0
			13	13				
4	A	1	Total	C	N	O	P	0
			47	37	1	8	1	
4	A	1	Total	C	N	O	P	0
			44	34	1	8	1	
4	A	1	Total	C	N	O	P	0
			49	39	1	8	1	
4	A	1	Total	C				0
			13	13				
4	A	1	Total	C	N	O	P	0
			43	33	1	8	1	
4	A	1	Total	C	N	O	P	0
			24	15	1	7	1	
4	A	1	Total	C	N	O	P	0
			39	29	1	8	1	
4	A	1	Total	C	N	O	P	0
			34	24	1	8	1	

Continued on next page...

Continued from previous page...

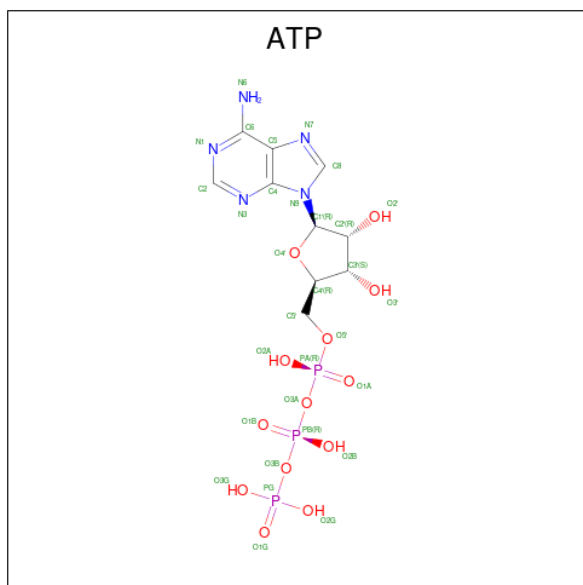
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			49	39	1	8	1	
4	A	1	Total	C	N	O	P	0
			41	31	1	8	1	
4	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
4	C	1	Total	C	N	O	P	0
			44	34	1	8	1	
4	C	1	Total	C	N	O	P	0
			43	33	1	8	1	
4	C	1	Total	C	N	O	P	0
			24	15	1	7	1	
4	C	1	Total	C	N	O	P	0
			39	29	1	8	1	
4	C	1	Total	C	N	O	P	0
			34	24	1	8	1	
4	C	1	Total	C	N	O	P	0
			41	31	1	8	1	
4	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	G	1	Total	C	N	O	P	0
			47	37	1	8	1	
4	G	1	Total	C	N	O	P	0
			44	34	1	8	1	
4	G	1	Total	C				0
			13	13				
4	G	1	Total	C	N	O	P	0
			43	33	1	8	1	
4	G	1	Total	C	N	O	P	0
			24	15	1	7	1	
4	G	1	Total	C	N	O	P	0
			39	29	1	8	1	
4	G	1	Total	C	N	O	P	0
			34	24	1	8	1	
4	G	1	Total	C	N	O	P	0
			49	39	1	8	1	
4	G	1	Total	C	N	O	P	0
			41	31	1	8	1	
4	G	1	Total	C	N	O	P	0
			52	42	1	8	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
4	J	1	Total	C	N	O	P	0
			49	39	1	8	1	
4	J	1	Total	C	N	O	P	0
			41	31	1	8	1	
4	J	1	Total	C	N	O	P	0
			52	42	1	8	1	
4	J	1	Total	C	N	O	P	0
			47	37	1	8	1	
4	J	1	Total	C	N	O	P	0
			44	34	1	8	1	
4	J	1	Total	C				0
			13	13				
4	J	1	Total	C	N	O	P	0
			43	33	1	8	1	
4	J	1	Total	C	N	O	P	0
			24	15	1	7	1	
4	J	1	Total	C	N	O	P	0
			39	29	1	8	1	
4	J	1	Total	C	N	O	P	0
			34	24	1	8	1	

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



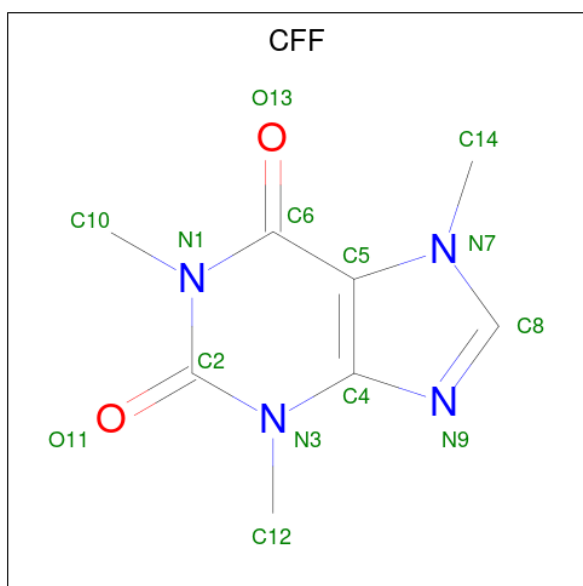
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

Continued on next page...

Continued from previous page...

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

- Molecule 6 is CAFFEINE (CCD ID: CFF) (formula: $C_8H_{10}N_4O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Ca	
			1	1	0

Continued on next page...

Continued from previous page...

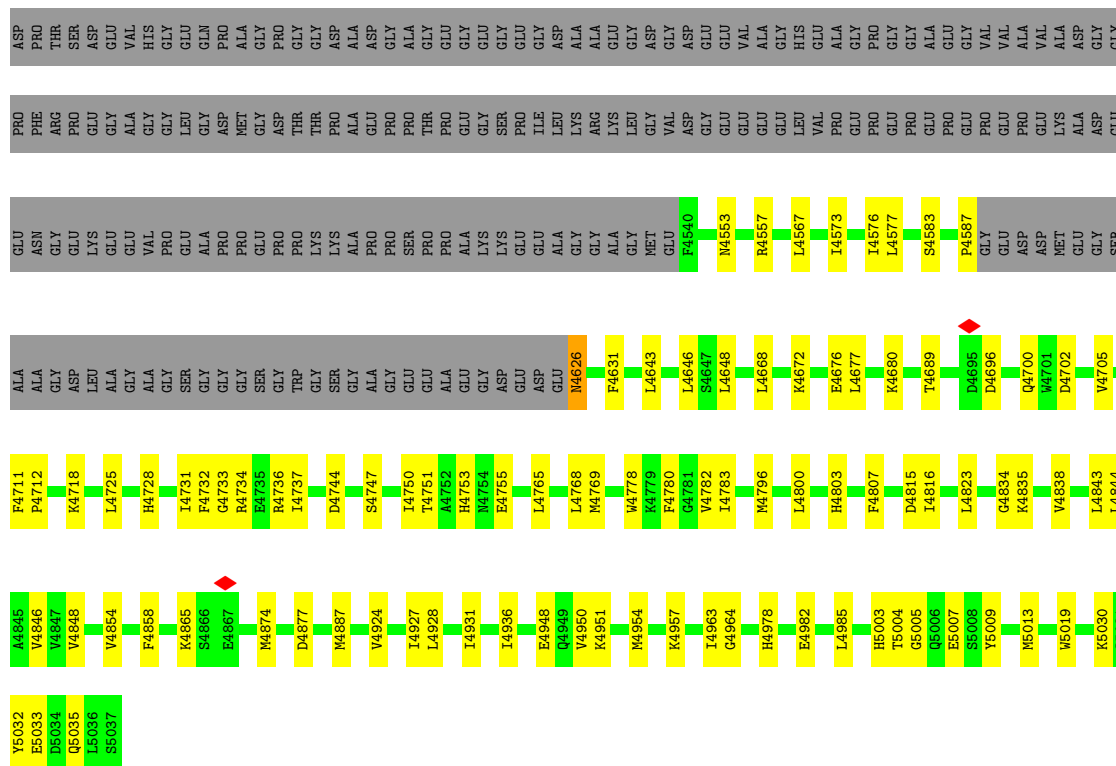
Mol	Chain	Residues	Atoms		AltConf
7	C	1	Total 1	Ca 1	0
7	G	1	Total 1	Ca 1	0
7	J	1	Total 1	Ca 1	0

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

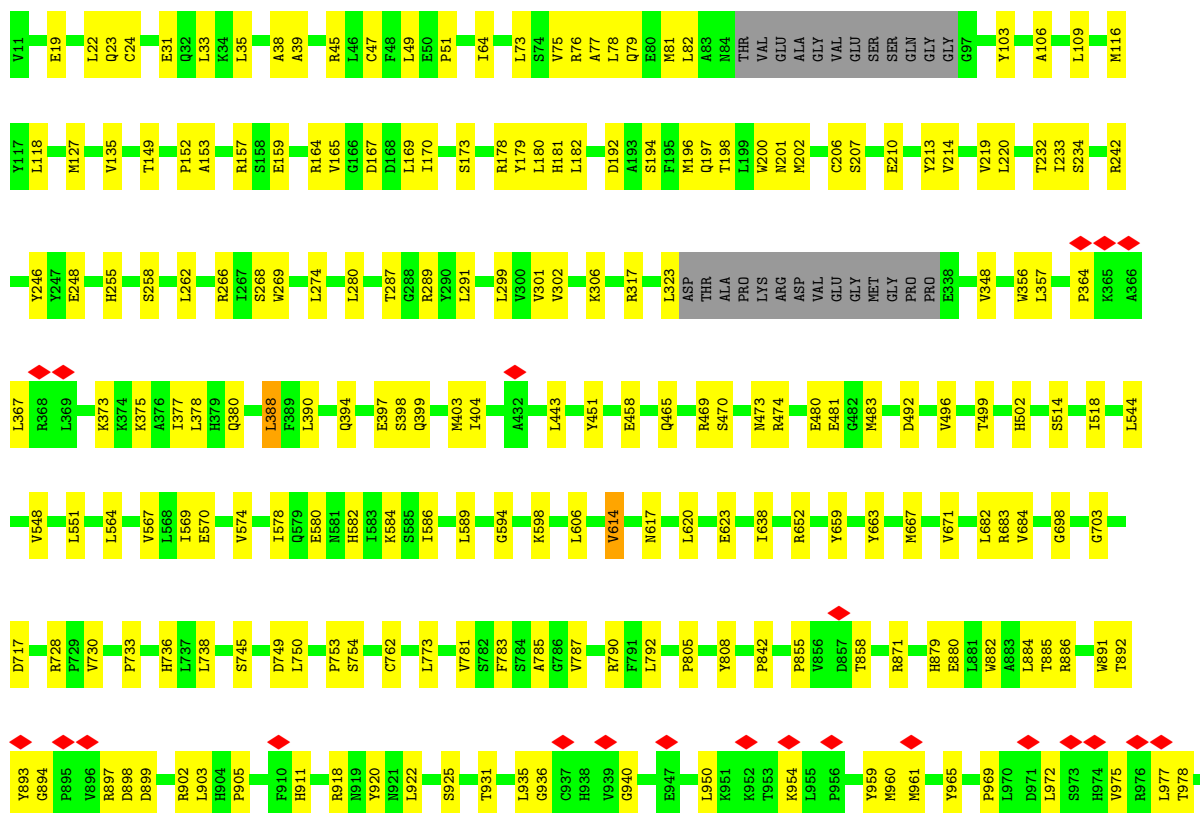
Mol	Chain	Residues	Atoms		AltConf
8	A	1	Total 1	Zn 1	0
8	C	1	Total 1	Zn 1	0
8	G	1	Total 1	Zn 1	0
8	J	1	Total 1	Zn 1	0







• Molecule 1: Ryanodine receptor 1





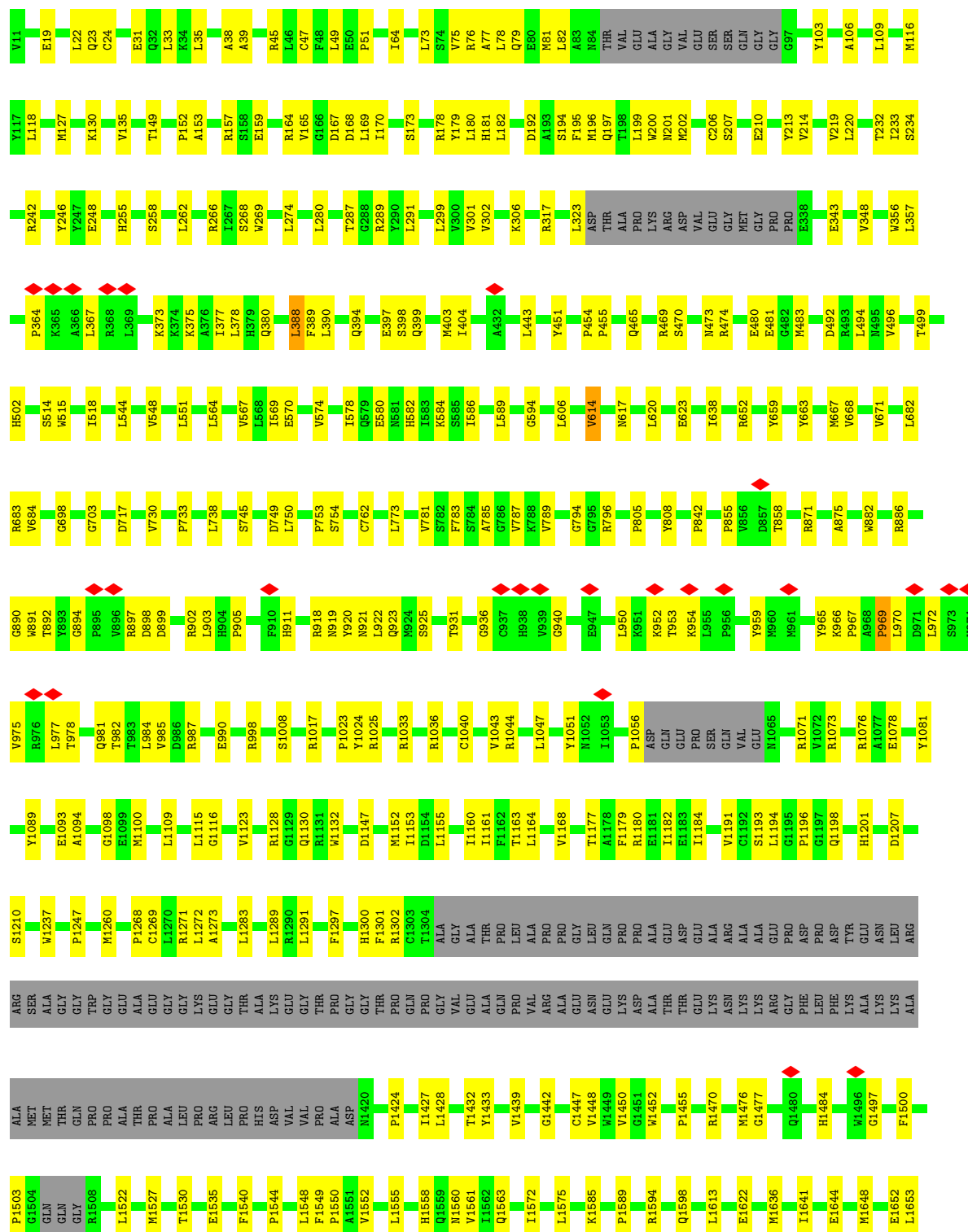
V3812	E3682	G3665	SER	L3322	LYS	G3027	R2939	A2879	W2819	W2819	A2769	L2682
V3826	Q3683	S3566	GLY	P3233	GLY	G3028	GLY	E2880	E2820	E2820	E2760	F2683
L3835	E3685	L3569	SER	V3236	GLY	H3029	LYS	Y2881	W2821	W2821	Y2761	D2692
L3842	E3686	R3570	ASP	V3239	GLY	H3030	ASP	T2882	T2822	T2822	T2762	Q2693
Q3850	E3687	R3582	GLN	M3239	L3129	K3036	ASP	H2883	T2823	T2823	H2763	E2694
E3688	E3688	E3583	GLU	V3245	T3132	T2885	ASP	H2884	E2824	E2824	E2764	L2695
E3689	E3689	E3584	THR	L3246	T3133	E3037	ASP	W2886	K2825	K2825	K2765	T2696
V3690	V3690	D3585	LYS	D3247	V3134	K3038	ASP	C2887	A2826	A2826	W2766	R2697
E3691	E3691	A3586	LYS	R3248	A3135	L3049	ASP	K2888	R2827	R2827	A2767	A2699
K3694	K3694	L3592	ARG	L3249	L3136	V3050	ASP	E2952	E2828	E2828	F2768	W2700
L3716	L3716	R3595	ARG	M3250	L3137	R3051	ASP	K2890	Q2829	Q2829	D2769	P2701
M3729	M3729	R3595	ASP	G3254	L3140	S3055	ASP	K2891	E2830	E2830	K2770	L2706
K3730	K3730	V3602	ARG	E3258	F3144	L3056	ASP	Q2892	GLU	GLU	I2771	L2710
K3731	K3731	V3603	TYR	E3268	Q3145	L3062	ASP	E2893	THR	THR	Q2772	P2711
S3732	S3732	H3605	THR	L3272	H3146	P3062	ASP	L2894	GLU	GLU	N2773	P2712
C3733	C3733	L3606	LYS	T3273	H3150	A3063	ASP	E2895	LYS	LYS	N2774	D2713
H3734	H3734	E3607	LYS	L3274	G3153	V3065	ASP	A2896	LYS	LYS	W2775	Y2714
G3739	G3739	Q3608	LYS	P3275	G3153	N3066	ASP	K2897	THR	THR	Y2777	K2722
E3740	E3740	T3609	LYS	M3276	L3277	C3067	ASP	G2898	ARG	ARG	E2778	A2723
ASN	ASN	P3612	LYS	L3282	V3163	L3068	ASP	G2900	ILE	ILE	E2779	E2724
GLY	GLY	TRP	LYS	P3293	R3167	I3070	ASP	T2901	SER	SER	N2780	K2725
GLU	GLU	LYS	LYS	P3294	S3171	R3073	ASP	H2902	GLN	GLN	V2781	LYS
ALA	ALA	LYS	LYS	A3295	I3172	S3074	ASP	P2903	THR	THR	D2782	ALA
GLU	GLU	LYS	LYS	L3296	L3176	A3077	ASP	L2904	ALA	ALA	E2783	THR
E3747	E3747	ALA	ALA	P3297	G3176	V3080	ASP	L2905	GLN	GLN	E2784	VAL
S3752	S3752	VAL	VAL	A3298	K3179	P3085	ASP	V2906	THR	THR	E2784	ASP
F3756	F3756	TRP	TRP	A3299	V3183	E3086	ASP	V2908	TVR	TVR	L2785	ALA
K3758	K3758	LEU	LEU	A3300	V3183	K3089	ASP	T2909	PRO	PRO	K2786	GLU
M3758	M3758	LEU	LEU	T3308	R3187	K3089	ASP	T2910	ARG	ARG	T2787	GLY
R3762	R3762	LYS	LYS	H3311	P3188	E3097	ASP	L2911	GLY	GLY	H2788	K2734
Q3766	Q3766	ARG	ARG	L3315	A3189	E3097	ASP	A2913	N2855	N2855	P2789	D2736
Q3767	Q3767	ARG	ARG	L3316	A3189	E3097	ASP	E2913	N2856	N2856	M2790	P2737
S3768	S3768	ALA	ALA	L3319	L3190	D3102	ASP	K2914	P2857	P2857	L2791	R2738
R3769	R3769	ALA	ALA	L3345	L3190	D3102	ASP	E2915	Q2858	Q2858	R2792	P2739
L3770	L3770	VAL	VAL	L3346	A3195	K3105	ASP	K2916	P2859	P2859	P2793	E2740
H3771	H3771	VAL	VAL	D3330	R3196	K3106	ASP	A2917	P2860	P2860	E2741	V2740
M3778	M3778	ALA	ALA	F3341	L3197	V3107	ASP	R2918	D2861	D2861	K2795	T2742
M3782	M3782	ARG	ARG	F3342	P3202	R3111	ASP	D2919	L2862	L2862	T2796	L2743
M3793	M3793	ARG	ARG	L3345	Q3209	GLY	ASP	R2920	Q2863	Q2863	F2797	N2744
V3794	V3794	MET	MET	V3346	N3211	VAL	ASP	E2921	V2865	V2865	S2798	V2745
S3803	S3803	LYS	LYS	E3352	Y3219	ALA	ASP	K2922	T2866	T2866	E2799	L2746
L3804	L3804	ALA	ALA	L3353	R3225	GLN	ASP	Q2924	L2867	L2867	K2800	L2747
L3805	L3805	GLY	GLY	L3354	E3226	THR	ASP	E2925	L2868	L2868	D2801	P2748
N3809	N3809	ASP	ASP	F3358	R3227	VAL	ASP	L2926	R2869	R2869	K2802	E2749
				I3362		GLN	ASP	L2927	E2870	E2870	E2803	K2750
							ASP	K2928	L2871	L2871	L2751	L2751
							ALA	F2929	Q2872	Q2872	D2752	D2752
							GLN	L2930	A2873	A2873	S2753	S2753
							GLN	Q2931	M2874	M2874	Q2757	Q2757
							GLN	M2932	E2876	E2876	K2757	K2757
							VAL	N2933	Q2877	Q2877	L2755	L2755
								G2934	L2878	L2878	S2812	S2812
								Y2935			L2813	L2813
								A2936			A2815	A2815
								V2937			M2816	M2816
								T2938			L2817	L2817
											A2818	A2818







• Molecule 1: Ryanodine receptor 1

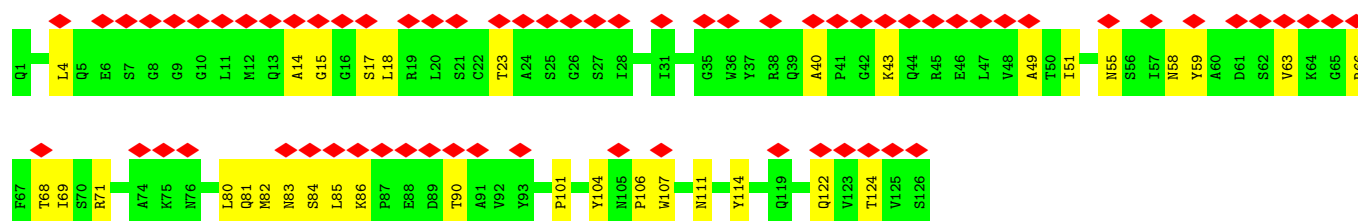




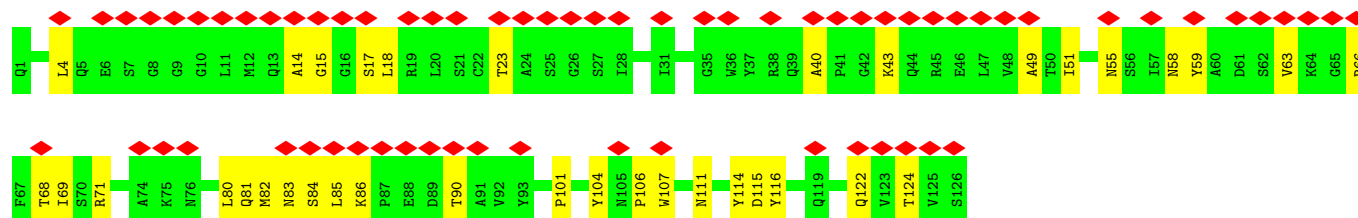
GLY	VAL	GLY	Q3127	N3128	L3129	T3132	T3133	V3134	A3135	L3136	L3137	L3140	F3144	Q3145	H3146	H3150	G3153	V3163	R3167	S3171	I3172	L3175	G3176	R3179	V3183	R3187	F3188	A3189	L3190	L3194	A3195	R3196	L3197	P3202	L3206	Q3209	L3210	N3211	Y3219	R3225	E3226				
R3227																																													
		F3358																																											
		K3367																																											
		V3372																																											
		L3379																																											
		R3380																																											
		L3381																																											
		E3382																																											
		A3383																																											
		K3384																																											
		A3385																																											
		E3386																																											
		A3387																																											
		E3391																																											
		L3392																																											
		L3393																																											
		E3397																																											
		F3398																																											
		R3403																																											
		Y3406																																											
		Y3409																																											
		P3410																																											
		R3420																																											
		W3423																																											
		E3433																																											
		L3434																																											
		F3435																																											
		R3436																																											
		M3437																																											
		V3438																																											
		G3439																																											
		A3536																																											
		T3537																																											
		R3538																																											



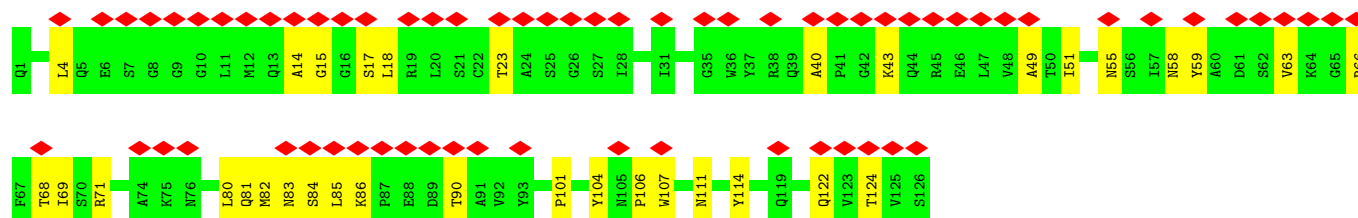
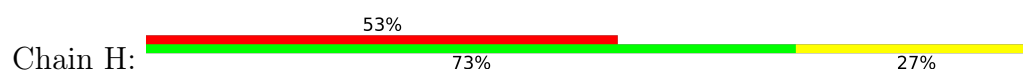
• Molecule 2: Nanobody 9657



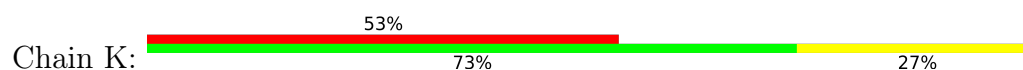
• Molecule 2: Nanobody 9657

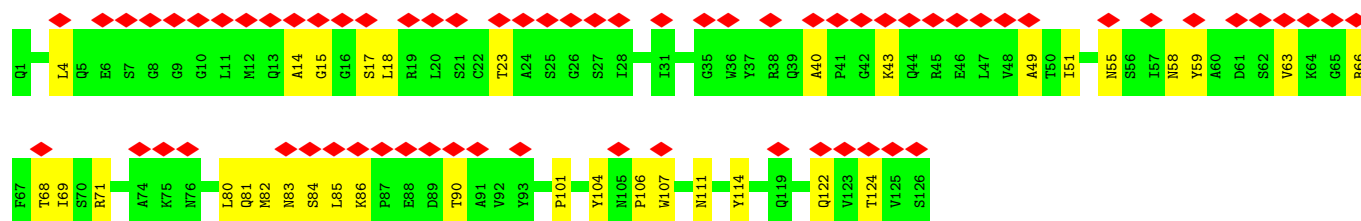


• Molecule 2: Nanobody 9657

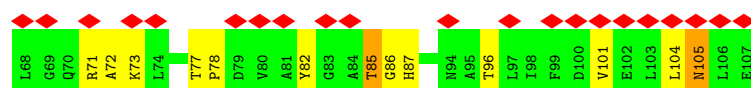
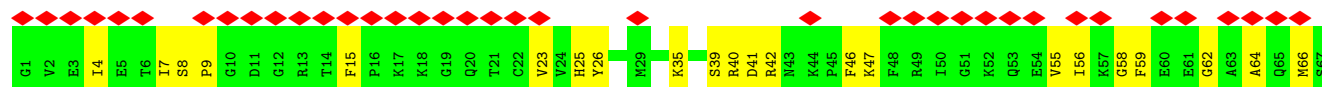


• Molecule 2: Nanobody 9657

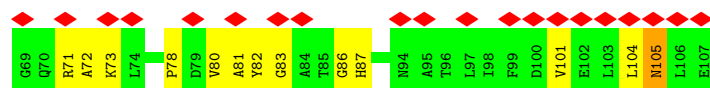
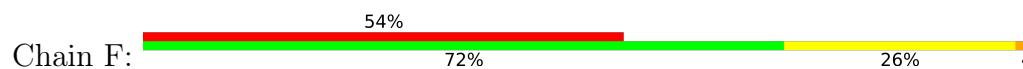




• Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B



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

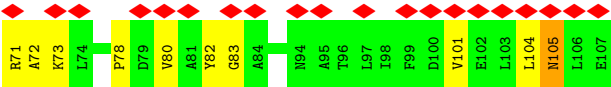


• Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B



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





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	80709	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	4.326	Depositor
Minimum map value	-0.162	Depositor
Average map value	0.056	Depositor
Map value standard deviation	0.123	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	488.544, 488.544, 488.544	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.454, 1.454, 1.454	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, POV, CA, CFF, 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	0.22	0/34909	0.44	1/47317 (0.0%)
1	C	0.22	0/34926	0.44	1/47340 (0.0%)
1	G	0.22	0/34909	0.43	1/47317 (0.0%)
1	J	0.23	0/34909	0.44	3/47317 (0.0%)
2	B	0.18	0/987	0.49	0/1340
2	D	0.27	0/987	0.54	0/1340
2	H	0.18	0/987	0.49	0/1340
2	K	0.18	0/987	0.49	0/1340
3	E	0.33	0/834	0.73	0/1123
3	F	0.38	0/834	0.74	0/1123
3	I	0.39	0/834	0.72	0/1123
3	L	0.40	0/834	0.73	0/1123
All	All	0.23	0/146937	0.45	6/199143 (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	C	0	1
1	J	0	1
All	All	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1503	PRO	N-CA-CB	6.00	110.16	103.44
1	G	1503	PRO	N-CA-CB	6.00	110.16	103.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1503	PRO	N-CA-CB	5.98	110.14	103.44
1	J	1503	PRO	N-CA-CB	5.97	110.13	103.44
1	J	794	GLY	CA-C-O	-5.69	118.22	122.37
1	J	969	PRO	N-CA-CB	-5.07	97.92	103.25

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	1020	ARG	Sidechain
1	J	987	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	34138	0	33528	683	0
1	C	34154	0	33553	690	0
1	G	34138	0	33528	682	0
1	J	34138	0	33528	683	0
2	B	967	0	916	28	0
2	D	967	0	916	28	0
2	H	967	0	916	27	0
2	K	967	0	916	27	0
3	E	818	0	824	25	0
3	F	818	0	824	24	0
3	I	818	0	824	24	0
3	L	818	0	824	23	0
4	A	448	0	640	12	0
4	C	324	0	448	10	0
4	G	386	0	544	9	0
4	J	386	0	544	13	0
5	A	31	0	12	0	0
5	C	31	0	12	0	0
5	G	31	0	12	0	0
5	J	31	0	12	0	0
6	A	14	0	10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	14	0	10	0	0
6	G	14	0	10	0	0
6	J	14	0	10	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
7	G	1	0	0	0	0
7	J	1	0	0	0	0
8	A	1	0	0	0	0
8	C	1	0	0	0	0
8	G	1	0	0	0	0
8	J	1	0	0	0	0
All	All	145440	0	143361	2925	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 (2925) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:959:TYR:HA	1:J:965:TYR:HA	1.31	1.06
1:A:959:TYR:HA	1:A:965:TYR:HA	1.38	1.05
1:C:181:HIS:HD2	1:C:194:SER:HB2	1.42	0.84
1:A:181:HIS:HD2	1:A:194:SER:HB2	1.41	0.84
1:G:181:HIS:HD2	1:G:194:SER:HB2	1.41	0.83
3:F:78:PRO:HA	3:F:83:GLY:HA3	1.62	0.82
1:G:181:HIS:CD2	1:G:194:SER:HB2	2.17	0.78
2:K:101:PRO:HG2	2:K:104:TYR:HB3	1.65	0.78
1:A:181:HIS:CD2	1:A:194:SER:HB2	2.17	0.78
1:C:2627:VAL:HG22	1:C:2678:LEU:HB2	1.65	0.78
1:J:181:HIS:HD2	1:J:194:SER:HB2	1.48	0.78
1:C:181:HIS:CD2	1:C:194:SER:HB2	2.18	0.78
2:K:122:GLN:HE21	2:K:124:THR:HG22	1.49	0.78
1:A:2627:VAL:HG22	1:A:2678:LEU:HB2	1.65	0.77
2:B:122:GLN:HE21	2:B:124:THR:HG22	1.49	0.77
1:C:3195:ALA:HB2	1:C:3275:PRO:HB3	1.67	0.77
2:D:101:PRO:HG2	2:D:104:TYR:HB3	1.65	0.77
1:J:2627:VAL:HG22	1:J:2678:LEU:HB2	1.65	0.77
1:A:2423:MET:HE1	1:A:2494:PHE:HA	1.68	0.76
2:H:101:PRO:HG2	2:H:104:TYR:HB3	1.65	0.76
1:J:2423:MET:HE1	1:J:2494:PHE:HA	1.68	0.76
1:A:2770:LYS:HD3	1:A:2787:THR:HB	1.68	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:PRO:HG2	2:B:104:TYR:HB3	1.65	0.76
2:D:122:GLN:HE21	2:D:124:THR:HG22	1.49	0.76
1:G:2627:VAL:HG22	1:G:2678:LEU:HB2	1.65	0.76
1:G:3195:ALA:HB2	1:G:3275:PRO:HB3	1.67	0.76
1:J:2770:LYS:HD3	1:J:2787:THR:HB	1.68	0.76
1:A:3195:ALA:HB2	1:A:3275:PRO:HB3	1.67	0.76
1:G:730:VAL:HA	1:G:1476:MET:HE1	1.66	0.76
1:G:2770:LYS:HD3	1:G:2787:THR:HB	1.68	0.76
1:C:2423:MET:HE1	1:C:2494:PHE:HA	1.67	0.76
1:C:2770:LYS:HD3	1:C:2787:THR:HB	1.68	0.76
1:J:3195:ALA:HB2	1:J:3275:PRO:HB3	1.67	0.76
1:G:2423:MET:HE1	1:G:2494:PHE:HA	1.68	0.75
1:J:730:VAL:HA	1:J:1476:MET:HE1	1.66	0.75
1:C:730:VAL:HA	1:C:1476:MET:HE1	1.66	0.75
1:J:1089:TYR:HD1	1:J:1152:MET:HG2	1.51	0.75
1:J:959:TYR:HA	1:J:965:TYR:CA	2.14	0.75
2:H:122:GLN:HE21	2:H:124:THR:HG22	1.49	0.75
1:C:1089:TYR:HD1	1:C:1152:MET:HG2	1.51	0.75
1:A:2797:PHE:HB3	1:A:2802:LYS:HE3	1.69	0.75
1:C:2797:PHE:HB3	1:C:2802:LYS:HE3	1.69	0.75
1:A:730:VAL:HA	1:A:1476:MET:HE1	1.66	0.75
1:G:2797:PHE:HB3	1:G:2802:LYS:HE3	1.69	0.75
1:J:2797:PHE:HB3	1:J:2802:LYS:HE3	1.69	0.75
1:A:2604:GLU:HB2	1:A:2639:MET:HG3	1.69	0.74
1:C:891:TRP:HA	1:C:902:ARG:HB3	1.67	0.74
1:A:2883:HIS:HD1	1:A:2908:TYR:HB2	1.52	0.74
1:J:2469:ILE:HB	1:J:2502:MET:HE1	1.69	0.74
1:C:2604:GLU:HB2	1:C:2639:MET:HG3	1.69	0.74
1:A:1089:TYR:HD1	1:A:1152:MET:HG2	1.51	0.74
1:C:2469:ILE:HB	1:C:2502:MET:HE1	1.69	0.74
1:G:1089:TYR:HD1	1:G:1152:MET:HG2	1.51	0.74
3:L:78:PRO:HA	3:L:83:GLY:HA3	1.69	0.74
1:C:173:SER:HB3	1:C:178:ARG:H	1.53	0.74
1:A:173:SER:HB3	1:A:178:ARG:H	1.53	0.73
1:J:173:SER:HB3	1:J:178:ARG:H	1.53	0.73
1:J:2604:GLU:HB2	1:J:2639:MET:HG3	1.69	0.73
1:J:181:HIS:CD2	1:J:194:SER:HB2	2.23	0.73
1:J:2883:HIS:HD1	1:J:2908:TYR:HB2	1.52	0.73
1:A:2469:ILE:HB	1:A:2502:MET:HE1	1.69	0.73
1:C:2883:HIS:HD1	1:C:2908:TYR:HB2	1.52	0.73
1:G:2604:GLU:HB2	1:G:2639:MET:HG3	1.69	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:858:THR:HG21	1:A:931:THR:HG22	1.71	0.72
1:G:858:THR:HG21	1:G:931:THR:HG22	1.71	0.72
1:G:2883:HIS:HD1	1:G:2908:TYR:HB2	1.52	0.72
1:C:638:ILE:HD11	1:C:1636:MET:HE2	1.71	0.72
1:A:1116:GLY:HA3	1:A:1132:TRP:HB3	1.71	0.72
1:C:858:THR:HG21	1:C:931:THR:HG22	1.71	0.72
1:C:1116:GLY:HA3	1:C:1132:TRP:HB3	1.72	0.72
3:F:23:VAL:HG22	3:F:47:LYS:HG2	1.72	0.72
1:G:173:SER:HB3	1:G:178:ARG:H	1.53	0.72
1:G:2231:SER:HA	1:G:2234:ARG:HD2	1.70	0.72
1:A:3106:MET:HG2	1:A:3132:THR:HG21	1.72	0.72
1:G:2469:ILE:HB	1:G:2502:MET:HE1	1.69	0.72
3:I:23:VAL:HG22	3:I:47:LYS:HG2	1.72	0.72
1:J:638:ILE:HD11	1:J:1636:MET:HE2	1.71	0.72
1:J:858:THR:HG21	1:J:931:THR:HG22	1.71	0.72
3:E:23:VAL:HG22	3:E:47:LYS:HG2	1.72	0.71
1:A:638:ILE:HD11	1:A:1636:MET:HE2	1.71	0.71
1:C:246:TYR:HB3	1:C:373:LYS:HB3	1.72	0.71
1:G:246:TYR:HB3	1:G:373:LYS:HB3	1.72	0.71
1:J:246:TYR:HB3	1:J:373:LYS:HB3	1.72	0.71
3:E:105:ASN:C	3:E:105:ASN:HD22	1.99	0.71
1:A:246:TYR:HB3	1:A:373:LYS:HB3	1.72	0.71
1:J:1116:GLY:HA3	1:J:1132:TRP:HB3	1.71	0.71
1:G:3106:MET:HG2	1:G:3132:THR:HG21	1.72	0.71
1:J:891:TRP:HA	1:J:902:ARG:HB3	1.71	0.71
1:G:1116:GLY:HA3	1:G:1132:TRP:HB3	1.71	0.71
3:L:105:ASN:HD22	3:L:105:ASN:C	1.99	0.71
3:I:105:ASN:HD22	3:I:105:ASN:C	1.99	0.71
1:J:3106:MET:HG2	1:J:3132:THR:HG21	1.72	0.70
3:L:23:VAL:HG22	3:L:47:LYS:HG2	1.72	0.70
1:A:891:TRP:HA	1:A:902:ARG:HB3	1.71	0.70
1:G:1738:LEU:HB2	1:G:2146:PRO:HD3	1.73	0.70
3:F:105:ASN:HD22	3:F:105:ASN:C	1.99	0.70
1:G:638:ILE:HD11	1:G:1636:MET:HE2	1.72	0.70
1:A:168:ASP:HB3	1:A:199:LEU:HD12	1.73	0.70
1:C:3106:MET:HG2	1:C:3132:THR:HG21	1.72	0.70
1:G:940:GLY:HA3	1:G:1051:TYR:HA	1.74	0.70
1:J:940:GLY:HA3	1:J:1051:TYR:HA	1.74	0.69
1:J:3250:MET:HE1	1:J:3277:LEU:HD22	1.73	0.69
1:G:3951:PHE:O	1:G:3955:MET:HB2	1.93	0.69
1:A:1738:LEU:HB2	1:A:2146:PRO:HD3	1.73	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1738:LEU:HB2	1:C:2146:PRO:HD3	1.73	0.69
1:J:3951:PHE:O	1:J:3955:MET:HB2	1.93	0.69
1:G:127:MET:HE3	1:G:127:MET:H	1.58	0.69
1:C:3951:PHE:O	1:C:3955:MET:HB2	1.93	0.69
2:D:111:ASN:HA	2:D:114:TYR:HD2	1.57	0.69
1:G:3250:MET:HE1	1:G:3277:LEU:HD22	1.73	0.69
1:A:3250:MET:HE1	1:A:3277:LEU:HD22	1.73	0.69
1:A:3951:PHE:O	1:A:3955:MET:HB2	1.93	0.69
1:A:940:GLY:HA3	1:A:1051:TYR:HA	1.74	0.69
1:C:3250:MET:HE1	1:C:3277:LEU:HD22	1.73	0.68
1:J:1738:LEU:HB2	1:J:2146:PRO:HD3	1.73	0.68
1:C:544:LEU:HD11	1:C:574:VAL:HB	1.75	0.68
1:C:940:GLY:HA3	1:C:1051:TYR:HA	1.74	0.68
1:C:3530:GLN:HA	1:C:3533:ILE:HG12	1.76	0.68
1:A:544:LEU:HD11	1:A:574:VAL:HB	1.75	0.68
1:A:984:LEU:HD13	1:A:987:ARG:HD2	1.76	0.68
1:C:127:MET:HE3	1:C:127:MET:H	1.58	0.68
1:G:3530:GLN:HA	1:G:3533:ILE:HG12	1.76	0.68
1:A:3530:GLN:HA	1:A:3533:ILE:HG12	1.76	0.67
1:J:127:MET:HE3	1:J:127:MET:H	1.58	0.67
1:J:2803:GLU:HA	1:J:2806:ARG:HB3	1.77	0.67
1:G:544:LEU:HD11	1:G:574:VAL:HB	1.75	0.67
1:J:544:LEU:HD11	1:J:574:VAL:HB	1.75	0.67
1:J:3530:GLN:HA	1:J:3533:ILE:HG12	1.76	0.67
1:A:127:MET:H	1:A:127:MET:HE3	1.58	0.67
1:G:2803:GLU:HA	1:G:2806:ARG:HB3	1.77	0.67
1:A:2496:PRO:HG3	1:A:2550:LEU:HD22	1.77	0.67
1:G:4071:ILE:HG21	1:G:4097:MET:HE1	1.77	0.67
1:J:2496:PRO:HG3	1:J:2550:LEU:HD22	1.77	0.66
1:A:578:ILE:HG13	1:A:606:LEU:HD11	1.77	0.66
1:C:2803:GLU:HA	1:C:2806:ARG:HB3	1.76	0.66
1:C:4071:ILE:HG21	1:C:4097:MET:HE1	1.76	0.66
1:G:2496:PRO:HG3	1:G:2550:LEU:HD22	1.77	0.66
1:C:578:ILE:HG13	1:C:606:LEU:HD11	1.77	0.66
1:A:985:VAL:HG11	1:A:1040:CYS:SG	2.36	0.66
1:C:2496:PRO:HG3	1:C:2550:LEU:HD22	1.77	0.66
1:A:2874:MET:HE1	1:A:2937:VAL:HB	1.77	0.66
1:C:73:LEU:HD13	1:C:77:ALA:HB1	1.77	0.66
1:C:4090:LYS:HG3	1:C:4112:LEU:HD22	1.78	0.66
1:C:871:ARG:HG3	1:C:925:SER:HB2	1.78	0.66
1:A:1147:ASP:HB3	1:A:1164:LEU:HD11	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2803:GLU:HA	1:A:2806:ARG:HB3	1.77	0.66
1:J:578:ILE:HG13	1:J:606:LEU:HD11	1.77	0.66
1:C:2874:MET:HE1	1:C:2937:VAL:HB	1.77	0.65
1:G:871:ARG:HG3	1:G:925:SER:HB2	1.78	0.65
1:G:1147:ASP:HB3	1:G:1164:LEU:HD11	1.78	0.65
1:J:4081:VAL:HG22	1:J:4088:ILE:HB	1.78	0.65
1:C:4081:VAL:HG22	1:C:4088:ILE:HB	1.78	0.65
1:A:73:LEU:HD13	1:A:77:ALA:HB1	1.77	0.65
1:A:4071:ILE:HG21	1:A:4097:MET:HE1	1.77	0.65
1:C:684:VAL:HG22	1:C:781:VAL:HG12	1.79	0.65
1:J:1786:LEU:HB2	3:L:82:TYR:HB3	1.78	0.65
1:A:4081:VAL:HG22	1:A:4088:ILE:HB	1.78	0.65
1:J:73:LEU:HD13	1:J:77:ALA:HB1	1.77	0.65
1:G:4090:LYS:HG3	1:G:4112:LEU:HD22	1.78	0.65
1:A:684:VAL:HG22	1:A:781:VAL:HG12	1.79	0.65
1:A:3510:ILE:H	1:A:3510:ILE:HD12	1.60	0.65
1:C:1115:LEU:HD23	1:C:1123:VAL:HG11	1.78	0.65
1:C:2208:MET:HA	1:C:2211:MET:HG2	1.79	0.65
1:G:578:ILE:HG13	1:G:606:LEU:HD11	1.77	0.65
1:G:3410:PRO:HD3	1:G:3509:LEU:HD21	1.79	0.65
1:J:2874:MET:HE1	1:J:2937:VAL:HB	1.77	0.65
1:A:4090:LYS:HG3	1:A:4112:LEU:HD22	1.78	0.65
1:J:3410:PRO:HD3	1:J:3509:LEU:HD21	1.79	0.65
1:A:2208:MET:HA	1:A:2211:MET:HG2	1.79	0.65
1:J:2208:MET:HA	1:J:2211:MET:HG2	1.79	0.65
1:J:4071:ILE:HG21	1:J:4097:MET:HE1	1.77	0.65
1:A:3716:LEU:HD21	1:A:3793:MET:HG2	1.79	0.64
1:G:1271:ARG:HH12	1:G:1273:ALA:HB2	1.62	0.64
1:J:3716:LEU:HD21	1:J:3793:MET:HG2	1.79	0.64
1:C:3196:ARG:HH12	1:C:3341:PHE:HE1	1.44	0.64
1:C:3409:TYR:HB2	1:C:3509:LEU:HD11	1.79	0.64
1:C:3716:LEU:HD21	1:C:3793:MET:HG2	1.79	0.64
1:G:73:LEU:HD13	1:G:77:ALA:HB1	1.77	0.64
1:G:2208:MET:HA	1:G:2211:MET:HG2	1.79	0.64
1:J:2155:LEU:HD21	1:J:2198:MET:HE1	1.79	0.64
1:J:3196:ARG:HH12	1:J:3341:PHE:HE1	1.44	0.64
1:C:1147:ASP:HB3	1:C:1164:LEU:HD11	1.78	0.64
1:G:2874:MET:HE1	1:G:2937:VAL:HB	1.77	0.64
1:G:3716:LEU:HD21	1:G:3793:MET:HG2	1.79	0.64
1:J:1147:ASP:HB3	1:J:1164:LEU:HD11	1.78	0.64
1:J:4090:LYS:HG3	1:J:4112:LEU:HD22	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:871:ARG:HG3	1:A:925:SER:HB2	1.78	0.64
1:C:594:GLY:HA2	1:C:1594:ARG:HD3	1.80	0.64
1:C:959:TYR:HA	1:C:965:TYR:HA	1.80	0.64
1:G:2755:ILE:HD12	1:G:2813:LEU:HB3	1.78	0.64
1:G:4081:VAL:HG22	1:G:4088:ILE:HB	1.78	0.64
1:C:2534:ALA:HB1	1:C:2588:ARG:HE	1.62	0.64
1:G:2821:TRP:HB3	1:G:2939:ARG:HB3	1.80	0.64
1:A:2002:PRO:HD2	1:A:3863:GLY:HA2	1.79	0.64
1:A:2155:LEU:HD21	1:A:2198:MET:HE1	1.79	0.64
1:G:1115:LEU:HD23	1:G:1123:VAL:HG11	1.78	0.64
2:H:68:THR:HB	2:H:81:GLN:HB2	1.80	0.64
1:C:2755:ILE:HD12	1:C:2813:LEU:HB3	1.78	0.64
1:G:2534:ALA:HB1	1:G:2588:ARG:HE	1.62	0.64
1:J:684:VAL:HG22	1:J:781:VAL:HG12	1.79	0.64
1:C:2002:PRO:HD2	1:C:3863:GLY:HA2	1.79	0.64
1:G:594:GLY:HA2	1:G:1594:ARG:HD3	1.80	0.64
1:J:1271:ARG:HH12	1:J:1273:ALA:HB2	1.62	0.64
1:A:1115:LEU:HD23	1:A:1123:VAL:HG11	1.78	0.64
1:J:2591:ARG:HH12	1:J:2625:ARG:HH21	1.46	0.64
1:J:2755:ILE:HD12	1:J:2813:LEU:HB3	1.78	0.64
1:C:2155:LEU:HD21	1:C:2198:MET:HE1	1.79	0.63
1:C:2917:ALA:HA	1:C:2920:ARG:HB3	1.80	0.63
1:J:2002:PRO:HD2	1:J:3863:GLY:HA2	1.79	0.63
2:K:68:THR:HB	2:K:81:GLN:HB2	1.80	0.63
1:A:2233:CYS:SG	1:A:2275:VAL:HB	2.38	0.63
1:G:2002:PRO:HD2	1:G:3863:GLY:HA2	1.79	0.63
1:C:1094:ALA:HB1	1:C:1100:MET:HE1	1.80	0.63
1:J:2534:ALA:HB1	1:J:2588:ARG:HE	1.62	0.63
1:J:2821:TRP:HB3	1:J:2939:ARG:HB3	1.80	0.63
1:A:2755:ILE:HD12	1:A:2813:LEU:HB3	1.78	0.63
1:G:684:VAL:HG22	1:G:781:VAL:HG12	1.79	0.63
1:J:1115:LEU:HD23	1:J:1123:VAL:HG11	1.79	0.63
1:G:2155:LEU:HD21	1:G:2198:MET:HE1	1.79	0.63
3:I:78:PRO:HA	3:I:83:GLY:HA3	1.81	0.63
1:J:871:ARG:HG3	1:J:925:SER:HB2	1.78	0.63
1:J:2917:ALA:HA	1:J:2920:ARG:HB3	1.80	0.63
1:A:3196:ARG:HH12	1:A:3341:PHE:HE1	1.44	0.63
1:C:2591:ARG:HH12	1:C:2625:ARG:HH21	1.46	0.63
1:G:1094:ALA:HB1	1:G:1100:MET:HE1	1.79	0.63
1:J:1094:ALA:HB1	1:J:1100:MET:HE1	1.80	0.63
1:J:2001:PRO:HB3	1:J:3864:THR:H	1.64	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:66:ARG:HD2	2:K:83:ASN:HB2	1.81	0.63
2:B:68:THR:HB	2:B:81:GLN:HB2	1.80	0.63
1:A:1094:ALA:HB1	1:A:1100:MET:HE1	1.79	0.63
1:A:2821:TRP:HB3	1:A:2939:ARG:HB3	1.80	0.63
1:A:2917:ALA:HA	1:A:2920:ARG:HB3	1.80	0.63
1:G:3196:ARG:HH12	1:G:3341:PHE:HE1	1.44	0.63
1:A:2534:ALA:HB1	1:A:2588:ARG:HE	1.62	0.63
1:C:2233:CYS:SG	1:C:2275:VAL:HB	2.39	0.63
2:D:68:THR:HB	2:D:81:GLN:HB2	1.80	0.63
1:G:894:GLY:HA3	1:G:903:LEU:HD22	1.80	0.63
1:G:3510:ILE:H	1:G:3510:ILE:HD12	1.62	0.63
1:J:936:GLY:H	1:J:1056:PRO:HB3	1.64	0.63
1:A:1271:ARG:HH12	1:A:1273:ALA:HB2	1.62	0.62
1:A:3536:ALA:HA	1:A:3539:ARG:HE	1.64	0.62
2:B:66:ARG:HD2	2:B:83:ASN:HB2	1.81	0.62
1:G:2001:PRO:HB3	1:G:3864:THR:H	1.64	0.62
1:G:2591:ARG:HH12	1:G:2625:ARG:HH21	1.46	0.62
1:G:2876:GLU:HG3	1:G:2908:TYR:HE2	1.64	0.62
1:G:4843:LEU:HD22	1:J:4823:LEU:HD11	1.81	0.62
2:H:66:ARG:HD2	2:H:83:ASN:HB2	1.81	0.62
1:C:936:GLY:H	1:C:1056:PRO:HB3	1.64	0.62
1:C:1271:ARG:HH12	1:C:1273:ALA:HB2	1.62	0.62
1:G:936:GLY:H	1:G:1056:PRO:HB3	1.64	0.62
1:G:2611:CYS:HA	1:G:2614:ILE:HG12	1.81	0.62
1:J:594:GLY:HA2	1:J:1594:ARG:HD3	1.80	0.62
1:A:936:GLY:H	1:A:1056:PRO:HB3	1.64	0.62
1:C:3510:ILE:H	1:C:3510:ILE:HD12	1.63	0.62
1:G:1078:GLU:HG3	1:G:1237:TRP:HE1	1.64	0.62
1:J:3536:ALA:HA	1:J:3539:ARG:HE	1.64	0.62
1:A:594:GLY:HA2	1:A:1594:ARG:HD3	1.80	0.62
2:B:15:GLY:H	2:B:85:LEU:HB2	1.64	0.62
1:A:2876:GLU:HG3	1:A:2908:TYR:HE2	1.64	0.62
1:A:4843:LEU:HD22	1:G:4823:LEU:HD11	1.81	0.62
1:J:1926:LEU:HG	1:J:1939:MET:HE1	1.81	0.62
1:J:2170:MET:HE1	1:J:2178:MET:HE1	1.82	0.62
1:A:2170:MET:HE1	1:A:2178:MET:HE1	1.82	0.62
1:C:3372:VAL:HG11	1:C:3398:PHE:HB3	1.81	0.62
3:E:82:TYR:HB2	3:E:86:GLY:HA2	1.82	0.62
1:G:3069:HIS:HB3	1:G:3073:ARG:HH12	1.65	0.62
1:J:950:LEU:HD11	1:J:972:LEU:HA	1.81	0.62
1:J:2876:GLU:HG3	1:J:2908:TYR:HE2	1.64	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2591:ARG:HH12	1:A:2625:ARG:HH21	1.46	0.62
1:C:2001:PRO:HB3	1:C:3864:THR:H	1.64	0.62
1:C:2170:MET:HE1	1:C:2178:MET:HE1	1.82	0.62
1:C:2611:CYS:HA	1:C:2614:ILE:HG12	1.81	0.62
1:G:49:LEU:HD21	1:G:182:LEU:HD11	1.82	0.62
1:J:2611:CYS:HA	1:J:2614:ILE:HG12	1.81	0.62
1:A:2611:CYS:HA	1:A:2614:ILE:HG12	1.81	0.62
2:B:51:ILE:HG13	2:B:71:ARG:HH21	1.64	0.62
2:B:51:ILE:HD11	2:B:71:ARG:HB3	1.82	0.62
1:C:2821:TRP:HB3	1:C:2939:ARG:HB3	1.80	0.62
1:C:2980:VAL:HB	1:C:2986:VAL:HB	1.82	0.62
1:G:2980:VAL:HB	1:G:2986:VAL:HB	1.82	0.62
1:J:3372:VAL:HG11	1:J:3398:PHE:HB3	1.81	0.62
2:K:15:GLY:H	2:K:85:LEU:HB2	1.64	0.62
2:K:51:ILE:HG13	2:K:71:ARG:HH21	1.64	0.62
1:A:3069:HIS:HB3	1:A:3073:ARG:HH12	1.65	0.62
1:G:2519:LEU:HB3	1:G:2575:ARG:HH12	1.64	0.62
1:G:2917:ALA:HA	1:G:2920:ARG:HB3	1.80	0.62
1:J:2615:ARG:HG3	1:J:2617:SER:H	1.65	0.62
1:C:2449:GLU:HA	1:C:2452:ARG:HE	1.65	0.61
1:A:2001:PRO:HB3	1:A:3864:THR:H	1.64	0.61
1:A:3372:VAL:HG11	1:A:3398:PHE:HB3	1.81	0.61
2:D:66:ARG:HD2	2:D:83:ASN:HB2	1.81	0.61
1:G:2170:MET:HE1	1:G:2178:MET:HE1	1.82	0.61
1:G:3372:VAL:HG11	1:G:3398:PHE:HB3	1.81	0.61
1:J:985:VAL:HG22	1:J:1043:VAL:HG21	1.82	0.61
1:J:2519:LEU:HB3	1:J:2575:ARG:HH12	1.64	0.61
1:J:2710:LEU:HD12	1:J:2711:PRO:HD2	1.82	0.61
1:A:2519:LEU:HB3	1:A:2575:ARG:HH12	1.64	0.61
1:A:2710:LEU:HD12	1:A:2711:PRO:HD2	1.82	0.61
1:C:3536:ALA:HA	1:C:3539:ARG:HE	1.64	0.61
2:D:15:GLY:H	2:D:85:LEU:HB2	1.64	0.61
2:D:51:ILE:HG13	2:D:71:ARG:HH21	1.64	0.61
1:G:106:ALA:HA	1:G:149:THR:HA	1.82	0.61
1:G:1926:LEU:HG	1:G:1939:MET:HE1	1.81	0.61
2:H:15:GLY:H	2:H:85:LEU:HB2	1.64	0.61
1:A:1926:LEU:HG	1:A:1939:MET:HE1	1.81	0.61
1:A:2980:VAL:HB	1:A:2986:VAL:HB	1.82	0.61
1:C:1078:GLU:HG3	1:C:1237:TRP:HE1	1.64	0.61
1:C:2615:ARG:HG3	1:C:2617:SER:H	1.64	0.61
1:C:4823:LEU:HD11	1:J:4843:LEU:HD22	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3536:ALA:HA	1:G:3539:ARG:HE	1.64	0.61
1:A:2799:GLU:HA	1:A:2802:LYS:HD2	1.83	0.61
1:C:4834:GLY:HA3	4:C:5106:POV:H1	1.83	0.61
1:A:4823:LEU:HD11	1:C:4843:LEU:HD22	1.83	0.61
1:C:2799:GLU:HA	1:C:2802:LYS:HD2	1.83	0.61
2:H:51:ILE:HG13	2:H:71:ARG:HH21	1.64	0.61
1:J:153:ALA:HB2	1:J:170:ILE:HG13	1.82	0.61
1:C:317:ARG:HH11	1:C:323:LEU:HB2	1.66	0.61
2:D:51:ILE:HD11	2:D:71:ARG:HB3	1.82	0.61
1:G:2799:GLU:HA	1:G:2802:LYS:HD2	1.83	0.61
1:J:317:ARG:HH11	1:J:323:LEU:HB2	1.66	0.61
1:J:1078:GLU:HG3	1:J:1237:TRP:HE1	1.64	0.61
1:J:2980:VAL:HB	1:J:2986:VAL:HB	1.82	0.61
1:J:3510:ILE:HD12	1:J:3510:ILE:H	1.65	0.61
1:A:1078:GLU:HG3	1:A:1237:TRP:HE1	1.64	0.61
1:C:49:LEU:HD21	1:C:182:LEU:HD11	1.82	0.61
1:C:2519:LEU:HB3	1:C:2575:ARG:HH12	1.64	0.61
1:A:2010:LEU:HD22	1:A:3656:SER:HB2	1.82	0.61
1:J:49:LEU:HD21	1:J:182:LEU:HD11	1.82	0.61
1:J:106:ALA:HA	1:J:149:THR:HA	1.82	0.61
1:J:2010:LEU:HD22	1:J:3656:SER:HB2	1.82	0.61
1:C:2876:GLU:HG3	1:C:2908:TYR:HE2	1.64	0.61
2:H:51:ILE:HD11	2:H:71:ARG:HB3	1.82	0.61
1:A:4059:LEU:HD13	1:A:4167:ALA:HB2	1.83	0.60
1:C:153:ALA:HB2	1:C:170:ILE:HG13	1.82	0.60
1:G:2615:ARG:HG3	1:G:2617:SER:H	1.65	0.60
1:J:2799:GLU:HA	1:J:2802:LYS:HD2	1.83	0.60
1:J:3069:HIS:HB3	1:J:3073:ARG:HH12	1.65	0.60
1:A:49:LEU:HD21	1:A:182:LEU:HD11	1.82	0.60
1:A:153:ALA:HB2	1:A:170:ILE:HG13	1.82	0.60
1:A:234:SER:HB2	1:A:242:ARG:HA	1.83	0.60
1:C:106:ALA:HA	1:C:149:THR:HA	1.82	0.60
1:C:234:SER:HB2	1:C:242:ARG:HA	1.83	0.60
1:C:4059:LEU:HD13	1:C:4167:ALA:HB2	1.83	0.60
1:G:2710:LEU:HD12	1:G:2711:PRO:HD2	1.82	0.60
1:G:4059:LEU:HD13	1:G:4167:ALA:HB2	1.83	0.60
1:C:671:VAL:HG22	1:C:787:VAL:HG12	1.83	0.60
1:J:2624:ARG:HD2	1:J:2906:VAL:HG11	1.83	0.60
1:J:4059:LEU:HD13	1:J:4167:ALA:HB2	1.83	0.60
4:J:5101:POV:H23	4:J:5102:POV:H34A	1.83	0.60
1:A:3097:GLU:HG2	1:A:3167:ARG:HH12	1.66	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2989:SER:HB2	1:C:2992:GLU:HB2	1.83	0.60
1:C:3097:GLU:HG2	1:C:3167:ARG:HH12	1.66	0.60
4:A:5107:POV:H23	4:C:5111:POV:H34A	1.82	0.60
1:J:671:VAL:HG22	1:J:787:VAL:HG12	1.83	0.60
1:A:299:LEU:HD22	1:A:378:LEU:HG	1.84	0.60
1:A:2615:ARG:HG3	1:A:2617:SER:H	1.65	0.60
1:C:3227:ARG:HG2	1:C:3232:LEU:HD12	1.84	0.60
1:G:22:LEU:HG	1:G:202:MET:HE1	1.84	0.60
1:J:959:TYR:CA	1:J:965:TYR:HA	2.19	0.60
1:C:2010:LEU:HD22	1:C:3656:SER:HB2	1.83	0.60
1:C:2624:ARG:HD2	1:C:2906:VAL:HG11	1.83	0.60
1:G:317:ARG:HH11	1:G:323:LEU:HB2	1.66	0.60
2:K:51:ILE:HD11	2:K:71:ARG:HB3	1.82	0.60
1:A:152:PRO:HA	1:A:169:LEU:HD22	1.84	0.60
1:C:1926:LEU:HG	1:C:1939:MET:HE1	1.81	0.60
1:C:3442:PHE:HE1	1:C:3511:VAL:HG22	1.67	0.60
1:G:299:LEU:HD22	1:G:378:LEU:HG	1.84	0.60
1:G:2272:PRO:HA	1:G:2275:VAL:HG12	1.83	0.60
1:G:2989:SER:HB2	1:G:2992:GLU:HB2	1.83	0.60
1:G:3227:ARG:HG2	1:G:3232:LEU:HD12	1.84	0.60
1:J:2449:GLU:HA	1:J:2452:ARG:HE	1.65	0.60
1:J:3097:GLU:HG2	1:J:3167:ARG:HH12	1.66	0.60
1:A:22:LEU:HG	1:A:202:MET:HE1	1.84	0.60
1:C:152:PRO:HA	1:C:169:LEU:HD22	1.84	0.60
1:C:2710:LEU:HD12	1:C:2711:PRO:HD2	1.82	0.60
1:G:153:ALA:HB2	1:G:170:ILE:HG13	1.82	0.60
1:A:2116:LEU:O	1:A:2120:MET:HG2	2.02	0.60
1:A:2624:ARG:HD2	1:A:2906:VAL:HG11	1.83	0.60
1:J:234:SER:HB2	1:J:242:ARG:HA	1.83	0.60
1:A:106:ALA:HA	1:A:149:THR:HA	1.82	0.59
1:A:317:ARG:HH11	1:A:323:LEU:HB2	1.66	0.59
1:A:2449:GLU:HA	1:A:2452:ARG:HE	1.66	0.59
1:G:3097:GLU:HG2	1:G:3167:ARG:HH12	1.66	0.59
1:A:899:ASP:H	2:B:58:ASN:HD21	1.51	0.59
1:C:3069:HIS:HB3	1:C:3073:ARG:HH12	1.65	0.59
1:G:2116:LEU:O	1:G:2120:MET:HG2	2.02	0.59
1:J:2272:PRO:HA	1:J:2275:VAL:HG12	1.84	0.59
1:A:3227:ARG:HG2	1:A:3232:LEU:HD12	1.84	0.59
1:G:954:LYS:HA	1:G:969:PRO:HG2	1.84	0.59
1:G:2010:LEU:HD22	1:G:3656:SER:HB2	1.83	0.59
1:J:22:LEU:HG	1:J:202:MET:HE1	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1694:LEU:HB3	1:J:1715:LEU:HD12	1.85	0.59
1:A:2989:SER:HB2	1:A:2992:GLU:HB2	1.83	0.59
4:G:5112:POV:H23	4:G:5113:POV:H34A	1.82	0.59
3:I:8:SER:H	3:I:71:ARG:HB2	1.68	0.59
1:J:2477:PRO:HG3	1:J:2544:THR:HG21	1.85	0.59
1:J:3227:ARG:HG2	1:J:3232:LEU:HD12	1.84	0.59
1:C:981:GLN:HG3	1:C:1047:LEU:HD21	1.85	0.59
1:G:152:PRO:HA	1:G:169:LEU:HD22	1.84	0.59
1:A:2272:PRO:HA	1:A:2275:VAL:HG12	1.84	0.59
1:A:3442:PHE:HE1	1:A:3511:VAL:HG22	1.67	0.59
1:G:671:VAL:HG22	1:G:787:VAL:HG12	1.83	0.59
1:G:2477:PRO:HG3	1:G:2544:THR:HG21	1.85	0.59
1:G:2449:GLU:HA	1:G:2452:ARG:HE	1.66	0.59
1:G:2624:ARG:HD2	1:G:2906:VAL:HG11	1.83	0.59
1:J:152:PRO:HA	1:J:169:LEU:HD22	1.84	0.59
1:A:981:GLN:HG3	1:A:1047:LEU:HD21	1.85	0.59
1:C:22:LEU:HG	1:C:202:MET:HE1	1.84	0.59
1:C:2477:PRO:HG3	1:C:2544:THR:HG21	1.85	0.59
1:C:2645:THR:HB	1:C:2702:CYS:HA	1.85	0.59
3:F:8:SER:H	3:F:71:ARG:HB2	1.68	0.59
1:G:3406:TYR:HA	1:G:3509:LEU:HD22	1.84	0.59
1:A:671:VAL:HG22	1:A:787:VAL:HG12	1.83	0.59
2:D:111:ASN:HA	2:D:114:TYR:CD2	2.36	0.59
1:G:234:SER:HB2	1:G:242:ARG:HA	1.83	0.59
1:G:981:GLN:HG3	1:G:1047:LEU:HD21	1.85	0.59
1:J:2989:SER:HB2	1:J:2992:GLU:HB2	1.83	0.59
1:C:4677:LEU:HD21	1:C:4702:ASP:HB3	1.85	0.59
1:J:981:GLN:HG3	1:J:1047:LEU:HD21	1.85	0.59
1:J:2766:TRP:O	1:J:2770:LYS:HG2	2.03	0.59
4:A:5114:POV:H23	4:A:5115:POV:H34A	1.82	0.58
1:C:3683:GLN:HB2	1:C:3694:LYS:HE3	1.85	0.58
1:J:299:LEU:HD22	1:J:378:LEU:HG	1.84	0.58
1:J:2645:THR:HB	1:J:2702:CYS:HA	1.85	0.58
1:J:3219:TYR:HA	1:J:3227:ARG:HD3	1.85	0.58
1:A:2477:PRO:HG3	1:A:2544:THR:HG21	1.84	0.58
1:C:2272:PRO:HA	1:C:2275:VAL:HG12	1.83	0.58
1:J:4567:LEU:HD13	1:J:4815:ASP:HB3	1.85	0.58
1:J:4677:LEU:HD21	1:J:4702:ASP:HB3	1.85	0.58
1:A:1155:LEU:HD12	1:A:1184:ILE:HG13	1.86	0.58
1:C:299:LEU:HD22	1:C:378:LEU:HG	1.84	0.58
1:C:1000:ARG:HH22	2:D:115:ASP:H	1.49	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2766:TRP:O	1:C:2770:LYS:HG2	2.03	0.58
1:G:891:TRP:HA	1:G:902:ARG:HB3	1.84	0.58
1:J:2894:LEU:HD22	1:J:2905:LEU:HD12	1.86	0.58
1:A:2645:THR:HB	1:A:2702:CYS:HA	1.85	0.58
1:A:2766:TRP:O	1:A:2770:LYS:HG2	2.03	0.58
1:A:4677:LEU:HD21	1:A:4702:ASP:HB3	1.85	0.58
1:C:3219:TYR:HA	1:C:3227:ARG:HD3	1.86	0.58
3:E:8:SER:H	3:E:71:ARG:HB2	1.68	0.58
1:G:2894:LEU:HD22	1:G:2905:LEU:HD12	1.86	0.58
1:G:4677:LEU:HD21	1:G:4702:ASP:HB3	1.85	0.58
1:J:220:LEU:HD23	1:J:390:LEU:HB3	1.86	0.58
1:J:899:ASP:H	2:K:58:ASN:HD21	1.51	0.58
3:L:8:SER:H	3:L:71:ARG:HB2	1.68	0.58
1:A:2894:LEU:HD22	1:A:2905:LEU:HD12	1.86	0.58
1:G:1694:LEU:HB3	1:G:1715:LEU:HD12	1.85	0.58
1:G:4567:LEU:HD13	1:G:4815:ASP:HB3	1.85	0.58
1:A:683:ARG:HG2	1:A:717:ASP:HB3	1.85	0.58
1:A:1694:LEU:HB3	1:A:1715:LEU:HD12	1.85	0.58
1:A:3219:TYR:HA	1:A:3227:ARG:HD3	1.85	0.58
1:J:2116:LEU:O	1:J:2120:MET:HG2	2.02	0.58
1:C:1694:LEU:HB3	1:C:1715:LEU:HD12	1.85	0.58
1:G:220:LEU:HD23	1:G:390:LEU:HB3	1.86	0.58
1:G:683:ARG:HG2	1:G:717:ASP:HB3	1.85	0.58
1:A:2554:LEU:HA	1:A:2558:VAL:HG22	1.86	0.58
1:A:2644:LEU:HD21	1:A:2678:LEU:HD21	1.86	0.58
1:A:3406:TYR:HA	1:A:3509:LEU:HD22	1.86	0.58
1:C:1447:CYS:HB3	1:C:1555:LEU:HB3	1.86	0.58
1:C:2644:LEU:HD21	1:C:2678:LEU:HD21	1.86	0.58
1:C:2894:LEU:HD22	1:C:2905:LEU:HD12	1.86	0.58
1:A:1780:PRO:HD3	1:A:1801:ALA:H	1.69	0.58
1:C:899:ASP:H	2:D:58:ASN:HD21	1.51	0.58
1:G:899:ASP:H	2:H:58:ASN:HD21	1.51	0.58
1:J:683:ARG:HG2	1:J:717:ASP:HB3	1.85	0.58
1:G:1780:PRO:HD3	1:G:1801:ALA:H	1.69	0.57
1:C:1780:PRO:HD3	1:C:1801:ALA:H	1.69	0.57
3:F:39:SER:HA	3:F:42:ARG:HE	1.69	0.57
1:G:2340:PHE:HB2	1:G:2435:ARG:HD3	1.86	0.57
1:C:683:ARG:HG2	1:C:717:ASP:HB3	1.85	0.57
1:C:1694:LEU:HD22	1:C:1715:LEU:HB2	1.86	0.57
1:C:2116:LEU:O	1:C:2120:MET:HG2	2.02	0.57
2:D:40:ALA:HB3	2:D:43:LYS:HB3	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3514:LEU:HD11	1:C:3602:VAL:HG13	1.87	0.57
1:G:3683:GLN:HB2	1:G:3694:LYS:HE3	1.85	0.57
2:H:40:ALA:HB3	2:H:43:LYS:HB3	1.87	0.57
2:B:40:ALA:HB3	2:B:43:LYS:HB3	1.87	0.57
1:G:3219:TYR:HA	1:G:3227:ARG:HD3	1.86	0.57
1:J:1155:LEU:HD12	1:J:1184:ILE:HG13	1.85	0.57
1:J:3406:TYR:HA	1:J:3509:LEU:HD22	1.85	0.57
2:K:40:ALA:HB3	2:K:43:LYS:HB3	1.87	0.57
1:A:3683:GLN:HB2	1:A:3694:LYS:HE3	1.85	0.57
1:A:4567:LEU:HD13	1:A:4815:ASP:HB3	1.85	0.57
1:C:4648:LEU:HD12	1:C:4803:HIS:HE1	1.70	0.57
1:C:4848:VAL:HG11	1:C:4887:MET:HG2	1.86	0.57
1:G:2554:LEU:HA	1:G:2558:VAL:HG22	1.86	0.57
1:G:2644:LEU:HD21	1:G:2678:LEU:HD21	1.86	0.57
1:J:1447:CYS:HB3	1:J:1555:LEU:HB3	1.86	0.57
1:J:3316:LEU:HD11	1:J:3346:VAL:HA	1.87	0.57
1:A:220:LEU:HD23	1:A:390:LEU:HB3	1.86	0.57
1:A:4780:PHE:HA	1:A:4783:ILE:HG22	1.87	0.57
1:G:1694:LEU:HD22	1:G:1715:LEU:HB2	1.87	0.57
1:G:2766:TRP:O	1:G:2770:LYS:HG2	2.03	0.57
1:J:2642:LYS:HE3	1:J:2646:ASN:HD21	1.70	0.57
1:A:1694:LEU:HD22	1:A:1715:LEU:HB2	1.86	0.57
1:A:4648:LEU:HD12	1:A:4803:HIS:HE1	1.70	0.57
1:G:2645:THR:HB	1:G:2702:CYS:HA	1.85	0.57
3:I:39:SER:HA	3:I:42:ARG:HE	1.69	0.57
1:J:2554:LEU:HA	1:J:2558:VAL:HG22	1.86	0.57
1:C:4567:LEU:HD13	1:C:4815:ASP:HB3	1.85	0.57
1:G:2861:ASP:HA	1:G:2932:MET:HE1	1.87	0.57
1:J:3683:GLN:HB2	1:J:3694:LYS:HE3	1.85	0.57
1:J:4848:VAL:HG11	1:J:4887:MET:HG2	1.87	0.57
1:C:3316:LEU:HD11	1:C:3346:VAL:HA	1.87	0.57
1:G:4780:PHE:HA	1:G:4783:ILE:HG22	1.87	0.57
1:J:1780:PRO:HD3	1:J:1801:ALA:H	1.69	0.57
1:J:2615:ARG:HD3	1:J:2616:PRO:HD2	1.87	0.57
1:J:4648:LEU:HD12	1:J:4803:HIS:HE1	1.70	0.57
1:J:2644:LEU:HD21	1:J:2678:LEU:HD21	1.86	0.56
1:A:1447:CYS:HB3	1:A:1555:LEU:HB3	1.86	0.56
1:A:2097:LEU:O	1:A:2101:MET:HB2	2.06	0.56
1:A:2642:LYS:HE3	1:A:2646:ASN:HD21	1.70	0.56
1:C:220:LEU:HD23	1:C:390:LEU:HB3	1.86	0.56
1:C:2340:PHE:HB2	1:C:2435:ARG:HD3	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2554:LEU:HA	1:C:2558:VAL:HG22	1.86	0.56
1:J:2861:ASP:HA	1:J:2932:MET:HE1	1.87	0.56
1:A:2340:PHE:HB2	1:A:2435:ARG:HD3	1.86	0.56
1:A:3282:PRO:HG3	1:A:3345:ILE:HD13	1.87	0.56
1:C:2097:LEU:O	1:C:2101:MET:HB2	2.06	0.56
1:C:2615:ARG:HD3	1:C:2616:PRO:HD2	1.87	0.56
1:C:3733:CYS:HA	1:C:3766:GLN:HB3	1.87	0.56
1:C:4677:LEU:HD13	1:C:4711:PHE:HE1	1.71	0.56
1:G:348:VAL:HB	1:G:357:LEU:HD21	1.88	0.56
1:G:985:VAL:HG11	1:G:1040:CYS:SG	2.46	0.56
1:G:2642:LYS:HE3	1:G:2646:ASN:HD21	1.70	0.56
1:G:3733:CYS:HA	1:G:3766:GLN:HB3	1.87	0.56
1:J:3282:PRO:HG3	1:J:3345:ILE:HD13	1.87	0.56
1:A:2238:TYR:HA	1:A:2241:ARG:HD2	1.87	0.56
1:A:3086:GLU:HA	1:A:3089:LYS:HE2	1.88	0.56
1:C:2635:GLU:HA	1:C:2638:LYS:HZ3	1.71	0.56
1:C:4780:PHE:HA	1:C:4783:ILE:HG22	1.87	0.56
1:G:2097:LEU:O	1:G:2101:MET:HB2	2.06	0.56
1:G:2615:ARG:HD3	1:G:2616:PRO:HD2	1.87	0.56
1:G:2960:LEU:HD22	1:G:3038:MET:HE1	1.88	0.56
1:G:4648:LEU:HD12	1:G:4803:HIS:HE1	1.70	0.56
1:J:1694:LEU:HD22	1:J:1715:LEU:HB2	1.86	0.56
1:J:2340:PHE:HB2	1:J:2435:ARG:HD3	1.86	0.56
3:L:39:SER:HA	3:L:42:ARG:HE	1.69	0.56
1:J:4712:PRO:HB2	1:J:4718:LYS:HA	1.88	0.56
1:A:2861:ASP:HA	1:A:2932:MET:HE1	1.87	0.56
1:A:2960:LEU:HD22	1:A:3038:MET:HE1	1.88	0.56
1:C:954:LYS:HA	1:C:969:PRO:HG2	1.88	0.56
1:J:2097:LEU:O	1:J:2101:MET:HB2	2.06	0.56
1:A:348:VAL:HB	1:A:357:LEU:HD21	1.88	0.56
1:A:954:LYS:HA	1:A:969:PRO:HG2	1.88	0.56
1:A:2233:CYS:O	1:A:2237:CYS:N	2.39	0.56
1:A:4848:VAL:HG11	1:A:4887:MET:HG2	1.86	0.56
3:E:39:SER:HA	3:E:42:ARG:HE	1.69	0.56
1:J:2960:LEU:HD22	1:J:3038:MET:HE1	1.88	0.56
1:J:4677:LEU:HD13	1:J:4711:PHE:HE1	1.71	0.56
1:A:2615:ARG:HD3	1:A:2616:PRO:HD2	1.87	0.56
2:B:111:ASN:HA	2:B:114:TYR:HD1	1.71	0.56
1:C:3086:GLU:HA	1:C:3089:LYS:HE2	1.88	0.56
1:C:4712:PRO:HB2	1:C:4718:LYS:HA	1.88	0.56
1:G:4848:VAL:HG11	1:G:4887:MET:HG2	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:82:TYR:HB2	3:I:86:GLY:HA2	1.88	0.56
1:J:3733:CYS:HA	1:J:3766:GLN:HB3	1.87	0.56
2:K:111:ASN:HA	2:K:114:TYR:HD1	1.71	0.56
1:C:1179:PHE:HB2	1:C:1182:ILE:HD11	1.88	0.56
1:G:578:ILE:HG21	1:G:606:LEU:HD21	1.88	0.56
1:G:1447:CYS:HB3	1:G:1555:LEU:HB3	1.86	0.56
1:G:3514:LEU:HD11	1:G:3602:VAL:HG13	1.87	0.56
1:A:4677:LEU:HD13	1:A:4711:PHE:HE1	1.71	0.55
1:C:2233:CYS:O	1:C:2237:CYS:N	2.37	0.55
1:C:2507:ASP:HB3	1:C:2561:LEU:HD12	1.88	0.55
1:G:3316:LEU:HD11	1:G:3346:VAL:HA	1.87	0.55
1:G:4712:PRO:HB2	1:G:4718:LYS:HA	1.88	0.55
1:J:4780:PHE:HA	1:J:4783:ILE:HG22	1.87	0.55
1:J:4874:MET:HB3	1:J:4877:ASP:HB2	1.88	0.55
1:A:4712:PRO:HB2	1:A:4718:LYS:HA	1.88	0.55
1:C:1155:LEU:HD12	1:C:1184:ILE:HG13	1.88	0.55
1:C:2642:LYS:HE3	1:C:2646:ASN:HD21	1.70	0.55
1:C:3945:GLU:HG3	1:C:3949:ARG:HH11	1.71	0.55
1:G:1155:LEU:HD12	1:G:1184:ILE:HG13	1.88	0.55
1:J:3406:TYR:HA	1:J:3509:LEU:CD2	2.36	0.55
1:A:3316:LEU:HD11	1:A:3346:VAL:HA	1.87	0.55
1:C:2861:ASP:HA	1:C:2932:MET:HE1	1.87	0.55
1:G:3524:MET:HA	1:G:3582:ARG:HH22	1.72	0.55
1:G:3945:GLU:HG3	1:G:3949:ARG:HH11	1.71	0.55
1:J:348:VAL:HB	1:J:357:LEU:HD21	1.88	0.55
1:J:578:ILE:HG21	1:J:606:LEU:HD21	1.88	0.55
1:J:952:LYS:HE2	1:J:969:PRO:HD2	1.88	0.55
1:J:2974:ILE:HD11	1:J:3049:LEU:HD22	1.88	0.55
1:A:3733:CYS:HA	1:A:3766:GLN:HB3	1.87	0.55
1:C:3282:PRO:HG3	1:C:3345:ILE:HD13	1.87	0.55
1:G:1179:PHE:HB2	1:G:1182:ILE:HD11	1.88	0.55
1:G:4948:GLU:HA	1:G:4951:LYS:HE2	1.88	0.55
1:J:4039:MET:HE2	1:J:4039:MET:HA	1.89	0.55
1:G:2507:ASP:HB3	1:G:2561:LEU:HD12	1.88	0.55
1:G:2974:ILE:HD11	1:G:3049:LEU:HD22	1.88	0.55
1:J:3945:GLU:HG3	1:J:3949:ARG:HH11	1.71	0.55
1:A:1735:ILE:HG22	1:A:1771:LEU:HD13	1.89	0.55
1:A:2233:CYS:HA	1:A:2236:LEU:HB2	1.89	0.55
1:C:2960:LEU:HD22	1:C:3038:MET:HE1	1.88	0.55
1:G:4874:MET:HB3	1:G:4877:ASP:HB2	1.88	0.55
1:A:1100:MET:HA	1:A:1193:SER:O	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1098:GLY:HA3	1:C:1198:GLN:NE2	2.22	0.55
1:C:1100:MET:HA	1:C:1193:SER:O	2.07	0.55
1:C:1786:LEU:HB2	3:E:82:TYR:HB3	1.89	0.55
1:G:2751:LEU:O	1:G:2755:ILE:HG12	2.07	0.55
1:J:2507:ASP:HB3	1:J:2561:LEU:HD12	1.88	0.55
1:A:3524:MET:HA	1:A:3582:ARG:HH22	1.72	0.55
1:G:1098:GLY:HA3	1:G:1198:GLN:NE2	2.22	0.55
1:G:4039:MET:HE2	1:G:4039:MET:HA	1.89	0.55
2:H:111:ASN:HA	2:H:114:TYR:HD1	1.71	0.55
1:A:1098:GLY:HA3	1:A:1198:GLN:NE2	2.22	0.55
1:C:1558:HIS:CD2	1:C:1560:ASN:H	2.25	0.55
1:C:2449:GLU:HB3	1:C:2452:ARG:HH21	1.72	0.55
1:C:2758:PHE:HD2	1:C:2813:LEU:HD11	1.72	0.55
1:C:4039:MET:HA	1:C:4039:MET:HE2	1.89	0.55
1:G:1735:ILE:HG22	1:G:1771:LEU:HD13	1.89	0.55
1:G:2758:PHE:HD2	1:G:2813:LEU:HD11	1.72	0.55
1:G:3282:PRO:HG3	1:G:3345:ILE:HD13	1.87	0.55
1:J:3524:MET:HA	1:J:3582:ARG:HH22	1.72	0.55
1:C:348:VAL:HB	1:C:357:LEU:HD21	1.88	0.55
1:C:578:ILE:HG21	1:C:606:LEU:HD21	1.88	0.55
1:J:1098:GLY:HA3	1:J:1198:GLN:NE2	2.22	0.55
1:J:2758:PHE:HD2	1:J:2813:LEU:HD11	1.72	0.55
3:L:56:ILE:HB	3:L:59:PHE:HB2	1.89	0.55
1:A:1530:THR:HG22	1:A:1535:GLU:HA	1.90	0.54
1:C:1735:ILE:HG22	1:C:1771:LEU:HD13	1.89	0.54
1:G:1100:MET:HA	1:G:1193:SER:O	2.07	0.54
1:G:2765:LYS:HG2	1:G:2857:PRO:HG2	1.90	0.54
1:G:3086:GLU:HA	1:G:3089:LYS:HE2	1.88	0.54
1:J:1735:ILE:HG22	1:J:1771:LEU:HD13	1.89	0.54
1:J:2635:GLU:HA	1:J:2638:LYS:HZ3	1.72	0.54
1:J:2765:LYS:HG2	1:J:2857:PRO:HG2	1.90	0.54
1:A:4005:GLN:HA	1:A:4114:CYS:HA	1.89	0.54
1:C:985:VAL:HG22	1:C:1043:VAL:HG21	1.88	0.54
1:J:2702:CYS:O	1:J:2706:ILE:HG12	2.08	0.54
1:J:4948:GLU:HA	1:J:4951:LYS:HE2	1.88	0.54
1:A:164:ARG:HB2	1:A:167:ASP:HB2	1.90	0.54
1:A:1093:GLU:HB3	1:A:1201:HIS:HB3	1.90	0.54
1:A:2758:PHE:HD2	1:A:2813:LEU:HD11	1.72	0.54
1:C:2233:CYS:HA	1:C:2236:LEU:HB2	1.89	0.54
1:C:4874:MET:HB3	1:C:4877:ASP:HB2	1.88	0.54
1:G:894:GLY:O	1:G:903:LEU:HB3	2.06	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1093:GLU:HB3	1:G:1201:HIS:HB3	1.90	0.54
1:G:1558:HIS:CD2	1:G:1560:ASN:H	2.25	0.54
1:J:1093:GLU:HB3	1:J:1201:HIS:HB3	1.89	0.54
1:J:1558:HIS:CD2	1:J:1560:ASN:H	2.25	0.54
1:J:3086:GLU:HA	1:J:3089:LYS:HE2	1.88	0.54
1:A:1694:LEU:HD11	1:A:1718:ILE:HD11	1.90	0.54
1:A:3410:PRO:HD3	1:A:3509:LEU:HD21	1.89	0.54
1:C:1530:THR:HG22	1:C:1535:GLU:HA	1.90	0.54
1:C:4005:GLN:HA	1:C:4114:CYS:HA	1.89	0.54
1:G:753:PRO:HG3	1:G:773:LEU:HD21	1.90	0.54
1:A:1558:HIS:CD2	1:A:1560:ASN:H	2.25	0.54
1:A:2507:ASP:HB3	1:A:2561:LEU:HD12	1.88	0.54
1:A:4948:GLU:HA	1:A:4951:LYS:HE2	1.88	0.54
1:C:2751:LEU:O	1:C:2755:ILE:HG12	2.07	0.54
1:G:164:ARG:HB2	1:G:167:ASP:HB2	1.90	0.54
1:G:2702:CYS:O	1:G:2706:ILE:HG12	2.08	0.54
1:G:2816:MET:HB2	1:G:2878:LEU:HD13	1.90	0.54
1:J:2751:LEU:O	1:J:2755:ILE:HG12	2.07	0.54
1:A:39:ALA:HB2	1:A:47:CYS:HA	1.90	0.54
1:A:4874:MET:HB3	1:A:4877:ASP:HB2	1.88	0.54
1:C:39:ALA:HB2	1:C:47:CYS:HA	1.90	0.54
3:E:56:ILE:HB	3:E:59:PHE:HB2	1.89	0.54
1:G:4677:LEU:HD13	1:G:4711:PHE:HE1	1.71	0.54
1:J:2792:ARG:HB3	1:J:2796:THR:HG23	1.90	0.54
1:A:578:ILE:HG21	1:A:606:LEU:HD21	1.88	0.54
1:A:753:PRO:HG3	1:A:773:LEU:HD21	1.90	0.54
1:A:2449:GLU:HB3	1:A:2452:ARG:HH21	1.72	0.54
1:A:2751:LEU:O	1:A:2755:ILE:HG12	2.07	0.54
1:A:2974:ILE:HD11	1:A:3049:LEU:HD22	1.89	0.54
1:A:4039:MET:HE2	1:A:4039:MET:HA	1.89	0.54
1:C:4948:GLU:HA	1:C:4951:LYS:HE2	1.88	0.54
2:K:111:ASN:HA	2:K:114:TYR:CD1	2.43	0.54
1:C:1093:GLU:HB3	1:C:1201:HIS:HB3	1.90	0.54
1:G:2823:ILE:HD13	1:G:2937:VAL:HG22	1.89	0.54
1:G:3971:GLY:HA2	1:G:5005:GLY:HA3	1.90	0.54
1:J:39:ALA:HB2	1:J:47:CYS:HA	1.90	0.54
1:J:1100:MET:HA	1:J:1193:SER:O	2.07	0.54
1:J:2816:MET:HB2	1:J:2878:LEU:HD13	1.90	0.54
1:A:364:PRO:HD2	1:A:367:LEU:HD12	1.90	0.54
1:A:1786:LEU:HB2	3:F:82:TYR:HB3	1.90	0.54
1:A:2816:MET:HB2	1:A:2878:LEU:HD13	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3971:GLY:HA2	1:A:5005:GLY:HA3	1.90	0.54
1:C:364:PRO:HD2	1:C:367:LEU:HD12	1.90	0.54
1:C:2702:CYS:O	1:C:2706:ILE:HG12	2.08	0.54
1:C:2974:ILE:HD11	1:C:3049:LEU:HD22	1.89	0.54
1:G:918:ARG:O	1:G:922:LEU:HG	2.08	0.54
1:G:1694:LEU:HD11	1:G:1718:ILE:HD11	1.90	0.54
1:J:364:PRO:HD2	1:J:367:LEU:HD12	1.90	0.54
1:A:2722:LYS:HD3	1:A:2877:GLN:HE21	1.73	0.54
1:A:2792:ARG:HB3	1:A:2796:THR:HG23	1.90	0.54
1:G:3768:SER:HA	1:G:3771:HIS:CD2	2.43	0.54
2:H:111:ASN:HA	2:H:114:TYR:CD1	2.43	0.54
1:J:753:PRO:HG3	1:J:773:LEU:HD21	1.90	0.54
1:J:1694:LEU:HD11	1:J:1718:ILE:HD11	1.90	0.54
1:J:4045:VAL:HG12	1:J:4159:ARG:HH21	1.73	0.54
2:K:55:ASN:H	2:K:71:ARG:HH22	1.56	0.54
1:A:918:ARG:O	1:A:922:LEU:HG	2.08	0.53
1:A:2470:ILE:HG22	1:A:2525:GLY:HA3	1.90	0.53
1:A:2765:LYS:HG2	1:A:2857:PRO:HG2	1.90	0.53
1:A:3945:GLU:HG3	1:A:3949:ARG:HH11	1.71	0.53
1:C:2470:ILE:HG22	1:C:2525:GLY:HA3	1.90	0.53
1:C:2765:LYS:HG2	1:C:2857:PRO:HG2	1.90	0.53
1:C:2792:ARG:HB3	1:C:2796:THR:HG23	1.90	0.53
1:C:3245:VAL:HG12	1:C:3248:ARG:HG2	1.90	0.53
1:G:4045:VAL:HG12	1:G:4159:ARG:HH21	1.73	0.53
1:J:2759:ALA:HB1	1:J:2806:ARG:HG3	1.89	0.53
1:A:977:LEU:HD23	1:A:982:THR:HG22	1.91	0.53
1:A:3406:TYR:HA	1:A:3509:LEU:CD2	2.38	0.53
2:B:111:ASN:HA	2:B:114:TYR:CD1	2.43	0.53
1:C:2883:HIS:ND1	1:C:2908:TYR:HB2	2.23	0.53
1:G:1530:THR:HG22	1:G:1535:GLU:HA	1.90	0.53
1:G:1786:LEU:HD12	1:G:1787:PRO:HD2	1.91	0.53
3:I:56:ILE:HB	3:I:59:PHE:HB2	1.89	0.53
1:J:2887:GLY:HA2	1:J:2890:LYS:HD3	1.91	0.53
1:A:2702:CYS:O	1:A:2706:ILE:HG12	2.08	0.53
1:A:3768:SER:HA	1:A:3771:HIS:CD2	2.44	0.53
1:C:3524:MET:HA	1:C:3582:ARG:HH22	1.72	0.53
1:C:4765:LEU:HA	1:C:4768:LEU:HD12	1.91	0.53
1:G:364:PRO:HD2	1:G:367:LEU:HD12	1.90	0.53
1:J:1758:ARG:HH12	1:J:2037:ASP:HA	1.73	0.53
1:J:1786:LEU:HD12	1:J:1787:PRO:HD2	1.91	0.53
1:J:2470:ILE:HG22	1:J:2525:GLY:HA3	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:2882:TYR:HD2	1:J:2919:ASP:HB3	1.74	0.53
1:J:3794:VAL:HG21	1:J:3835:LEU:HD21	1.91	0.53
1:A:4045:VAL:HG12	1:A:4159:ARG:HH21	1.73	0.53
1:C:2722:LYS:HD3	1:C:2877:GLN:HE21	1.73	0.53
1:C:2759:ALA:HB1	1:C:2806:ARG:HG3	1.89	0.53
1:G:977:LEU:HD23	1:G:982:THR:HG22	1.91	0.53
1:G:2449:GLU:HB3	1:G:2452:ARG:HH21	1.72	0.53
1:J:2823:ILE:HD13	1:J:2937:VAL:HG22	1.89	0.53
1:A:1786:LEU:HD12	1:A:1787:PRO:HD2	1.91	0.53
1:C:3794:VAL:HG21	1:C:3835:LEU:HD21	1.91	0.53
1:C:3971:GLY:HA2	1:C:5005:GLY:HA3	1.90	0.53
1:G:2759:ALA:HB1	1:G:2806:ARG:HG3	1.89	0.53
1:J:3245:VAL:HG12	1:J:3248:ARG:HG2	1.91	0.53
1:A:2823:ILE:HD13	1:A:2937:VAL:HG22	1.89	0.53
1:C:935:LEU:HD11	1:C:987:ARG:HD2	1.91	0.53
1:C:1272:LEU:HD22	1:C:1289:LEU:HD11	1.91	0.53
1:C:2882:TYR:HD2	1:C:2919:ASP:HB3	1.74	0.53
1:C:2902:HIS:CE1	1:C:2904:LEU:HB2	2.44	0.53
1:G:882:TRP:HH2	2:H:104:TYR:HA	1.72	0.53
1:J:918:ARG:O	1:J:922:LEU:HG	2.08	0.53
1:J:1530:THR:HG22	1:J:1535:GLU:HA	1.90	0.53
1:J:4765:LEU:HA	1:J:4768:LEU:HD12	1.91	0.53
1:A:2759:ALA:HB1	1:A:2806:ARG:HG3	1.89	0.53
1:A:2902:HIS:CE1	1:A:2904:LEU:HB2	2.44	0.53
2:B:55:ASN:H	2:B:71:ARG:HH22	1.56	0.53
1:C:164:ARG:HB2	1:C:167:ASP:HB2	1.90	0.53
1:C:977:LEU:HD23	1:C:982:THR:HG22	1.91	0.53
1:C:1758:ARG:HH12	1:C:2037:ASP:HA	1.73	0.53
1:G:2882:TYR:HD2	1:G:2919:ASP:HB3	1.74	0.53
1:G:3794:VAL:HG21	1:G:3835:LEU:HD21	1.91	0.53
1:G:4005:GLN:HA	1:G:4114:CYS:HA	1.89	0.53
1:A:1813:ARG:O	1:A:1817:GLU:HG2	2.09	0.53
1:A:2882:TYR:HD2	1:A:2919:ASP:HB3	1.74	0.53
1:C:753:PRO:HG3	1:C:773:LEU:HD21	1.90	0.53
1:C:1694:LEU:HD11	1:C:1718:ILE:HD11	1.90	0.53
1:C:1786:LEU:HD12	1:C:1787:PRO:HD2	1.91	0.53
1:C:1813:ARG:O	1:C:1817:GLU:HG2	2.09	0.53
1:C:2816:MET:HB2	1:C:2878:LEU:HD13	1.90	0.53
1:C:3768:SER:HA	1:C:3771:HIS:CD2	2.43	0.53
1:C:4725:LEU:HD21	1:C:4734:ARG:HG3	1.91	0.53
1:G:1758:ARG:HH12	1:G:2037:ASP:HA	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4765:LEU:HA	1:G:4768:LEU:HD12	1.91	0.53
1:J:2449:GLU:HB3	1:J:2452:ARG:HH21	1.72	0.53
1:J:3768:SER:HA	1:J:3771:HIS:CD2	2.44	0.53
1:A:4765:LEU:HA	1:A:4768:LEU:HD12	1.91	0.53
1:C:548:VAL:HG21	1:C:582:HIS:HD2	1.74	0.53
3:F:56:ILE:HB	3:F:59:PHE:HB2	1.89	0.53
1:G:39:ALA:HB2	1:G:47:CYS:HA	1.90	0.53
1:G:1813:ARG:O	1:G:1817:GLU:HG2	2.09	0.53
1:C:638:ILE:HD13	1:C:703:GLY:HA2	1.91	0.53
1:G:45:ARG:HE	1:G:116:MET:HE1	1.74	0.53
2:H:55:ASN:H	2:H:71:ARG:HH22	1.56	0.53
1:J:45:ARG:HE	1:J:116:MET:HE1	1.74	0.53
1:J:164:ARG:HB2	1:J:167:ASP:HB2	1.90	0.53
1:J:548:VAL:HG21	1:J:582:HIS:HD2	1.74	0.53
1:J:638:ILE:HD13	1:J:703:GLY:HA2	1.91	0.53
1:J:2722:LYS:HD3	1:J:2877:GLN:HE21	1.73	0.53
1:J:4005:GLN:HA	1:J:4114:CYS:HA	1.89	0.53
1:A:548:VAL:HG21	1:A:582:HIS:HD2	1.74	0.52
1:C:181:HIS:NE2	1:C:196:MET:HB3	2.24	0.52
1:C:2559:LEU:HG	1:C:2603:ILE:HD13	1.91	0.52
1:C:2823:ILE:HD13	1:C:2937:VAL:HG22	1.89	0.52
1:C:2887:GLY:HA2	1:C:2890:LYS:HD3	1.91	0.52
1:G:891:TRP:HE1	1:G:904:HIS:HA	1.75	0.52
1:G:2722:LYS:HD3	1:G:2877:GLN:HE21	1.73	0.52
1:G:2902:HIS:CE1	1:G:2904:LEU:HB2	2.44	0.52
1:J:1272:LEU:HD22	1:J:1289:LEU:HD11	1.91	0.52
1:A:2887:GLY:HA2	1:A:2890:LYS:HD3	1.90	0.52
1:A:3794:VAL:HG21	1:A:3835:LEU:HD21	1.91	0.52
1:G:4087:LEU:HA	1:G:4125:PHE:HE1	1.74	0.52
1:G:4725:LEU:HD21	1:G:4734:ARG:HG3	1.91	0.52
1:J:3971:GLY:HA2	1:J:5005:GLY:HA3	1.90	0.52
1:A:1758:ARG:HH12	1:A:2037:ASP:HA	1.73	0.52
1:A:2418:LEU:O	1:A:2422:ILE:HG12	2.10	0.52
1:A:3245:VAL:HG12	1:A:3248:ARG:HG2	1.91	0.52
1:C:45:ARG:HE	1:C:116:MET:HE1	1.74	0.52
1:C:892:THR:HB	1:C:903:LEU:HD23	1.91	0.52
1:C:3951:PHE:HB3	1:C:4012:LEU:HD11	1.92	0.52
1:J:2928:LYS:O	1:J:2932:MET:HG3	2.10	0.52
1:A:45:ARG:HE	1:A:116:MET:HE1	1.74	0.52
1:A:1272:LEU:HD22	1:A:1289:LEU:HD11	1.91	0.52
1:A:5032:TYR:HB3	1:A:5035:GLN:HB2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:348:VAL:HG23	1:C:388:LEU:HD23	1.91	0.52
1:C:3106:MET:HA	1:C:3106:MET:HE2	1.92	0.52
1:C:4750:ILE:HA	1:C:4753:HIS:CD2	2.45	0.52
1:G:1676:LEU:HD22	1:G:2167:ILE:HD12	1.92	0.52
1:G:2470:ILE:HG22	1:G:2525:GLY:HA3	1.90	0.52
1:G:2792:ARG:HB3	1:G:2796:THR:HG23	1.90	0.52
3:I:86:GLY:O	3:I:87:HIS:C	2.51	0.52
1:J:977:LEU:HD23	1:J:982:THR:HG22	1.91	0.52
1:J:1676:LEU:HD22	1:J:2167:ILE:HD12	1.92	0.52
1:J:2902:HIS:CE1	1:J:2904:LEU:HB2	2.44	0.52
1:C:985:VAL:HG11	1:C:1040:CYS:SG	2.49	0.52
1:C:4045:VAL:HG12	1:C:4159:ARG:HH21	1.73	0.52
2:D:55:ASN:H	2:D:71:ARG:HH22	1.56	0.52
1:G:2418:LEU:O	1:G:2422:ILE:HG12	2.10	0.52
1:G:2866:THR:HA	1:G:2928:LYS:HZ2	1.74	0.52
1:G:3354:LEU:HA	1:G:3358:PHE:CD1	2.45	0.52
1:G:3937:TYR:HB3	1:G:4002:LYS:HZ1	1.75	0.52
1:G:4750:ILE:HA	1:G:4753:HIS:CD2	2.45	0.52
1:J:3937:TYR:HB3	1:J:4002:LYS:HZ1	1.75	0.52
1:A:3106:MET:HE2	1:A:3106:MET:HA	1.92	0.52
1:A:3536:ALA:HB2	1:A:3539:ARG:HH21	1.75	0.52
1:C:3937:TYR:HB3	1:C:4002:LYS:HZ1	1.75	0.52
1:G:3245:VAL:HG12	1:G:3248:ARG:HG2	1.91	0.52
1:J:897:ARG:HG2	1:J:905:PRO:HA	1.91	0.52
1:J:2559:LEU:HG	1:J:2603:ILE:HD13	1.92	0.52
1:J:3106:MET:HE2	1:J:3106:MET:HA	1.92	0.52
1:A:638:ILE:HD13	1:A:703:GLY:HA2	1.91	0.52
1:G:2928:LYS:O	1:G:2932:MET:HG3	2.10	0.52
1:C:897:ARG:HG2	1:C:905:PRO:HA	1.91	0.52
1:G:348:VAL:HG23	1:G:388:LEU:HD23	1.91	0.52
1:G:1786:LEU:HB2	3:I:82:TYR:HB3	1.92	0.52
1:G:2883:HIS:ND1	1:G:2908:TYR:HB2	2.23	0.52
1:G:3406:TYR:HA	1:G:3509:LEU:CD2	2.39	0.52
1:J:783:PHE:HB2	1:J:787:VAL:HG21	1.92	0.52
1:J:1813:ARG:O	1:J:1817:GLU:HG2	2.09	0.52
1:J:4183:ILE:O	1:J:4190:ILE:HA	2.10	0.52
1:A:2928:LYS:O	1:A:2932:MET:HG3	2.10	0.52
1:A:4854:VAL:HG11	4:A:5114:POV:H21B	1.92	0.52
4:A:5107:POV:H21B	1:C:4854:VAL:HG11	1.91	0.52
1:C:3051:ARG:HH22	1:C:3102:ASP:HB2	1.75	0.52
1:C:4808:PHE:HZ	4:C:5105:POV:H32A	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2012:PHE:CZ	1:G:2031:LEU:HD23	2.45	0.52
1:G:3051:ARG:HH22	1:G:3102:ASP:HB2	1.75	0.52
1:G:3106:MET:HE2	1:G:3106:MET:HA	1.92	0.52
1:G:4854:VAL:HG11	4:G:5112:POV:H21B	1.92	0.52
1:J:985:VAL:HG11	1:J:1040:CYS:SG	2.49	0.52
1:J:2377:LEU:HD22	1:J:2465:ASP:HA	1.92	0.52
1:J:3354:LEU:HA	1:J:3358:PHE:CD1	2.45	0.52
1:A:897:ARG:HG2	1:A:905:PRO:HA	1.91	0.52
1:A:2233:CYS:O	1:A:2234:ARG:C	2.53	0.52
1:A:4750:ILE:HA	1:A:4753:HIS:CD2	2.45	0.52
1:C:2233:CYS:O	1:C:2234:ARG:C	2.53	0.52
1:C:4087:LEU:HA	1:C:4125:PHE:HE1	1.74	0.52
1:C:4088:ILE:HG23	1:C:4123:ILE:HG22	1.92	0.52
1:C:4183:ILE:O	1:C:4190:ILE:HA	2.10	0.52
1:C:4781:GLY:HA2	4:C:5109:POV:H28	1.92	0.52
1:G:638:ILE:HD13	1:G:703:GLY:HA2	1.91	0.52
1:G:3931:SER:O	1:G:3935:TRP:HB3	2.11	0.52
1:J:3951:PHE:HB3	1:J:4012:LEU:HD11	1.92	0.52
1:J:4087:LEU:HA	1:J:4125:PHE:HE1	1.74	0.52
1:A:4219:PHE:HA	1:A:4950:VAL:HG11	1.92	0.51
1:A:4725:LEU:HD21	1:A:4734:ARG:HG3	1.91	0.51
1:C:3055:SER:HB2	1:C:3127:GLN:HG2	1.92	0.51
1:G:1272:LEU:HD22	1:G:1289:LEU:HD11	1.91	0.51
1:G:2755:ILE:HG23	1:G:2813:LEU:HB2	1.92	0.51
1:G:3962:PHE:O	1:G:3966:THR:HG23	2.10	0.51
1:J:348:VAL:HG23	1:J:388:LEU:HD23	1.91	0.51
1:J:3187:ARG:HG2	1:J:3272:ILE:HD11	1.93	0.51
1:J:4088:ILE:HG23	1:J:4123:ILE:HG22	1.92	0.51
1:A:2012:PHE:CZ	1:A:2031:LEU:HD23	2.45	0.51
1:A:3354:LEU:HA	1:A:3358:PHE:CD1	2.45	0.51
1:A:3962:PHE:O	1:A:3966:THR:HG23	2.10	0.51
1:G:2887:GLY:HA2	1:G:2890:LYS:HD3	1.91	0.51
1:G:5032:TYR:HB3	1:G:5035:GLN:HB2	1.91	0.51
1:J:3051:ARG:HH22	1:J:3102:ASP:HB2	1.75	0.51
1:J:4750:ILE:HA	1:J:4753:HIS:CD2	2.45	0.51
1:A:3466:ASN:O	1:A:3470:LEU:HD22	2.11	0.51
1:A:4087:LEU:HA	1:A:4125:PHE:HE1	1.74	0.51
1:C:918:ARG:O	1:C:922:LEU:HG	2.08	0.51
1:C:3931:SER:O	1:C:3935:TRP:HB3	2.11	0.51
3:E:105:ASN:C	3:E:105:ASN:ND2	2.68	0.51
1:G:548:VAL:HG21	1:G:582:HIS:HD2	1.74	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2257:LEU:HD13	1:G:2275:VAL:HG13	1.93	0.51
1:G:3187:ARG:HG2	1:G:3272:ILE:HD11	1.93	0.51
1:J:289:ARG:HB3	1:J:301:VAL:HB	1.92	0.51
1:J:2012:PHE:CZ	1:J:2031:LEU:HD23	2.45	0.51
1:J:2866:THR:HA	1:J:2928:LYS:HZ2	1.75	0.51
1:J:3962:PHE:O	1:J:3966:THR:HG23	2.10	0.51
1:A:1676:LEU:HD22	1:A:2167:ILE:HD12	1.92	0.51
1:A:2559:LEU:HG	1:A:2603:ILE:HD13	1.91	0.51
1:C:3536:ALA:HB2	1:C:3539:ARG:HH21	1.75	0.51
1:G:181:HIS:NE2	1:G:196:MET:HB2	2.26	0.51
1:G:897:ARG:HG2	1:G:905:PRO:HA	1.91	0.51
1:G:2559:LEU:HG	1:G:2603:ILE:HD13	1.91	0.51
1:G:3466:ASN:O	1:G:3470:LEU:HD22	2.11	0.51
3:I:86:GLY:HA3	3:I:91:ILE:HB	1.92	0.51
1:A:4183:ILE:O	1:A:4190:ILE:HA	2.10	0.51
1:C:2257:LEU:HD13	1:C:2275:VAL:HG13	1.93	0.51
1:C:3962:PHE:O	1:C:3966:THR:HG23	2.10	0.51
1:G:4183:ILE:O	1:G:4190:ILE:HA	2.10	0.51
1:A:2257:LEU:HD13	1:A:2275:VAL:HG13	1.92	0.51
1:A:2883:HIS:ND1	1:A:2908:TYR:HB2	2.23	0.51
1:A:3055:SER:HB2	1:A:3127:GLN:HG2	1.92	0.51
1:C:2012:PHE:CZ	1:C:2031:LEU:HD23	2.45	0.51
1:C:2377:LEU:HD22	1:C:2465:ASP:HA	1.92	0.51
1:C:2418:LEU:O	1:C:2422:ILE:HG12	2.10	0.51
1:G:1428:LEU:HD13	1:G:1585:LYS:HE2	1.93	0.51
1:G:3056:LEU:H	1:G:3056:LEU:HD23	1.76	0.51
1:J:4219:PHE:HA	1:J:4950:VAL:HG11	1.92	0.51
1:J:5032:TYR:HB3	1:J:5035:GLN:HB2	1.91	0.51
1:A:289:ARG:HB3	1:A:301:VAL:HB	1.92	0.51
1:A:3539:ARG:HB3	1:A:3549:VAL:HG12	1.93	0.51
1:C:2928:LYS:O	1:C:2932:MET:HG3	2.10	0.51
1:C:5032:TYR:HB3	1:C:5035:GLN:HB2	1.91	0.51
1:G:289:ARG:HB3	1:G:301:VAL:HB	1.92	0.51
1:G:499:THR:HG23	1:G:502:HIS:H	1.76	0.51
1:G:783:PHE:HB2	1:G:787:VAL:HG21	1.92	0.51
1:G:3539:ARG:HB3	1:G:3549:VAL:HG12	1.93	0.51
1:J:3931:SER:O	1:J:3935:TRP:HB3	2.11	0.51
1:A:499:THR:HG23	1:A:502:HIS:H	1.76	0.51
1:A:783:PHE:HB2	1:A:787:VAL:HG21	1.92	0.51
1:A:3951:PHE:HB3	1:A:4012:LEU:HD11	1.91	0.51
1:C:1152:MET:HE3	1:C:1161:ILE:HB	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1676:LEU:HD22	1:C:2167:ILE:HD12	1.92	0.51
1:C:3245:VAL:O	1:C:3249:LEU:HD12	2.11	0.51
1:C:3354:LEU:HA	1:C:3358:PHE:CD1	2.45	0.51
1:G:2792:ARG:NH2	1:G:2798:SER:H	2.08	0.51
1:G:3682:GLU:HA	1:G:3685:GLU:HB3	1.93	0.51
1:G:4219:PHE:HA	1:G:4950:VAL:HG11	1.92	0.51
1:J:1152:MET:HE3	1:J:1161:ILE:HB	1.92	0.51
1:J:2755:ILE:HG23	1:J:2813:LEU:HB2	1.92	0.51
1:J:3055:SER:HB2	1:J:3127:GLN:HG2	1.92	0.51
1:J:3466:ASN:O	1:J:3470:LEU:HD22	2.11	0.51
1:J:3682:GLU:HA	1:J:3685:GLU:HB3	1.93	0.51
1:A:348:VAL:HG23	1:A:388:LEU:HD23	1.91	0.51
1:A:3056:LEU:HD23	1:A:3056:LEU:H	1.76	0.51
1:A:3245:VAL:O	1:A:3249:LEU:HD12	2.11	0.51
1:A:3931:SER:O	1:A:3935:TRP:HB3	2.11	0.51
1:A:3967:GLU:HA	1:A:3970:GLN:HG2	1.93	0.51
1:C:990:GLU:CD	1:C:1024:TYR:HB3	2.36	0.51
1:C:2347:GLU:CD	1:C:2347:GLU:H	2.19	0.51
1:C:3770:LEU:HD12	1:C:3804:ILE:HD11	1.93	0.51
1:G:2377:LEU:HD22	1:G:2465:ASP:HA	1.92	0.51
1:J:499:THR:HG23	1:J:502:HIS:H	1.76	0.51
1:J:1428:LEU:HD13	1:J:1585:LYS:HE2	1.92	0.51
1:J:2770:LYS:HD3	1:J:2788:HIS:H	1.76	0.51
1:J:3536:ALA:HB2	1:J:3539:ARG:HH21	1.75	0.51
1:A:3682:GLU:HA	1:A:3685:GLU:HB3	1.93	0.51
1:A:3937:TYR:HB3	1:A:4002:LYS:HZ1	1.75	0.51
1:C:2792:ARG:NH2	1:C:2798:SER:H	2.08	0.51
1:C:3038:MET:C	1:C:3038:MET:HE2	2.36	0.51
1:G:2233:CYS:O	1:G:2237:CYS:N	2.36	0.51
1:G:3967:GLU:HA	1:G:3970:GLN:HG2	1.93	0.51
2:H:90:THR:HG23	2:H:124:THR:HA	1.93	0.51
1:J:2418:LEU:O	1:J:2422:ILE:HG12	2.10	0.51
1:J:2792:ARG:NH2	1:J:2798:SER:H	2.08	0.51
1:J:3770:LEU:HD12	1:J:3804:ILE:HD11	1.93	0.51
1:A:1450:VAL:HA	1:A:1552:VAL:HG12	1.93	0.50
1:A:2792:ARG:NH2	1:A:2798:SER:H	2.08	0.50
1:A:3038:MET:C	1:A:3038:MET:HE2	2.36	0.50
2:B:90:THR:HG23	2:B:124:THR:HA	1.93	0.50
1:C:783:PHE:HB2	1:C:787:VAL:HG21	1.92	0.50
2:D:90:THR:HG23	2:D:124:THR:HA	1.93	0.50
1:G:3055:SER:HB2	1:G:3127:GLN:HG2	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3951:PHE:HB3	1:G:4012:LEU:HD11	1.91	0.50
1:J:2960:LEU:HD23	1:J:2963:LEU:HD21	1.94	0.50
1:J:4725:LEU:HD21	1:J:4734:ARG:HG3	1.91	0.50
1:A:2755:ILE:HG23	1:A:2813:LEU:HB2	1.92	0.50
1:A:3511:VAL:HG21	1:A:3609:THR:HG21	1.92	0.50
1:C:3187:ARG:HG2	1:C:3272:ILE:HD11	1.93	0.50
1:C:3995:VAL:O	1:C:3999:MET:HB2	2.12	0.50
1:G:3038:MET:C	1:G:3038:MET:HE2	2.36	0.50
1:J:1527:MET:HE2	1:J:1540:PHE:HB2	1.94	0.50
1:A:1152:MET:HE3	1:A:1161:ILE:HB	1.92	0.50
1:A:3187:ARG:HG2	1:A:3272:ILE:HD11	1.93	0.50
1:A:4088:ILE:HG23	1:A:4123:ILE:HG22	1.92	0.50
1:C:289:ARG:HB3	1:C:301:VAL:HB	1.92	0.50
1:C:2615:ARG:HG2	1:C:2618:MET:HE3	1.94	0.50
1:C:4219:PHE:HA	1:C:4950:VAL:HG11	1.92	0.50
1:C:4887:MET:HE2	4:J:5103:POV:H210	1.92	0.50
1:G:2347:GLU:H	1:G:2347:GLU:CD	2.19	0.50
1:G:3245:VAL:O	1:G:3249:LEU:HD12	2.11	0.50
1:J:4769:MET:HE3	1:J:4769:MET:O	2.12	0.50
1:A:2347:GLU:CD	1:A:2347:GLU:H	2.19	0.50
1:C:1477:GLY:HA2	1:C:1484:HIS:H	1.77	0.50
1:C:3466:ASN:O	1:C:3470:LEU:HD22	2.11	0.50
1:C:4841:VAL:HG12	4:J:5103:POV:H21D	1.94	0.50
1:G:2960:LEU:HD23	1:G:2963:LEU:HD21	1.94	0.50
1:G:3007:ASN:HB2	1:G:3067:CYS:SG	2.51	0.50
1:G:3536:ALA:HB2	1:G:3539:ARG:HH21	1.75	0.50
2:K:90:THR:HG23	2:K:124:THR:HA	1.93	0.50
1:A:959:TYR:CA	1:A:965:TYR:HA	2.26	0.50
1:A:2377:LEU:HD22	1:A:2465:ASP:HA	1.92	0.50
1:A:2770:LYS:HD3	1:A:2788:HIS:H	1.76	0.50
1:A:3007:ASN:HB2	1:A:3067:CYS:SG	2.51	0.50
1:G:1152:MET:HE3	1:G:1161:ILE:HB	1.92	0.50
1:G:1450:VAL:HA	1:G:1552:VAL:HG12	1.94	0.50
1:G:1527:MET:HE2	1:G:1540:PHE:HB2	1.94	0.50
1:G:2203:MET:HG3	1:G:2235:PHE:HZ	1.76	0.50
1:A:1428:LEU:HD13	1:A:1585:LYS:HE2	1.93	0.50
1:A:3051:ARG:HH22	1:A:3102:ASP:HB2	1.75	0.50
1:A:3107:VAL:HA	1:A:3175:LEU:HD21	1.94	0.50
1:C:1428:LEU:HD13	1:C:1585:LYS:HE2	1.92	0.50
1:C:2755:ILE:HG23	1:C:2813:LEU:HB2	1.93	0.50
1:G:3770:LEU:HD12	1:G:3804:ILE:HD11	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4088:ILE:HG23	1:G:4123:ILE:HG22	1.92	0.50
4:G:5110:POV:H32	4:G:5110:POV:H13B	1.94	0.50
1:J:2257:LEU:HD13	1:J:2275:VAL:HG13	1.93	0.50
1:A:181:HIS:NE2	1:A:196:MET:HB2	2.27	0.50
1:A:2635:GLU:HA	1:A:2638:LYS:HZ3	1.77	0.50
1:A:3995:VAL:O	1:A:3999:MET:HB2	2.11	0.50
1:C:179:TYR:CB	1:C:197:GLN:HA	2.41	0.50
1:C:894:GLY:HA3	1:C:903:LEU:HD22	1.93	0.50
1:C:2960:LEU:HD23	1:C:2963:LEU:HD21	1.94	0.50
1:C:3539:ARG:HB3	1:C:3549:VAL:HG12	1.93	0.50
1:G:959:TYR:HD1	1:G:965:TYR:HA	1.75	0.50
1:G:1477:GLY:HA2	1:G:1484:HIS:H	1.77	0.50
1:G:2693:GLN:HG3	1:G:2697:ARG:HH21	1.77	0.50
1:J:2186:MET:HA	1:J:2186:MET:HE3	1.94	0.50
1:J:2211:MET:SD	1:J:2232:CYS:HB3	2.52	0.50
3:L:105:ASN:C	3:L:105:ASN:ND2	2.69	0.50
1:A:3153:GLY:O	1:A:3202:PRO:HG3	2.12	0.50
1:A:3943:ILE:HD11	1:A:4002:LYS:HE2	1.94	0.50
1:G:4769:MET:O	1:G:4769:MET:HE3	2.12	0.50
1:J:614:VAL:HG22	1:J:617:ASN:H	1.77	0.50
1:J:3245:VAL:O	1:J:3249:LEU:HD12	2.11	0.50
1:J:3539:ARG:HB3	1:J:3549:VAL:HG12	1.93	0.50
1:A:614:VAL:HG22	1:A:617:ASN:H	1.77	0.50
1:A:1477:GLY:HA2	1:A:1484:HIS:H	1.77	0.50
1:A:2615:ARG:HG2	1:A:2618:MET:HE3	1.94	0.50
1:A:3107:VAL:HG21	1:A:3171:SER:HB2	1.94	0.50
1:C:499:THR:HG23	1:C:502:HIS:H	1.76	0.50
1:C:614:VAL:HG22	1:C:617:ASN:H	1.77	0.50
1:C:3682:GLU:HA	1:C:3685:GLU:HB3	1.93	0.50
1:G:2823:ILE:HD11	1:G:2935:TYR:HB3	1.94	0.50
1:G:3943:ILE:HD11	1:G:4002:LYS:HE2	1.94	0.50
1:G:3995:VAL:O	1:G:3999:MET:HB2	2.11	0.50
1:J:2823:ILE:HD11	1:J:2935:TYR:HB3	1.94	0.50
1:J:3943:ILE:HD11	1:J:4002:LYS:HE2	1.94	0.50
1:A:2186:MET:HE3	1:A:2186:MET:HA	1.94	0.49
1:A:2211:MET:HA	1:A:2211:MET:HE3	1.94	0.49
1:C:960:MET:O	1:C:961:MET:C	2.55	0.49
1:C:1439:VAL:HG21	1:C:1448:VAL:HG11	1.94	0.49
1:C:1527:MET:HE2	1:C:1540:PHE:HB2	1.94	0.49
1:C:3211:ASN:HD22	1:C:3236:VAL:HG23	1.77	0.49
3:I:105:ASN:C	3:I:105:ASN:ND2	2.69	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:2347:GLU:H	1:J:2347:GLU:CD	2.19	0.49
1:J:3038:MET:C	1:J:3038:MET:HE2	2.36	0.49
1:J:3211:ASN:HD22	1:J:3236:VAL:HG23	1.77	0.49
1:A:3770:LEU:HD12	1:A:3804:ILE:HD11	1.93	0.49
1:C:1450:VAL:HA	1:C:1552:VAL:HG12	1.94	0.49
1:C:1802:ILE:HD13	1:C:1807:LEU:HD11	1.93	0.49
1:C:3007:ASN:HB2	1:C:3067:CYS:SG	2.51	0.49
1:C:3056:LEU:HD23	1:C:3056:LEU:H	1.76	0.49
1:C:3107:VAL:HG21	1:C:3171:SER:HB2	1.94	0.49
1:C:3943:ILE:HD11	1:C:4002:LYS:HE2	1.94	0.49
3:E:105:ASN:ND2	3:E:105:ASN:O	2.35	0.49
1:G:990:GLU:CD	1:G:1024:TYR:HB3	2.38	0.49
1:G:2211:MET:HA	1:G:2211:MET:HE3	1.94	0.49
1:J:990:GLU:CD	1:J:1024:TYR:HB3	2.37	0.49
1:J:1450:VAL:HA	1:J:1552:VAL:HG12	1.94	0.49
1:J:3353:LEU:HG	1:J:3358:PHE:HE1	1.76	0.49
1:A:2693:GLN:HG3	1:A:2697:ARG:HH21	1.77	0.49
1:A:2960:LEU:HD23	1:A:2963:LEU:HD21	1.94	0.49
1:C:2211:MET:HA	1:C:2211:MET:HE3	1.94	0.49
1:C:2770:LYS:HD3	1:C:2788:HIS:H	1.76	0.49
1:G:614:VAL:HG22	1:G:617:ASN:H	1.77	0.49
1:G:2770:LYS:HD3	1:G:2788:HIS:H	1.76	0.49
1:G:3107:VAL:HA	1:G:3175:LEU:HD21	1.94	0.49
1:J:274:LEU:HD13	1:J:280:LEU:HD22	1.95	0.49
1:J:1439:VAL:HG21	1:J:1448:VAL:HG11	1.94	0.49
1:J:2211:MET:HE3	1:J:2211:MET:HA	1.94	0.49
1:J:2615:ARG:HG2	1:J:2618:MET:HE3	1.94	0.49
1:J:3007:ASN:HB2	1:J:3067:CYS:SG	2.51	0.49
1:G:3353:LEU:HG	1:G:3358:PHE:HE1	1.76	0.49
1:J:1802:ILE:HD13	1:J:1807:LEU:HD11	1.93	0.49
1:J:3995:VAL:O	1:J:3999:MET:HB2	2.12	0.49
1:A:2208:MET:O	1:A:2212:VAL:HG23	2.13	0.49
1:A:2431:ASP:HB2	1:A:2501:SER:HB2	1.93	0.49
1:A:4769:MET:O	1:A:4769:MET:HE3	2.12	0.49
1:C:894:GLY:O	1:C:903:LEU:HB3	2.12	0.49
1:C:1297:PHE:HE1	1:C:1548:LEU:HD12	1.77	0.49
1:G:2584:HIS:CE1	1:G:2588:ARG:HH22	2.31	0.49
1:G:4957:LYS:HG2	1:G:4964:GLY:HA2	1.95	0.49
1:J:1297:PHE:HE1	1:J:1548:LEU:HD12	1.77	0.49
1:J:2380:ILE:O	1:J:2384:ILE:HG12	2.13	0.49
1:J:3056:LEU:HD23	1:J:3056:LEU:H	1.76	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:3967:GLU:HA	1:J:3970:GLN:HG2	1.93	0.49
1:A:179:TYR:CB	1:A:197:GLN:HA	2.43	0.49
1:A:2195:PRO:HB3	1:A:2242:ILE:CG2	2.41	0.49
1:C:2431:ASP:HB2	1:C:2501:SER:HB2	1.94	0.49
1:C:3967:GLU:HA	1:C:3970:GLN:HG2	1.93	0.49
1:C:4978:HIS:HA	1:C:4982:GLU:HG3	1.95	0.49
1:G:38:ALA:HB1	1:G:64:ILE:HG13	1.94	0.49
1:G:2208:MET:O	1:G:2212:VAL:HG23	2.13	0.49
1:J:45:ARG:NE	1:J:116:MET:HE1	2.28	0.49
1:J:953:THR:O	1:J:969:PRO:HG3	2.12	0.49
1:J:3153:GLY:O	1:J:3202:PRO:HG3	2.12	0.49
4:J:5113:POV:H32	4:J:5113:POV:H13B	1.94	0.49
1:A:614:VAL:HG11	1:A:617:ASN:HD22	1.78	0.49
1:A:1802:ILE:HD13	1:A:1807:LEU:HD11	1.93	0.49
1:A:3435:PHE:CD2	1:A:3521:GLY:HA3	2.48	0.49
1:A:4744:ASP:HB3	1:A:4747:SER:HB3	1.95	0.49
1:C:3107:VAL:HA	1:C:3175:LEU:HD21	1.94	0.49
1:C:4769:MET:O	1:C:4769:MET:HE3	2.12	0.49
1:G:1297:PHE:HE1	1:G:1548:LEU:HD12	1.77	0.49
1:G:2265:LEU:HB2	1:G:2330:ARG:HD2	1.94	0.49
1:G:4978:HIS:HA	1:G:4982:GLU:HG3	1.95	0.49
1:J:1477:GLY:HA2	1:J:1484:HIS:H	1.77	0.49
1:A:2380:ILE:O	1:A:2384:ILE:HG12	2.13	0.49
1:C:3153:GLY:O	1:C:3202:PRO:HG3	2.12	0.49
2:D:59:TYR:HD2	2:D:63:VAL:HG11	1.78	0.49
1:G:3183:VAL:O	1:G:3187:ARG:HG3	2.12	0.49
1:J:1979:LEU:HG	1:J:1982:ARG:HH21	1.78	0.49
1:J:2208:MET:O	1:J:2212:VAL:HG23	2.13	0.49
1:J:2265:LEU:HB2	1:J:2330:ARG:HD2	1.94	0.49
1:J:3107:VAL:HA	1:J:3175:LEU:HD21	1.94	0.49
2:K:59:TYR:HD2	2:K:63:VAL:HG11	1.78	0.49
1:A:1527:MET:HE2	1:A:1540:PHE:HB2	1.94	0.49
1:A:3140:LEU:HG	1:A:3144:PHE:CE2	2.48	0.49
4:A:5112:POV:H13B	4:A:5112:POV:H32	1.94	0.49
1:C:2380:ILE:O	1:C:2384:ILE:HG12	2.13	0.49
1:C:4957:LYS:HG2	1:C:4964:GLY:HA2	1.95	0.49
4:C:5109:POV:H32	4:C:5109:POV:H13B	1.94	0.49
1:G:2615:ARG:HG2	1:G:2618:MET:HE3	1.94	0.49
1:J:3183:VAL:O	1:J:3187:ARG:HG3	2.12	0.49
1:J:3435:PHE:CD2	1:J:3521:GLY:HA3	2.48	0.49
1:A:75:VAL:O	1:A:78:LEU:HB3	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1297:PHE:HE1	1:A:1548:LEU:HD12	1.78	0.49
1:A:3353:LEU:HG	1:A:3358:PHE:HE1	1.76	0.49
1:A:4978:HIS:HA	1:A:4982:GLU:HG3	1.95	0.49
1:C:3435:PHE:CD2	1:C:3521:GLY:HA3	2.48	0.49
1:G:75:VAL:O	1:G:78:LEU:HB3	2.13	0.49
1:G:3107:VAL:HG21	1:G:3171:SER:HB2	1.94	0.49
1:J:614:VAL:HG11	1:J:617:ASN:HD22	1.78	0.49
1:J:2693:GLN:HG3	1:J:2697:ARG:HH21	1.77	0.49
1:J:3592:ILE:HG12	1:J:3595:ARG:HH21	1.78	0.49
1:J:4744:ASP:HB3	1:J:4747:SER:HB3	1.95	0.49
1:J:4978:HIS:HA	1:J:4982:GLU:HG3	1.95	0.49
1:A:274:LEU:HD13	1:A:280:LEU:HD22	1.95	0.48
1:A:652:ARG:HB2	1:A:750:LEU:HD13	1.95	0.48
1:A:842:PRO:HD3	1:A:1073:ARG:HB2	1.95	0.48
1:A:3592:ILE:HG12	1:A:3595:ARG:HH21	1.78	0.48
1:C:652:ARG:HB2	1:C:750:LEU:HD13	1.95	0.48
1:C:2186:MET:HA	1:C:2186:MET:HE3	1.94	0.48
1:C:2823:ILE:HD11	1:C:2935:TYR:HB3	1.94	0.48
1:C:3353:LEU:HG	1:C:3358:PHE:HE1	1.76	0.48
3:F:26:TYR:HB3	3:F:101:VAL:HG12	1.95	0.48
1:G:1439:VAL:HG21	1:G:1448:VAL:HG11	1.94	0.48
1:G:1979:LEU:HG	1:G:1982:ARG:HH21	1.78	0.48
1:G:3211:ASN:HD22	1:G:3236:VAL:HG23	1.77	0.48
2:H:59:TYR:HD2	2:H:63:VAL:HG11	1.78	0.48
1:J:2431:ASP:HB2	1:J:2501:SER:HB2	1.94	0.48
1:J:3140:LEU:HG	1:J:3144:PHE:CE2	2.48	0.48
1:A:157:ARG:HH21	1:A:164:ARG:HG3	1.78	0.48
1:C:614:VAL:HG11	1:C:617:ASN:HD22	1.78	0.48
1:C:3354:LEU:HA	1:C:3358:PHE:HD1	1.78	0.48
1:C:4744:ASP:HB3	1:C:4747:SER:HB3	1.95	0.48
1:C:4936:ILE:HD12	1:J:4927:ILE:HD11	1.96	0.48
1:G:2380:ILE:O	1:G:2384:ILE:HG12	2.13	0.48
1:J:38:ALA:HB1	1:J:64:ILE:HG13	1.94	0.48
1:J:842:PRO:HD3	1:J:1073:ARG:HB2	1.95	0.48
1:J:2883:HIS:ND1	1:J:2908:TYR:HB2	2.23	0.48
1:A:38:ALA:HB1	1:A:64:ILE:HG13	1.94	0.48
1:A:1439:VAL:HG21	1:A:1448:VAL:HG11	1.94	0.48
1:A:1729:SER:O	1:A:1730:MET:HG2	2.14	0.48
1:A:2211:MET:SD	1:A:2232:CYS:HB3	2.53	0.48
1:A:2584:HIS:CE1	1:A:2588:ARG:HH22	2.31	0.48
1:A:2823:ILE:HD11	1:A:2935:TYR:HB3	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3211:ASN:HD22	1:A:3236:VAL:HG23	1.77	0.48
1:A:4577:LEU:HD13	1:A:4807:PHE:HD1	1.79	0.48
1:C:1979:LEU:HG	1:C:1982:ARG:HH21	1.78	0.48
1:C:2102:VAL:HG13	1:C:2120:MET:HB2	1.96	0.48
1:C:4577:LEU:HD13	1:C:4807:PHE:HD1	1.79	0.48
1:G:45:ARG:NE	1:G:116:MET:HE1	2.28	0.48
1:G:2635:GLU:HA	1:G:2638:LYS:HZ3	1.78	0.48
1:J:1729:SER:O	1:J:1730:MET:HG2	2.14	0.48
1:J:2102:VAL:HG13	1:J:2120:MET:HB2	1.96	0.48
1:J:3514:LEU:HD11	1:J:3602:VAL:HG13	1.94	0.48
1:J:4696:ASP:O	1:J:4700:GLN:HG2	2.14	0.48
1:A:1071:ARG:HG2	1:A:1196:PRO:HD3	1.95	0.48
1:A:2866:THR:HA	1:A:2928:LYS:HZ2	1.78	0.48
1:C:274:LEU:HD13	1:C:280:LEU:HD22	1.95	0.48
1:G:1071:ARG:HG2	1:G:1196:PRO:HD3	1.96	0.48
1:G:2186:MET:HA	1:G:2186:MET:HE3	1.94	0.48
1:G:3153:GLY:O	1:G:3202:PRO:HG3	2.12	0.48
1:G:3996:PHE:HZ	1:G:4019:LEU:HG	1.78	0.48
1:J:181:HIS:CD2	1:J:196:MET:HB2	2.48	0.48
1:J:966:LYS:N	1:J:967:PRO:HD3	2.27	0.48
1:A:45:ARG:NE	1:A:116:MET:HE1	2.28	0.48
1:A:698:GLY:H	1:A:1636:MET:HE1	1.79	0.48
1:C:38:ALA:HB1	1:C:64:ILE:HG13	1.94	0.48
1:C:3183:VAL:O	1:C:3187:ARG:HG3	2.12	0.48
1:C:3592:ILE:HG12	1:C:3595:ARG:HH21	1.78	0.48
1:C:3850:GLN:HE22	1:C:3872:GLU:HA	1.79	0.48
1:G:1802:ILE:HD13	1:G:1807:LEU:HD11	1.93	0.48
1:G:3140:LEU:HG	1:G:3144:PHE:CE2	2.48	0.48
3:I:26:TYR:HB3	3:I:101:VAL:HG12	1.95	0.48
1:J:75:VAL:O	1:J:78:LEU:HB3	2.13	0.48
1:J:232:THR:HG22	1:J:258:SER:HB3	1.96	0.48
1:J:404:ILE:HD13	1:J:481:GLU:HG3	1.95	0.48
1:J:2584:HIS:CE1	1:J:2588:ARG:HH22	2.31	0.48
1:J:3680:ALA:HB1	1:J:3683:GLN:HG2	1.96	0.48
1:A:2203:MET:HG3	1:A:2235:PHE:HZ	1.78	0.48
1:A:2265:LEU:HB2	1:A:2330:ARG:HD2	1.94	0.48
1:A:3850:GLN:HE22	1:A:3872:GLU:HA	1.79	0.48
1:A:3996:PHE:HZ	1:A:4019:LEU:HG	1.78	0.48
2:B:59:TYR:HD2	2:B:63:VAL:HG11	1.78	0.48
1:C:75:VAL:O	1:C:78:LEU:HB3	2.13	0.48
1:C:1071:ARG:HG2	1:C:1196:PRO:HD3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2265:LEU:HB2	1:C:2330:ARG:HD2	1.94	0.48
1:C:4696:ASP:O	1:C:4700:GLN:HG2	2.14	0.48
1:G:79:GLN:HA	1:G:82:LEU:HD12	1.96	0.48
1:G:2431:ASP:HB2	1:G:2501:SER:HB2	1.93	0.48
1:G:3066:ASN:O	1:G:3070:ILE:HG12	2.14	0.48
1:G:3435:PHE:CD2	1:G:3521:GLY:HA3	2.48	0.48
1:G:3680:ALA:HB1	1:G:3683:GLN:HG2	1.96	0.48
1:G:4577:LEU:HD13	1:G:4807:PHE:HD1	1.79	0.48
1:G:4744:ASP:HB3	1:G:4747:SER:HB3	1.95	0.48
1:J:1071:ARG:HG2	1:J:1196:PRO:HD3	1.95	0.48
1:J:3354:LEU:HA	1:J:3358:PHE:HD1	1.79	0.48
1:J:3850:GLN:HE22	1:J:3872:GLU:HA	1.79	0.48
1:J:4577:LEU:HD13	1:J:4807:PHE:HD1	1.78	0.48
1:A:232:THR:HG22	1:A:258:SER:HB3	1.96	0.48
1:C:842:PRO:HD3	1:C:1073:ARG:HB2	1.95	0.48
1:C:1301:PHE:CG	1:C:1544:PRO:HG3	2.49	0.48
1:C:2693:GLN:HG3	1:C:2697:ARG:HH21	1.77	0.48
1:G:274:LEU:HD13	1:G:280:LEU:HD22	1.95	0.48
1:G:2233:CYS:O	1:G:2234:ARG:C	2.57	0.48
1:G:4696:ASP:O	1:G:4700:GLN:HG2	2.14	0.48
1:J:157:ARG:HH21	1:J:164:ARG:HG3	1.78	0.48
1:J:954:LYS:HB2	1:J:967:PRO:HA	1.96	0.48
1:J:3209:GLN:CD	1:J:3209:GLN:H	2.21	0.48
1:J:4957:LYS:HG2	1:J:4964:GLY:HA2	1.95	0.48
4:J:5101:POV:H21A	4:J:5102:POV:H313	1.95	0.48
1:A:3183:VAL:O	1:A:3187:ARG:HG3	2.12	0.48
1:C:2584:HIS:CE1	1:C:2588:ARG:HH22	2.31	0.48
1:C:2952:GLU:HG2	1:C:2961:GLN:HE22	1.78	0.48
1:G:698:GLY:H	1:G:1636:MET:HE1	1.79	0.48
1:G:984:LEU:HD21	1:G:1056:PRO:HD2	1.95	0.48
1:J:3107:VAL:HG21	1:J:3171:SER:HB2	1.94	0.48
1:A:1979:LEU:HG	1:A:1982:ARG:HH21	1.78	0.48
1:C:45:ARG:NE	1:C:116:MET:HE1	2.28	0.48
1:C:698:GLY:H	1:C:1636:MET:HE1	1.79	0.48
1:C:3996:PHE:HZ	1:C:4019:LEU:HG	1.78	0.48
1:G:4733:GLY:O	1:G:4737:ILE:HG12	2.14	0.48
4:G:5112:POV:H21A	4:G:5113:POV:H313	1.95	0.48
1:J:3066:ASN:O	1:J:3070:ILE:HG12	2.14	0.48
3:L:26:TYR:HB3	3:L:101:VAL:HG12	1.95	0.48
1:A:2922:LYS:O	1:A:2925:GLU:HG3	2.14	0.48
1:A:3680:ALA:HB1	1:A:3683:GLN:HG2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1729:SER:O	1:C:1730:MET:HG2	2.14	0.48
1:C:2922:LYS:O	1:C:2925:GLU:HG3	2.14	0.48
3:E:26:TYR:HB3	3:E:101:VAL:HG12	1.95	0.48
1:G:232:THR:HG22	1:G:258:SER:HB3	1.96	0.48
1:G:842:PRO:HD3	1:G:1073:ARG:HB2	1.95	0.48
1:J:698:GLY:H	1:J:1636:MET:HE1	1.79	0.48
1:J:1179:PHE:HB2	1:J:1182:ILE:HD11	1.96	0.48
1:J:2233:CYS:O	1:J:2237:CYS:N	2.39	0.48
1:A:404:ILE:HD13	1:A:481:GLU:HG3	1.95	0.47
4:A:5114:POV:H21A	4:A:5115:POV:H313	1.95	0.47
1:C:3209:GLN:H	1:C:3209:GLN:CD	2.21	0.47
1:C:4844:LEU:HD11	1:C:4924:VAL:HG13	1.96	0.47
1:G:1729:SER:O	1:G:1730:MET:HG2	2.14	0.47
1:J:1301:PHE:CG	1:J:1544:PRO:HG3	2.49	0.47
1:J:2669:GLU:HG2	1:J:2714:TYR:HE1	1.79	0.47
1:J:4733:GLY:O	1:J:4737:ILE:HG12	2.14	0.47
1:A:357:LEU:HD23	1:A:357:LEU:H	1.79	0.47
1:A:1969:LEU:HD12	1:A:2009:LEU:HD13	1.96	0.47
4:A:5107:POV:H21A	4:C:5111:POV:H313	1.95	0.47
2:B:82:MET:HG3	2:B:84:SER:O	2.14	0.47
1:C:1000:ARG:NH2	2:D:115:ASP:H	2.11	0.47
1:C:2208:MET:O	1:C:2212:VAL:HG23	2.13	0.47
1:C:2758:PHE:HA	1:C:2761:TYR:HB3	1.97	0.47
1:C:3066:ASN:O	1:C:3070:ILE:HG12	2.14	0.47
1:C:3680:ALA:HB1	1:C:3683:GLN:HG2	1.96	0.47
3:F:82:TYR:HB2	3:F:86:GLY:HA2	1.96	0.47
1:J:2758:PHE:HA	1:J:2761:TYR:HB3	1.97	0.47
1:J:5009:TYR:O	1:J:5013:MET:HG2	2.14	0.47
1:A:1424:PRO:HA	1:A:1427:ILE:HG22	1.97	0.47
1:A:2669:GLU:HG2	1:A:2714:TYR:HE1	1.79	0.47
1:A:3564:GLU:HA	1:A:3570:ARG:HH12	1.80	0.47
1:C:404:ILE:HD13	1:C:481:GLU:HG3	1.95	0.47
1:C:1283:LEU:HD23	1:C:1283:LEU:H	1.80	0.47
1:C:3140:LEU:HG	1:C:3144:PHE:CE2	2.48	0.47
2:D:69:ILE:HB	2:D:80:LEU:HD13	1.96	0.47
1:G:357:LEU:H	1:G:357:LEU:HD23	1.79	0.47
1:G:614:VAL:HG11	1:G:617:ASN:HD22	1.78	0.47
1:G:3752:SER:O	1:G:3756:LYS:HG3	2.14	0.47
1:J:2512:ILE:HG21	1:J:2518:LEU:HD13	1.97	0.47
1:J:2922:LYS:O	1:J:2925:GLU:HG3	2.14	0.47
1:J:2960:LEU:HA	1:J:2963:LEU:HG	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:3009:TYR:HE1	1:J:3017:PHE:HZ	1.63	0.47
1:J:4231:MET:HE3	1:J:4231:MET:HA	1.97	0.47
3:L:105:ASN:ND2	3:L:105:ASN:O	2.35	0.47
1:A:2952:GLU:HG2	1:A:2961:GLN:HE22	1.79	0.47
1:C:357:LEU:HD23	1:C:357:LEU:H	1.79	0.47
1:C:3511:VAL:HG21	1:C:3609:THR:HG21	1.95	0.47
1:C:3564:GLU:HA	1:C:3570:ARG:HH12	1.80	0.47
1:C:3752:SER:O	1:C:3756:LYS:HG3	2.14	0.47
1:C:5009:TYR:O	1:C:5013:MET:HG2	2.14	0.47
1:G:920:TYR:HE2	2:H:106:PRO:HD2	1.80	0.47
1:G:1301:PHE:CG	1:G:1544:PRO:HG3	2.49	0.47
1:G:2669:GLU:HG2	1:G:2714:TYR:HE1	1.79	0.47
1:G:2737:PRO:HB3	1:G:2884:ASN:HA	1.96	0.47
1:G:2952:GLU:HG2	1:G:2961:GLN:HE22	1.79	0.47
1:G:3209:GLN:CD	1:G:3209:GLN:H	2.21	0.47
1:G:3354:LEU:HA	1:G:3358:PHE:HD1	1.78	0.47
1:G:3850:GLN:HE22	1:G:3872:GLU:HA	1.79	0.47
1:G:5009:TYR:O	1:G:5013:MET:HG2	2.14	0.47
1:J:652:ARG:HB2	1:J:750:LEU:HD13	1.95	0.47
1:A:79:GLN:HA	1:A:82:LEU:HD12	1.96	0.47
1:A:4733:GLY:O	1:A:4737:ILE:HG12	2.14	0.47
1:A:4927:ILE:HD11	1:G:4936:ILE:HD12	1.97	0.47
1:A:4957:LYS:HG2	1:A:4964:GLY:HA2	1.95	0.47
1:C:1424:PRO:HA	1:C:1427:ILE:HG22	1.97	0.47
1:C:2737:PRO:HB3	1:C:2884:ASN:HA	1.96	0.47
1:C:4162:ASN:O	1:C:4166:LEU:HG	2.15	0.47
1:G:157:ARG:HH21	1:G:164:ARG:HG3	1.78	0.47
1:G:404:ILE:HD13	1:G:481:GLU:HG3	1.95	0.47
1:G:3009:TYR:HE1	1:G:3017:PHE:HZ	1.63	0.47
1:J:1128:ARG:HD2	1:J:1130:GLN:HE21	1.80	0.47
1:A:1301:PHE:CG	1:A:1544:PRO:HG3	2.49	0.47
1:A:1939:MET:HE3	1:A:1939:MET:HB2	1.72	0.47
1:A:2512:ILE:HG21	1:A:2518:LEU:HD13	1.97	0.47
1:A:2667:THR:HG21	1:A:2672:LEU:HD21	1.96	0.47
1:A:3409:TYR:HB2	1:A:3509:LEU:HD21	1.96	0.47
1:A:3729:MET:HE1	1:A:3778:MET:HE1	1.96	0.47
1:A:4104:THR:O	1:A:4108:ILE:HG13	2.14	0.47
2:B:69:ILE:HB	2:B:80:LEU:HD13	1.96	0.47
1:C:157:ARG:HH21	1:C:164:ARG:HG3	1.78	0.47
1:C:219:VAL:HG21	1:C:398:SER:HB2	1.96	0.47
1:C:892:THR:N	1:C:902:ARG:O	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1128:ARG:HD2	1:C:1130:GLN:HE21	1.80	0.47
1:C:2211:MET:SD	1:C:2232:CYS:HB3	2.55	0.47
1:C:3409:TYR:CB	1:C:3509:LEU:HD11	2.43	0.47
1:G:1424:PRO:HA	1:G:1427:ILE:HG22	1.97	0.47
1:G:2102:VAL:HG13	1:G:2120:MET:HB2	1.96	0.47
1:G:3885:PHE:HE1	1:G:3919:THR:HG23	1.80	0.47
1:J:79:GLN:HA	1:J:82:LEU:HD12	1.96	0.47
1:J:2737:PRO:HB3	1:J:2884:ASN:HA	1.96	0.47
1:J:3018:LEU:HD21	1:J:3150:HIS:NE2	2.30	0.47
1:J:3996:PHE:HZ	1:J:4019:LEU:HG	1.78	0.47
1:J:4104:THR:O	1:J:4108:ILE:HG13	2.14	0.47
1:J:4912:TYR:CD1	4:J:5101:POV:H25	2.49	0.47
1:A:659:TYR:HB2	1:A:1017:ARG:HH12	1.79	0.47
1:A:2241:ARG:O	1:A:2242:ILE:C	2.57	0.47
1:A:2737:PRO:HB3	1:A:2884:ASN:HA	1.96	0.47
1:A:3354:LEU:HA	1:A:3358:PHE:HD1	1.79	0.47
1:A:4648:LEU:HG	4:A:5105:POV:H27A	1.97	0.47
1:A:4696:ASP:O	1:A:4700:GLN:HG2	2.14	0.47
1:C:2336:ARG:HB3	1:C:2435:ARG:HH11	1.80	0.47
1:C:2512:ILE:HG21	1:C:2518:LEU:HD13	1.97	0.47
1:C:3536:ALA:HA	1:C:3539:ARG:NE	2.30	0.47
1:C:4733:GLY:O	1:C:4737:ILE:HG12	2.14	0.47
3:F:4:ILE:HG23	3:F:72:ALA:HB1	1.97	0.47
3:F:56:ILE:HG22	3:F:59:PHE:H	1.80	0.47
1:G:652:ARG:HB2	1:G:750:LEU:HD13	1.95	0.47
1:G:1741:GLU:O	1:G:1745:ILE:HG13	2.15	0.47
1:G:2667:THR:HG21	1:G:2672:LEU:HD21	1.96	0.47
1:G:2722:LYS:HD3	1:G:2877:GLN:HG2	1.97	0.47
1:G:3018:LEU:HD21	1:G:3150:HIS:NE2	2.30	0.47
1:G:3062:PRO:HA	1:G:3065:VAL:HG22	1.97	0.47
1:G:3564:GLU:HA	1:G:3570:ARG:HH12	1.80	0.47
1:G:3592:ILE:HG12	1:G:3595:ARG:HH21	1.78	0.47
2:H:4:LEU:HA	2:H:23:THR:O	2.15	0.47
2:H:82:MET:HG3	2:H:84:SER:O	2.14	0.47
3:I:56:ILE:HG22	3:I:59:PHE:H	1.80	0.47
1:J:45:ARG:NH1	1:J:443:LEU:HD11	2.30	0.47
1:J:181:HIS:NE2	1:J:196:MET:HB2	2.30	0.47
1:J:357:LEU:H	1:J:357:LEU:HD23	1.79	0.47
1:J:2233:CYS:O	1:J:2234:ARG:C	2.58	0.47
1:J:2238:TYR:O	1:J:2242:ILE:HG12	2.15	0.47
1:J:2952:GLU:HG2	1:J:2961:GLN:HE22	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:3062:PRO:HA	1:J:3065:VAL:HG22	1.97	0.47
1:J:3536:ALA:HA	1:J:3539:ARG:NE	2.30	0.47
2:K:69:ILE:HB	2:K:80:LEU:HD13	1.96	0.47
1:A:219:VAL:HG21	1:A:398:SER:HB2	1.96	0.47
1:A:3066:ASN:O	1:A:3070:ILE:HG12	2.14	0.47
1:A:3209:GLN:H	1:A:3209:GLN:CD	2.21	0.47
1:A:3935:TRP:CZ3	1:C:76:ARG:HB3	2.50	0.47
1:C:210:GLU:HG3	1:C:213:TYR:HB2	1.97	0.47
1:C:2608:MET:HA	1:C:2643:LEU:HD13	1.97	0.47
1:C:2960:LEU:HA	1:C:2963:LEU:HG	1.96	0.47
1:G:682:LEU:HG	1:G:738:LEU:HD12	1.96	0.47
1:G:2512:ILE:HG21	1:G:2518:LEU:HD13	1.97	0.47
1:G:2908:TYR:CZ	1:G:2916:LYS:HE2	2.50	0.47
1:J:3003:LEU:HB3	1:J:3004:PRO:HD3	1.97	0.47
1:J:3868:ARG:HH12	1:J:3869:GLN:HB3	1.80	0.47
1:A:109:LEU:HD12	1:A:118:LEU:HD23	1.97	0.47
1:A:1078:GLU:HB3	1:A:1081:TYR:CD2	2.50	0.47
1:A:2102:VAL:HG13	1:A:2120:MET:HB2	1.96	0.47
1:A:3868:ARG:HH12	1:A:3869:GLN:HB3	1.80	0.47
1:A:4162:ASN:O	1:A:4166:LEU:HG	2.15	0.47
1:C:232:THR:HG22	1:C:258:SER:HB3	1.96	0.47
1:C:1969:LEU:HD12	1:C:2009:LEU:HD13	1.96	0.47
1:C:2582:MET:HE3	1:C:2582:MET:HB3	1.86	0.47
1:G:659:TYR:HB2	1:G:1017:ARG:HH12	1.80	0.47
1:G:2922:LYS:O	1:G:2925:GLU:HG3	2.14	0.47
1:G:3868:ARG:HH12	1:G:3869:GLN:HB3	1.80	0.47
1:J:1283:LEU:HD23	1:J:1283:LEU:H	1.80	0.47
1:J:1969:LEU:HD12	1:J:2009:LEU:HD13	1.96	0.47
1:J:3885:PHE:HE1	1:J:3919:THR:HG23	1.80	0.47
1:J:5013:MET:HE2	1:J:5013:MET:HB3	1.74	0.47
2:K:107:TRP:HB3	2:K:111:ASN:HB3	1.97	0.47
1:A:892:THR:N	1:A:902:ARG:O	2.48	0.47
1:A:1128:ARG:HD2	1:A:1130:GLN:HE21	1.80	0.47
1:A:3003:LEU:HB3	1:A:3004:PRO:HD3	1.97	0.47
1:A:3209:GLN:HE22	1:A:3245:VAL:HG21	1.80	0.47
1:A:3533:ILE:O	1:A:3537:LYS:HG3	2.15	0.47
1:C:1023:PRO:HB3	1:C:1025:ARG:HH21	1.80	0.47
1:C:2722:LYS:HD3	1:C:2877:GLN:HG2	1.97	0.47
1:C:3868:ARG:HH12	1:C:3869:GLN:HB3	1.80	0.47
1:C:3885:PHE:HE1	1:C:3919:THR:HG23	1.80	0.47
1:C:4104:THR:O	1:C:4108:ILE:HG13	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1128:ARG:HD2	1:G:1130:GLN:HE21	1.80	0.47
1:G:1756:ASN:HA	1:G:1759:ARG:HB2	1.97	0.47
1:G:2758:PHE:HA	1:G:2761:TYR:HB3	1.97	0.47
1:G:3442:PHE:HE1	1:G:3511:VAL:HG22	1.80	0.47
3:I:4:ILE:HD11	3:I:62:GLY:HA2	1.97	0.47
1:J:2722:LYS:HD3	1:J:2877:GLN:HG2	1.97	0.47
1:J:4834:GLY:O	1:J:4838:VAL:HG22	2.15	0.47
3:L:56:ILE:HG22	3:L:59:PHE:H	1.80	0.47
1:A:45:ARG:NH1	1:A:443:LEU:HD11	2.30	0.46
1:A:993:HIS:CE1	1:A:996:TRP:HZ3	2.34	0.46
1:A:1741:GLU:O	1:A:1745:ILE:HG13	2.15	0.46
1:A:2960:LEU:HA	1:A:2963:LEU:HG	1.96	0.46
1:A:4834:GLY:O	1:A:4838:VAL:HG22	2.16	0.46
1:A:5009:TYR:O	1:A:5013:MET:HG2	2.14	0.46
2:B:4:LEU:HA	2:B:23:THR:O	2.15	0.46
1:C:79:GLN:HA	1:C:82:LEU:HD12	1.96	0.46
1:C:790:ARG:NH1	1:C:792:LEU:HD21	2.30	0.46
1:C:1078:GLU:HB3	1:C:1081:TYR:CD2	2.50	0.46
1:C:3003:LEU:HB3	1:C:3004:PRO:HD3	1.97	0.46
1:C:3209:GLN:HE22	1:C:3245:VAL:HG21	1.80	0.46
2:D:82:MET:HG3	2:D:84:SER:O	2.14	0.46
3:E:56:ILE:HG22	3:E:59:PHE:H	1.80	0.46
1:G:45:ARG:NH1	1:G:443:LEU:HD11	2.30	0.46
1:G:109:LEU:HD12	1:G:118:LEU:HD23	1.97	0.46
1:G:214:VAL:HG13	1:G:220:LEU:HD21	1.97	0.46
1:G:219:VAL:HG21	1:G:398:SER:HB2	1.96	0.46
1:G:3137:LEU:HD22	1:G:3189:ALA:HB1	1.97	0.46
1:G:4162:ASN:O	1:G:4166:LEU:HG	2.14	0.46
1:G:4231:MET:HA	1:G:4231:MET:HE3	1.97	0.46
2:H:107:TRP:HB3	2:H:111:ASN:HB3	1.97	0.46
1:J:733:PRO:HG2	1:J:762:CYS:HB3	1.97	0.46
1:J:920:TYR:HE2	2:K:106:PRO:HD2	1.80	0.46
1:J:1023:PRO:HB3	1:J:1025:ARG:HH21	1.81	0.46
1:J:3752:SER:O	1:J:3756:LYS:HG3	2.14	0.46
3:L:4:ILE:HG23	3:L:72:ALA:HB1	1.97	0.46
1:A:214:VAL:HG13	1:A:220:LEU:HD21	1.97	0.46
1:A:955:LEU:HD12	1:A:956:PRO:HD2	1.97	0.46
1:A:3752:SER:O	1:A:3756:LYS:HG3	2.14	0.46
1:A:3966:THR:HG22	1:A:4026:MET:HA	1.97	0.46
1:C:659:TYR:HB2	1:C:1017:ARG:HH12	1.79	0.46
1:C:950:LEU:HD11	1:C:972:LEU:HA	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3062:PRO:HA	1:C:3065:VAL:HG22	1.97	0.46
3:F:105:ASN:C	3:F:105:ASN:ND2	2.68	0.46
1:G:210:GLU:HG3	1:G:213:TYR:HB2	1.97	0.46
1:G:1078:GLU:HB3	1:G:1081:TYR:CD2	2.50	0.46
1:G:2336:ARG:HB3	1:G:2435:ARG:HH11	1.80	0.46
1:G:3019:SER:HB3	1:G:3030:HIS:HA	1.97	0.46
1:G:3077:ALA:HA	1:G:3080:VAL:HG12	1.97	0.46
1:G:3533:ILE:O	1:G:3537:LYS:HG3	2.15	0.46
1:G:4576:ILE:HG21	1:G:4643:LEU:HB2	1.97	0.46
1:G:4844:LEU:HD11	1:G:4924:VAL:HG13	1.96	0.46
1:G:4927:ILE:HD11	1:J:4936:ILE:HD12	1.97	0.46
1:J:31:GLU:HG3	1:J:33:LEU:HD21	1.98	0.46
1:J:3019:SER:HB3	1:J:3030:HIS:HA	1.97	0.46
3:L:4:ILE:HD11	3:L:62:GLY:HA2	1.97	0.46
1:A:682:LEU:HG	1:A:738:LEU:HD12	1.96	0.46
1:A:950:LEU:HD11	1:A:972:LEU:HA	1.97	0.46
1:A:2368:LEU:HD13	1:A:2460:LEU:HD12	1.98	0.46
4:A:5116:POV:H38	4:A:5116:POV:H311	1.68	0.46
1:C:214:VAL:HG13	1:C:220:LEU:HD21	1.97	0.46
1:C:2325:PRO:HB2	1:C:2421:ALA:HB1	1.98	0.46
1:C:3009:TYR:CZ	1:C:3013:HIS:HD2	2.33	0.46
2:D:17:SER:HA	2:D:83:ASN:HA	1.98	0.46
1:G:781:VAL:HG22	1:G:791:PHE:HE2	1.80	0.46
1:G:1076:ARG:HB3	1:G:1191:VAL:HG23	1.98	0.46
1:G:4104:THR:O	1:G:4108:ILE:HG13	2.14	0.46
1:J:1076:ARG:HB3	1:J:1191:VAL:HG23	1.98	0.46
1:J:1424:PRO:HA	1:J:1427:ILE:HG22	1.97	0.46
1:J:2667:THR:HG21	1:J:2672:LEU:HD21	1.96	0.46
1:J:3077:ALA:HA	1:J:3080:VAL:HG12	1.97	0.46
1:J:4728:HIS:HD2	1:J:4731:ILE:HD12	1.81	0.46
1:A:31:GLU:HG3	1:A:33:LEU:HD21	1.98	0.46
1:A:2758:PHE:HA	1:A:2761:TYR:HB3	1.97	0.46
1:A:2908:TYR:CZ	1:A:2916:LYS:HE2	2.50	0.46
1:A:4576:ILE:HG21	1:A:4643:LEU:HB2	1.97	0.46
1:A:4844:LEU:HD11	1:A:4924:VAL:HG13	1.96	0.46
1:A:4936:ILE:HD12	1:C:4927:ILE:HD11	1.97	0.46
1:C:682:LEU:HG	1:C:738:LEU:HD12	1.96	0.46
1:C:2927:LEU:HA	1:C:2930:LEU:HD12	1.97	0.46
1:C:3018:LEU:HD21	1:C:3150:HIS:NE2	2.30	0.46
1:C:3019:SER:HB3	1:C:3030:HIS:HA	1.97	0.46
1:G:1283:LEU:HD23	1:G:1283:LEU:H	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2960:LEU:HA	1:G:2963:LEU:HG	1.96	0.46
3:I:4:ILE:HG23	3:I:72:ALA:HB1	1.97	0.46
1:J:219:VAL:HG21	1:J:398:SER:HB2	1.96	0.46
1:J:3533:ILE:O	1:J:3537:LYS:HG3	2.15	0.46
1:J:4844:LEU:HD11	1:J:4924:VAL:HG13	1.96	0.46
2:K:4:LEU:HA	2:K:23:THR:O	2.15	0.46
1:A:733:PRO:HG2	1:A:762:CYS:HB3	1.96	0.46
1:A:1023:PRO:HB3	1:A:1025:ARG:HH21	1.80	0.46
1:A:1730:MET:HE2	1:A:1730:MET:HB3	1.77	0.46
1:A:1756:ASN:HA	1:A:1759:ARG:HB2	1.97	0.46
1:A:3009:TYR:HE1	1:A:3017:PHE:HZ	1.63	0.46
1:A:3062:PRO:HA	1:A:3065:VAL:HG22	1.97	0.46
1:A:4001:MET:HG3	1:A:4057:MET:HE2	1.97	0.46
1:C:2667:THR:HG21	1:C:2672:LEU:HD21	1.97	0.46
1:C:2908:TYR:CZ	1:C:2916:LYS:HE2	2.50	0.46
1:C:3009:TYR:HE1	1:C:3017:PHE:HZ	1.63	0.46
1:C:4803:HIS:CE1	4:C:5104:POV:H23A	2.51	0.46
1:G:993:HIS:CE1	1:G:996:TRP:HZ3	2.34	0.46
1:G:1730:MET:HE2	1:G:1730:MET:HB3	1.77	0.46
1:G:1969:LEU:HD12	1:G:2009:LEU:HD13	1.96	0.46
1:J:214:VAL:HG13	1:J:220:LEU:HD21	1.98	0.46
1:J:659:TYR:HB2	1:J:1017:ARG:HH12	1.79	0.46
1:J:2325:PRO:HB2	1:J:2421:ALA:HB1	1.98	0.46
1:J:2368:LEU:HD13	1:J:2460:LEU:HD12	1.98	0.46
1:J:3564:GLU:HA	1:J:3570:ARG:HH12	1.80	0.46
2:K:59:TYR:HB2	2:K:63:VAL:HG21	1.98	0.46
2:K:82:MET:HG3	2:K:84:SER:O	2.14	0.46
1:A:2325:PRO:HB2	1:A:2421:ALA:HB1	1.98	0.46
1:A:2998:PHE:HA	1:A:3002:LEU:HB2	1.98	0.46
1:A:3885:PHE:HE1	1:A:3919:THR:HG23	1.80	0.46
1:A:4728:HIS:HD2	1:A:4731:ILE:HD12	1.81	0.46
1:C:2669:GLU:HG2	1:C:2714:TYR:HE1	1.79	0.46
1:C:3533:ILE:O	1:C:3537:LYS:HG3	2.15	0.46
1:G:3003:LEU:HB3	1:G:3004:PRO:HD3	1.97	0.46
1:G:4728:HIS:HD2	1:G:4731:ILE:HD12	1.81	0.46
2:H:59:TYR:HB2	2:H:63:VAL:HG21	1.98	0.46
2:H:69:ILE:HB	2:H:80:LEU:HD13	1.96	0.46
1:J:1078:GLU:HB3	1:J:1081:TYR:HD2	1.81	0.46
1:J:1756:ASN:HA	1:J:1759:ARG:HB2	1.97	0.46
1:J:3209:GLN:HE22	1:J:3245:VAL:HG21	1.80	0.46
1:J:3966:THR:HG22	1:J:4026:MET:HA	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1432:THR:HG23	1:A:1572:ILE:HG23	1.98	0.46
1:A:2336:ARG:HB3	1:A:2435:ARG:HH11	1.80	0.46
1:A:3273:THR:HA	1:A:3276:MET:HG2	1.98	0.46
1:A:3514:LEU:HD11	1:A:3602:VAL:HG13	1.97	0.46
1:C:31:GLU:HG3	1:C:33:LEU:HD21	1.98	0.46
1:C:2368:LEU:HD13	1:C:2460:LEU:HD12	1.98	0.46
1:C:2866:THR:HA	1:C:2928:LYS:HZ2	1.81	0.46
2:D:4:LEU:HA	2:D:23:THR:O	2.15	0.46
3:E:4:ILE:HA	3:E:73:LYS:O	2.16	0.46
1:G:31:GLU:HG3	1:G:33:LEU:HD21	1.98	0.46
1:G:2368:LEU:HD13	1:G:2460:LEU:HD12	1.98	0.46
1:G:3729:MET:HE1	1:G:3778:MET:HE1	1.96	0.46
1:J:2908:TYR:CZ	1:J:2916:LYS:HE2	2.50	0.46
1:J:3009:TYR:CZ	1:J:3013:HIS:HD2	2.34	0.46
1:J:3137:LEU:HD22	1:J:3189:ALA:HB1	1.97	0.46
1:A:887:ILE:HG12	1:A:960:MET:SD	2.56	0.46
1:A:978:THR:HB	1:A:981:GLN:HG2	1.98	0.46
1:A:2608:MET:HA	1:A:2643:LEU:HD13	1.97	0.46
1:A:2722:LYS:HD3	1:A:2877:GLN:HG2	1.97	0.46
1:A:3009:TYR:CZ	1:A:3013:HIS:HD2	2.33	0.46
1:C:233:ILE:HD13	1:C:287:THR:HG21	1.98	0.46
1:C:470:SER:HA	1:C:473:ASN:HD21	1.80	0.46
1:C:733:PRO:HG2	1:C:762:CYS:HB3	1.97	0.46
1:C:1078:GLU:HB3	1:C:1081:TYR:HD2	1.81	0.46
1:C:1741:GLU:O	1:C:1745:ILE:HG13	2.15	0.46
1:C:3435:PHE:CG	1:C:3521:GLY:HA3	2.51	0.46
1:G:233:ILE:HD13	1:G:287:THR:HG21	1.98	0.46
1:G:1023:PRO:HB3	1:G:1025:ARG:HH21	1.80	0.46
1:G:1078:GLU:HB3	1:G:1081:TYR:HD2	1.81	0.46
1:G:3209:GLN:HE22	1:G:3245:VAL:HG21	1.80	0.46
1:J:168:ASP:HB3	1:J:199:LEU:HD12	1.98	0.46
1:J:470:SER:HA	1:J:473:ASN:ND2	2.31	0.46
1:J:892:THR:N	1:J:902:ARG:O	2.48	0.46
1:J:1470:ARG:HD3	1:J:1470:ARG:HA	1.72	0.46
1:J:2927:LEU:HA	1:J:2930:LEU:HD12	1.98	0.46
1:J:3729:MET:HE1	1:J:3778:MET:HE1	1.96	0.46
1:C:19:GLU:HB3	1:C:206:CYS:HB2	1.98	0.46
1:C:45:ARG:NH1	1:C:443:LEU:HD11	2.30	0.46
1:C:109:LEU:HD12	1:C:118:LEU:HD23	1.97	0.46
1:C:2754:PHE:HA	1:C:2757:LYS:HB3	1.98	0.46
1:C:2998:PHE:HA	1:C:3002:LEU:HB2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3273:THR:HA	1:C:3276:MET:HG2	1.98	0.46
1:C:3511:VAL:HG12	1:C:3515:LYS:HE3	1.97	0.46
1:C:3546:ASP:HA	1:C:3549:VAL:HG22	1.97	0.46
1:C:3966:THR:HG22	1:C:4026:MET:HA	1.97	0.46
1:C:4231:MET:HA	1:C:4231:MET:HE3	1.97	0.46
1:C:4834:GLY:O	1:C:4838:VAL:HG22	2.15	0.46
1:G:733:PRO:HG2	1:G:762:CYS:HB3	1.97	0.46
1:G:1432:THR:HG23	1:G:1572:ILE:HG23	1.98	0.46
1:G:2325:PRO:HB2	1:G:2421:ALA:HB1	1.98	0.46
1:G:2355:ARG:O	1:G:2359:ARG:HG2	2.16	0.46
1:G:2608:MET:HA	1:G:2643:LEU:HD13	1.97	0.46
1:G:3423:TRP:HB2	1:G:3520:ILE:HD12	1.98	0.46
1:G:3966:THR:HG22	1:G:4026:MET:HA	1.97	0.46
1:G:4001:MET:HG3	1:G:4057:MET:HE2	1.97	0.46
2:H:17:SER:HA	2:H:83:ASN:HA	1.97	0.46
1:J:1008:SER:HB2	1:J:1017:ARG:CZ	2.46	0.46
1:J:1078:GLU:HB3	1:J:1081:TYR:CD2	2.50	0.46
1:J:2336:ARG:HB3	1:J:2435:ARG:HH11	1.80	0.46
1:J:2902:HIS:HE1	1:J:2904:LEU:HB2	1.81	0.46
1:J:4750:ILE:HA	1:J:4753:HIS:HD2	1.81	0.46
1:A:210:GLU:HG3	1:A:213:TYR:HB2	1.97	0.46
1:A:470:SER:HA	1:A:473:ASN:ND2	2.31	0.46
1:A:920:TYR:HE2	2:B:106:PRO:HD2	1.80	0.46
1:A:990:GLU:CD	1:A:1024:TYR:HB3	2.41	0.46
1:A:1179:PHE:HB2	1:A:1182:ILE:HD11	1.97	0.46
1:A:1283:LEU:HD23	1:A:1283:LEU:H	1.80	0.46
1:A:2875:ALA:HB2	1:A:2927:LEU:HD22	1.98	0.46
1:A:2902:HIS:HE1	1:A:2904:LEU:HB2	1.81	0.46
2:B:59:TYR:HB2	2:B:63:VAL:HG21	1.98	0.46
1:C:1756:ASN:HA	1:C:1759:ARG:HB2	1.98	0.46
1:C:3729:MET:HE1	1:C:3778:MET:HE1	1.96	0.46
1:C:4001:MET:HG3	1:C:4057:MET:HE2	1.97	0.46
1:C:4576:ILE:HG21	1:C:4643:LEU:HB2	1.98	0.46
3:E:4:ILE:HG23	3:E:72:ALA:HB1	1.97	0.46
1:G:19:GLU:HB3	1:G:206:CYS:HB2	1.98	0.46
1:G:179:TYR:CB	1:G:197:GLN:HA	2.46	0.46
1:G:1008:SER:HB2	1:G:1017:ARG:CZ	2.46	0.46
1:G:2765:LYS:HA	1:G:2765:LYS:HD3	1.73	0.46
1:G:2998:PHE:HA	1:G:3002:LEU:HB2	1.98	0.46
1:J:210:GLU:HG3	1:J:213:TYR:HB2	1.97	0.46
1:J:470:SER:HA	1:J:473:ASN:HD21	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:659:TYR:HB2	1:J:1017:ARG:NH1	2.31	0.46
1:J:682:LEU:HG	1:J:738:LEU:HD12	1.96	0.46
1:J:1432:THR:HG23	1:J:1572:ILE:HG23	1.98	0.46
1:J:2754:PHE:HA	1:J:2757:LYS:HB3	1.98	0.46
1:A:898:ASP:H	1:A:903:LEU:HB2	1.81	0.45
1:A:3018:LEU:HD21	1:A:3150:HIS:NE2	2.30	0.45
1:A:4231:MET:HA	1:A:4231:MET:HE3	1.97	0.45
2:B:17:SER:HA	2:B:83:ASN:HA	1.97	0.45
1:C:551:LEU:HD11	1:C:564:LEU:HD22	1.99	0.45
1:C:1008:SER:HB2	1:C:1017:ARG:CZ	2.46	0.45
1:C:1076:ARG:HB3	1:C:1191:VAL:HG23	1.98	0.45
1:C:4805:ASN:HD22	4:C:5105:POV:P	2.39	0.45
2:D:59:TYR:HB2	2:D:63:VAL:HG21	1.98	0.45
2:D:107:TRP:HB3	2:D:111:ASN:HB3	1.97	0.45
1:G:76:ARG:HB3	1:J:3935:TRP:CZ3	2.52	0.45
1:G:883:ALA:O	1:G:887:ILE:HG13	2.16	0.45
1:G:1098:GLY:HA3	1:G:1198:GLN:HE22	1.81	0.45
1:G:3009:TYR:CZ	1:G:3013:HIS:HD2	2.33	0.45
1:G:4648:LEU:HG	4:G:5104:POV:H27A	1.97	0.45
1:J:109:LEU:HD12	1:J:118:LEU:HD23	1.97	0.45
1:J:4162:ASN:O	1:J:4166:LEU:HG	2.15	0.45
1:A:233:ILE:HD13	1:A:287:THR:HG21	1.98	0.45
1:A:2913:ALA:HA	1:A:2916:LYS:HG2	1.98	0.45
1:A:3852:LYS:HE3	1:A:3852:LYS:HB2	1.79	0.45
1:C:179:TYR:HB2	1:C:197:GLN:HA	1.97	0.45
1:C:898:ASP:H	1:C:903:LEU:HB2	1.81	0.45
1:C:4218:ILE:O	1:C:4222:VAL:HG23	2.16	0.45
3:E:4:ILE:HD11	3:E:62:GLY:HA2	1.97	0.45
1:G:2902:HIS:HE1	1:G:2904:LEU:HB2	1.81	0.45
1:G:3511:VAL:HG21	1:G:3609:THR:HG21	1.98	0.45
1:G:4834:GLY:O	1:G:4838:VAL:HG22	2.16	0.45
1:J:2913:ALA:HA	1:J:2916:LYS:HG2	1.98	0.45
1:J:4001:MET:HG3	1:J:4057:MET:HE2	1.97	0.45
1:A:3019:SER:HB3	1:A:3030:HIS:HA	1.97	0.45
1:A:3137:LEU:HD22	1:A:3189:ALA:HB1	1.97	0.45
1:C:1432:THR:HG23	1:C:1572:ILE:HG23	1.98	0.45
1:G:551:LEU:HD11	1:G:564:LEU:HD22	1.99	0.45
1:G:898:ASP:H	1:G:903:LEU:HB2	1.81	0.45
1:G:1300:HIS:HB3	1:G:1302:ARG:NE	2.31	0.45
1:G:2871:LEU:HA	1:G:2874:MET:HE3	1.99	0.45
1:G:3435:PHE:CG	1:G:3521:GLY:HA3	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3566:SER:HB3	1:G:3569:LEU:HD12	1.99	0.45
3:I:4:ILE:HA	3:I:73:LYS:O	2.16	0.45
1:J:24:CYS:HB2	1:J:200:TRP:CE3	2.51	0.45
1:J:220:LEU:HD13	1:J:262:LEU:HG	1.98	0.45
1:J:551:LEU:HD11	1:J:564:LEU:HD22	1.99	0.45
1:J:1741:GLU:O	1:J:1745:ILE:HG13	2.15	0.45
1:J:3423:TRP:HB2	1:J:3520:ILE:HD12	1.98	0.45
1:A:1076:ARG:HB3	1:A:1191:VAL:HG23	1.98	0.45
1:A:1078:GLU:HB3	1:A:1081:TYR:HD2	1.81	0.45
1:A:1098:GLY:HA3	1:A:1198:GLN:HE22	1.82	0.45
1:A:2871:LEU:HA	1:A:2874:MET:HE3	1.99	0.45
1:A:3423:TRP:HB2	1:A:3520:ILE:HD12	1.98	0.45
1:A:3435:PHE:CG	1:A:3521:GLY:HA3	2.51	0.45
1:A:3536:ALA:HA	1:A:3539:ARG:NE	2.30	0.45
1:A:4750:ILE:HA	1:A:4753:HIS:HD2	1.81	0.45
1:A:5003:HIS:HD2	1:A:5007:GLU:HB3	1.82	0.45
1:C:2875:ALA:HB2	1:C:2927:LEU:HD22	1.98	0.45
1:C:3010:PHE:O	1:C:3014:CYS:HB3	2.16	0.45
1:C:4108:ILE:O	1:C:4112:LEU:HG	2.17	0.45
3:F:4:ILE:HD11	3:F:62:GLY:HA2	1.97	0.45
1:G:4835:LYS:H	1:G:4835:LYS:HD2	1.82	0.45
1:G:5003:HIS:HD2	1:G:5007:GLU:HB3	1.82	0.45
2:H:14:ALA:HA	2:H:85:LEU:HB2	1.99	0.45
1:J:2006:ILE:HG21	1:J:3652:MET:HB3	1.99	0.45
1:J:3010:PHE:O	1:J:3014:CYS:HB3	2.16	0.45
1:J:3546:ASP:HA	1:J:3549:VAL:HG22	1.97	0.45
1:J:4218:ILE:O	1:J:4222:VAL:HG23	2.16	0.45
1:A:1008:SER:HB2	1:A:1017:ARG:CZ	2.46	0.45
1:A:1455:PRO:HG3	1:A:1549:PHE:HE1	1.82	0.45
1:A:3077:ALA:HA	1:A:3080:VAL:HG12	1.97	0.45
1:A:3546:ASP:HA	1:A:3549:VAL:HG22	1.98	0.45
1:A:4218:ILE:HD13	1:A:4954:MET:HE2	1.97	0.45
1:C:1455:PRO:HG3	1:C:1549:PHE:HE1	1.82	0.45
1:C:2754:PHE:CE2	1:C:2825:LYS:HB3	2.52	0.45
1:C:2902:HIS:HE1	1:C:2904:LEU:HB2	1.81	0.45
1:C:3137:LEU:HD22	1:C:3189:ALA:HB1	1.97	0.45
1:C:3423:TRP:HB2	1:C:3520:ILE:HD12	1.98	0.45
1:C:4750:ILE:HA	1:C:4753:HIS:HD2	1.81	0.45
1:G:3536:ALA:HA	1:G:3539:ARG:NE	2.30	0.45
1:G:4218:ILE:O	1:G:4222:VAL:HG23	2.16	0.45
1:G:4218:ILE:HD13	1:G:4954:MET:HE2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:233:ILE:HD13	1:J:287:THR:HG21	1.98	0.45
1:J:1300:HIS:HB3	1:J:1302:ARG:NE	2.31	0.45
1:J:2608:MET:HA	1:J:2643:LEU:HD13	1.97	0.45
1:A:19:GLU:HB3	1:A:206:CYS:HB2	1.98	0.45
1:A:551:LEU:HD11	1:A:564:LEU:HD22	1.99	0.45
1:A:3018:LEU:HD13	1:A:3074:SER:HA	1.98	0.45
1:A:4108:ILE:O	1:A:4112:LEU:HG	2.17	0.45
2:B:107:TRP:HB3	2:B:111:ASN:HB3	1.97	0.45
1:C:181:HIS:CD2	1:C:196:MET:HB3	2.52	0.45
1:C:987:ARG:HD3	1:C:987:ARG:C	2.42	0.45
1:C:2867:LEU:H	1:C:2928:LYS:HZ2	1.65	0.45
1:C:3352:GLU:H	1:C:3352:GLU:CD	2.25	0.45
1:C:3935:TRP:CZ3	1:J:76:ARG:HB3	2.51	0.45
4:C:5112:POV:H311	4:C:5112:POV:H38	1.68	0.45
1:G:181:HIS:CD2	1:G:196:MET:HB2	2.52	0.45
1:G:470:SER:HA	1:G:473:ASN:HD21	1.80	0.45
1:G:887:ILE:HG12	1:G:960:MET:SD	2.57	0.45
1:G:2913:ALA:HA	1:G:2916:LYS:HG2	1.98	0.45
1:J:19:GLU:HB3	1:J:206:CYS:HB2	1.98	0.45
1:J:1455:PRO:HG3	1:J:1549:PHE:HE1	1.82	0.45
1:J:2355:ARG:O	1:J:2359:ARG:HG2	2.16	0.45
1:J:2871:LEU:HA	1:J:2874:MET:HE3	1.99	0.45
1:J:4648:LEU:HG	4:J:5107:POV:H27A	1.97	0.45
1:A:659:TYR:HB2	1:A:1017:ARG:NH1	2.31	0.45
1:A:2238:TYR:HD1	1:A:2241:ARG:HD2	1.81	0.45
1:A:4835:LYS:H	1:A:4835:LYS:HD2	1.82	0.45
1:C:3018:LEU:HD13	1:C:3074:SER:HA	1.98	0.45
1:G:659:TYR:HB2	1:G:1017:ARG:NH1	2.31	0.45
1:G:2226:PRO:O	1:G:2230:THR:HG23	2.16	0.45
1:G:3010:PHE:O	1:G:3014:CYS:HB3	2.16	0.45
1:G:3133:THR:HG22	1:G:3134:VAL:HG13	1.99	0.45
1:J:2998:PHE:HA	1:J:3002:LEU:HB2	1.98	0.45
1:J:3435:PHE:CG	1:J:3521:GLY:HA3	2.51	0.45
1:J:4576:ILE:HG21	1:J:4643:LEU:HB2	1.97	0.45
1:C:180:LEU:HD23	1:C:200:TRP:CE2	2.52	0.45
1:C:4728:HIS:HD2	1:C:4731:ILE:HD12	1.81	0.45
3:F:4:ILE:HA	3:F:73:LYS:O	2.16	0.45
1:G:3273:THR:HA	1:G:3276:MET:HG2	1.98	0.45
1:G:3546:ASP:HA	1:G:3549:VAL:HG22	1.98	0.45
2:H:82:MET:HE2	2:H:82:MET:HA	1.98	0.45
1:J:551:LEU:HD13	1:J:589:LEU:HD11	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1674:CYS:HB3	1:J:1685:LEU:HD12	1.99	0.45
1:J:1931:LEU:HD22	1:J:1935:VAL:HG11	1.99	0.45
2:K:86:LYS:HE2	2:K:86:LYS:HB2	1.84	0.45
1:A:470:SER:HA	1:A:473:ASN:HD21	1.80	0.45
1:A:1247:PRO:HA	1:A:1598:GLN:HG2	1.99	0.45
1:A:2355:ARG:O	1:A:2359:ARG:HG2	2.16	0.45
1:C:920:TYR:HE2	2:D:106:PRO:HD2	1.81	0.45
1:C:2355:ARG:O	1:C:2359:ARG:HG2	2.16	0.45
1:C:2619:LEU:O	1:C:2623:LEU:HB3	2.17	0.45
1:C:2871:LEU:HA	1:C:2874:MET:HE3	1.99	0.45
1:C:3077:ALA:HA	1:C:3080:VAL:HG12	1.97	0.45
1:G:470:SER:HA	1:G:473:ASN:ND2	2.31	0.45
1:G:950:LEU:HD11	1:G:972:LEU:HA	1.97	0.45
1:G:1931:LEU:HD22	1:G:1935:VAL:HG11	1.99	0.45
1:G:2927:LEU:HD23	1:G:2928:LYS:HZ1	1.81	0.45
1:G:3556:ASN:HA	1:G:3559:LEU:HD13	1.99	0.45
1:G:3842:LEU:HB2	1:G:3929:SER:HB2	1.99	0.45
1:J:978:THR:HB	1:J:981:GLN:HG2	1.98	0.45
1:J:1433:TYR:CE2	1:J:1522:LEU:HD22	2.52	0.45
1:J:1730:MET:HE2	1:J:1730:MET:HB3	1.77	0.45
1:J:2156:LEU:HD23	1:J:2156:LEU:HA	1.86	0.45
1:J:2875:ALA:HB2	1:J:2927:LEU:HD22	1.98	0.45
1:J:3133:THR:HG22	1:J:3134:VAL:HG13	1.99	0.45
1:J:3442:PHE:HE1	1:J:3511:VAL:HG22	1.82	0.45
3:L:4:ILE:HA	3:L:73:LYS:O	2.16	0.45
1:A:76:ARG:HB3	1:G:3935:TRP:CZ3	2.52	0.45
1:A:180:LEU:HD23	1:A:200:TRP:CE2	2.52	0.45
1:A:1728:ARG:HH11	1:A:1850:VAL:HG21	1.82	0.45
1:A:2927:LEU:HA	1:A:2930:LEU:HD12	1.97	0.45
1:C:470:SER:HA	1:C:473:ASN:ND2	2.31	0.45
1:C:1300:HIS:HB3	1:C:1302:ARG:NE	2.31	0.45
1:C:1433:TYR:CE2	1:C:1522:LEU:HD22	2.52	0.45
1:C:2913:ALA:HA	1:C:2916:LYS:HG2	1.98	0.45
1:C:3133:THR:HG22	1:C:3134:VAL:HG13	1.99	0.45
1:C:3835:LEU:HG	1:C:3880:PHE:HZ	1.82	0.45
1:C:5003:HIS:HD2	1:C:5007:GLU:HB3	1.82	0.45
1:C:5004:THR:HG22	1:C:5007:GLU:HG3	1.99	0.45
1:G:1247:PRO:HA	1:G:1598:GLN:HG2	1.99	0.45
1:G:1433:TYR:CE2	1:G:1522:LEU:HD22	2.52	0.45
1:G:2288:LEU:HD21	1:G:3852:LYS:HB3	1.99	0.45
1:J:2288:LEU:HD21	1:J:3852:LYS:HB3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:3556:ASN:HA	1:J:3559:LEU:HD13	1.99	0.45
1:J:3835:LEU:HG	1:J:3880:PHE:HZ	1.82	0.45
2:K:82:MET:HE2	2:K:82:MET:HA	1.98	0.45
1:A:1433:TYR:CE2	1:A:1522:LEU:HD22	2.52	0.44
1:A:2619:LEU:O	1:A:2623:LEU:HB3	2.17	0.44
1:A:2882:TYR:HA	1:A:2886:TRP:CD1	2.52	0.44
1:A:3556:ASN:HA	1:A:3559:LEU:HD13	1.99	0.44
1:A:3566:SER:HB3	1:A:3569:LEU:HD12	1.99	0.44
2:B:14:ALA:HA	2:B:85:LEU:HB2	1.99	0.44
1:C:659:TYR:HB2	1:C:1017:ARG:NH1	2.31	0.44
1:C:2288:LEU:HD21	1:C:3852:LYS:HB3	1.99	0.44
1:C:2735:PHE:O	1:C:2737:PRO:HD3	2.17	0.44
1:C:2765:LYS:HA	1:C:2765:LYS:HD3	1.73	0.44
1:C:3556:ASN:HA	1:C:3559:LEU:HD13	1.99	0.44
2:D:82:MET:HE2	2:D:82:MET:HA	1.98	0.44
3:F:23:VAL:HB	3:F:104:LEU:O	2.17	0.44
1:G:978:THR:HB	1:G:981:GLN:HG2	1.98	0.44
1:G:2006:ILE:HG21	1:G:3652:MET:HB3	1.99	0.44
1:G:2166:LEU:HD21	1:G:2206:THR:HG23	1.99	0.44
1:G:2754:PHE:CE2	1:G:2825:LYS:HB3	2.52	0.44
1:G:3537:LYS:NZ	1:G:3607:GLU:HG2	2.32	0.44
1:G:3835:LEU:HG	1:G:3880:PHE:HZ	1.82	0.44
1:J:2359:ARG:NH1	1:J:2359:ARG:HA	2.33	0.44
1:J:2559:LEU:O	1:J:2563:THR:HG23	2.17	0.44
1:J:2619:LEU:O	1:J:2623:LEU:HB3	2.17	0.44
1:J:2735:PHE:O	1:J:2737:PRO:HD3	2.17	0.44
1:J:3273:THR:HA	1:J:3276:MET:HG2	1.98	0.44
1:J:3537:LYS:NZ	1:J:3607:GLU:HG2	2.32	0.44
1:J:4108:ILE:O	1:J:4112:LEU:HG	2.17	0.44
1:J:4218:ILE:HD13	1:J:4954:MET:HE2	1.97	0.44
1:J:5003:HIS:HD2	1:J:5007:GLU:HB3	1.82	0.44
2:K:17:SER:HA	2:K:83:ASN:HA	1.97	0.44
1:A:220:LEU:HD13	1:A:262:LEU:HG	1.98	0.44
1:A:3994:HIS:HA	1:A:4054:ASN:OD1	2.18	0.44
1:A:4068:LEU:HD12	1:A:4068:LEU:HA	1.81	0.44
1:C:978:THR:HB	1:C:981:GLN:HG2	1.98	0.44
1:C:2692:ASP:HB3	1:C:2695:LEU:HD23	2.00	0.44
1:C:3852:LYS:HB2	1:C:3852:LYS:HE3	1.79	0.44
1:C:4218:ILE:HD13	1:C:4954:MET:HE2	1.98	0.44
1:G:180:LEU:HD23	1:G:200:TRP:CE2	2.52	0.44
1:G:551:LEU:HD13	1:G:589:LEU:HD11	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1939:MET:HE3	1:G:1939:MET:HB2	1.72	0.44
1:G:2559:LEU:O	1:G:2563:THR:HG23	2.17	0.44
1:G:5013:MET:HE2	1:G:5013:MET:HB3	1.74	0.44
1:J:1247:PRO:HA	1:J:1598:GLN:HG2	1.99	0.44
1:J:2882:TYR:HA	1:J:2886:TRP:CD1	2.52	0.44
1:J:4705:VAL:HB	1:J:4778:TRP:CG	2.53	0.44
3:L:23:VAL:HB	3:L:104:LEU:O	2.17	0.44
1:A:894:GLY:H	1:A:903:LEU:HD22	1.81	0.44
1:A:1078:GLU:HG3	1:A:1237:TRP:NE1	2.32	0.44
1:A:1300:HIS:HB3	1:A:1302:ARG:NE	2.31	0.44
1:A:2519:LEU:HA	1:A:2522:LEU:HD12	2.00	0.44
1:A:2930:LEU:HB3	1:A:2935:TYR:HB2	1.99	0.44
1:A:3010:PHE:O	1:A:3014:CYS:HB3	2.16	0.44
1:A:3352:GLU:H	1:A:3352:GLU:CD	2.25	0.44
1:A:3393:LEU:O	1:A:3397:GLU:HB2	2.18	0.44
1:A:3842:LEU:HB2	1:A:3929:SER:HB2	1.99	0.44
1:C:1931:LEU:HD22	1:C:1935:VAL:HG11	1.99	0.44
1:C:3443:ILE:HG22	1:C:3605:HIS:CG	2.53	0.44
2:D:14:ALA:HA	2:D:85:LEU:HB2	1.99	0.44
3:F:105:ASN:ND2	3:F:105:ASN:O	2.35	0.44
1:G:103:TYR:HB2	1:G:159:GLU:HA	1.99	0.44
1:G:892:THR:N	1:G:902:ARG:O	2.50	0.44
1:G:2210:VAL:O	1:G:2214:VAL:HG12	2.18	0.44
1:G:2519:LEU:HA	1:G:2522:LEU:HD12	2.00	0.44
1:G:2754:PHE:HA	1:G:2757:LYS:HB3	1.98	0.44
1:G:4705:VAL:HB	1:G:4778:TRP:CG	2.53	0.44
1:G:4796:MET:HE3	1:G:4800:LEU:HG	1.99	0.44
4:G:5114:POV:H311	4:G:5114:POV:H38	1.68	0.44
1:J:1476:MET:HE3	1:J:1476:MET:HB3	1.85	0.44
1:J:2210:VAL:O	1:J:2214:VAL:HG12	2.18	0.44
1:J:2214:VAL:HG13	1:J:2215:LEU:HD13	2.00	0.44
1:J:2692:ASP:HB3	1:J:2695:LEU:HD23	2.00	0.44
1:J:2754:PHE:CE2	1:J:2825:LYS:HB3	2.52	0.44
1:J:3352:GLU:CD	1:J:3352:GLU:H	2.25	0.44
1:A:1931:LEU:HD22	1:A:1935:VAL:HG11	1.99	0.44
1:A:2162:ILE:O	1:A:2166:LEU:HD13	2.18	0.44
1:A:2754:PHE:CE2	1:A:2825:LYS:HB3	2.52	0.44
1:A:2754:PHE:HA	1:A:2757:LYS:HB3	1.98	0.44
1:A:3531:ASP:HA	1:A:3534:MET:HE1	2.00	0.44
1:A:3537:LYS:NZ	1:A:3607:GLU:HG2	2.32	0.44
1:A:4218:ILE:O	1:A:4222:VAL:HG23	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:551:LEU:HD13	1:C:589:LEU:HD11	1.99	0.44
1:C:855:PRO:HD2	1:C:998:ARG:CZ	2.46	0.44
1:C:1098:GLY:HA3	1:C:1198:GLN:HE22	1.81	0.44
1:C:2214:VAL:HG13	1:C:2215:LEU:HD13	2.00	0.44
1:C:2882:TYR:HA	1:C:2886:TRP:CD1	2.52	0.44
1:C:2882:TYR:O	1:C:2886:TRP:HB2	2.18	0.44
1:C:4705:VAL:HB	1:C:4778:TRP:CG	2.53	0.44
1:C:4835:LYS:H	1:C:4835:LYS:HD2	1.82	0.44
1:G:2162:ILE:O	1:G:2166:LEU:HD13	2.18	0.44
1:G:2619:LEU:O	1:G:2623:LEU:HB3	2.17	0.44
1:G:2875:ALA:HB2	1:G:2927:LEU:HD22	1.98	0.44
1:G:3758:MET:O	1:G:3762:ARG:HG3	2.18	0.44
1:J:4835:LYS:H	1:J:4835:LYS:HD2	1.82	0.44
1:A:750:LEU:HD23	1:A:750:LEU:HA	1.75	0.44
1:A:4705:VAL:HB	1:A:4778:TRP:CG	2.53	0.44
2:B:82:MET:HE2	2:B:82:MET:HA	1.98	0.44
1:C:1939:MET:HE3	1:C:1939:MET:HB2	1.72	0.44
1:C:2930:LEU:HB3	1:C:2935:TYR:HB2	1.99	0.44
1:C:3842:LEU:HB2	1:C:3929:SER:HB2	1.99	0.44
1:G:220:LEU:HD13	1:G:262:LEU:HG	1.98	0.44
1:G:1033:ARG:HA	1:G:1036:ARG:HG2	2.00	0.44
1:G:2214:VAL:HG13	1:G:2215:LEU:HD13	2.00	0.44
1:G:2882:TYR:HA	1:G:2886:TRP:CD1	2.52	0.44
1:G:2927:LEU:HA	1:G:2930:LEU:HD12	1.97	0.44
1:G:3206:LEU:HD23	1:G:3206:LEU:HA	1.75	0.44
3:I:23:VAL:HB	3:I:104:LEU:O	2.17	0.44
1:J:3566:SER:HB3	1:J:3569:LEU:HD12	1.99	0.44
1:J:3809:ASN:OD1	1:J:3812:VAL:HG12	2.18	0.44
1:J:4003:LEU:HD22	1:J:4009:GLN:HB3	2.00	0.44
2:B:18:LEU:HB2	2:B:82:MET:HB3	2.00	0.44
1:C:220:LEU:HD13	1:C:262:LEU:HG	1.98	0.44
1:C:248:GLU:HG3	1:C:373:LYS:HG2	2.00	0.44
1:C:1247:PRO:HA	1:C:1598:GLN:HG2	1.99	0.44
1:C:2359:ARG:NH1	1:C:2359:ARG:HA	2.33	0.44
1:C:2559:LEU:O	1:C:2563:THR:HG23	2.17	0.44
1:G:3994:HIS:HA	1:G:4054:ASN:OD1	2.18	0.44
1:G:4750:ILE:HA	1:G:4753:HIS:HD2	1.81	0.44
1:G:4813:LEU:HD23	1:G:4813:LEU:HA	1.88	0.44
1:J:248:GLU:HG3	1:J:373:LYS:HG2	2.00	0.44
1:J:855:PRO:HD2	1:J:998:ARG:CZ	2.48	0.44
1:J:898:ASP:H	1:J:903:LEU:HB2	1.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:2166:LEU:HD21	1:J:2206:THR:HG23	2.00	0.44
1:J:2882:TYR:O	1:J:2886:TRP:HB2	2.18	0.44
1:A:2210:VAL:O	1:A:2214:VAL:HG12	2.18	0.44
1:A:2293:GLN:O	1:A:2297:LYS:HG3	2.18	0.44
1:A:3133:THR:HG22	1:A:3134:VAL:HG13	1.99	0.44
1:A:3758:MET:O	1:A:3762:ARG:HG3	2.18	0.44
1:A:3924:LEU:O	1:A:3927:GLN:HG3	2.18	0.44
1:C:1674:CYS:HB3	1:C:1685:LEU:HD12	1.99	0.44
1:C:2359:ARG:NH1	1:J:195:PHE:O	2.43	0.44
1:G:248:GLU:HG3	1:G:373:LYS:HG2	2.00	0.44
1:G:663:TYR:CE1	1:G:745:SER:HB3	2.53	0.44
1:G:985:VAL:HG22	1:G:1043:VAL:HG21	2.00	0.44
1:G:1728:ARG:HH11	1:G:1850:VAL:HG21	1.82	0.44
1:G:3352:GLU:CD	1:G:3352:GLU:H	2.25	0.44
1:G:3393:LEU:O	1:G:3397:GLU:HB2	2.18	0.44
1:J:1098:GLY:HA3	1:J:1198:GLN:HE22	1.82	0.44
1:J:1153:ILE:HG13	1:J:1160:ILE:HG12	2.00	0.44
1:J:1728:ARG:HH11	1:J:1850:VAL:HG21	1.82	0.44
1:J:2293:GLN:O	1:J:2297:LYS:HG3	2.18	0.44
1:J:3511:VAL:HG21	1:J:3609:THR:HG21	2.00	0.44
1:J:3852:LYS:HB2	1:J:3852:LYS:HE3	1.79	0.44
1:J:4124:ASN:HB2	1:J:4128:PHE:HB2	2.00	0.44
1:A:115:ARG:HD2	1:A:115:ARG:HA	1.88	0.44
1:A:302:VAL:HB	1:A:306:LYS:HE3	2.00	0.44
1:A:663:TYR:CE1	1:A:745:SER:HB3	2.53	0.44
1:A:2006:ILE:HG21	1:A:3652:MET:HB3	1.99	0.44
1:A:2759:ALA:HB2	1:A:2810:LYS:HG3	2.00	0.44
1:A:3074:SER:H	1:A:3146:HIS:CD2	2.36	0.44
1:A:3570:ARG:HH21	1:C:1825:HIS:CE1	2.36	0.44
1:C:663:TYR:CE1	1:C:745:SER:HB3	2.53	0.44
1:C:1728:ARG:HH11	1:C:1850:VAL:HG21	1.82	0.44
1:C:3010:PHE:HE1	1:C:3074:SER:HB2	1.83	0.44
1:C:3074:SER:H	1:C:3146:HIS:CD2	2.36	0.44
1:C:3994:HIS:HA	1:C:4054:ASN:OD1	2.18	0.44
1:C:4003:LEU:HD22	1:C:4009:GLN:HB3	2.00	0.44
1:C:4796:MET:HE3	1:C:4800:LEU:HG	1.99	0.44
1:C:5013:MET:HE2	1:C:5013:MET:HB3	1.74	0.44
3:E:23:VAL:HB	3:E:104:LEU:O	2.17	0.44
1:G:2735:PHE:O	1:G:2737:PRO:HD3	2.17	0.44
1:G:2951:ILE:H	1:G:2951:ILE:HD12	1.83	0.44
1:G:4108:ILE:O	1:G:4112:LEU:HG	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:663:TYR:CE1	1:J:745:SER:HB3	2.53	0.44
1:J:882:TRP:CH2	2:K:104:TYR:HA	2.53	0.44
1:J:2928:LYS:HA	1:J:2928:LYS:HD3	1.80	0.44
2:K:14:ALA:HA	2:K:85:LEU:HB2	1.99	0.44
1:A:179:TYR:HB2	1:A:197:GLN:HA	1.99	0.44
1:A:181:HIS:CD2	1:A:196:MET:HB2	2.53	0.44
1:A:1291:LEU:HD12	1:A:1550:PRO:HB2	2.00	0.44
1:A:1825:HIS:CE1	1:G:3570:ARG:HH21	2.36	0.44
1:A:2288:LEU:HD21	1:A:3852:LYS:HB3	1.99	0.44
1:A:2559:LEU:O	1:A:2563:THR:HG23	2.17	0.44
1:A:2735:PHE:O	1:A:2737:PRO:HD3	2.17	0.44
1:A:5004:THR:HG22	1:A:5007:GLU:HG3	1.99	0.44
2:B:86:LYS:HB2	2:B:86:LYS:HE2	1.84	0.44
1:C:1733:GLU:HG2	1:C:2201:LEU:HD23	2.00	0.44
1:C:2162:ILE:O	1:C:2166:LEU:HD13	2.18	0.44
1:C:2928:LYS:HA	1:C:2928:LYS:HD3	1.80	0.44
1:C:3393:LEU:O	1:C:3397:GLU:HB2	2.18	0.44
1:C:3970:GLN:OE1	1:C:5004:THR:HA	2.18	0.44
1:C:4124:ASN:HB2	1:C:4128:PHE:HB2	2.00	0.44
1:G:302:VAL:HB	1:G:306:LYS:HE3	2.00	0.44
1:J:894:GLY:H	1:J:903:LEU:HD22	1.81	0.44
1:J:984:LEU:HD21	1:J:1056:PRO:HD2	1.99	0.44
1:J:3018:LEU:HD13	1:J:3074:SER:HA	1.98	0.44
1:A:551:LEU:HD13	1:A:589:LEU:HD11	1.99	0.43
1:A:2882:TYR:O	1:A:2886:TRP:HB2	2.18	0.43
1:A:3835:LEU:HG	1:A:3880:PHE:HZ	1.82	0.43
1:A:4124:ASN:HB2	1:A:4128:PHE:HB2	2.00	0.43
1:A:4626:ASN:HD22	1:A:4626:ASN:N	2.16	0.43
1:C:2519:LEU:HA	1:C:2522:LEU:HD12	2.00	0.43
1:C:2747:ILE:HG13	1:C:2814:LYS:HG2	1.99	0.43
1:C:3433:GLU:HA	1:C:3436:ARG:HD2	2.00	0.43
1:C:4091:LYS:HE2	1:C:4091:LYS:HA	2.00	0.43
1:C:4626:ASN:HD22	1:C:4626:ASN:N	2.16	0.43
1:G:182:LEU:HB2	1:G:198:THR:HG21	2.00	0.43
1:G:1455:PRO:HG3	1:G:1549:PHE:HE1	1.82	0.43
1:G:1674:CYS:HB3	1:G:1685:LEU:HD12	1.99	0.43
1:G:2211:MET:SD	1:G:2232:CYS:HB3	2.58	0.43
1:G:2747:ILE:HG13	1:G:2814:LYS:HG2	1.99	0.43
1:G:3010:PHE:HE1	1:G:3074:SER:HB2	1.83	0.43
1:G:3018:LEU:HD13	1:G:3074:SER:HA	1.98	0.43
1:G:3924:LEU:O	1:G:3927:GLN:HG3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1452:TRP:CZ3	1:J:1550:PRO:HG3	2.53	0.43
1:J:3010:PHE:HE1	1:J:3074:SER:HB2	1.83	0.43
1:A:3562:LYS:HB3	1:A:3564:GLU:OE1	2.19	0.43
1:C:103:TYR:HB2	1:C:159:GLU:HA	2.00	0.43
1:C:2241:ARG:O	1:C:2242:ILE:C	2.60	0.43
1:C:2292:GLU:HB2	1:C:2352:VAL:HG11	2.00	0.43
1:C:2876:GLU:HG3	1:C:2908:TYR:CE2	2.51	0.43
1:C:3924:LEU:O	1:C:3927:GLN:HG3	2.18	0.43
2:D:18:LEU:HB2	2:D:82:MET:HB3	2.00	0.43
1:G:3734:HIS:HB3	1:G:3803:SER:HB2	2.00	0.43
1:G:4003:LEU:HD22	1:G:4009:GLN:HB3	2.00	0.43
1:G:4626:ASN:HD22	1:G:4626:ASN:N	2.16	0.43
1:G:5030:LYS:HA	1:G:5033:GLU:HG3	2.00	0.43
2:H:86:LYS:HE2	2:H:86:LYS:HB2	1.84	0.43
1:J:1100:MET:HB3	1:J:1194:LEU:HG	2.00	0.43
1:J:2930:LEU:HB3	1:J:2935:TYR:HB2	1.99	0.43
1:J:2951:ILE:H	1:J:2951:ILE:HD12	1.83	0.43
1:J:5004:THR:HG22	1:J:5007:GLU:HG3	1.99	0.43
1:A:248:GLU:HG3	1:A:373:LYS:HG2	2.00	0.43
1:A:886:ARG:HB3	1:A:891:TRP:CD1	2.53	0.43
1:A:2166:LEU:HD21	1:A:2206:THR:HG23	2.00	0.43
1:A:2214:VAL:HG13	1:A:2215:LEU:HD13	2.00	0.43
1:A:2292:GLU:HB2	1:A:2352:VAL:HG11	2.00	0.43
1:A:3245:VAL:HG22	1:A:3246:LEU:HD23	2.01	0.43
1:A:4003:LEU:HD22	1:A:4009:GLN:HB3	2.00	0.43
1:C:77:ALA:O	1:C:81:MET:HG3	2.18	0.43
1:C:1033:ARG:HA	1:C:1036:ARG:HG2	2.00	0.43
1:C:1291:LEU:HD12	1:C:1550:PRO:HB2	2.00	0.43
1:C:1452:TRP:CZ3	1:C:1550:PRO:HG3	2.54	0.43
1:C:3537:LYS:NZ	1:C:3607:GLU:HG2	2.32	0.43
1:C:3809:ASN:OD1	1:C:3812:VAL:HG12	2.18	0.43
1:C:5030:LYS:HA	1:C:5033:GLU:HG3	2.00	0.43
1:G:875:ALA:HB1	1:G:921:ASN:HB3	2.00	0.43
1:G:876:GLU:O	1:G:880:GLU:HG3	2.18	0.43
1:G:1291:LEU:HD12	1:G:1550:PRO:HB2	2.00	0.43
1:G:1470:ARG:HA	1:G:1470:ARG:HD3	1.71	0.43
1:G:2359:ARG:NH1	1:G:2359:ARG:HA	2.33	0.43
1:G:3245:VAL:HG22	1:G:3246:LEU:HD23	2.01	0.43
1:J:785:ALA:HB2	1:J:1613:LEU:HD11	2.00	0.43
1:J:972:LEU:HD11	1:J:1044:ARG:HG3	2.00	0.43
1:J:2519:LEU:HA	1:J:2522:LEU:HD12	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:3758:MET:O	1:J:3762:ARG:HG3	2.18	0.43
1:J:3994:HIS:HA	1:J:4054:ASN:OD1	2.18	0.43
1:A:2951:ILE:H	1:A:2951:ILE:HD12	1.83	0.43
1:A:3443:ILE:HG22	1:A:3605:HIS:CG	2.53	0.43
1:A:3734:HIS:HB3	1:A:3803:SER:HB2	2.00	0.43
1:A:3809:ASN:OD1	1:A:3812:VAL:HG12	2.18	0.43
1:A:4796:MET:HE3	1:A:4800:LEU:HG	1.99	0.43
1:C:3531:ASP:HA	1:C:3534:MET:HE1	2.00	0.43
1:C:4105:GLY:O	1:C:4109:GLN:HG2	2.19	0.43
3:E:7:ILE:HB	3:E:71:ARG:HD2	2.00	0.43
3:F:7:ILE:HB	3:F:71:ARG:HD2	2.00	0.43
1:G:785:ALA:HB2	1:G:1613:LEU:HD11	2.00	0.43
1:G:2293:GLN:O	1:G:2297:LYS:HG3	2.18	0.43
1:G:2591:ARG:HH22	1:G:2625:ARG:NH2	2.17	0.43
1:G:2678:LEU:O	1:G:2682:ILE:HG12	2.19	0.43
1:G:2758:PHE:CD2	1:G:2813:LEU:HD11	2.53	0.43
1:G:3081:MET:HE2	1:G:3081:MET:HB3	1.88	0.43
1:G:3443:ILE:HG22	1:G:3605:HIS:CG	2.53	0.43
1:G:3934:TYR:CE2	1:G:3935:TRP:HB2	2.54	0.43
1:J:179:TYR:CD2	1:J:197:GLN:HG2	2.53	0.43
1:J:2678:LEU:O	1:J:2682:ILE:HG12	2.19	0.43
1:J:2747:ILE:HG13	1:J:2814:LYS:HG2	1.99	0.43
1:J:3132:THR:HA	1:J:3136:LEU:HB3	2.00	0.43
1:J:4909:TYR:HE1	4:J:5101:POV:H22A	1.82	0.43
1:A:1674:CYS:HB3	1:A:1685:LEU:HD12	1.99	0.43
1:A:4091:LYS:HE2	1:A:4091:LYS:HA	2.00	0.43
1:A:4232:GLU:HG3	1:A:5019:TRP:CD1	2.54	0.43
1:C:598:LYS:HE2	1:C:598:LYS:HB2	1.90	0.43
1:C:3566:SER:HB3	1:C:3569:LEU:HD12	1.99	0.43
1:C:3758:MET:O	1:C:3762:ARG:HG3	2.18	0.43
1:G:77:ALA:O	1:G:81:MET:HG3	2.18	0.43
1:G:668:VAL:HA	1:G:789:VAL:HG12	2.00	0.43
1:G:1497:GLY:HA2	1:G:1500:PHE:HB2	2.01	0.43
1:G:1733:GLU:HG2	1:G:2201:LEU:HD23	2.00	0.43
1:G:1825:HIS:CE1	1:J:3570:ARG:HH21	2.36	0.43
1:G:3562:LYS:HB3	1:G:3564:GLU:OE1	2.18	0.43
3:I:7:ILE:HB	3:I:71:ARG:HD2	2.00	0.43
1:J:2759:ALA:HB2	1:J:2810:LYS:HG3	2.00	0.43
1:J:3179:LYS:HG2	1:J:3187:ARG:HH22	1.84	0.43
1:J:3433:GLU:HA	1:J:3436:ARG:HD2	2.00	0.43
1:J:3934:TYR:CE2	1:J:3935:TRP:HB2	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4105:GLY:O	1:J:4109:GLN:HG2	2.19	0.43
1:A:77:ALA:O	1:A:81:MET:HG3	2.18	0.43
1:A:399:GLN:O	1:A:403:MET:HG3	2.19	0.43
1:A:1100:MET:HB3	1:A:1194:LEU:HG	2.01	0.43
1:A:2346:VAL:HG13	1:A:2349:ASN:HB2	2.00	0.43
1:A:3233:PRO:HG2	1:A:3239:MET:HA	2.01	0.43
1:C:302:VAL:HB	1:C:306:LYS:HE3	2.00	0.43
1:C:2006:ILE:HG21	1:C:3652:MET:HB3	1.99	0.43
1:C:2293:GLN:O	1:C:2297:LYS:HG3	2.18	0.43
1:C:2827:ARG:HH22	1:C:2830:GLU:HB3	1.83	0.43
1:C:4778:TRP:O	1:C:4782:VAL:HG13	2.19	0.43
1:C:4816:ILE:HD11	1:J:4846:VAL:HG21	2.00	0.43
1:G:750:LEU:HD23	1:G:750:LEU:HA	1.75	0.43
1:G:2759:ALA:HB2	1:G:2810:LYS:HG3	2.00	0.43
1:G:3233:PRO:HG2	1:G:3239:MET:HA	2.01	0.43
1:G:4056:GLU:HG2	1:G:4166:LEU:HD12	2.01	0.43
1:G:4124:ASN:HB2	1:G:4128:PHE:HB2	2.00	0.43
1:G:4567:LEU:HD21	1:G:4816:ILE:HG22	2.01	0.43
2:H:18:LEU:HB2	2:H:82:MET:HB3	2.00	0.43
1:J:2827:ARG:HH22	1:J:2830:GLU:HB3	1.83	0.43
1:J:3443:ILE:HG22	1:J:3605:HIS:CG	2.53	0.43
1:J:3531:ASP:HA	1:J:3534:MET:HE1	2.00	0.43
1:J:3842:LEU:HB2	1:J:3929:SER:HB2	1.99	0.43
1:J:3924:LEU:O	1:J:3927:GLN:HG3	2.18	0.43
1:A:1153:ILE:HG13	1:A:1160:ILE:HG12	2.00	0.43
1:A:2692:ASP:HB3	1:A:2695:LEU:HD23	2.00	0.43
1:A:3433:GLU:HA	1:A:3436:ARG:HD2	2.00	0.43
1:A:4567:LEU:HD21	1:A:4816:ILE:HG22	2.01	0.43
1:A:4778:TRP:O	1:A:4782:VAL:HG13	2.19	0.43
1:C:1100:MET:HB3	1:C:1194:LEU:HG	2.01	0.43
1:C:1153:ILE:HG13	1:C:1160:ILE:HG12	2.00	0.43
1:C:1163:THR:HG22	1:C:1168:VAL:HA	2.01	0.43
1:C:2210:VAL:O	1:C:2214:VAL:HG12	2.18	0.43
1:C:2678:LEU:O	1:C:2682:ILE:HG12	2.19	0.43
1:C:3562:LYS:HB3	1:C:3564:GLU:OE1	2.19	0.43
1:G:911:HIS:CD2	1:G:918:ARG:HG2	2.54	0.43
1:G:1153:ILE:HG13	1:G:1160:ILE:HG12	2.00	0.43
1:G:1163:THR:HG22	1:G:1168:VAL:HA	2.01	0.43
1:G:1452:TRP:CZ3	1:G:1550:PRO:HG3	2.53	0.43
1:G:2692:ASP:HB3	1:G:2695:LEU:HD23	2.00	0.43
1:G:2930:LEU:HB3	1:G:2935:TYR:HB2	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3809:ASN:OD1	1:G:3812:VAL:HG12	2.18	0.43
1:G:4963:ILE:HD13	1:G:5030:LYS:HD2	2.01	0.43
1:J:103:TYR:HB2	1:J:159:GLU:HA	2.00	0.43
1:J:1033:ARG:HA	1:J:1036:ARG:HG2	2.00	0.43
1:J:2738:ARG:H	1:J:2738:ARG:HG3	1.57	0.43
1:J:3074:SER:H	1:J:3146:HIS:CD2	2.36	0.43
1:J:4056:GLU:HG2	1:J:4166:LEU:HD12	2.01	0.43
1:J:4778:TRP:O	1:J:4782:VAL:HG13	2.18	0.43
4:J:5112:POV:H31E	4:J:5112:POV:H311	1.88	0.43
1:A:103:TYR:HB2	1:A:159:GLU:HA	2.00	0.43
1:A:356:TRP:H	1:A:380:GLN:HA	1.83	0.43
1:A:1452:TRP:CZ3	1:A:1550:PRO:HG3	2.53	0.43
1:A:2359:ARG:NH1	1:A:2359:ARG:HA	2.33	0.43
1:A:2678:LEU:O	1:A:2682:ILE:HG12	2.19	0.43
1:A:3010:PHE:HE1	1:A:3074:SER:HB2	1.83	0.43
1:A:3163:VAL:O	1:A:3167:ARG:HG2	2.19	0.43
1:A:4202:ARG:O	1:A:4206:GLU:HG2	2.19	0.43
1:C:35:LEU:HG	1:C:51:PRO:HA	2.01	0.43
1:C:399:GLN:O	1:C:403:MET:HG3	2.19	0.43
1:C:984:LEU:HD21	1:C:1056:PRO:HD2	1.99	0.43
1:C:1123:VAL:HG23	1:C:1132:TRP:HB2	2.01	0.43
1:C:2166:LEU:HD21	1:C:2206:THR:HG23	1.99	0.43
1:C:2346:VAL:HG13	1:C:2349:ASN:HB2	2.01	0.43
1:C:2700:MET:HE3	1:C:2701:PRO:HD3	2.01	0.43
1:C:2823:ILE:HA	1:C:2937:VAL:HA	2.01	0.43
1:C:2951:ILE:HD12	1:C:2951:ILE:H	1.83	0.43
1:G:1100:MET:HB3	1:G:1194:LEU:HG	2.01	0.43
1:G:2582:MET:HE3	1:G:2582:MET:HB3	1.86	0.43
1:G:2735:PHE:CE1	1:G:2907:PRO:HG3	2.54	0.43
1:G:2827:ARG:HH22	1:G:2830:GLU:HB3	1.83	0.43
1:G:3074:SER:H	1:G:3146:HIS:CD2	2.36	0.43
1:G:3965:LEU:O	1:G:3969:ILE:HG12	2.19	0.43
1:G:4861:LYS:HE2	1:G:4861:LYS:HB3	1.89	0.43
1:J:465:GLN:O	1:J:469:ARG:HG3	2.18	0.43
1:J:1291:LEU:HD12	1:J:1550:PRO:HB2	2.00	0.43
1:J:1497:GLY:HA2	1:J:1500:PHE:HB2	2.01	0.43
1:J:3379:LEU:HD11	1:J:3391:GLU:HB2	2.01	0.43
1:J:3970:GLN:OE1	1:J:5004:THR:HA	2.18	0.43
1:A:24:CYS:HB2	1:A:200:TRP:CE3	2.54	0.43
1:A:1575:LEU:HD23	1:A:1575:LEU:HA	1.77	0.43
1:A:1634:LEU:HD12	1:A:1634:LEU:HA	1.90	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1733:GLU:HG2	1:A:2201:LEU:HD23	2.00	0.43
1:A:2700:MET:HE3	1:A:2701:PRO:HD3	2.01	0.43
1:A:2747:ILE:HG13	1:A:2814:LYS:HG2	1.99	0.43
1:A:3934:TYR:CE2	1:A:3935:TRP:HB2	2.54	0.43
1:A:4105:GLY:O	1:A:4109:GLN:HG2	2.19	0.43
1:C:291:LEU:HD11	1:C:299:LEU:HD12	2.00	0.43
1:C:2604:GLU:O	1:C:2608:MET:HG3	2.19	0.43
1:C:3163:VAL:O	1:C:3167:ARG:HG2	2.19	0.43
1:C:3379:LEU:HD11	1:C:3391:GLU:HB2	2.01	0.43
1:C:3570:ARG:HH21	1:J:1825:HIS:CE1	2.37	0.43
1:C:4202:ARG:O	1:C:4206:GLU:HG2	2.19	0.43
1:G:266:ARG:HG3	1:G:268:SER:HB3	2.01	0.43
1:G:394:GLN:HB2	1:G:397:GLU:OE1	2.19	0.43
1:G:1237:TRP:CH2	1:G:1652:GLU:HG3	2.54	0.43
1:G:2380:ILE:HG13	1:G:2469:ILE:HD13	2.01	0.43
1:G:3179:LYS:HG2	1:G:3187:ARG:HH22	1.84	0.43
1:G:4091:LYS:HE2	1:G:4091:LYS:HA	2.00	0.43
1:G:4232:GLU:HG3	1:G:5019:TRP:CD1	2.54	0.43
1:J:302:VAL:HB	1:J:306:LYS:HE3	2.00	0.43
1:J:1237:TRP:CH2	1:J:1652:GLU:HG3	2.54	0.43
1:J:1733:GLU:HG2	1:J:2201:LEU:HD23	2.00	0.43
1:J:2591:ARG:HH22	1:J:2625:ARG:NH2	2.17	0.43
1:A:404:ILE:HG23	1:A:483:MET:SD	2.59	0.43
1:A:1033:ARG:HA	1:A:1036:ARG:HG2	2.00	0.43
1:A:1163:THR:HG22	1:A:1168:VAL:HA	2.01	0.43
1:A:1717:SER:HA	1:A:1721:GLU:HB2	2.01	0.43
1:A:2515:GLN:HE22	1:A:2574:HIS:HE1	1.67	0.43
1:A:3282:PRO:HG3	1:A:3345:ILE:CD1	2.49	0.43
1:A:3420:ARG:HG3	1:A:3520:ILE:HD11	2.00	0.43
1:A:4056:GLU:HG2	1:A:4166:LEU:HD12	2.01	0.43
1:A:4172:GLU:HA	1:A:4175:ARG:HH12	1.84	0.43
1:C:207:SER:HB3	1:C:269:TRP:HE1	1.84	0.43
1:C:451:TYR:CZ	1:C:474:ARG:HD3	2.54	0.43
1:C:2474:LEU:HD13	1:C:2494:PHE:HD2	1.84	0.43
1:C:2515:GLN:HE22	1:C:2574:HIS:HE1	1.67	0.43
1:C:2759:ALA:HB2	1:C:2810:LYS:HG3	2.00	0.43
1:C:3039:ILE:HD12	1:C:3039:ILE:HA	1.88	0.43
1:C:3050:VAL:HG21	1:C:3064:VAL:HG11	2.01	0.43
1:G:2604:GLU:O	1:G:2608:MET:HG3	2.19	0.43
1:G:2882:TYR:O	1:G:2886:TRP:HB2	2.18	0.43
1:G:3020:THR:HB	1:G:3023:LYS:HG3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3107:VAL:HG22	1:G:3175:LEU:HG	2.01	0.43
1:G:3379:LEU:HD11	1:G:3391:GLU:HB2	2.01	0.43
1:G:3826:VAL:HA	1:G:3909:ASN:HD21	1.84	0.43
1:G:4105:GLY:O	1:G:4109:GLN:HG2	2.19	0.43
1:G:4202:ARG:O	1:G:4206:GLU:HG2	2.19	0.43
1:G:4778:TRP:O	1:G:4782:VAL:HG13	2.19	0.43
1:J:2162:ILE:O	1:J:2166:LEU:HD13	2.18	0.43
1:J:2380:ILE:HG13	1:J:2469:ILE:HD13	2.01	0.43
1:J:3233:PRO:HG2	1:J:3239:MET:HA	2.01	0.43
1:J:3393:LEU:O	1:J:3397:GLU:HB2	2.18	0.43
1:J:3420:ARG:HG3	1:J:3520:ILE:HD11	2.00	0.43
1:J:3965:LEU:O	1:J:3969:ILE:HG12	2.19	0.43
4:J:5103:POV:H38	4:J:5103:POV:H311	1.68	0.43
1:A:35:LEU:HG	1:A:51:PRO:HA	2.01	0.42
1:A:465:GLN:O	1:A:469:ARG:HG3	2.18	0.42
1:A:580:GLU:HG2	1:A:584:LYS:HE2	2.01	0.42
1:A:875:ALA:HB1	1:A:921:ASN:HB3	2.00	0.42
1:A:2144:ILE:HD11	1:A:2149:VAL:HG12	2.01	0.42
1:A:2534:ALA:HB1	1:A:2588:ARG:NE	2.33	0.42
1:A:2758:PHE:CD2	1:A:2813:LEU:HD11	2.53	0.42
1:A:2867:LEU:H	1:A:2928:LYS:HZ2	1.66	0.42
1:A:3050:VAL:HG21	1:A:3064:VAL:HG11	2.01	0.42
1:A:3179:LYS:HG2	1:A:3187:ARG:HH22	1.84	0.42
1:A:5030:LYS:HA	1:A:5033:GLU:HG3	2.00	0.42
1:C:356:TRP:H	1:C:380:GLN:HA	1.83	0.42
1:C:569:ILE:HG13	1:C:570:GLU:HG2	2.01	0.42
1:C:1177:THR:O	1:C:1180:ARG:NH2	2.52	0.42
1:C:1260:MET:HE2	1:C:1269:CYS:SG	2.59	0.42
1:C:1268:PRO:HD2	1:C:1589:PRO:HB2	2.01	0.42
1:C:2758:PHE:CD2	1:C:2813:LEU:HD11	2.53	0.42
1:C:3934:TYR:CE2	1:C:3935:TRP:HB2	2.54	0.42
1:G:465:GLN:O	1:G:469:ARG:HG3	2.18	0.42
1:G:1123:VAL:HG23	1:G:1132:TRP:HB2	2.01	0.42
1:G:3039:ILE:HD12	1:G:3039:ILE:HA	1.88	0.42
1:G:3190:LEU:O	1:G:3194:LEU:HB3	2.19	0.42
1:G:3420:ARG:HG3	1:G:3520:ILE:HD11	2.00	0.42
1:G:3531:ASP:HA	1:G:3534:MET:HE1	2.00	0.42
1:G:4172:GLU:HA	1:G:4175:ARG:HH12	1.84	0.42
1:J:77:ALA:O	1:J:81:MET:HG3	2.18	0.42
1:J:451:TYR:CZ	1:J:474:ARG:HD3	2.54	0.42
1:J:1163:THR:HG22	1:J:1168:VAL:HA	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1260:MET:HE2	1:J:1269:CYS:SG	2.59	0.42
1:J:3020:THR:HB	1:J:3023:LYS:HG3	2.00	0.42
1:J:3353:LEU:HG	1:J:3358:PHE:CE1	2.54	0.42
1:J:4733:GLY:H	1:J:4736:ARG:HD2	1.84	0.42
1:J:4796:MET:HE3	1:J:4800:LEU:HG	1.99	0.42
2:K:18:LEU:HB2	2:K:82:MET:HB3	2.00	0.42
1:A:291:LEU:HD11	1:A:299:LEU:HD12	2.00	0.42
1:A:569:ILE:HG13	1:A:570:GLU:HG2	2.01	0.42
1:A:785:ALA:HB2	1:A:1613:LEU:HD11	2.00	0.42
1:A:855:PRO:HD2	1:A:998:ARG:CZ	2.48	0.42
1:A:2195:PRO:HB3	1:A:2242:ILE:HG21	2.00	0.42
1:A:2339:VAL:O	1:A:2346:VAL:HG12	2.19	0.42
1:A:2735:PHE:CE1	1:A:2907:PRO:HG3	2.54	0.42
1:A:3965:LEU:O	1:A:3969:ILE:HG12	2.19	0.42
1:A:3970:GLN:OE1	1:A:5004:THR:HA	2.18	0.42
1:C:24:CYS:HB2	1:C:200:TRP:CE3	2.54	0.42
1:C:394:GLN:HB2	1:C:397:GLU:OE1	2.19	0.42
1:C:1641:ILE:HG22	1:C:1644:GLU:H	1.84	0.42
1:C:2735:PHE:CE1	1:C:2907:PRO:HG3	2.54	0.42
1:C:4865:LYS:HE2	1:C:4865:LYS:HB3	1.87	0.42
1:G:24:CYS:HB2	1:G:200:TRP:CE3	2.54	0.42
1:G:404:ILE:HG23	1:G:483:MET:SD	2.59	0.42
1:G:881:LEU:O	1:G:885:THR:HG23	2.18	0.42
1:G:2144:ILE:HD11	1:G:2149:VAL:HG12	2.01	0.42
1:G:3050:VAL:HG21	1:G:3064:VAL:HG11	2.01	0.42
1:G:3132:THR:HA	1:G:3136:LEU:HB3	2.00	0.42
1:G:4248:ALA:HA	1:G:4251:ILE:HG12	2.02	0.42
1:G:5004:THR:HG22	1:G:5007:GLU:HG3	1.99	0.42
1:J:255:HIS:CD2	1:J:480:GLU:HG3	2.55	0.42
1:J:356:TRP:H	1:J:380:GLN:HA	1.83	0.42
1:J:569:ILE:HG13	1:J:570:GLU:HG2	2.01	0.42
1:J:875:ALA:HB1	1:J:921:ASN:HB3	2.00	0.42
1:J:2292:GLU:HB2	1:J:2352:VAL:HG11	2.00	0.42
1:J:2339:VAL:O	1:J:2346:VAL:HG12	2.19	0.42
1:J:2474:LEU:HD13	1:J:2494:PHE:HD2	1.84	0.42
1:J:2735:PHE:CE1	1:J:2907:PRO:HG3	2.54	0.42
1:J:2823:ILE:HA	1:J:2937:VAL:HA	2.01	0.42
1:J:3245:VAL:HG22	1:J:3246:LEU:HD23	2.01	0.42
1:J:4172:GLU:HA	1:J:4175:ARG:NH1	2.35	0.42
1:A:1123:VAL:HG23	1:A:1132:TRP:HB2	2.01	0.42
1:A:1237:TRP:CH2	1:A:1652:GLU:HG3	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1763:PRO:HD2	1:A:1863:LEU:HD21	2.01	0.42
1:A:3132:THR:HA	1:A:3136:LEU:HB3	2.01	0.42
1:A:3850:GLN:NE2	1:A:3874:VAL:HG12	2.34	0.42
1:A:4846:VAL:HG21	1:G:4816:ILE:HD11	2.01	0.42
1:C:1717:SER:HA	1:C:1721:GLU:HB2	2.01	0.42
1:C:3245:VAL:HG22	1:C:3246:LEU:HD23	2.01	0.42
1:C:3353:LEU:HG	1:C:3358:PHE:CE1	2.54	0.42
1:C:3965:LEU:O	1:C:3969:ILE:HG12	2.19	0.42
1:C:4232:GLU:HG3	1:C:5019:TRP:CD1	2.54	0.42
1:G:569:ILE:HG13	1:G:570:GLU:HG2	2.01	0.42
1:G:1078:GLU:HG3	1:G:1237:TRP:NE1	2.32	0.42
1:G:3850:GLN:NE2	1:G:3874:VAL:HG12	2.35	0.42
3:I:62:GLY:O	3:I:66:MET:HG3	2.19	0.42
1:J:404:ILE:HG23	1:J:483:MET:SD	2.59	0.42
1:J:749:ASP:OD2	1:J:754:SER:HB3	2.20	0.42
1:J:1078:GLU:HG3	1:J:1237:TRP:NE1	2.32	0.42
1:J:2680:TRP:CE3	1:J:2683:PHE:HB3	2.54	0.42
1:J:3562:LYS:HB3	1:J:3564:GLU:OE1	2.19	0.42
1:J:4232:GLU:HG3	1:J:5019:TRP:CD1	2.54	0.42
1:J:4567:LEU:HD21	1:J:4816:ILE:HG22	2.01	0.42
1:A:394:GLN:HB2	1:A:397:GLU:OE1	2.19	0.42
1:A:2680:TRP:CE3	1:A:2683:PHE:HB3	2.54	0.42
1:A:3107:VAL:HG22	1:A:3175:LEU:HG	2.01	0.42
1:A:3379:LEU:HD11	1:A:3391:GLU:HB2	2.01	0.42
1:A:3826:VAL:HA	1:A:3909:ASN:HD21	1.84	0.42
1:A:3836:MET:HE2	1:A:3836:MET:HB2	1.89	0.42
1:A:4085:ARG:HD2	1:A:4085:ARG:HA	1.88	0.42
1:A:4172:GLU:HA	1:A:4175:ARG:NH1	2.35	0.42
1:C:1003:GLN:HB2	1:C:1005:TRP:HD1	1.83	0.42
1:C:1237:TRP:CH2	1:C:1652:GLU:HG3	2.54	0.42
1:C:1763:PRO:HD2	1:C:1863:LEU:HD21	2.01	0.42
1:C:2339:VAL:O	1:C:2346:VAL:HG12	2.19	0.42
1:C:2680:TRP:CE3	1:C:2683:PHE:HB3	2.54	0.42
3:F:62:GLY:O	3:F:66:MET:HG3	2.19	0.42
1:G:399:GLN:O	1:G:403:MET:HG3	2.19	0.42
1:G:1297:PHE:HA	1:G:1522:LEU:HG	2.01	0.42
1:G:3282:PRO:HG3	1:G:3345:ILE:CD1	2.49	0.42
1:G:3353:LEU:HG	1:G:3358:PHE:CE1	2.54	0.42
1:G:4823:LEU:HD12	1:G:4823:LEU:HA	1.75	0.42
1:J:35:LEU:HG	1:J:51:PRO:HA	2.01	0.42
1:J:394:GLN:HB2	1:J:397:GLU:OE1	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:890:GLY:O	1:J:891:TRP:C	2.62	0.42
1:J:1109:LEU:HD21	1:J:1115:LEU:HD11	2.02	0.42
1:J:2250:MET:HE2	1:J:2250:MET:HA	2.01	0.42
1:J:2582:MET:HE3	1:J:2582:MET:HB3	1.86	0.42
1:J:3367:LYS:HE2	1:J:3367:LYS:HB2	1.93	0.42
1:J:3850:GLN:NE2	1:J:3874:VAL:HG12	2.34	0.42
1:J:4091:LYS:HE2	1:J:4091:LYS:HA	2.01	0.42
1:J:4172:GLU:HA	1:J:4175:ARG:HH12	1.84	0.42
3:L:62:GLY:O	3:L:66:MET:HG3	2.19	0.42
1:A:451:TYR:CZ	1:A:474:ARG:HD3	2.54	0.42
1:A:883:ALA:O	1:A:887:ILE:HG13	2.20	0.42
1:A:911:HIS:CD2	1:A:918:ARG:HG2	2.54	0.42
1:A:2765:LYS:HD3	1:A:2765:LYS:HA	1.73	0.42
1:A:2799:GLU:O	1:A:2803:GLU:HG2	2.20	0.42
1:A:2827:ARG:HH22	1:A:2830:GLU:HB3	1.83	0.42
1:C:255:HIS:CD2	1:C:480:GLU:HG3	2.55	0.42
1:C:1476:MET:HE3	1:C:1476:MET:HB3	1.85	0.42
1:C:3132:THR:HA	1:C:3136:LEU:HB3	2.01	0.42
1:C:3233:PRO:HG2	1:C:3239:MET:HA	2.01	0.42
1:C:4172:GLU:HA	1:C:4175:ARG:NH1	2.35	0.42
1:C:4668:LEU:O	1:C:4672:LYS:HG2	2.19	0.42
1:G:255:HIS:CD2	1:G:480:GLU:HG3	2.55	0.42
1:G:1653:LEU:HD23	1:G:1660:GLN:HA	2.02	0.42
1:G:2250:MET:HE2	1:G:2250:MET:HA	2.01	0.42
1:G:2292:GLU:HB2	1:G:2352:VAL:HG11	2.00	0.42
1:G:2339:VAL:O	1:G:2346:VAL:HG12	2.19	0.42
1:G:2623:LEU:O	1:G:2627:VAL:HG23	2.20	0.42
1:G:2680:TRP:CE3	1:G:2683:PHE:HB3	2.54	0.42
1:G:2816:MET:SD	1:G:2878:LEU:HD22	2.60	0.42
1:G:3163:VAL:O	1:G:3167:ARG:HG2	2.19	0.42
1:G:4846:VAL:HG21	1:J:4816:ILE:HD11	2.01	0.42
1:J:2346:VAL:HG13	1:J:2349:ASN:HB2	2.01	0.42
1:J:3163:VAL:O	1:J:3167:ARG:HG2	2.19	0.42
1:J:3190:LEU:O	1:J:3194:LEU:HB3	2.19	0.42
1:J:3734:HIS:HB3	1:J:3803:SER:HB2	2.00	0.42
1:J:4626:ASN:HD22	1:J:4626:ASN:N	2.16	0.42
1:A:1653:LEU:HD23	1:A:1660:GLN:HA	2.02	0.42
1:A:2816:MET:SD	1:A:2878:LEU:HD22	2.60	0.42
1:A:3353:LEU:HG	1:A:3358:PHE:CE1	2.54	0.42
1:A:3782:MET:HA	1:A:3782:MET:HE3	2.02	0.42
1:A:4248:ALA:HA	1:A:4251:ILE:HG12	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4963:ILE:HD13	1:A:5030:LYS:HD2	2.01	0.42
1:C:465:GLN:O	1:C:469:ARG:HG3	2.18	0.42
1:C:785:ALA:HB2	1:C:1613:LEU:HD11	2.00	0.42
1:C:911:HIS:CD2	1:C:918:ARG:HG2	2.54	0.42
1:C:2250:MET:HA	1:C:2250:MET:HE2	2.01	0.42
1:C:3020:THR:HB	1:C:3023:LYS:HG3	2.00	0.42
1:C:3129:LEU:HD23	1:C:3129:LEU:H	1.85	0.42
2:D:49:ALA:HB2	2:D:63:VAL:HG23	2.01	0.42
1:G:179:TYR:HB2	1:G:197:GLN:HA	2.00	0.42
1:G:214:VAL:HG21	1:G:390:LEU:HD12	2.02	0.42
1:G:291:LEU:HD11	1:G:299:LEU:HD12	2.00	0.42
1:G:1476:MET:HE3	1:G:1476:MET:HB3	1.85	0.42
1:G:2515:GLN:HE22	1:G:2574:HIS:HE1	1.67	0.42
1:G:2976:HIS:CE1	1:G:2990:PRO:HD2	2.55	0.42
1:G:3433:GLU:HA	1:G:3436:ARG:HD2	2.01	0.42
1:G:4172:GLU:HA	1:G:4175:ARG:NH1	2.35	0.42
1:G:4733:GLY:H	1:G:4736:ARG:HD2	1.84	0.42
2:H:49:ALA:HB2	2:H:63:VAL:HG23	2.01	0.42
1:J:399:GLN:O	1:J:403:MET:HG3	2.19	0.42
1:J:668:VAL:HA	1:J:789:VAL:HG12	2.02	0.42
1:J:1641:ILE:HG22	1:J:1644:GLU:H	1.84	0.42
1:J:2700:MET:HE3	1:J:2701:PRO:HD3	2.01	0.42
1:A:454:PRO:HA	1:A:455:PRO:HD3	1.97	0.42
1:A:1207:ASP:HB2	1:A:1210:SER:HB2	2.02	0.42
1:A:1297:PHE:HA	1:A:1522:LEU:HG	2.01	0.42
1:A:2474:LEU:HD13	1:A:2494:PHE:HD2	1.84	0.42
1:A:2623:LEU:O	1:A:2627:VAL:HG23	2.20	0.42
1:A:2823:ILE:HA	1:A:2937:VAL:HA	2.01	0.42
1:A:4668:LEU:O	1:A:4672:LYS:HG2	2.19	0.42
1:A:4816:ILE:HD11	1:C:4846:VAL:HG21	2.01	0.42
2:B:49:ALA:HB2	2:B:63:VAL:HG23	2.01	0.42
1:C:404:ILE:HG23	1:C:483:MET:SD	2.59	0.42
1:C:2816:MET:SD	1:C:2878:LEU:HD22	2.60	0.42
1:C:2976:HIS:CE1	1:C:2990:PRO:HD2	2.55	0.42
1:C:3179:LYS:HG2	1:C:3187:ARG:HH22	1.84	0.42
1:C:3850:GLN:NE2	1:C:3874:VAL:HG12	2.35	0.42
1:G:35:LEU:HG	1:G:51:PRO:HA	2.01	0.42
1:G:207:SER:HB3	1:G:269:TRP:HE1	1.84	0.42
1:G:883:ALA:HB1	1:G:967:PRO:HG2	2.01	0.42
1:G:1558:HIS:HD2	1:G:1560:ASN:H	1.67	0.42
1:G:2236:LEU:HD23	1:G:2236:LEU:HA	1.89	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:266:ARG:HG3	1:J:268:SER:HB3	2.01	0.42
1:J:2350:ALA:O	1:J:2354:VAL:HG12	2.20	0.42
1:J:2976:HIS:CE1	1:J:2990:PRO:HD2	2.55	0.42
1:J:3826:VAL:HA	1:J:3909:ASN:HD21	1.84	0.42
1:J:4668:LEU:O	1:J:4672:LYS:HG2	2.19	0.42
1:J:5030:LYS:HA	1:J:5033:GLU:HG3	2.00	0.42
1:A:73:LEU:HA	1:A:73:LEU:HD23	1.84	0.42
1:A:207:SER:HB3	1:A:269:TRP:HE1	1.84	0.42
1:A:1260:MET:HE2	1:A:1269:CYS:SG	2.59	0.42
1:A:1268:PRO:HD2	1:A:1589:PRO:HB2	2.01	0.42
1:A:1641:ILE:HG22	1:A:1644:GLU:H	1.84	0.42
1:A:2591:ARG:HH22	1:A:2625:ARG:NH2	2.17	0.42
1:A:5013:MET:HE2	1:A:5013:MET:HB3	1.74	0.42
4:A:5115:POV:H25A	4:A:5115:POV:H22	1.94	0.42
1:C:580:GLU:HG2	1:C:584:LYS:HE2	2.01	0.42
1:C:1207:ASP:HB2	1:C:1210:SER:HB2	2.02	0.42
1:C:2380:ILE:HG13	1:C:2469:ILE:HD13	2.01	0.42
1:C:3420:ARG:HG3	1:C:3520:ILE:HD11	2.00	0.42
1:C:4055:VAL:O	1:C:4059:LEU:HG	2.20	0.42
1:C:4056:GLU:HG2	1:C:4166:LEU:HD12	2.01	0.42
1:C:4567:LEU:HD21	1:C:4816:ILE:HG22	2.01	0.42
3:E:56:ILE:HG22	3:E:58:GLY:N	2.35	0.42
3:F:56:ILE:HG22	3:F:58:GLY:N	2.35	0.42
3:F:58:GLY:HA3	3:F:80:VAL:HG11	2.02	0.42
1:G:451:TYR:CZ	1:G:474:ARG:HD3	2.54	0.42
1:G:1109:LEU:HD21	1:G:1115:LEU:HD11	2.02	0.42
1:G:2238:TYR:O	1:G:2242:ILE:HG12	2.20	0.42
1:G:2346:VAL:HG13	1:G:2349:ASN:HB2	2.01	0.42
1:G:2700:MET:HE3	1:G:2701:PRO:HD3	2.01	0.42
1:G:3868:ARG:NH1	1:G:3869:GLN:HB3	2.35	0.42
1:G:4668:LEU:O	1:G:4672:LYS:HG2	2.19	0.42
1:J:882:TRP:O	1:J:886:ARG:HG2	2.20	0.42
1:J:1297:PHE:HA	1:J:1522:LEU:HG	2.01	0.42
1:J:3330:ASP:HA	1:J:3403:ARG:HH22	1.85	0.42
1:A:214:VAL:HG21	1:A:390:LEU:HD12	2.02	0.42
1:A:2185:ILE:HD12	1:A:2203:MET:HE1	2.02	0.42
1:A:3330:ASP:HA	1:A:3403:ARG:HH22	1.85	0.42
1:A:4044:MET:HE3	1:A:4044:MET:HB3	1.82	0.42
1:C:882:TRP:O	1:C:885:THR:OG1	2.37	0.42
1:C:2208:MET:HE1	1:C:2253:HIS:ND1	2.35	0.42
1:C:3564:GLU:HA	1:C:3570:ARG:NH1	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1641:ILE:HG22	1:G:1644:GLU:H	1.84	0.42
1:G:2185:ILE:HD12	1:G:2203:MET:HE1	2.02	0.42
1:G:2208:MET:HE1	1:G:2253:HIS:ND1	2.35	0.42
1:G:2522:LEU:HA	1:G:2526:PHE:HB2	2.02	0.42
1:G:2799:GLU:O	1:G:2803:GLU:HG2	2.20	0.42
1:G:3782:MET:HA	1:G:3782:MET:HE3	2.02	0.42
1:G:3970:GLN:OE1	1:G:5004:THR:HA	2.18	0.42
1:J:291:LEU:HD11	1:J:299:LEU:HD12	2.00	0.42
1:J:911:HIS:CD2	1:J:918:ARG:HG2	2.54	0.42
1:J:1862:ILE:O	1:J:1866:ILE:HG12	2.20	0.42
1:J:2515:GLN:HE22	1:J:2574:HIS:HE1	1.67	0.42
1:J:3050:VAL:HG21	1:J:3064:VAL:HG11	2.01	0.42
1:J:3966:THR:O	1:J:3970:GLN:HG2	2.20	0.42
3:L:7:ILE:HB	3:L:71:ARG:HD2	2.00	0.42
1:A:890:GLY:O	1:A:891:TRP:C	2.62	0.42
1:A:2177:LEU:HD13	1:A:2177:LEU:HA	1.96	0.42
1:A:2380:ILE:HG13	1:A:2469:ILE:HD13	2.01	0.42
1:A:2515:GLN:HE22	1:A:2574:HIS:CE1	2.38	0.42
1:A:2976:HIS:CE1	1:A:2990:PRO:HD2	2.55	0.42
1:A:3020:THR:HB	1:A:3023:LYS:HG3	2.00	0.42
1:A:3868:ARG:NH1	1:A:3869:GLN:HB3	2.35	0.42
1:C:1692:ALA:HB2	3:E:41:ASP:HB2	2.02	0.42
1:C:3506:GLN:H	1:C:3506:GLN:HG3	1.67	0.42
1:C:3734:HIS:HB3	1:C:3803:SER:HB2	2.00	0.42
1:C:4813:LEU:HA	1:C:4813:LEU:HD23	1.88	0.42
1:G:1758:ARG:HD3	1:G:1758:ARG:HA	1.85	0.42
1:G:2474:LEU:HD13	1:G:2494:PHE:HD2	1.84	0.42
4:G:5104:POV:H38A	4:G:5104:POV:H31B	1.78	0.42
1:J:567:VAL:HG12	1:J:574:VAL:HG21	2.02	0.42
1:J:2623:LEU:O	1:J:2627:VAL:HG23	2.20	0.42
1:J:3282:PRO:HG3	1:J:3345:ILE:CD1	2.49	0.42
1:J:3782:MET:HA	1:J:3782:MET:HE3	2.02	0.42
1:J:4583:SER:HB3	1:J:4631:PHE:HE1	1.85	0.42
1:J:4834:GLY:HA3	4:J:5110:POV:H1	2.02	0.42
1:A:266:ARG:HG3	1:A:268:SER:HB3	2.01	0.41
1:A:4928:LEU:HD23	1:A:4931:ILE:HD12	2.02	0.41
1:C:805:PRO:HB2	1:C:808:TYR:CD1	2.55	0.41
1:C:1497:GLY:HA2	1:C:1500:PHE:HB2	2.01	0.41
1:C:1862:ILE:O	1:C:1866:ILE:HG12	2.20	0.41
1:C:2144:ILE:HD11	1:C:2149:VAL:HG12	2.01	0.41
1:C:2522:LEU:HA	1:C:2526:PHE:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4963:ILE:HD13	1:C:5030:LYS:HD2	2.01	0.41
1:G:356:TRP:H	1:G:380:GLN:HA	1.83	0.41
1:G:749:ASP:OD2	1:G:754:SER:HB3	2.20	0.41
1:G:2350:ALA:O	1:G:2354:VAL:HG12	2.20	0.41
1:G:3330:ASP:HA	1:G:3403:ARG:HH22	1.85	0.41
1:G:4068:LEU:HD12	1:G:4068:LEU:HA	1.81	0.41
1:J:981:GLN:O	1:J:985:VAL:HG23	2.20	0.41
1:J:1123:VAL:HG23	1:J:1132:TRP:HB2	2.01	0.41
1:J:1717:SER:HA	1:J:1721:GLU:HB2	2.01	0.41
1:J:2469:ILE:HA	1:J:2472:LEU:HB2	2.02	0.41
1:J:2604:GLU:O	1:J:2608:MET:HG3	2.19	0.41
1:J:2816:MET:SD	1:J:2878:LEU:HD22	2.60	0.41
1:J:2879:ALA:HA	1:J:2882:TYR:CD2	2.55	0.41
1:J:3107:VAL:HG22	1:J:3175:LEU:HG	2.01	0.41
1:J:3129:LEU:HD23	1:J:3129:LEU:H	1.85	0.41
1:J:4085:ARG:HD2	1:J:4085:ARG:HA	1.88	0.41
4:J:5103:POV:H13B	4:J:5103:POV:H11A	1.89	0.41
2:K:49:ALA:HB2	2:K:63:VAL:HG23	2.01	0.41
3:L:56:ILE:HG22	3:L:58:GLY:N	2.35	0.41
1:A:255:HIS:CD2	1:A:480:GLU:HG3	2.55	0.41
1:A:567:VAL:HG12	1:A:574:VAL:HG21	2.02	0.41
1:A:882:TRP:CH2	2:B:104:TYR:HA	2.55	0.41
1:A:2244:ARG:HH21	1:A:2283:ASN:HA	1.85	0.41
1:A:2350:ALA:O	1:A:2354:VAL:HG12	2.20	0.41
1:A:4646:LEU:HD13	1:A:4646:LEU:HA	1.91	0.41
1:C:1109:LEU:HD21	1:C:1115:LEU:HD11	2.02	0.41
1:C:2515:GLN:HE22	1:C:2574:HIS:CE1	2.38	0.41
1:C:3107:VAL:HG22	1:C:3175:LEU:HG	2.01	0.41
1:C:3539:ARG:HD3	1:C:3552:PHE:CD2	2.56	0.41
1:C:4583:SER:HB3	1:C:4631:PHE:HE1	1.85	0.41
1:C:4733:GLY:H	1:C:4736:ARG:HD2	1.84	0.41
2:D:86:LYS:HE2	2:D:86:LYS:HB2	1.84	0.41
1:G:1177:THR:O	1:G:1180:ARG:NH2	2.53	0.41
1:G:1260:MET:HE2	1:G:1269:CYS:SG	2.59	0.41
1:G:1717:SER:HA	1:G:1721:GLU:HB2	2.01	0.41
1:G:2823:ILE:HA	1:G:2937:VAL:HA	2.01	0.41
1:G:2954:ARG:HG2	1:G:2956:ALA:H	1.85	0.41
1:G:3731:LYS:HA	1:G:3734:HIS:ND1	2.36	0.41
1:G:4573:ILE:O	1:G:4577:LEU:HG	2.20	0.41
3:I:56:ILE:HG22	3:I:58:GLY:N	2.35	0.41
1:J:23:GLN:HG3	1:J:201:ASN:OD1	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:514:SER:O	1:J:518:ILE:HG13	2.21	0.41
1:J:1268:PRO:HD2	1:J:1589:PRO:HB2	2.01	0.41
1:J:1763:PRO:HD2	1:J:1863:LEU:HD21	2.01	0.41
1:J:2025:GLU:HA	1:J:2028:ARG:HG2	2.02	0.41
1:J:4573:ILE:O	1:J:4577:LEU:HG	2.20	0.41
1:A:23:GLN:HG3	1:A:201:ASN:OD1	2.21	0.41
1:A:1476:MET:HE3	1:A:1476:MET:HB3	1.85	0.41
1:A:1497:GLY:HA2	1:A:1500:PHE:HB2	2.01	0.41
1:A:3276:MET:HA	1:A:3276:MET:HE3	2.02	0.41
1:A:3439:GLY:O	1:A:3443:ILE:HG12	2.20	0.41
1:A:4587:PRO:HG3	1:A:4631:PHE:HB3	2.02	0.41
1:C:182:LEU:HB2	1:C:198:THR:HG21	2.00	0.41
1:C:567:VAL:HG12	1:C:574:VAL:HG21	2.02	0.41
1:C:614:VAL:HG13	1:C:617:ASN:HB2	2.03	0.41
1:C:1863:LEU:HD12	1:C:1863:LEU:HA	1.93	0.41
1:C:2712:PRO:HD3	1:C:3013:HIS:CE1	2.56	0.41
1:C:2799:GLU:O	1:C:2803:GLU:HG2	2.20	0.41
1:C:3172:ILE:HD12	1:C:3194:LEU:HB2	2.02	0.41
1:C:3276:MET:HA	1:C:3276:MET:HE3	2.02	0.41
1:C:3782:MET:HA	1:C:3782:MET:HE3	2.02	0.41
1:C:4172:GLU:HA	1:C:4175:ARG:HH12	1.84	0.41
1:C:4928:LEU:HD23	1:C:4931:ILE:HD12	2.02	0.41
3:E:62:GLY:O	3:E:66:MET:HG3	2.19	0.41
1:G:567:VAL:HG12	1:G:574:VAL:HG21	2.02	0.41
1:G:580:GLU:HG2	1:G:584:LYS:HE2	2.01	0.41
1:G:614:VAL:HG13	1:G:617:ASN:HB2	2.03	0.41
1:G:1763:PRO:HD2	1:G:1863:LEU:HD21	2.01	0.41
1:G:2712:PRO:HD3	1:G:3013:HIS:CE1	2.56	0.41
1:G:2879:ALA:HA	1:G:2882:TYR:CD2	2.55	0.41
1:G:3037:GLU:CD	1:G:3085:PRO:HG2	2.45	0.41
3:I:25:HIS:HB3	3:I:40:ARG:CZ	2.50	0.41
1:J:180:LEU:HD23	1:J:200:TRP:CE2	2.55	0.41
1:J:614:VAL:HG13	1:J:617:ASN:HB2	2.03	0.41
1:J:620:LEU:HA	1:J:623:GLU:HG2	2.02	0.41
1:J:620:LEU:HA	1:J:620:LEU:HD23	1.87	0.41
1:J:2522:LEU:HA	1:J:2526:PHE:HB2	2.02	0.41
1:J:2799:GLU:O	1:J:2803:GLU:HG2	2.20	0.41
1:J:2867:LEU:H	1:J:2928:LYS:HZ2	1.68	0.41
1:J:3439:GLY:O	1:J:3443:ILE:HG12	2.20	0.41
1:A:582:HIS:O	1:A:586:ILE:HG13	2.21	0.41
1:A:1106:ARG:HH22	1:A:1183:GLU:HG3	1.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3190:LEU:O	1:A:3194:LEU:HB3	2.19	0.41
1:A:3539:ARG:HD3	1:A:3552:PHE:CD2	2.56	0.41
1:C:266:ARG:HG3	1:C:268:SER:HB3	2.01	0.41
1:C:1639:LEU:HD12	1:C:1639:LEU:HA	1.94	0.41
1:C:1648:MET:HG3	1:C:1652:GLU:HB3	2.02	0.41
1:C:2623:LEU:O	1:C:2627:VAL:HG23	2.20	0.41
1:C:3731:LYS:HA	1:C:3734:HIS:ND1	2.36	0.41
1:C:4248:ALA:HA	1:C:4251:ILE:HG12	2.02	0.41
3:E:78:PRO:HD3	3:E:96:THR:OG1	2.21	0.41
1:G:1268:PRO:HD2	1:G:1589:PRO:HB2	2.01	0.41
1:G:1648:MET:HG3	1:G:1652:GLU:HB3	2.02	0.41
1:G:2177:LEU:HD13	1:G:2177:LEU:HA	1.96	0.41
1:G:2641:LEU:HD11	1:G:2698:MET:SD	2.61	0.41
1:G:3194:LEU:HA	1:G:3197:LEU:HG	2.03	0.41
1:G:3564:GLU:HA	1:G:3570:ARG:NH1	2.35	0.41
1:J:207:SER:HB3	1:J:269:TRP:HE1	1.84	0.41
1:J:796:ARG:HB3	1:J:1622:GLU:OE1	2.20	0.41
1:J:805:PRO:HB2	1:J:808:TYR:CD1	2.55	0.41
1:J:2144:ILE:HD11	1:J:2149:VAL:HG12	2.01	0.41
1:J:2203:MET:HG3	1:J:2235:PHE:HZ	1.85	0.41
1:J:2954:ARG:HG2	1:J:2956:ALA:H	1.85	0.41
1:J:3206:LEU:HD23	1:J:3206:LEU:HA	1.75	0.41
1:J:3564:GLU:HA	1:J:3570:ARG:NH1	2.35	0.41
1:A:494:LEU:HD22	1:A:515:TRP:CD1	2.56	0.41
1:A:749:ASP:OD2	1:A:754:SER:HB3	2.20	0.41
1:A:805:PRO:HB2	1:A:808:TYR:CD1	2.55	0.41
1:A:2250:MET:HE2	1:A:2250:MET:HA	2.01	0.41
1:A:2604:GLU:O	1:A:2608:MET:HG3	2.19	0.41
1:A:2856:ASN:HA	1:A:2857:PRO:HD3	1.96	0.41
1:A:3731:LYS:HA	1:A:3734:HIS:ND1	2.36	0.41
1:A:4014:LYS:HB2	1:A:4014:LYS:HE3	1.85	0.41
1:A:4573:ILE:O	1:A:4577:LEU:HG	2.20	0.41
1:A:4583:SER:HB3	1:A:4631:PHE:HE1	1.86	0.41
1:C:214:VAL:HG21	1:C:390:LEU:HD12	2.02	0.41
1:C:1297:PHE:HA	1:C:1522:LEU:HG	2.01	0.41
1:C:1575:LEU:HD23	1:C:1575:LEU:HA	1.77	0.41
1:C:1653:LEU:HD23	1:C:1660:GLN:HA	2.02	0.41
1:C:2244:ARG:HH21	1:C:2283:ASN:HA	1.85	0.41
1:C:3194:LEU:HA	1:C:3197:LEU:HG	2.03	0.41
3:F:25:HIS:HB3	3:F:40:ARG:CZ	2.50	0.41
1:G:4583:SER:HB3	1:G:4631:PHE:HE1	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1271:ARG:HG3	1:J:1563:GLN:HB2	2.03	0.41
1:J:2382:GLU:O	1:J:2386:ILE:HG13	2.21	0.41
1:J:2641:LEU:HD11	1:J:2698:MET:SD	2.61	0.41
1:J:3036:LYS:O	1:J:3039:ILE:HG22	2.20	0.41
1:J:3194:LEU:HA	1:J:3197:LEU:HG	2.03	0.41
1:J:3539:ARG:HD3	1:J:3552:PHE:CD2	2.56	0.41
1:J:4055:VAL:O	1:J:4059:LEU:HG	2.20	0.41
1:J:4107:GLU:O	1:J:4111:LEU:HG	2.21	0.41
1:J:4202:ARG:O	1:J:4206:GLU:HG2	2.19	0.41
1:A:2469:ILE:HA	1:A:2472:LEU:HB2	2.02	0.41
1:A:3302:PRO:HA	1:A:3303:PRO:HD3	1.97	0.41
1:A:3564:GLU:HA	1:A:3570:ARG:NH1	2.35	0.41
1:A:3966:THR:O	1:A:3970:GLN:HG2	2.20	0.41
1:A:4021:LYS:HG3	1:A:4142:ASN:ND2	2.36	0.41
1:A:4733:GLY:H	1:A:4736:ARG:HD2	1.84	0.41
1:A:4928:LEU:HD23	1:A:4928:LEU:HA	1.88	0.41
1:C:620:LEU:HA	1:C:623:GLU:HG2	2.02	0.41
1:C:736:HIS:HB2	3:E:9:PRO:CG	2.50	0.41
1:C:996:TRP:O	1:C:1000:ARG:HG2	2.21	0.41
1:C:1271:ARG:HG3	1:C:1563:GLN:HB2	2.03	0.41
1:C:2641:LEU:HD11	1:C:2698:MET:SD	2.61	0.41
1:C:2924:GLN:O	1:C:2928:LYS:HG2	2.21	0.41
1:C:3362:ILE:HD12	1:C:3362:ILE:HA	1.95	0.41
1:C:3439:GLY:O	1:C:3443:ILE:HG12	2.20	0.41
1:C:4107:GLU:O	1:C:4111:LEU:HG	2.21	0.41
1:G:23:GLN:HG3	1:G:201:ASN:OD1	2.21	0.41
1:G:514:SER:O	1:G:518:ILE:HG13	2.21	0.41
1:G:582:HIS:O	1:G:586:ILE:HG13	2.21	0.41
1:G:2310:CYS:SG	1:G:2312:MET:HG2	2.61	0.41
1:G:2856:ASN:HA	1:G:2857:PRO:HD3	1.96	0.41
1:G:3276:MET:HE3	1:G:3276:MET:HA	2.02	0.41
1:G:3316:LEU:HD21	1:G:3345:ILE:O	2.21	0.41
1:G:3966:THR:O	1:G:3970:GLN:HG2	2.20	0.41
1:G:4055:VAL:O	1:G:4059:LEU:HG	2.20	0.41
1:G:4689:THR:HA	1:G:4732:PHE:CZ	2.55	0.41
1:G:4751:THR:O	1:G:4755:GLU:HG2	2.20	0.41
3:I:35:LYS:H	3:I:35:LYS:HD2	1.86	0.41
1:J:582:HIS:O	1:J:586:ILE:HG13	2.21	0.41
1:J:1207:ASP:HB2	1:J:1210:SER:HB2	2.02	0.41
1:J:2208:MET:HE1	1:J:2253:HIS:ND1	2.35	0.41
1:J:2336:ARG:HB3	1:J:2435:ARG:NH1	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:2534:ALA:HB1	1:J:2588:ARG:NE	2.33	0.41
1:J:3172:ILE:HD12	1:J:3194:LEU:HB2	2.02	0.41
1:J:3308:THR:H	1:J:3311:HIS:CE1	2.39	0.41
1:J:3868:ARG:NH1	1:J:3869:GLN:HB3	2.35	0.41
3:L:25:HIS:HB3	3:L:40:ARG:CZ	2.50	0.41
1:A:2025:GLU:HA	1:A:2028:ARG:HG2	2.02	0.41
1:A:2641:LEU:HD11	1:A:2698:MET:SD	2.61	0.41
1:A:2712:PRO:HD3	1:A:3013:HIS:CE1	2.56	0.41
1:A:2876:GLU:HG3	1:A:2908:TYR:CE2	2.51	0.41
1:A:3254:GLY:O	1:A:3258:GLU:HG2	2.21	0.41
1:A:4751:THR:O	1:A:4755:GLU:HG2	2.20	0.41
1:C:749:ASP:OD2	1:C:754:SER:HB3	2.20	0.41
1:C:886:ARG:HD3	1:C:891:TRP:CD1	2.56	0.41
1:C:3190:LEU:O	1:C:3194:LEU:HB3	2.19	0.41
1:C:3405:LEU:HD12	1:C:3509:LEU:HD12	2.03	0.41
1:C:3826:VAL:HA	1:C:3909:ASN:HD21	1.84	0.41
1:C:3868:ARG:NH1	1:C:3869:GLN:HB3	2.35	0.41
1:C:4573:ILE:O	1:C:4577:LEU:HG	2.20	0.41
1:G:805:PRO:HB2	1:G:808:TYR:CD1	2.55	0.41
1:G:3254:GLY:O	1:G:3258:GLU:HG2	2.21	0.41
1:G:3308:THR:H	1:G:3311:HIS:CE1	2.39	0.41
1:G:4234:PHE:CE1	1:G:4985:LEU:HG	2.56	0.41
1:G:4587:PRO:HG3	1:G:4631:PHE:HB3	2.02	0.41
1:J:580:GLU:HG2	1:J:584:LYS:HE2	2.01	0.41
1:J:2677:LYS:HE3	1:J:2909:ASP:HB2	2.03	0.41
1:J:3276:MET:HA	1:J:3276:MET:HE3	2.02	0.41
1:J:4587:PRO:HG3	1:J:4631:PHE:HB3	2.02	0.41
1:J:4963:ILE:HD13	1:J:5030:LYS:HD2	2.01	0.41
3:L:35:LYS:HD2	3:L:35:LYS:H	1.86	0.41
1:A:2916:LYS:NZ	1:A:2920:ARG:HE	2.19	0.41
1:A:3194:LEU:HA	1:A:3197:LEU:HG	2.03	0.41
1:A:3308:THR:H	1:A:3311:HIS:CE1	2.39	0.41
1:A:4055:VAL:O	1:A:4059:LEU:HG	2.20	0.41
1:C:514:SER:O	1:C:518:ILE:HG13	2.21	0.41
1:C:582:HIS:O	1:C:586:ILE:HG13	2.21	0.41
1:C:977:LEU:HD12	1:C:1047:LEU:HD22	2.03	0.41
1:C:2012:PHE:HB2	1:C:2018:GLU:HA	2.03	0.41
1:C:2182:ILE:HD13	1:C:2182:ILE:HA	1.91	0.41
1:C:2591:ARG:HH22	1:C:2625:ARG:NH2	2.17	0.41
3:F:56:ILE:HG23	3:F:81:ALA:CB	2.50	0.41
1:G:1207:ASP:HB2	1:G:1210:SER:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2382:GLU:O	1:G:2386:ILE:HG13	2.21	0.41
1:G:2563:THR:HG22	1:G:2606:CYS:HA	2.03	0.41
1:G:4021:LYS:HG3	1:G:4142:ASN:ND2	2.36	0.41
1:G:4834:GLY:HA3	4:G:5107:POV:H1	2.02	0.41
4:G:5113:POV:H25	4:G:5113:POV:H35A	2.03	0.41
1:J:2515:GLN:HE22	1:J:2574:HIS:CE1	2.38	0.41
1:J:2916:LYS:NZ	1:J:2920:ARG:HE	2.19	0.41
1:J:3277:LEU:H	1:J:3277:LEU:HG	1.68	0.41
1:J:3731:LYS:HA	1:J:3734:HIS:ND1	2.36	0.41
1:J:4655:PHE:O	1:J:4659:ILE:HG12	2.21	0.41
1:J:4813:LEU:HD23	1:J:4813:LEU:HA	1.88	0.41
1:A:614:VAL:HG13	1:A:617:ASN:HB2	2.03	0.41
1:A:977:LEU:HD12	1:A:1047:LEU:HD22	2.03	0.41
1:A:1433:TYR:CD1	1:A:1578:ALA:HB2	2.56	0.41
1:A:2208:MET:HE1	1:A:2253:HIS:ND1	2.35	0.41
1:A:2233:CYS:C	1:A:2235:PHE:N	2.78	0.41
1:A:2310:CYS:SG	1:A:2312:MET:HG2	2.61	0.41
1:A:2336:ARG:HB3	1:A:2435:ARG:NH1	2.36	0.41
1:A:2522:LEU:HA	1:A:2526:PHE:HB2	2.02	0.41
1:A:3129:LEU:HD23	1:A:3129:LEU:H	1.85	0.41
1:A:3316:LEU:HD21	1:A:3345:ILE:O	2.21	0.41
1:A:4689:THR:HA	1:A:4732:PHE:CZ	2.56	0.41
1:A:4834:GLY:HA3	4:A:5109:POV:H1	2.02	0.41
1:C:135:VAL:HG22	1:C:192:ASP:HA	2.03	0.41
1:C:388:LEU:HD13	1:C:388:LEU:HA	1.88	0.41
1:C:1433:TYR:CD1	1:C:1578:ALA:HB2	2.56	0.41
1:C:2185:ILE:HD12	1:C:2203:MET:HE1	2.02	0.41
1:C:2233:CYS:C	1:C:2235:PHE:N	2.77	0.41
1:C:2310:CYS:SG	1:C:2312:MET:HG2	2.61	0.41
1:C:2350:ALA:O	1:C:2354:VAL:HG12	2.20	0.41
1:C:2469:ILE:HA	1:C:2472:LEU:HB2	2.02	0.41
1:C:3282:PRO:HG3	1:C:3345:ILE:CD1	2.49	0.41
1:C:3308:THR:H	1:C:3311:HIS:CE1	2.39	0.41
1:C:3966:THR:O	1:C:3970:GLN:HG2	2.20	0.41
1:C:4044:MET:HE3	1:C:4044:MET:HB3	1.82	0.41
3:E:15:PHE:HB3	3:E:64:ALA:O	2.21	0.41
3:E:25:HIS:HB3	3:E:40:ARG:CZ	2.50	0.41
1:G:959:TYR:CE2	1:G:961:MET:HA	2.56	0.41
1:G:1271:ARG:HG3	1:G:1563:GLN:HB2	2.03	0.41
1:G:2025:GLU:HA	1:G:2028:ARG:HG2	2.02	0.41
1:G:2916:LYS:NZ	1:G:2920:ARG:HE	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2924:GLN:O	1:G:2928:LYS:HG2	2.21	0.41
1:G:3129:LEU:HD23	1:G:3129:LEU:H	1.85	0.41
1:G:3315:LEU:HD12	1:G:3319:ILE:HD13	2.03	0.41
1:G:3439:GLY:O	1:G:3443:ILE:HG12	2.20	0.41
1:G:4107:GLU:O	1:G:4111:LEU:HG	2.21	0.41
1:G:4655:PHE:O	1:G:4659:ILE:HG12	2.21	0.41
1:G:4928:LEU:HD23	1:G:4931:ILE:HD12	2.02	0.41
1:J:492:ASP:O	1:J:496:VAL:HG23	2.21	0.41
1:J:894:GLY:HA3	1:J:903:LEU:HD22	2.03	0.41
1:J:1177:THR:O	1:J:1180:ARG:NH2	2.53	0.41
1:J:1442:GLY:HA3	1:J:1558:HIS:CG	2.56	0.41
1:J:1648:MET:HG3	1:J:1652:GLU:HB3	2.02	0.41
1:J:1712:TYR:O	1:J:1716:ILE:HG13	2.21	0.41
1:J:1867:GLU:O	1:J:1871:PHE:HB2	2.21	0.41
1:J:2186:MET:HE2	1:J:2238:TYR:HD2	1.85	0.41
1:J:2273:LEU:HD23	1:J:2330:ARG:HB3	2.03	0.41
1:J:2310:CYS:SG	1:J:2312:MET:HG2	2.61	0.41
1:J:2765:LYS:HD3	1:J:2765:LYS:HA	1.73	0.41
1:J:3037:GLU:CD	1:J:3085:PRO:HG2	2.45	0.41
1:J:3315:LEU:HD12	1:J:3319:ILE:HD13	2.03	0.41
1:J:3582:ARG:HD3	1:J:3582:ARG:HA	1.89	0.41
1:J:4837:LEU:HD23	1:J:4837:LEU:HA	1.96	0.41
1:A:620:LEU:HA	1:A:623:GLU:HG2	2.01	0.41
1:A:728:ARG:HE	1:A:1487:LEU:HD11	1.87	0.41
1:A:2382:GLU:O	1:A:2386:ILE:HG13	2.21	0.41
1:A:2779:GLU:HG3	1:A:2792:ARG:HG2	2.02	0.41
1:A:3036:LYS:O	1:A:3039:ILE:HG22	2.20	0.41
1:A:3437:MET:O	1:A:3441:ILE:HG13	2.21	0.41
1:A:4676:GLU:HG2	1:A:4680:LYS:HE2	2.03	0.41
1:C:1470:ARG:HD3	1:C:1470:ARG:HA	1.72	0.41
1:C:1786:LEU:HD22	3:E:85:THR:O	2.21	0.41
1:C:2954:ARG:HG2	1:C:2956:ALA:H	1.85	0.41
1:C:3037:GLU:CD	1:C:3085:PRO:HG2	2.45	0.41
1:C:3541:ALA:HA	1:C:3604:TYR:OH	2.21	0.41
1:C:4021:LYS:HG3	1:C:4142:ASN:ND2	2.36	0.41
1:C:4676:GLU:HG2	1:C:4680:LYS:HE2	2.03	0.41
1:G:1427:ILE:HD12	1:G:1427:ILE:HA	1.95	0.41
1:G:1712:TYR:O	1:G:1716:ILE:HG13	2.21	0.41
1:G:1867:GLU:O	1:G:1871:PHE:HB2	2.21	0.41
1:G:2336:ARG:HB3	1:G:2435:ARG:NH1	2.36	0.41
1:G:2876:GLU:HG3	1:G:2908:TYR:CE2	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3036:LYS:O	1:G:3039:ILE:HG22	2.20	0.41
1:G:3172:ILE:HD12	1:G:3194:LEU:HB2	2.02	0.41
1:G:4676:GLU:HG2	1:G:4680:LYS:HE2	2.03	0.41
1:J:977:LEU:HD12	1:J:1047:LEU:HD22	2.03	0.41
1:J:1653:LEU:HD23	1:J:1660:GLN:HA	2.02	0.41
1:J:2185:ILE:HD12	1:J:2203:MET:HE1	2.02	0.41
1:J:2236:LEU:HD23	1:J:2236:LEU:HA	1.89	0.41
1:J:2806:ARG:HG2	1:J:2810:LYS:HE2	2.03	0.41
1:J:2924:GLN:O	1:J:2928:LYS:HG2	2.21	0.41
1:J:4751:THR:O	1:J:4755:GLU:HG2	2.20	0.41
4:J:5102:POV:H25	4:J:5102:POV:H35A	2.03	0.41
3:L:15:PHE:HB3	3:L:64:ALA:O	2.21	0.41
1:A:479:GLN:HE21	1:A:539:LEU:HD22	1.86	0.40
1:A:514:SER:O	1:A:518:ILE:HG13	2.21	0.40
1:A:920:TYR:CZ	2:B:107:TRP:HD1	2.39	0.40
1:A:1109:LEU:HD21	1:A:1115:LEU:HD11	2.02	0.40
1:A:1271:ARG:HG3	1:A:1563:GLN:HB2	2.03	0.40
1:A:2879:ALA:HA	1:A:2882:TYR:CD2	2.55	0.40
1:A:4234:PHE:CE1	1:A:4985:LEU:HG	2.56	0.40
1:A:4553:ASN:O	1:A:4557:ARG:HG3	2.21	0.40
1:C:880:GLU:O	1:C:884:LEU:HG	2.20	0.40
1:C:1078:GLU:HG3	1:C:1237:TRP:NE1	2.32	0.40
1:C:1211:LEU:HD23	1:C:1211:LEU:HA	1.89	0.40
1:C:1712:TYR:O	1:C:1716:ILE:HG13	2.21	0.40
1:C:2336:ARG:HB3	1:C:2435:ARG:NH1	2.36	0.40
1:C:4068:LEU:HD12	1:C:4068:LEU:HA	1.81	0.40
1:C:4751:THR:O	1:C:4755:GLU:HG2	2.20	0.40
1:C:4800:LEU:HD13	4:C:5104:POV:H38	2.02	0.40
1:C:4861:LYS:HE2	1:C:4861:LYS:HB3	1.89	0.40
3:F:35:LYS:HD2	3:F:35:LYS:H	1.86	0.40
1:G:224:HIS:CE1	1:G:247:TYR:HE1	2.40	0.40
1:G:479:GLN:HE21	1:G:539:LEU:HD22	1.86	0.40
1:G:1442:GLY:HA3	1:G:1558:HIS:CG	2.56	0.40
1:G:2515:GLN:HE22	1:G:2574:HIS:CE1	2.38	0.40
1:G:3102:ASP:HA	1:G:3105:LYS:HE2	2.02	0.40
1:G:3539:ARG:HD3	1:G:3552:PHE:CD2	2.56	0.40
1:G:3541:ALA:HA	1:G:3604:TYR:OH	2.21	0.40
1:G:4865:LYS:HE2	1:G:4865:LYS:HB3	1.87	0.40
3:I:105:ASN:ND2	3:I:105:ASN:O	2.35	0.40
1:J:1558:HIS:HD2	1:J:1560:ASN:H	1.67	0.40
1:J:3102:ASP:HA	1:J:3105:LYS:HE2	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:3302:PRO:HA	1:J:3303:PRO:HD3	1.97	0.40
1:A:980:ALA:O	1:A:984:LEU:HD23	2.22	0.40
1:A:1041:GLN:HA	1:A:1044:ARG:HE	1.86	0.40
1:A:1712:TYR:O	1:A:1716:ILE:HG13	2.21	0.40
1:A:2012:PHE:HB2	1:A:2018:GLU:HA	2.03	0.40
1:A:3102:ASP:HA	1:A:3105:LYS:HE2	2.02	0.40
1:A:3232:LEU:HA	1:A:3233:PRO:HD3	1.96	0.40
1:A:3315:LEU:HD12	1:A:3319:ILE:HD13	2.03	0.40
1:A:3805:LEU:HB3	1:A:3890:LEU:HB3	2.03	0.40
1:A:4865:LYS:HE2	1:A:4865:LYS:HB3	1.87	0.40
1:C:23:GLN:HG3	1:C:201:ASN:OD1	2.21	0.40
1:C:458:GLU:H	1:C:458:GLU:HG3	1.70	0.40
1:C:2871:LEU:HD23	1:C:2927:LEU:HD11	2.03	0.40
1:C:2879:ALA:HA	1:C:2882:TYR:CD2	2.55	0.40
1:C:3254:GLY:O	1:C:3258:GLU:HG2	2.21	0.40
1:C:4234:PHE:CE1	1:C:4985:LEU:HG	2.56	0.40
1:C:4587:PRO:HG3	1:C:4631:PHE:HB3	2.02	0.40
1:C:4655:PHE:O	1:C:4659:ILE:HG12	2.21	0.40
1:C:4689:THR:HA	1:C:4732:PHE:CZ	2.56	0.40
1:C:4928:LEU:HD23	1:C:4928:LEU:HA	1.88	0.40
3:F:57:LYS:HE3	3:F:80:VAL:HG22	2.03	0.40
1:G:494:LEU:HD22	1:G:515:TRP:CD1	2.56	0.40
1:G:1238:PHE:HD1	1:G:1608:MET:HG3	1.87	0.40
1:G:1433:TYR:CD1	1:G:1578:ALA:HB2	2.56	0.40
1:J:214:VAL:HG21	1:J:390:LEU:HD12	2.02	0.40
1:J:919:ASN:O	1:J:923:GLN:HG2	2.22	0.40
1:J:1575:LEU:HD23	1:J:1575:LEU:HA	1.77	0.40
1:J:2779:GLU:HG3	1:J:2792:ARG:HG2	2.02	0.40
1:J:3437:MET:O	1:J:3441:ILE:HG13	2.21	0.40
1:J:4248:ALA:HA	1:J:4251:ILE:HG12	2.01	0.40
1:A:1648:MET:HG3	1:A:1652:GLU:HB3	2.02	0.40
1:A:2563:THR:HG22	1:A:2606:CYS:HA	2.03	0.40
1:A:2954:ARG:HG2	1:A:2956:ALA:H	1.85	0.40
4:A:5111:POV:H31E	4:A:5111:POV:H311	1.88	0.40
1:C:73:LEU:HA	1:C:73:LEU:HD23	1.84	0.40
1:C:2738:ARG:H	1:C:2738:ARG:HG3	1.57	0.40
1:C:2806:ARG:HG2	1:C:2810:LYS:HE2	2.03	0.40
1:C:3036:LYS:O	1:C:3039:ILE:HG22	2.20	0.40
1:C:3330:ASP:HA	1:C:3403:ARG:HH22	1.85	0.40
1:C:3437:MET:O	1:C:3441:ILE:HG13	2.21	0.40
1:C:4546:VAL:HA	1:C:4549:VAL:HG22	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:232:THR:O	1:G:245:VAL:HG23	2.22	0.40
1:G:909:ASN:HA	1:G:963:ASN:HD21	1.87	0.40
1:G:919:ASN:O	1:G:923:GLN:HG2	2.22	0.40
1:G:2244:ARG:HH21	1:G:2283:ASN:HA	1.85	0.40
1:G:2534:ALA:HB1	1:G:2588:ARG:NE	2.33	0.40
1:G:2637:ALA:C	1:G:2640:PRO:HD2	2.46	0.40
1:G:2806:ARG:HG2	1:G:2810:LYS:HE2	2.03	0.40
3:I:15:PHE:HB3	3:I:64:ALA:O	2.21	0.40
1:J:494:LEU:HD22	1:J:515:TRP:CD1	2.56	0.40
1:J:894:GLY:O	1:J:903:LEU:HB3	2.21	0.40
1:J:2712:PRO:HD3	1:J:3013:HIS:CE1	2.56	0.40
1:J:3053:ARG:HG3	1:J:3056:LEU:HG	2.04	0.40
1:J:3254:GLY:O	1:J:3258:GLU:HG2	2.21	0.40
1:J:3541:ALA:HA	1:J:3604:TYR:OH	2.21	0.40
1:J:4546:VAL:HA	1:J:4549:VAL:HG22	2.03	0.40
1:J:4928:LEU:HD23	1:J:4931:ILE:HD12	2.02	0.40
3:L:57:LYS:HE3	3:L:80:VAL:HG22	2.03	0.40
1:A:894:GLY:HA3	1:A:903:LEU:HD22	2.03	0.40
1:A:2203:MET:H	1:A:2203:MET:HG2	1.74	0.40
1:A:2871:LEU:HD23	1:A:2927:LEU:HD11	2.03	0.40
1:A:3037:GLU:CD	1:A:3085:PRO:HG2	2.45	0.40
1:A:3545:THR:HG23	1:A:3548:GLU:H	1.86	0.40
1:A:4823:LEU:HD12	1:A:4823:LEU:HA	1.75	0.40
1:C:492:ASP:O	1:C:496:VAL:HG23	2.21	0.40
1:C:1867:GLU:O	1:C:1871:PHE:HB2	2.21	0.40
1:C:2002:PRO:HA	1:C:2005:GLN:HG2	2.04	0.40
1:C:2273:LEU:HD23	1:C:2330:ARG:HB3	2.03	0.40
1:C:2677:LYS:HE3	1:C:2909:ASP:HB2	2.03	0.40
1:C:2758:PHE:HB2	1:C:2929:PHE:CE2	2.57	0.40
1:C:3102:ASP:HA	1:C:3105:LYS:HE2	2.02	0.40
1:C:3315:LEU:HD12	1:C:3319:ILE:HD13	2.03	0.40
1:C:3805:LEU:HB3	1:C:3890:LEU:HB3	2.03	0.40
1:C:4553:ASN:O	1:C:4557:ARG:HG3	2.21	0.40
1:G:492:ASP:O	1:G:496:VAL:HG23	2.21	0.40
1:G:620:LEU:HD23	1:G:620:LEU:HA	1.87	0.40
1:G:878:ILE:HD13	1:G:878:ILE:HA	1.92	0.40
1:G:1000:ARG:HB2	1:G:1021:LEU:HD11	2.03	0.40
1:G:2273:LEU:HD23	1:G:2330:ARG:HB3	2.03	0.40
1:G:2469:ILE:HA	1:G:2472:LEU:HB2	2.02	0.40
1:J:130:LYS:HE3	1:J:130:LYS:HB3	1.88	0.40
1:J:343:GLU:H	1:J:389:PHE:HE1	1.70	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:454:PRO:HA	1:J:455:PRO:HD3	1.97	0.40
1:J:2563:THR:HG22	1:J:2606:CYS:HA	2.03	0.40
1:J:2722:LYS:HG3	1:J:2724:GLU:HB2	2.03	0.40
1:J:2871:LEU:HD23	1:J:2927:LEU:HD11	2.03	0.40
1:J:2874:MET:HA	1:J:2877:GLN:HB2	2.04	0.40
1:J:4865:LYS:HB3	1:J:4865:LYS:HE2	1.87	0.40
1:A:232:THR:O	1:A:245:VAL:HG23	2.22	0.40
1:A:343:GLU:H	1:A:389:PHE:HE1	1.70	0.40
1:A:1119:GLU:H	1:A:1119:GLU:HG3	1.76	0.40
1:A:2582:MET:HE3	1:A:2582:MET:HB3	1.86	0.40
1:A:2874:MET:HA	1:A:2877:GLN:HB2	2.04	0.40
1:A:3187:ARG:CZ	1:A:3268:HIS:HB3	2.52	0.40
1:A:3930:ILE:HG22	1:A:3995:VAL:HG11	2.03	0.40
1:C:728:ARG:HE	1:C:1487:LEU:HD11	1.87	0.40
1:C:1300:HIS:HB3	1:C:1302:ARG:HE	1.87	0.40
1:C:4565:LEU:O	1:C:4569:LEU:HG	2.22	0.40
3:E:46:PHE:HE2	3:E:55:VAL:HG12	1.87	0.40
1:G:620:LEU:HA	1:G:623:GLU:HG2	2.02	0.40
1:G:1862:ILE:O	1:G:1866:ILE:HG12	2.20	0.40
1:G:3187:ARG:CZ	1:G:3268:HIS:HB3	2.52	0.40
1:G:3360:PRO:O	1:G:3364:ARG:HG2	2.22	0.40
1:G:3836:MET:HE2	1:G:3836:MET:HB2	1.89	0.40
1:G:4157:ASP:O	1:G:4161:ARG:HG2	2.22	0.40
1:G:4553:ASN:O	1:G:4557:ARG:HG3	2.21	0.40
1:J:135:VAL:HG22	1:J:192:ASP:HA	2.03	0.40
1:J:169:LEU:HD23	1:J:169:LEU:HA	1.92	0.40
1:J:1300:HIS:HB3	1:J:1302:ARG:HE	1.87	0.40
1:J:2244:ARG:HH21	1:J:2283:ASN:HA	1.85	0.40
1:J:3805:LEU:HB3	1:J:3890:LEU:HB3	2.03	0.40
1:J:3836:MET:HE2	1:J:3836:MET:HB2	1.89	0.40
1:J:4134:GLU:HB2	1:J:4135:PRO:HD3	2.04	0.40
1:J:4646:LEU:HD13	1:J:4646:LEU:HA	1.91	0.40
3:L:58:GLY:HA3	3:L:80:VAL:HG11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4279/5027 (85%)	4176 (98%)	101 (2%)	2 (0%)	100	100
1	C	4279/5027 (85%)	4174 (98%)	104 (2%)	1 (0%)	100	100
1	G	4279/5027 (85%)	4180 (98%)	98 (2%)	1 (0%)	100	100
1	J	4279/5027 (85%)	4179 (98%)	99 (2%)	1 (0%)	100	100
2	B	124/126 (98%)	120 (97%)	4 (3%)	0	100	100
2	D	124/126 (98%)	120 (97%)	4 (3%)	0	100	100
2	H	124/126 (98%)	120 (97%)	4 (3%)	0	100	100
2	K	124/126 (98%)	120 (97%)	4 (3%)	0	100	100
3	E	105/107 (98%)	98 (93%)	5 (5%)	2 (2%)	6	33
3	F	105/107 (98%)	100 (95%)	4 (4%)	1 (1%)	12	45
3	I	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
3	L	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
All	All	18032/21040 (86%)	17587 (98%)	437 (2%)	8 (0%)	100	100

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	375	LYS
1	C	375	LYS
3	E	85	THR
1	G	375	LYS
1	J	375	LYS
3	E	87	HIS
3	F	87	HIS
1	A	967	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3672/4270 (86%)	3648 (99%)	24 (1%)	76	78
1	C	3676/4270 (86%)	3650 (99%)	26 (1%)	76	78
1	G	3672/4270 (86%)	3645 (99%)	27 (1%)	76	78
1	J	3672/4270 (86%)	3648 (99%)	24 (1%)	76	78
2	B	104/104 (100%)	104 (100%)	0	100	100
2	D	104/104 (100%)	103 (99%)	1 (1%)	68	75
2	H	104/104 (100%)	104 (100%)	0	100	100
2	K	104/104 (100%)	104 (100%)	0	100	100
3	E	88/88 (100%)	85 (97%)	3 (3%)	32	57
3	F	88/88 (100%)	86 (98%)	2 (2%)	44	64
3	I	88/88 (100%)	85 (97%)	3 (3%)	32	57
3	L	88/88 (100%)	86 (98%)	2 (2%)	44	64
All	All	15460/17848 (87%)	15348 (99%)	112 (1%)	73	78

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	165	VAL
1	A	377	ILE
1	A	388	LEU
1	A	614	VAL
1	A	667	MET
1	A	975	VAL
1	A	1180	ARG
1	A	1561	VAL
1	A	1814	MET
1	A	1870	VAL
1	A	2166	LEU
1	A	2377	LEU
1	A	2460	LEU
1	A	2817	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2821	TRP
1	A	2827	ARG
1	A	2874	MET
1	A	2976	HIS
1	A	3194	LEU
1	A	3409	TYR
1	A	3508	SER
1	A	3934	TYR
1	A	4626	ASN
1	A	4858	PHE
1	C	165	VAL
1	C	377	ILE
1	C	388	LEU
1	C	614	VAL
1	C	667	MET
1	C	879	HIS
1	C	893	TYR
1	C	975	VAL
1	C	1561	VAL
1	C	1814	MET
1	C	1870	VAL
1	C	2166	LEU
1	C	2377	LEU
1	C	2460	LEU
1	C	2817	ILE
1	C	2821	TRP
1	C	2827	ARG
1	C	2874	MET
1	C	2976	HIS
1	C	3194	LEU
1	C	3409	TYR
1	C	3509	LEU
1	C	3514	LEU
1	C	3934	TYR
1	C	4626	ASN
1	C	4858	PHE
2	D	116	TYR
3	E	35	LYS
3	E	77	THR
3	E	105	ASN
3	F	35	LYS
3	F	105	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	165	VAL
1	G	377	ILE
1	G	388	LEU
1	G	614	VAL
1	G	667	MET
1	G	791	PHE
1	G	879	HIS
1	G	963	ASN
1	G	975	VAL
1	G	1561	VAL
1	G	1870	VAL
1	G	2166	LEU
1	G	2229	VAL
1	G	2233	CYS
1	G	2377	LEU
1	G	2460	LEU
1	G	2817	ILE
1	G	2821	TRP
1	G	2827	ARG
1	G	2874	MET
1	G	2976	HIS
1	G	3194	LEU
1	G	3409	TYR
1	G	3514	LEU
1	G	3934	TYR
1	G	4626	ASN
1	G	4858	PHE
3	I	35	LYS
3	I	77	THR
3	I	105	ASN
1	J	165	VAL
1	J	377	ILE
1	J	388	LEU
1	J	614	VAL
1	J	667	MET
1	J	970	LEU
1	J	975	VAL
1	J	1561	VAL
1	J	1814	MET
1	J	1870	VAL
1	J	2166	LEU
1	J	2233	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	2377	LEU
1	J	2460	LEU
1	J	2817	ILE
1	J	2821	TRP
1	J	2827	ARG
1	J	2874	MET
1	J	2976	HIS
1	J	3194	LEU
1	J	3409	TYR
1	J	3934	TYR
1	J	4626	ASN
1	J	4858	PHE
3	L	35	LYS
3	L	105	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (160) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	241	GLN
1	A	579	GLN
1	A	634	GLN
1	A	949	ASN
1	A	1066	GLN
1	A	1084	GLN
1	A	1429	ASN
1	A	1569	GLN
1	A	1590	GLN
1	A	1760	HIS
1	A	1952	GLN
1	A	2161	GLN
1	A	2169	GLN
1	A	2204	HIS
1	A	2417	HIS
1	A	2487	GLN
1	A	2574	HIS
1	A	2902	HIS
1	A	2971	GLN
1	A	2991	HIS
1	A	3013	HIS
1	A	3128	ASN
1	A	3146	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	3209	GLN
1	A	3430	ASN
1	A	3462	ASN
1	A	3850	GLN
1	A	3851	ASN
1	A	3897	ASN
1	A	3914	ASN
1	A	4109	GLN
1	A	4707	ASN
1	A	4803	HIS
1	A	5003	HIS
2	B	3	GLN
2	B	58	ASN
1	C	23	GLN
1	C	181	HIS
1	C	241	GLN
1	C	579	GLN
1	C	634	GLN
1	C	949	ASN
1	C	1003	GLN
1	C	1066	GLN
1	C	1084	GLN
1	C	1130	GLN
1	C	1429	ASN
1	C	1569	GLN
1	C	1590	GLN
1	C	1663	HIS
1	C	1952	GLN
1	C	2161	GLN
1	C	2169	GLN
1	C	2204	HIS
1	C	2247	GLN
1	C	2283	ASN
1	C	2291	GLN
1	C	2417	HIS
1	C	2574	HIS
1	C	2902	HIS
1	C	3013	HIS
1	C	3128	ASN
1	C	3146	HIS
1	C	3209	GLN
1	C	3430	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	3462	ASN
1	C	3850	GLN
1	C	3851	ASN
1	C	3897	ASN
1	C	3914	ASN
1	C	3998	HIS
1	C	4707	ASN
1	C	4803	HIS
1	C	5003	HIS
2	D	3	GLN
3	E	31	GLN
3	F	31	GLN
1	G	23	GLN
1	G	473	ASN
1	G	579	GLN
1	G	634	GLN
1	G	949	ASN
1	G	963	ASN
1	G	1066	GLN
1	G	1084	GLN
1	G	1429	ASN
1	G	1569	GLN
1	G	1590	GLN
1	G	1663	HIS
1	G	1952	GLN
1	G	2161	GLN
1	G	2169	GLN
1	G	2204	HIS
1	G	2247	GLN
1	G	2283	ASN
1	G	2291	GLN
1	G	2417	HIS
1	G	2574	HIS
1	G	2902	HIS
1	G	2971	GLN
1	G	2991	HIS
1	G	3013	HIS
1	G	3128	ASN
1	G	3146	HIS
1	G	3209	GLN
1	G	3430	ASN
1	G	3462	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	3850	GLN
1	G	3851	ASN
1	G	3897	ASN
1	G	3914	ASN
1	G	4094	GLN
1	G	4109	GLN
1	G	4707	ASN
1	G	4803	HIS
1	G	4857	ASN
1	G	5003	HIS
2	H	3	GLN
3	I	31	GLN
1	J	23	GLN
1	J	151	HIS
1	J	241	GLN
1	J	579	GLN
1	J	596	ASN
1	J	634	GLN
1	J	949	ASN
1	J	1066	GLN
1	J	1084	GLN
1	J	1130	GLN
1	J	1429	ASN
1	J	1569	GLN
1	J	1590	GLN
1	J	1760	HIS
1	J	1952	GLN
1	J	2161	GLN
1	J	2169	GLN
1	J	2204	HIS
1	J	2291	GLN
1	J	2417	HIS
1	J	2574	HIS
1	J	2902	HIS
1	J	2971	GLN
1	J	2991	HIS
1	J	3128	ASN
1	J	3146	HIS
1	J	3209	GLN
1	J	3430	ASN
1	J	3462	ASN
1	J	3850	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	3851	ASN
1	J	3897	ASN
1	J	3914	ASN
1	J	4094	GLN
1	J	4109	GLN
1	J	4707	ASN
1	J	4803	HIS
1	J	4857	ASN
2	K	3	GLN
3	L	31	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	$\# Z > 2$
4	POV	J	5102	-	40,40,51	0.55	0	46,48,59	0.52	0
4	POV	C	5111	-	40,40,51	0.55	0	46,48,59	0.51	0
4	POV	G	5113	-	40,40,51	0.55	0	46,48,59	0.51	0
4	POV	J	5112	-	38,38,51	0.56	0	44,46,59	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	POV	G	5114	-	51,51,51	0.50	0	57,59,59	0.45	0
4	POV	G	5112	-	48,48,51	0.52	0	54,56,59	0.48	0
4	POV	A	5109	-	42,42,51	0.54	0	48,50,59	0.48	0
4	POV	J	5101	-	48,48,51	0.51	0	54,56,59	0.48	0
4	POV	A	5101	-	12,12,51	0.22	0	11,11,59	0.25	0
4	POV	J	5108	-	43,43,51	0.54	0	49,51,59	0.50	0
4	POV	A	5111	-	38,38,51	0.56	0	44,46,59	0.52	0
4	POV	A	5108	-	12,12,51	0.22	0	11,11,59	0.25	0
4	POV	C	5105	-	43,43,51	0.54	0	49,51,59	0.50	0
4	POV	G	5104	-	46,46,51	0.52	0	52,54,59	0.48	0
5	ATP	A	5102	-	32,33,33	0.28	0	48,52,52	0.33	0
5	ATP	J	5104	-	32,33,33	0.28	0	48,52,52	0.33	0
4	POV	A	5105	-	46,46,51	0.52	0	52,54,59	0.48	0
4	POV	J	5103	-	51,51,51	0.50	0	57,59,59	0.45	0
4	POV	J	5110	-	42,42,51	0.54	0	48,50,59	0.48	0
4	POV	A	5107	-	48,48,51	0.52	0	54,56,59	0.48	0
4	POV	G	5109	-	38,38,51	0.56	0	44,46,59	0.52	0
4	POV	J	5107	-	46,46,51	0.52	0	52,54,59	0.48	0
4	POV	J	5109	-	12,12,51	0.22	0	11,11,59	0.25	0
4	POV	A	5112	-	33,33,51	0.60	0	39,41,59	0.54	0
5	ATP	C	5101	-	32,33,33	0.28	0	48,52,52	0.33	0
4	POV	C	5106	-	42,42,51	0.55	0	48,50,59	0.49	0
6	CFF	C	5102	-	15,15,15	0.52	0	23,23,23	0.74	1 (4%)
4	POV	G	5108	-	23,23,51	0.67	0	28,30,59	0.61	0
6	CFF	J	5105	-	15,15,15	0.54	0	23,23,23	0.74	1 (4%)
4	POV	C	5108	-	38,38,51	0.57	0	44,46,59	0.52	0
4	POV	C	5109	-	33,33,51	0.60	0	39,41,59	0.54	0
4	POV	A	5114	-	48,48,51	0.52	0	54,56,59	0.48	0
4	POV	C	5104	-	46,46,51	0.52	0	52,54,59	0.48	0
4	POV	G	5110	-	33,33,51	0.60	0	39,41,59	0.54	0
4	POV	J	5111	-	23,23,51	0.67	0	28,30,59	0.61	0
4	POV	G	5105	-	43,43,51	0.54	0	49,51,59	0.50	0
6	CFF	G	5102	-	15,15,15	0.54	0	23,23,23	0.74	1 (4%)
4	POV	C	5112	-	51,51,51	0.50	0	57,59,59	0.45	0
4	POV	J	5113	-	33,33,51	0.60	0	39,41,59	0.54	0
4	POV	G	5107	-	42,42,51	0.54	0	48,50,59	0.48	0
4	POV	A	5106	-	43,43,51	0.54	0	49,51,59	0.50	0
4	POV	C	5107	-	23,23,51	0.66	0	28,30,59	0.61	0
4	POV	A	5116	-	51,51,51	0.50	0	57,59,59	0.45	0
5	ATP	G	5101	-	32,33,33	0.28	0	48,52,52	0.33	0
6	CFF	A	5103	-	15,15,15	0.54	0	23,23,23	0.74	1 (4%)
4	POV	G	5106	-	12,12,51	0.22	0	11,11,59	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	POV	A	5115	-	40,40,51	0.55	0	46,48,59	0.51	0
4	POV	A	5110	-	23,23,51	0.67	0	28,30,59	0.61	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
4	POV	J	5102	-	-	6/44/44/55	-
4	POV	C	5111	-	-	6/44/44/55	-
4	POV	G	5113	-	-	6/44/44/55	-
4	POV	J	5112	-	-	12/42/42/55	-
4	POV	G	5114	-	-	21/55/55/55	-
4	POV	G	5112	-	-	18/52/52/55	-
4	POV	A	5109	-	-	12/46/46/55	-
4	POV	J	5101	-	-	18/52/52/55	-
4	POV	A	5101	-	-	2/10/10/55	-
4	POV	J	5108	-	-	9/47/47/55	-
4	POV	A	5111	-	-	12/42/42/55	-
4	POV	A	5108	-	-	2/10/10/55	-
4	POV	C	5105	-	-	9/47/47/55	-
4	POV	G	5104	-	-	16/50/50/55	-
5	ATP	A	5102	-	-	3/22/38/38	0/3/3/3
5	ATP	J	5104	-	-	3/22/38/38	0/3/3/3
4	POV	A	5105	-	-	16/50/50/55	-
4	POV	J	5103	-	-	21/55/55/55	-
4	POV	J	5110	-	-	12/46/46/55	-
4	POV	A	5107	-	-	18/52/52/55	-
4	POV	G	5109	-	-	12/42/42/55	-
4	POV	J	5107	-	-	16/50/50/55	-
4	POV	J	5109	-	-	2/10/10/55	-
4	POV	A	5112	-	-	10/37/37/55	-
5	ATP	C	5101	-	-	3/22/38/38	0/3/3/3
4	POV	C	5106	-	-	12/46/46/55	-
6	CFF	C	5102	-	-	-	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	POV	G	5108	-	-	10/26/26/55	-
6	CFF	J	5105	-	-	-	0/2/2/2
4	POV	C	5108	-	-	12/42/42/55	-
4	POV	C	5109	-	-	10/37/37/55	-
4	POV	A	5114	-	-	18/52/52/55	-
4	POV	C	5104	-	-	16/50/50/55	-
4	POV	G	5110	-	-	10/37/37/55	-
4	POV	J	5111	-	-	10/26/26/55	-
4	POV	G	5105	-	-	9/47/47/55	-
6	CFF	G	5102	-	-	-	0/2/2/2
4	POV	C	5112	-	-	21/55/55/55	-
4	POV	J	5113	-	-	10/37/37/55	-
4	POV	G	5107	-	-	12/46/46/55	-
4	POV	A	5106	-	-	9/47/47/55	-
4	POV	C	5107	-	-	10/26/26/55	-
4	POV	A	5116	-	-	21/55/55/55	-
5	ATP	G	5101	-	-	3/22/38/38	0/3/3/3
6	CFF	A	5103	-	-	-	0/2/2/2
4	POV	G	5106	-	-	2/10/10/55	-
4	POV	A	5115	-	-	6/44/44/55	-
4	POV	A	5110	-	-	10/26/26/55	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	5102	CFF	C12-N3-C2	2.28	121.30	117.33
6	A	5103	CFF	C12-N3-C2	2.26	121.27	117.33
6	G	5102	CFF	C12-N3-C2	2.26	121.27	117.33
6	J	5105	CFF	C12-N3-C2	2.26	121.27	117.33

There are no chirality outliers.

All (476) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5105	POV	C22-C21-O21-C2
4	A	5105	POV	O22-C21-O21-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	5106	POV	C1-O11-P-O14
4	A	5106	POV	C11-O12-P-O13
4	A	5106	POV	O12-C11-C12-N
4	A	5106	POV	C22-C21-O21-C2
4	A	5107	POV	C1-O11-P-O12
4	A	5107	POV	C1-O11-P-O14
4	A	5107	POV	C11-O12-P-O14
4	A	5107	POV	C2-C1-O11-P
4	A	5107	POV	O12-C11-C12-N
4	A	5109	POV	C1-O11-P-O12
4	A	5109	POV	C1-O11-P-O14
4	A	5110	POV	C1-O11-P-O12
4	A	5110	POV	C1-O11-P-O14
4	A	5110	POV	C11-O12-P-O11
4	A	5110	POV	C11-O12-P-O13
4	A	5110	POV	O12-C11-C12-N
4	A	5111	POV	C11-O12-P-O11
4	A	5111	POV	C11-O12-P-O13
4	A	5111	POV	O12-C11-C12-N
4	A	5111	POV	C22-C21-O21-C2
4	A	5112	POV	C1-O11-P-O14
4	A	5112	POV	C11-O12-P-O13
4	A	5114	POV	C1-O11-P-O12
4	A	5114	POV	C1-O11-P-O14
4	A	5114	POV	C11-O12-P-O14
4	A	5114	POV	C2-C1-O11-P
4	A	5114	POV	O12-C11-C12-N
4	A	5115	POV	C1-O11-P-O13
4	A	5115	POV	O12-C11-C12-N
4	A	5116	POV	C1-O11-P-O12
4	A	5116	POV	C1-O11-P-O13
4	A	5116	POV	C1-O11-P-O14
4	A	5116	POV	O12-C11-C12-N
4	C	5104	POV	C22-C21-O21-C2
4	C	5104	POV	O22-C21-O21-C2
4	C	5105	POV	C1-O11-P-O14
4	C	5105	POV	C11-O12-P-O13
4	C	5105	POV	O12-C11-C12-N
4	C	5105	POV	C22-C21-O21-C2
4	C	5106	POV	C1-O11-P-O12
4	C	5106	POV	C1-O11-P-O14
4	C	5107	POV	C1-O11-P-O12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C	5107	POV	C1-O11-P-O14
4	C	5107	POV	C11-O12-P-O11
4	C	5107	POV	C11-O12-P-O13
4	C	5107	POV	O12-C11-C12-N
4	C	5108	POV	C11-O12-P-O11
4	C	5108	POV	C11-O12-P-O13
4	C	5108	POV	O12-C11-C12-N
4	C	5108	POV	C22-C21-O21-C2
4	C	5109	POV	C1-O11-P-O14
4	C	5109	POV	C11-O12-P-O13
4	C	5111	POV	C1-O11-P-O13
4	C	5111	POV	O12-C11-C12-N
4	C	5112	POV	C1-O11-P-O12
4	C	5112	POV	C1-O11-P-O13
4	C	5112	POV	C1-O11-P-O14
4	C	5112	POV	O12-C11-C12-N
4	G	5104	POV	C22-C21-O21-C2
4	G	5104	POV	O22-C21-O21-C2
4	G	5105	POV	C1-O11-P-O14
4	G	5105	POV	C11-O12-P-O13
4	G	5105	POV	O12-C11-C12-N
4	G	5105	POV	C22-C21-O21-C2
4	G	5107	POV	C1-O11-P-O12
4	G	5107	POV	C1-O11-P-O14
4	G	5108	POV	C1-O11-P-O12
4	G	5108	POV	C1-O11-P-O14
4	G	5108	POV	C11-O12-P-O11
4	G	5108	POV	C11-O12-P-O13
4	G	5108	POV	O12-C11-C12-N
4	G	5109	POV	C11-O12-P-O11
4	G	5109	POV	C11-O12-P-O13
4	G	5109	POV	O12-C11-C12-N
4	G	5109	POV	C22-C21-O21-C2
4	G	5110	POV	C1-O11-P-O14
4	G	5110	POV	C11-O12-P-O13
4	G	5112	POV	C1-O11-P-O12
4	G	5112	POV	C1-O11-P-O14
4	G	5112	POV	C11-O12-P-O14
4	G	5112	POV	C2-C1-O11-P
4	G	5112	POV	O12-C11-C12-N
4	G	5113	POV	C1-O11-P-O13
4	G	5113	POV	O12-C11-C12-N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	G	5114	POV	C1-O11-P-O12
4	G	5114	POV	C1-O11-P-O13
4	G	5114	POV	C1-O11-P-O14
4	G	5114	POV	O12-C11-C12-N
4	J	5101	POV	C1-O11-P-O12
4	J	5101	POV	C1-O11-P-O14
4	J	5101	POV	C11-O12-P-O14
4	J	5101	POV	C2-C1-O11-P
4	J	5101	POV	O12-C11-C12-N
4	J	5102	POV	C1-O11-P-O13
4	J	5102	POV	O12-C11-C12-N
4	J	5103	POV	C1-O11-P-O12
4	J	5103	POV	C1-O11-P-O13
4	J	5103	POV	C1-O11-P-O14
4	J	5103	POV	O12-C11-C12-N
4	J	5107	POV	C22-C21-O21-C2
4	J	5107	POV	O22-C21-O21-C2
4	J	5108	POV	C1-O11-P-O14
4	J	5108	POV	C11-O12-P-O13
4	J	5108	POV	O12-C11-C12-N
4	J	5108	POV	C22-C21-O21-C2
4	J	5110	POV	C1-O11-P-O12
4	J	5110	POV	C1-O11-P-O14
4	J	5111	POV	C1-O11-P-O12
4	J	5111	POV	C1-O11-P-O14
4	J	5111	POV	C11-O12-P-O11
4	J	5111	POV	C11-O12-P-O13
4	J	5111	POV	O12-C11-C12-N
4	J	5112	POV	C11-O12-P-O11
4	J	5112	POV	C11-O12-P-O13
4	J	5112	POV	O12-C11-C12-N
4	J	5112	POV	C22-C21-O21-C2
4	J	5113	POV	C1-O11-P-O14
4	J	5113	POV	C11-O12-P-O13
4	A	5106	POV	O22-C21-O21-C2
4	C	5105	POV	O22-C21-O21-C2
4	G	5105	POV	O22-C21-O21-C2
4	J	5108	POV	O22-C21-O21-C2
4	A	5111	POV	O22-C21-O21-C2
4	C	5108	POV	O22-C21-O21-C2
4	G	5109	POV	O22-C21-O21-C2
4	J	5112	POV	O22-C21-O21-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	5110	POV	C2-C1-O11-P
4	C	5107	POV	C2-C1-O11-P
4	G	5108	POV	C2-C1-O11-P
4	J	5111	POV	C2-C1-O11-P
4	A	5116	POV	C31-C32-C33-C34
4	C	5112	POV	C31-C32-C33-C34
4	G	5114	POV	C31-C32-C33-C34
4	J	5103	POV	C31-C32-C33-C34
4	A	5107	POV	C21-C22-C23-C24
4	A	5114	POV	C21-C22-C23-C24
4	G	5112	POV	C21-C22-C23-C24
4	J	5101	POV	C21-C22-C23-C24
4	A	5109	POV	C31-C32-C33-C34
4	C	5106	POV	C31-C32-C33-C34
4	G	5107	POV	C31-C32-C33-C34
4	J	5110	POV	C31-C32-C33-C34
4	A	5105	POV	C311-C310-C39-C38
4	C	5104	POV	C311-C310-C39-C38
4	G	5104	POV	C311-C310-C39-C38
4	J	5107	POV	C311-C310-C39-C38
4	A	5109	POV	C211-C212-C213-C214
4	C	5106	POV	C211-C212-C213-C214
4	G	5107	POV	C211-C212-C213-C214
4	J	5110	POV	C211-C212-C213-C214
4	A	5116	POV	C212-C213-C214-C215
4	A	5116	POV	C37-C38-C39-C310
4	C	5112	POV	C212-C213-C214-C215
4	C	5112	POV	C37-C38-C39-C310
4	G	5114	POV	C212-C213-C214-C215
4	G	5114	POV	C37-C38-C39-C310
4	J	5103	POV	C37-C38-C39-C310
4	J	5103	POV	C212-C213-C214-C215
4	A	5105	POV	C32-C33-C34-C35
4	C	5104	POV	C32-C33-C34-C35
4	G	5104	POV	C32-C33-C34-C35
4	J	5103	POV	C32-C33-C34-C35
4	J	5107	POV	C32-C33-C34-C35
4	A	5116	POV	C32-C33-C34-C35
4	C	5112	POV	C32-C33-C34-C35
4	G	5114	POV	C32-C33-C34-C35
4	C	5104	POV	C39-C310-C311-C312
4	A	5105	POV	C39-C310-C311-C312

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	G	5104	POV	C39-C310-C311-C312
4	J	5107	POV	C39-C310-C311-C312
4	A	5107	POV	C35-C36-C37-C38
4	A	5114	POV	C35-C36-C37-C38
4	G	5112	POV	C35-C36-C37-C38
4	J	5101	POV	C35-C36-C37-C38
4	J	5103	POV	C311-C310-C39-C38
4	A	5116	POV	C311-C310-C39-C38
4	C	5112	POV	C311-C310-C39-C38
4	G	5114	POV	C311-C310-C39-C38
4	A	5109	POV	C21-C22-C23-C24
4	C	5106	POV	C21-C22-C23-C24
4	G	5107	POV	C21-C22-C23-C24
4	J	5110	POV	C21-C22-C23-C24
4	A	5111	POV	C37-C38-C39-C310
4	C	5108	POV	C37-C38-C39-C310
4	G	5109	POV	C37-C38-C39-C310
4	J	5112	POV	C37-C38-C39-C310
4	A	5110	POV	O11-C1-C2-C3
4	C	5107	POV	O11-C1-C2-C3
4	G	5108	POV	O11-C1-C2-C3
4	J	5111	POV	O11-C1-C2-C3
4	A	5112	POV	C22-C21-O21-C2
4	C	5109	POV	C22-C21-O21-C2
4	G	5110	POV	C22-C21-O21-C2
4	J	5113	POV	C22-C21-O21-C2
4	A	5105	POV	C35-C36-C37-C38
4	G	5104	POV	C35-C36-C37-C38
4	J	5107	POV	C35-C36-C37-C38
4	A	5101	POV	C26-C27-C28-C29
4	A	5108	POV	C26-C27-C28-C29
4	G	5106	POV	C26-C27-C28-C29
4	J	5109	POV	C26-C27-C28-C29
4	C	5104	POV	C35-C36-C37-C38
4	A	5109	POV	C212-C213-C214-C215
4	C	5106	POV	C212-C213-C214-C215
4	G	5107	POV	C212-C213-C214-C215
4	J	5110	POV	C212-C213-C214-C215
4	C	5108	POV	C34-C35-C36-C37
4	A	5111	POV	C34-C35-C36-C37
4	G	5109	POV	C34-C35-C36-C37
4	J	5112	POV	C34-C35-C36-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	5105	POV	C311-C312-C313-C314
4	C	5104	POV	C311-C312-C313-C314
4	G	5104	POV	C311-C312-C313-C314
4	J	5107	POV	C311-C312-C313-C314
4	A	5105	POV	C32-C31-O31-C3
4	C	5104	POV	C32-C31-O31-C3
4	G	5104	POV	C32-C31-O31-C3
4	J	5107	POV	C32-C31-O31-C3
4	A	5106	POV	C2-C1-O11-P
4	C	5105	POV	C2-C1-O11-P
4	G	5105	POV	C2-C1-O11-P
4	J	5108	POV	C2-C1-O11-P
4	A	5111	POV	C22-C23-C24-C25
4	G	5109	POV	C22-C23-C24-C25
4	J	5112	POV	C22-C23-C24-C25
4	A	5107	POV	O11-C1-C2-C3
4	A	5114	POV	O11-C1-C2-C3
4	G	5112	POV	O11-C1-C2-C3
4	J	5101	POV	O11-C1-C2-C3
4	C	5108	POV	C22-C23-C24-C25
4	A	5116	POV	C1-C2-C3-O31
4	C	5112	POV	C1-C2-C3-O31
4	G	5114	POV	C1-C2-C3-O31
4	J	5103	POV	C1-C2-C3-O31
4	A	5110	POV	O11-C1-C2-O21
4	C	5107	POV	O11-C1-C2-O21
4	G	5108	POV	O11-C1-C2-O21
4	J	5111	POV	O11-C1-C2-O21
4	A	5107	POV	C22-C23-C24-C25
4	A	5114	POV	C22-C23-C24-C25
4	G	5112	POV	C22-C23-C24-C25
4	J	5101	POV	C22-C23-C24-C25
4	A	5115	POV	C21-C22-C23-C24
4	C	5111	POV	C21-C22-C23-C24
4	G	5113	POV	C21-C22-C23-C24
4	J	5102	POV	C21-C22-C23-C24
4	A	5112	POV	O22-C21-O21-C2
4	C	5109	POV	O22-C21-O21-C2
4	G	5110	POV	O22-C21-O21-C2
4	J	5113	POV	O22-C21-O21-C2
4	A	5105	POV	O32-C31-O31-C3
4	C	5104	POV	O32-C31-O31-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	G	5104	POV	O32-C31-O31-C3
4	J	5107	POV	O32-C31-O31-C3
4	A	5107	POV	O11-C1-C2-O21
4	A	5114	POV	O11-C1-C2-O21
4	G	5112	POV	O11-C1-C2-O21
4	J	5101	POV	O11-C1-C2-O21
4	A	5107	POV	C12-C11-O12-P
4	A	5112	POV	C12-C11-O12-P
4	A	5114	POV	C12-C11-O12-P
4	C	5109	POV	C12-C11-O12-P
4	G	5110	POV	C12-C11-O12-P
4	G	5112	POV	C12-C11-O12-P
4	J	5101	POV	C12-C11-O12-P
4	J	5113	POV	C12-C11-O12-P
4	J	5101	POV	C34-C35-C36-C37
4	A	5107	POV	C34-C35-C36-C37
4	A	5114	POV	C34-C35-C36-C37
4	G	5112	POV	C34-C35-C36-C37
4	A	5106	POV	C36-C37-C38-C39
4	C	5105	POV	C36-C37-C38-C39
4	G	5105	POV	C36-C37-C38-C39
4	J	5108	POV	C36-C37-C38-C39
4	A	5105	POV	O12-C11-C12-N
4	C	5104	POV	O12-C11-C12-N
4	G	5104	POV	O12-C11-C12-N
4	J	5107	POV	O12-C11-C12-N
4	A	5116	POV	C36-C37-C38-C39
4	C	5112	POV	C36-C37-C38-C39
4	G	5114	POV	C36-C37-C38-C39
4	J	5103	POV	C36-C37-C38-C39
4	A	5111	POV	C31-C32-C33-C34
4	G	5109	POV	C31-C32-C33-C34
4	J	5112	POV	C31-C32-C33-C34
4	C	5108	POV	C31-C32-C33-C34
4	A	5116	POV	O21-C2-C3-O31
4	C	5112	POV	O21-C2-C3-O31
4	G	5114	POV	O21-C2-C3-O31
4	J	5103	POV	O21-C2-C3-O31
4	A	5111	POV	C32-C31-O31-C3
4	C	5108	POV	C32-C31-O31-C3
4	G	5109	POV	C32-C31-O31-C3
4	J	5112	POV	C32-C31-O31-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	5115	POV	C311-C312-C313-C314
4	C	5111	POV	C311-C312-C313-C314
4	G	5113	POV	C311-C312-C313-C314
4	J	5102	POV	C311-C312-C313-C314
4	A	5109	POV	C1-O11-P-O13
4	A	5110	POV	C11-O12-P-O14
4	A	5112	POV	C1-O11-P-O12
4	A	5112	POV	C1-O11-P-O13
4	A	5112	POV	C11-O12-P-O11
4	A	5115	POV	C11-O12-P-O14
4	A	5116	POV	C11-O12-P-O14
4	C	5106	POV	C1-O11-P-O13
4	C	5107	POV	C11-O12-P-O14
4	C	5109	POV	C1-O11-P-O12
4	C	5109	POV	C1-O11-P-O13
4	C	5109	POV	C11-O12-P-O11
4	C	5111	POV	C11-O12-P-O14
4	C	5112	POV	C11-O12-P-O14
4	G	5107	POV	C1-O11-P-O13
4	G	5108	POV	C11-O12-P-O14
4	G	5110	POV	C1-O11-P-O12
4	G	5110	POV	C1-O11-P-O13
4	G	5110	POV	C11-O12-P-O11
4	G	5113	POV	C11-O12-P-O14
4	G	5114	POV	C11-O12-P-O14
4	J	5102	POV	C11-O12-P-O14
4	J	5103	POV	C11-O12-P-O14
4	J	5110	POV	C1-O11-P-O13
4	J	5111	POV	C11-O12-P-O14
4	J	5113	POV	C1-O11-P-O12
4	J	5113	POV	C1-O11-P-O13
4	J	5113	POV	C11-O12-P-O11
5	A	5102	ATP	C5'-O5'-PA-O1A
5	C	5101	ATP	C5'-O5'-PA-O1A
5	G	5101	ATP	C5'-O5'-PA-O1A
5	J	5104	ATP	C5'-O5'-PA-O1A
4	C	5108	POV	O32-C31-O31-C3
4	A	5111	POV	O32-C31-O31-C3
4	G	5109	POV	O32-C31-O31-C3
4	J	5112	POV	O32-C31-O31-C3
4	A	5109	POV	C24-C25-C26-C27
4	G	5107	POV	C24-C25-C26-C27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	J	5110	POV	C24-C25-C26-C27
4	C	5106	POV	C24-C25-C26-C27
4	A	5105	POV	C11-C12-N-C13
4	C	5104	POV	C11-C12-N-C13
4	G	5104	POV	C11-C12-N-C13
4	J	5107	POV	C11-C12-N-C13
4	A	5109	POV	C22-C21-O21-C2
4	C	5106	POV	C22-C21-O21-C2
4	G	5107	POV	C22-C21-O21-C2
4	J	5110	POV	C22-C21-O21-C2
4	A	5109	POV	O22-C21-O21-C2
4	C	5106	POV	O22-C21-O21-C2
4	G	5107	POV	O22-C21-O21-C2
4	J	5110	POV	O22-C21-O21-C2
4	A	5116	POV	C213-C214-C215-C216
4	C	5112	POV	C213-C214-C215-C216
4	G	5114	POV	C213-C214-C215-C216
4	J	5103	POV	C213-C214-C215-C216
5	A	5102	ATP	O4'-C4'-C5'-O5'
5	C	5101	ATP	O4'-C4'-C5'-O5'
5	G	5101	ATP	O4'-C4'-C5'-O5'
5	J	5104	ATP	O4'-C4'-C5'-O5'
4	J	5101	POV	C32-C33-C34-C35
4	A	5107	POV	C32-C33-C34-C35
4	A	5114	POV	C32-C33-C34-C35
4	G	5112	POV	C32-C33-C34-C35
4	J	5102	POV	C311-C310-C39-C38
4	A	5115	POV	C311-C310-C39-C38
4	C	5111	POV	C311-C310-C39-C38
4	G	5113	POV	C311-C310-C39-C38
4	A	5109	POV	C210-C211-C212-C213
4	G	5107	POV	C210-C211-C212-C213
4	J	5110	POV	C210-C211-C212-C213
4	A	5105	POV	C11-C12-N-C14
4	C	5104	POV	C11-C12-N-C14
4	G	5104	POV	C11-C12-N-C14
4	J	5107	POV	C11-C12-N-C14
4	A	5110	POV	C1-C2-C3-O31
4	C	5107	POV	C1-C2-C3-O31
4	G	5108	POV	C1-C2-C3-O31
4	J	5111	POV	C1-C2-C3-O31
4	C	5106	POV	C210-C211-C212-C213

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	5105	POV	C11-C12-N-C15
4	C	5104	POV	C11-C12-N-C15
4	G	5104	POV	C11-C12-N-C15
4	J	5107	POV	C11-C12-N-C15
4	J	5103	POV	C211-C212-C213-C214
4	A	5116	POV	C211-C212-C213-C214
4	C	5112	POV	C211-C212-C213-C214
4	G	5114	POV	C211-C212-C213-C214
4	J	5103	POV	C33-C34-C35-C36
4	A	5116	POV	C33-C34-C35-C36
4	C	5112	POV	C33-C34-C35-C36
4	G	5114	POV	C33-C34-C35-C36
4	C	5104	POV	C33-C34-C35-C36
4	A	5105	POV	C33-C34-C35-C36
4	G	5104	POV	C33-C34-C35-C36
4	J	5107	POV	C33-C34-C35-C36
4	A	5116	POV	C39-C310-C311-C312
4	C	5112	POV	C39-C310-C311-C312
4	G	5114	POV	C39-C310-C311-C312
4	J	5103	POV	C39-C310-C311-C312
4	A	5116	POV	C11-C12-N-C13
4	C	5112	POV	C11-C12-N-C13
4	G	5114	POV	C11-C12-N-C13
4	J	5103	POV	C11-C12-N-C13
4	A	5101	POV	C211-C212-C213-C214
4	A	5105	POV	C36-C37-C38-C39
4	G	5104	POV	C36-C37-C38-C39
4	J	5107	POV	C36-C37-C38-C39
4	C	5104	POV	C36-C37-C38-C39
4	A	5108	POV	C211-C212-C213-C214
4	G	5106	POV	C211-C212-C213-C214
4	J	5109	POV	C211-C212-C213-C214
4	A	5111	POV	C311-C312-C313-C314
4	G	5109	POV	C311-C312-C313-C314
4	J	5112	POV	C311-C312-C313-C314
4	C	5108	POV	C311-C312-C313-C314
4	A	5116	POV	C11-C12-N-C15
4	C	5112	POV	C11-C12-N-C15
4	G	5114	POV	C11-C12-N-C15
4	J	5103	POV	C11-C12-N-C15
4	A	5106	POV	O32-C31-O31-C3
4	C	5105	POV	O32-C31-O31-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	G	5105	POV	O32-C31-O31-C3
4	J	5108	POV	O32-C31-O31-C3
4	A	5107	POV	O32-C31-O31-C3
4	A	5114	POV	O32-C31-O31-C3
4	G	5112	POV	O32-C31-O31-C3
4	J	5101	POV	O32-C31-O31-C3
4	A	5116	POV	C11-C12-N-C14
4	C	5112	POV	C11-C12-N-C14
4	G	5114	POV	C11-C12-N-C14
4	J	5103	POV	C11-C12-N-C14
4	C	5109	POV	C23-C24-C25-C26
4	A	5112	POV	C23-C24-C25-C26
4	G	5110	POV	C23-C24-C25-C26
4	J	5113	POV	C23-C24-C25-C26
4	A	5106	POV	C32-C31-O31-C3
4	G	5105	POV	C32-C31-O31-C3
4	J	5108	POV	C32-C31-O31-C3
4	C	5105	POV	C32-C31-O31-C3
4	A	5112	POV	C27-C28-C29-C210
4	A	5116	POV	C27-C28-C29-C210
4	C	5109	POV	C27-C28-C29-C210
4	C	5112	POV	C27-C28-C29-C210
4	G	5110	POV	C27-C28-C29-C210
4	G	5114	POV	C27-C28-C29-C210
4	J	5103	POV	C27-C28-C29-C210
4	J	5113	POV	C27-C28-C29-C210
4	J	5101	POV	C32-C31-O31-C3
4	A	5107	POV	O31-C31-C32-C33
4	A	5114	POV	O31-C31-C32-C33
4	G	5112	POV	O31-C31-C32-C33
4	J	5101	POV	O31-C31-C32-C33
4	A	5107	POV	C32-C31-O31-C3
4	A	5114	POV	C32-C31-O31-C3
4	G	5112	POV	C32-C31-O31-C3
4	J	5101	POV	O21-C21-C22-C23
4	A	5107	POV	O32-C31-C32-C33
4	A	5114	POV	O32-C31-C32-C33
4	G	5112	POV	O32-C31-C32-C33
4	J	5101	POV	O32-C31-C32-C33
4	A	5107	POV	O21-C21-C22-C23
4	A	5114	POV	O21-C21-C22-C23
4	G	5112	POV	O21-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	5105	POV	C310-C311-C312-C313
4	G	5104	POV	C310-C311-C312-C313
4	J	5107	POV	C310-C311-C312-C313
4	A	5109	POV	O31-C31-C32-C33
4	G	5107	POV	O31-C31-C32-C33
4	J	5110	POV	O31-C31-C32-C33
4	C	5104	POV	C310-C311-C312-C313
5	A	5102	ATP	O4'-C1'-N9-C8
5	C	5101	ATP	O4'-C1'-N9-C8
5	G	5101	ATP	O4'-C1'-N9-C8
5	J	5104	ATP	O4'-C1'-N9-C8
4	C	5106	POV	O31-C31-C32-C33

There are no ring outliers.

27 monomers are involved in 42 short contacts:

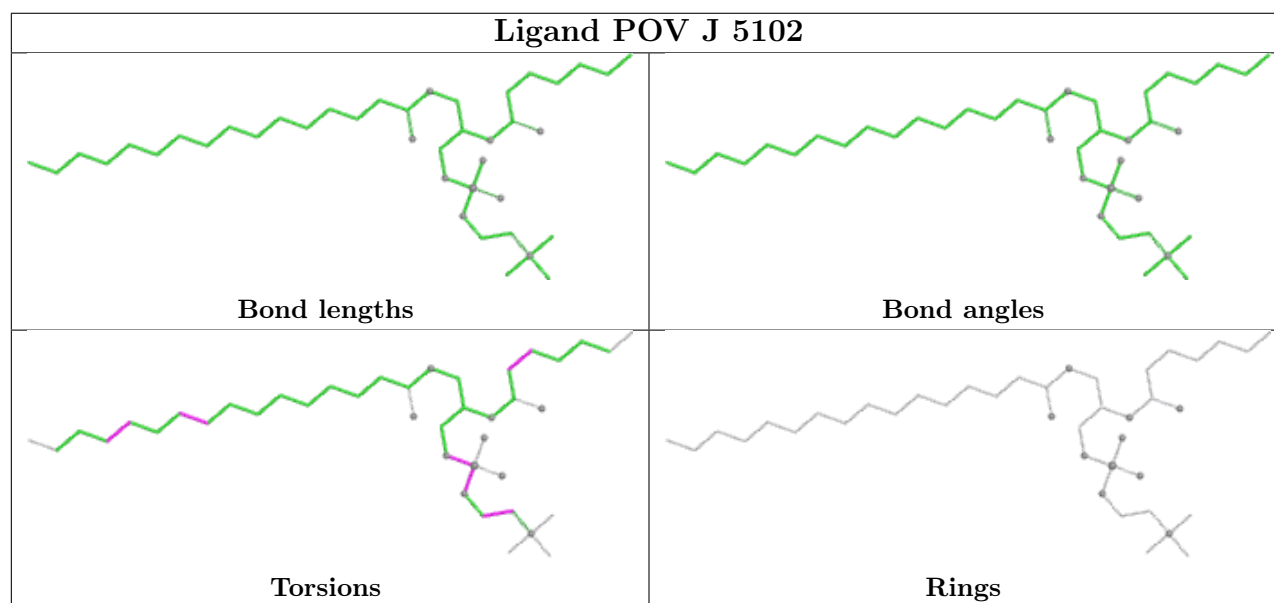
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	5102	POV	3	0
4	C	5111	POV	2	0
4	G	5113	POV	3	0
4	J	5112	POV	1	0
4	G	5114	POV	1	0
4	G	5112	POV	3	0
4	A	5109	POV	1	0
4	J	5101	POV	4	0
4	A	5111	POV	1	0
4	C	5105	POV	2	0
4	G	5104	POV	2	0
4	A	5105	POV	1	0
4	J	5103	POV	4	0
4	J	5110	POV	1	0
4	A	5107	POV	3	0
4	J	5107	POV	1	0
4	A	5112	POV	1	0
4	C	5106	POV	1	0
4	C	5109	POV	2	0
4	A	5114	POV	3	0
4	C	5104	POV	2	0
4	G	5110	POV	1	0
4	C	5112	POV	1	0
4	J	5113	POV	1	0
4	G	5107	POV	1	0

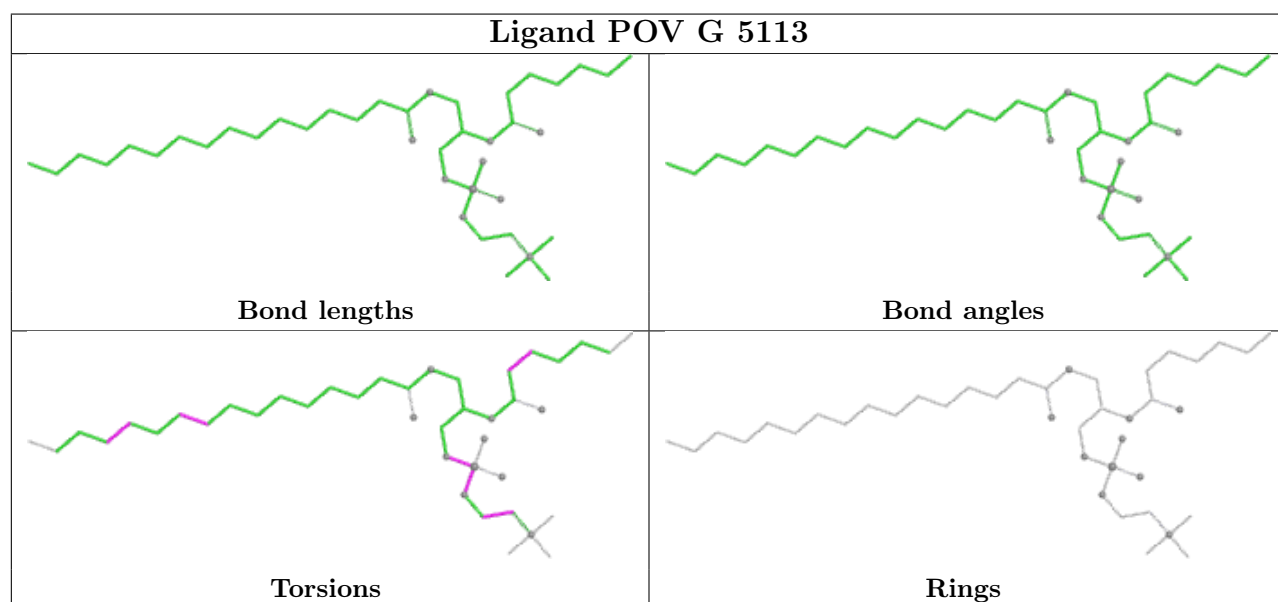
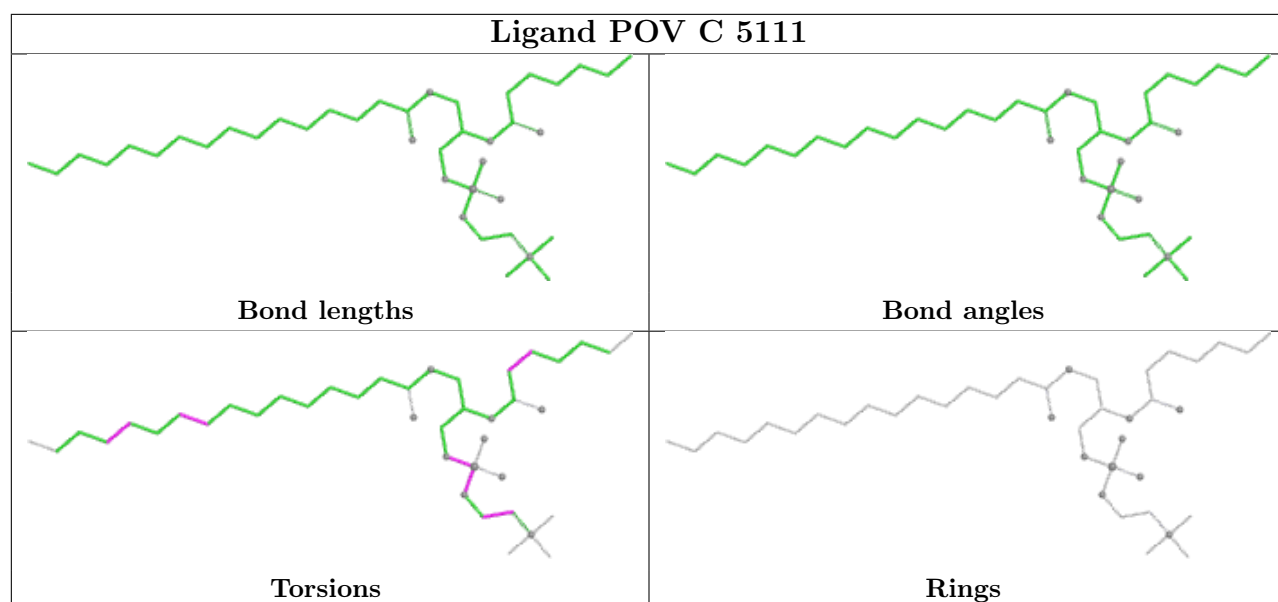
Continued on next page...

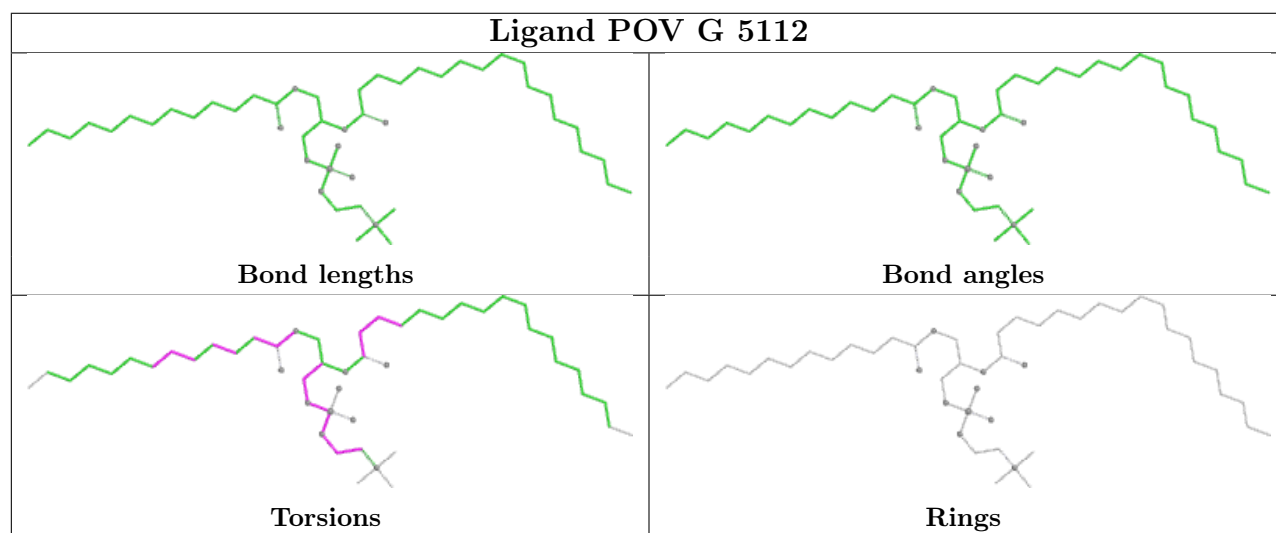
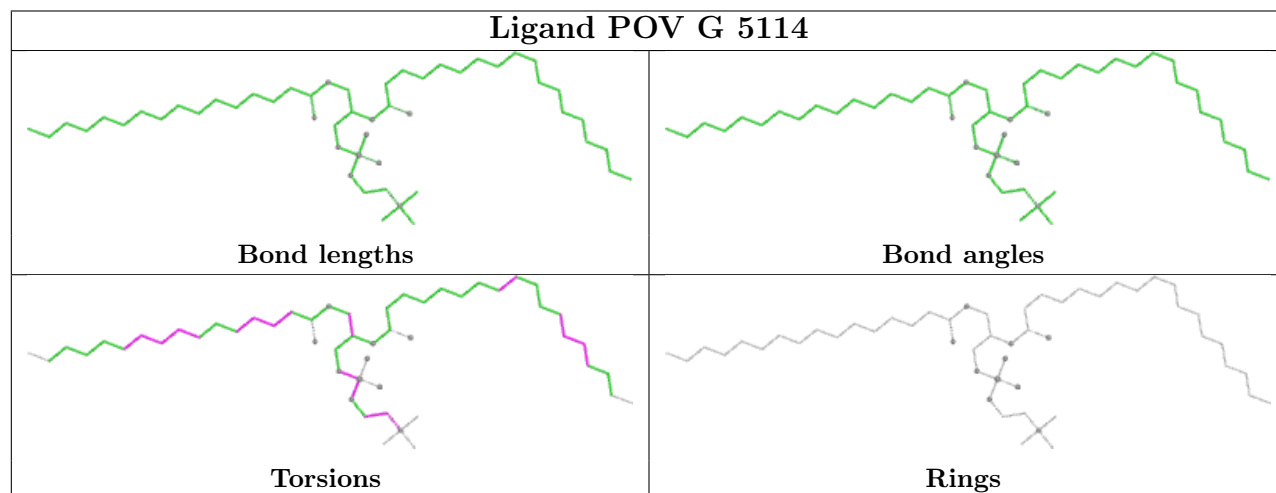
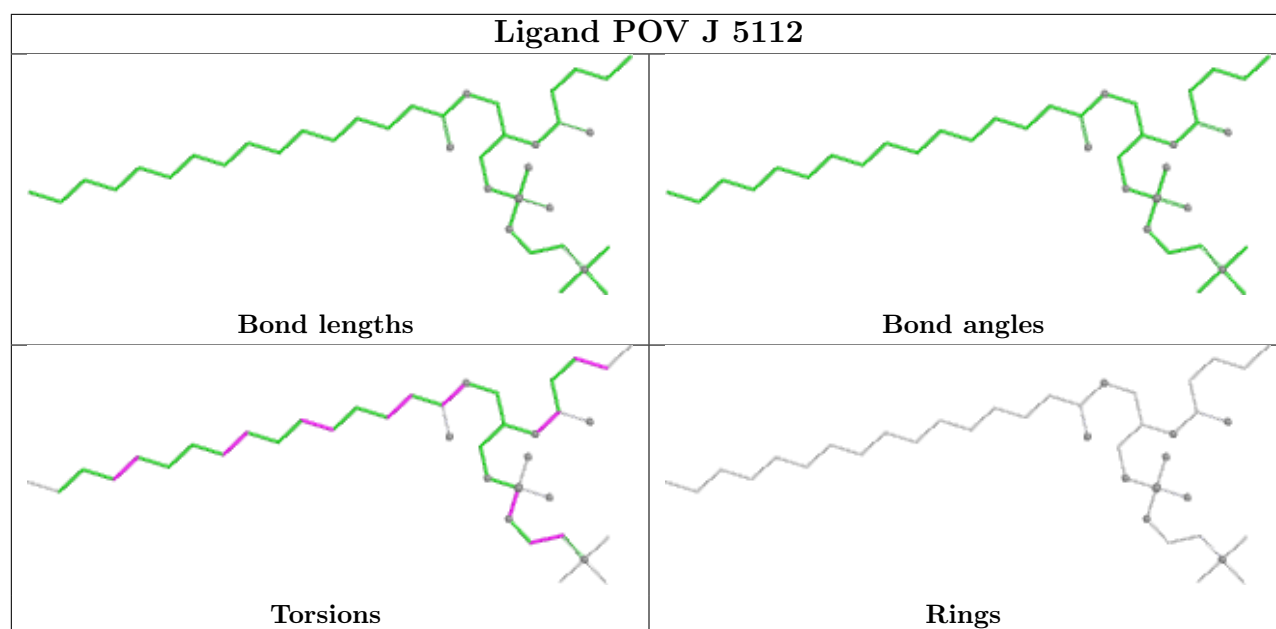
Continued from previous page...

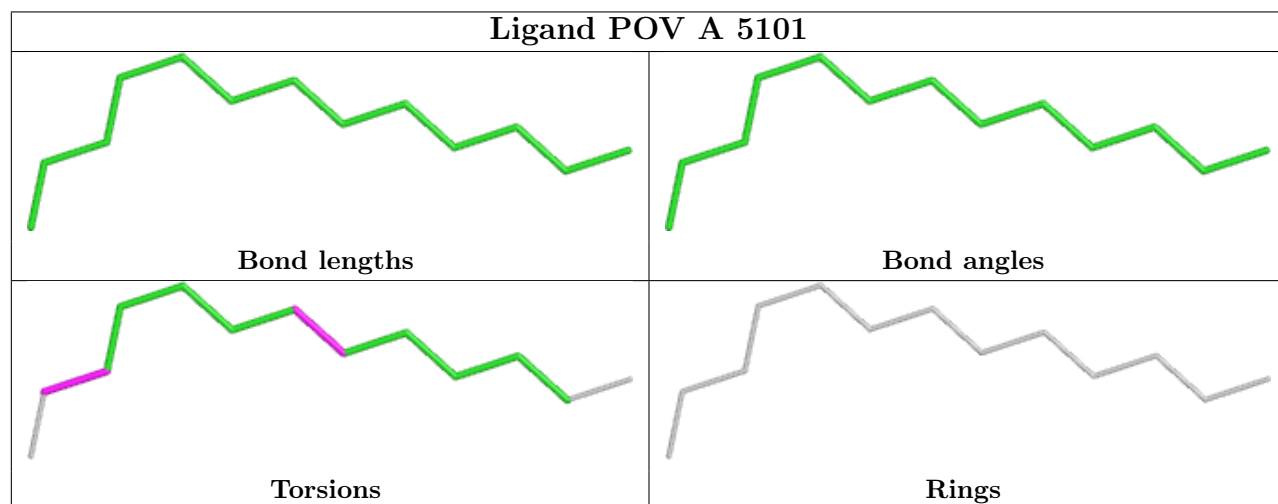
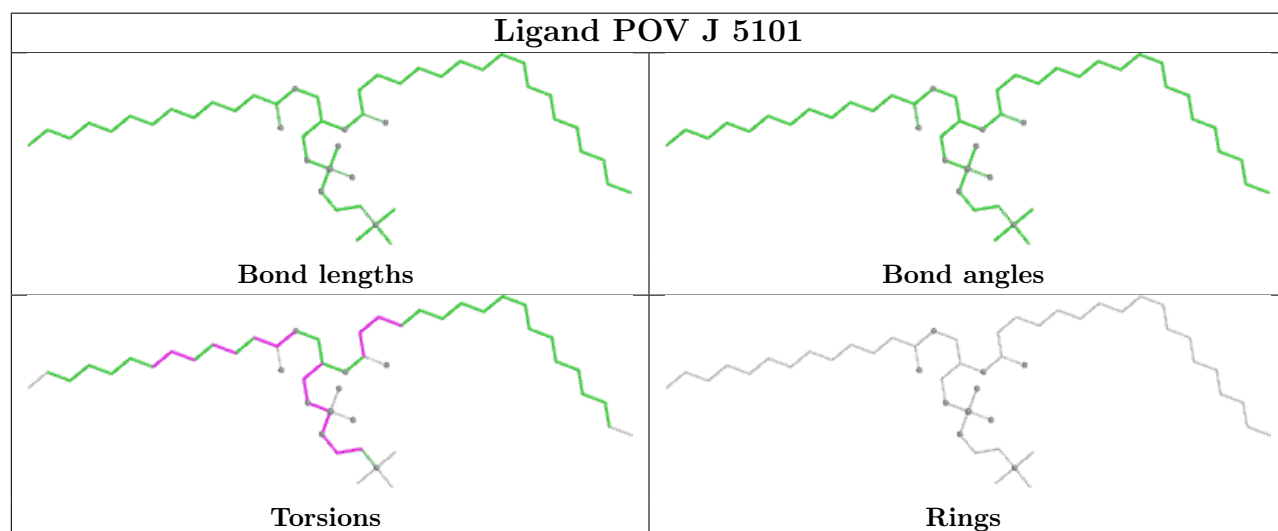
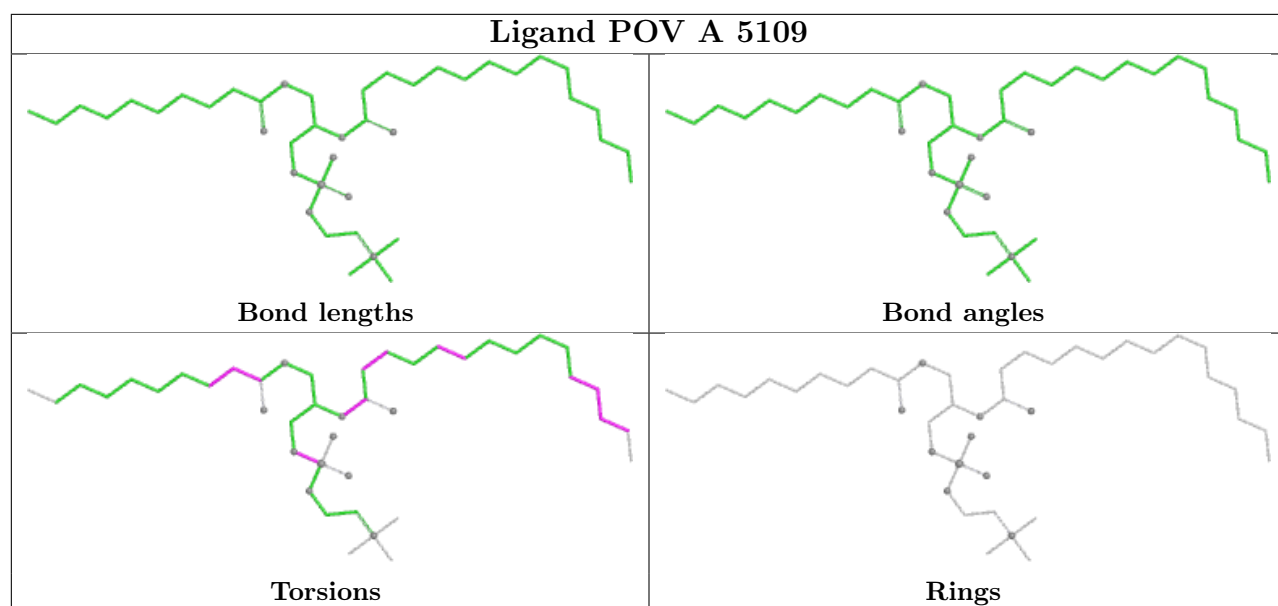
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	5116	POV	1	0
4	A	5115	POV	3	0

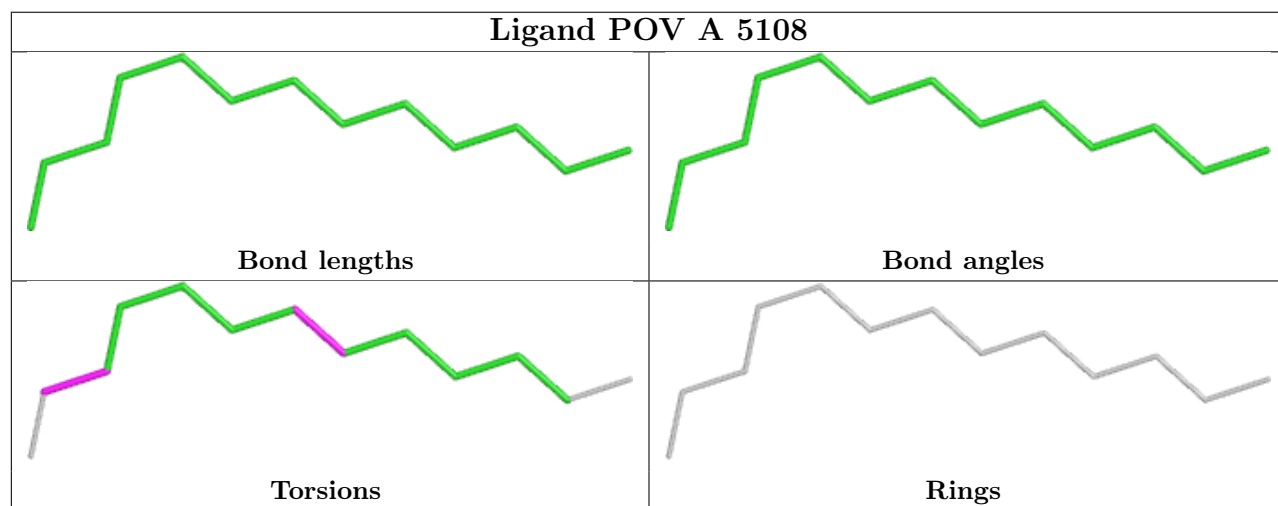
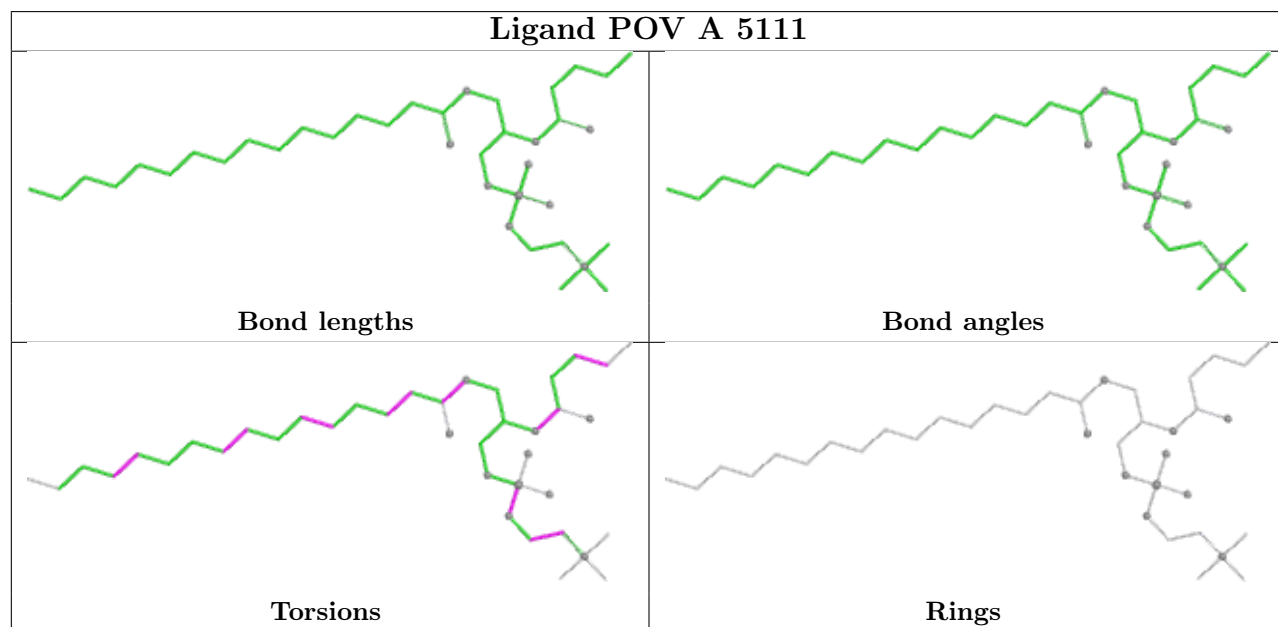
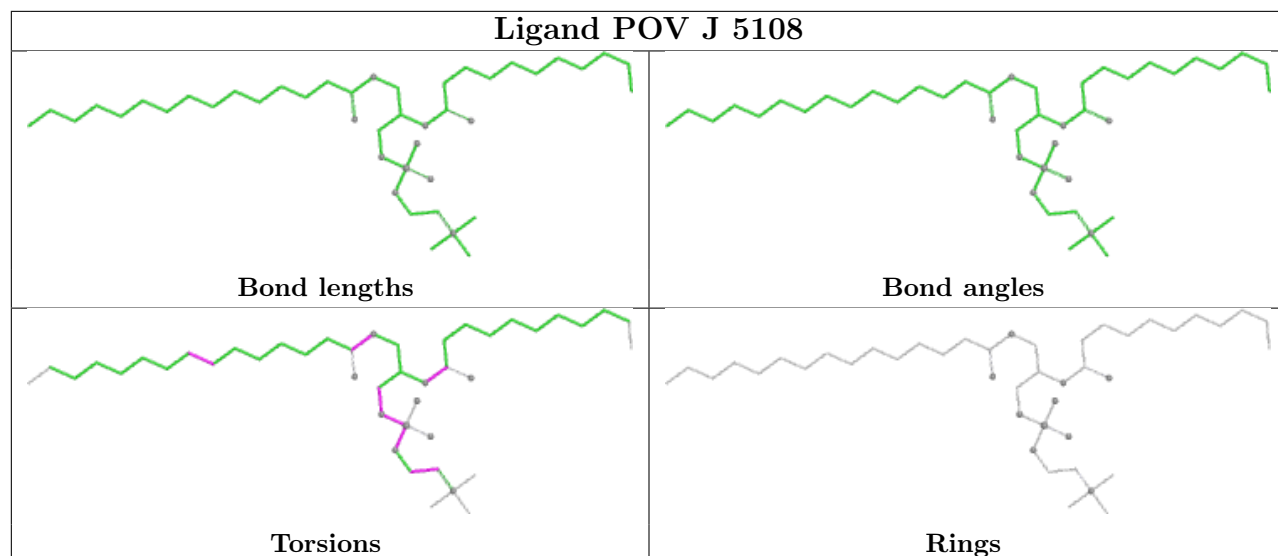
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

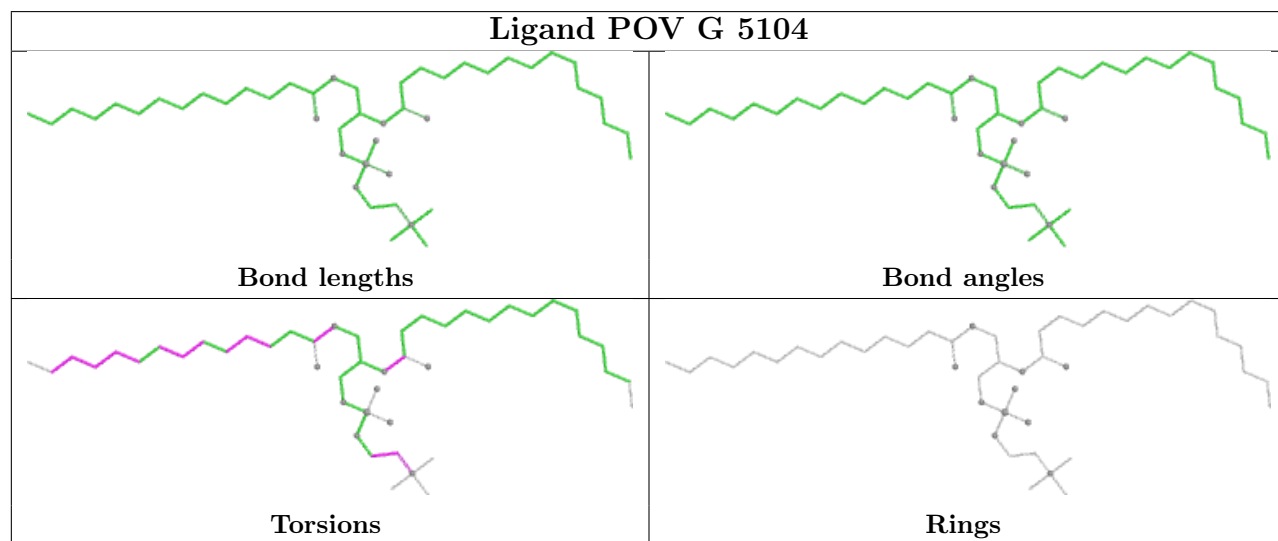
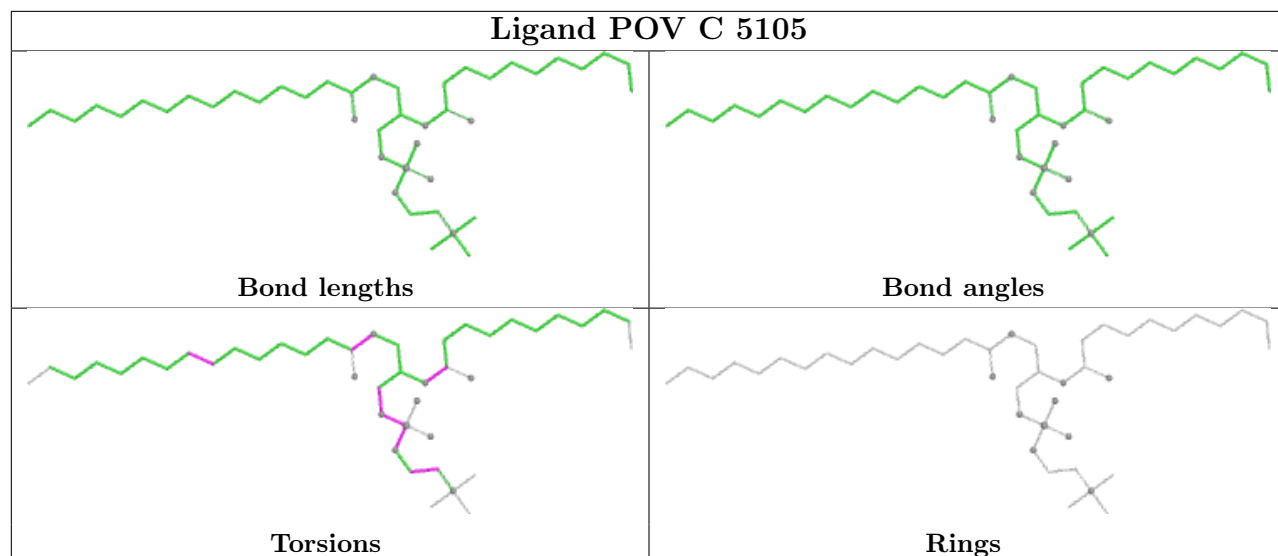


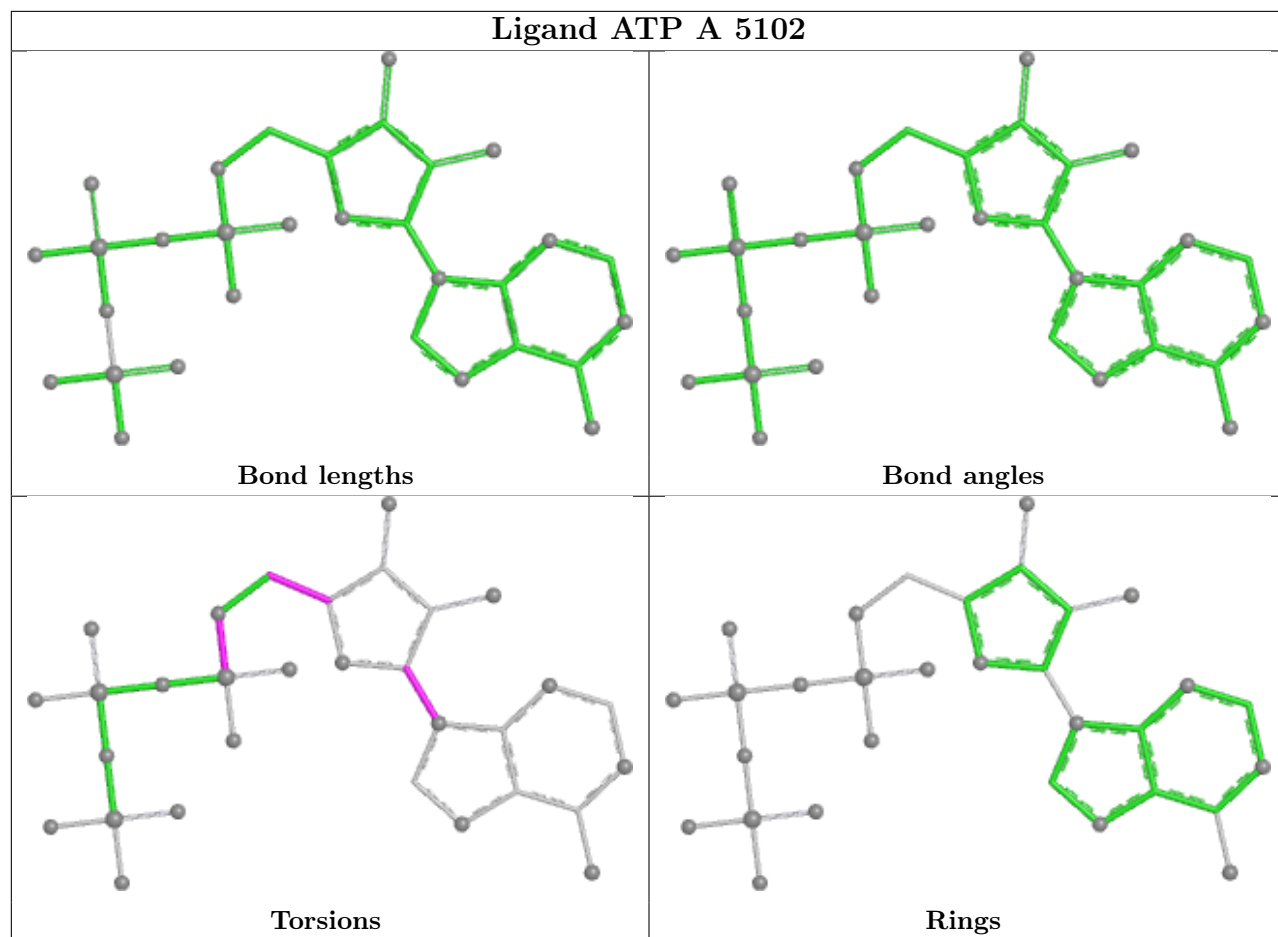


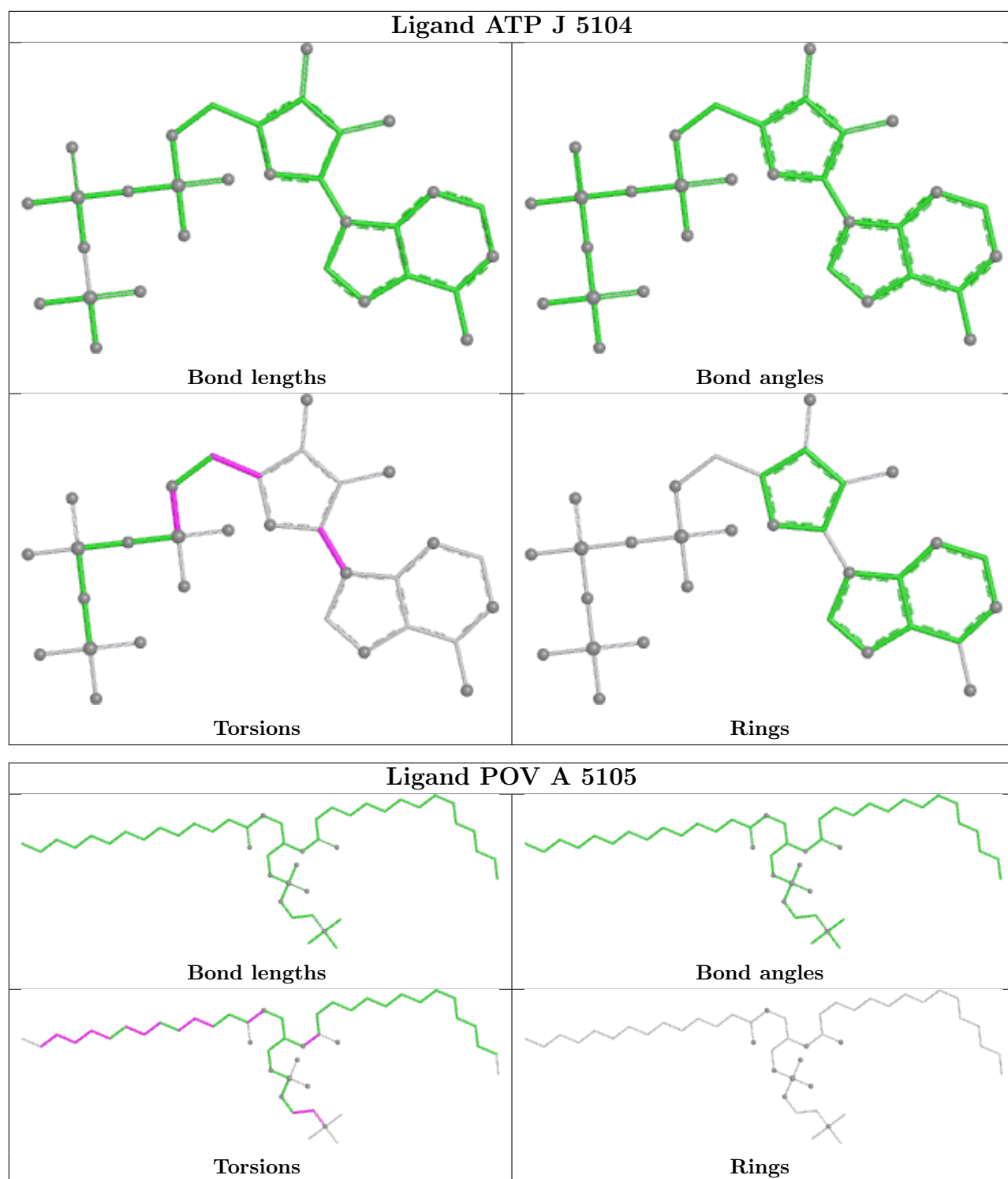


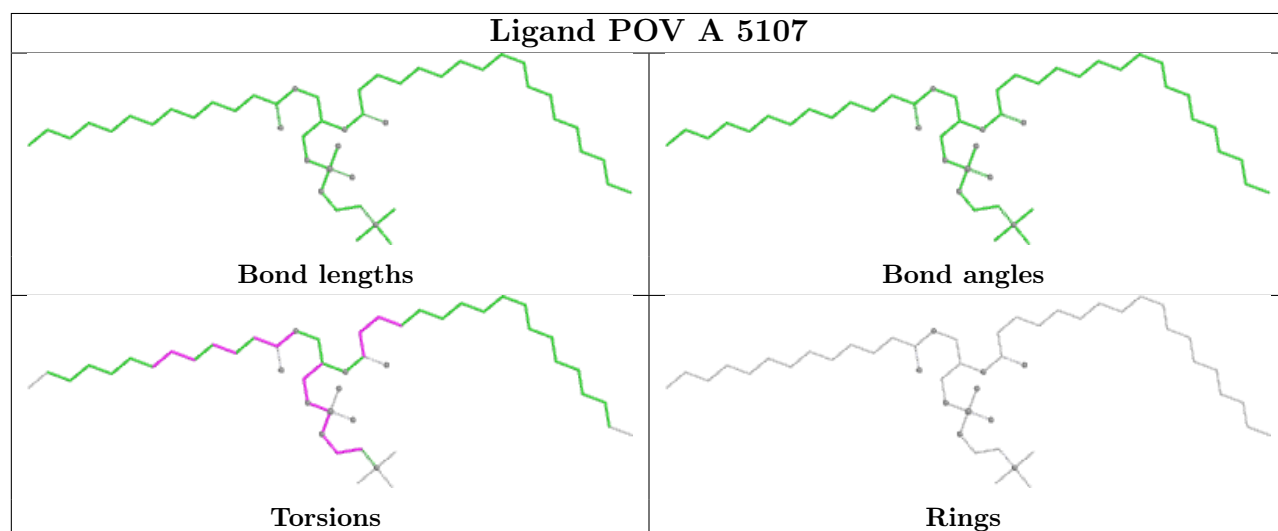
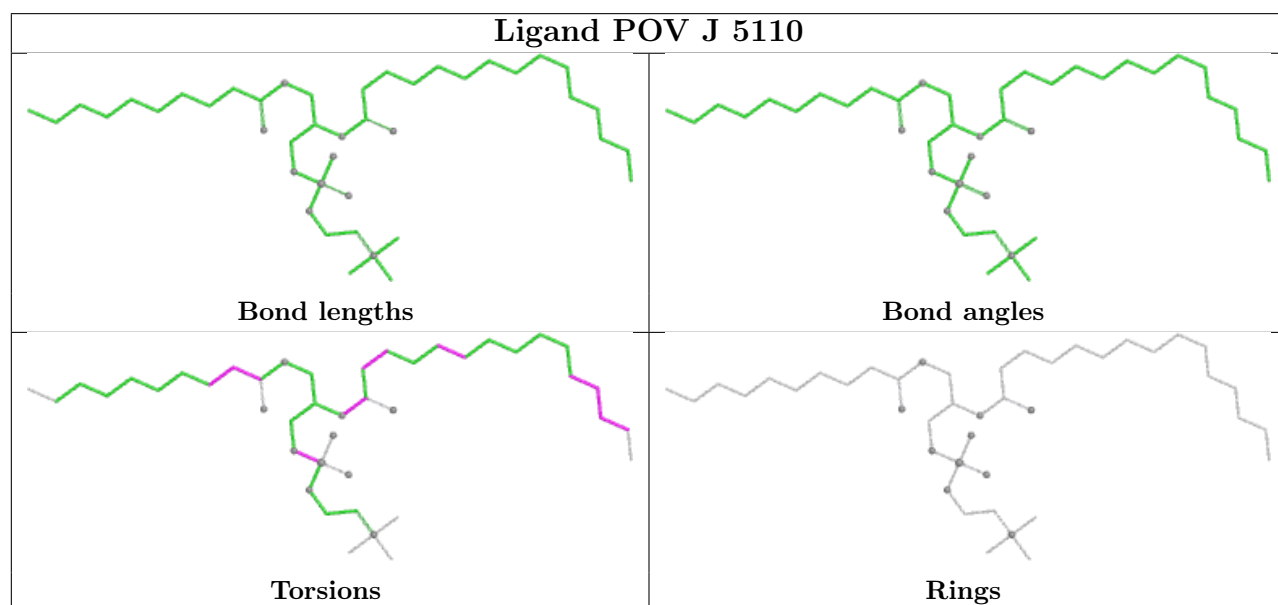
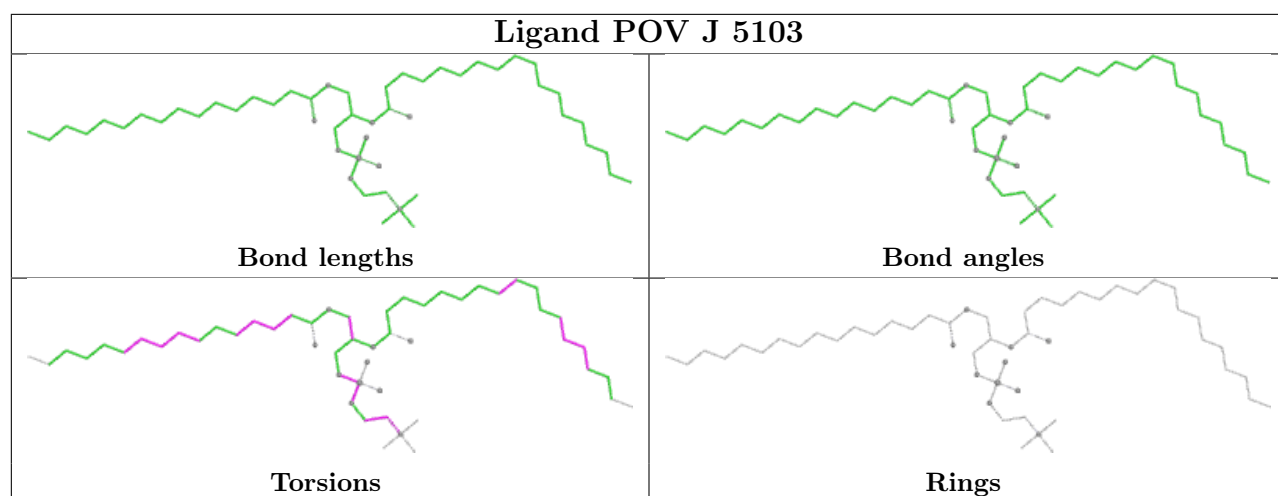


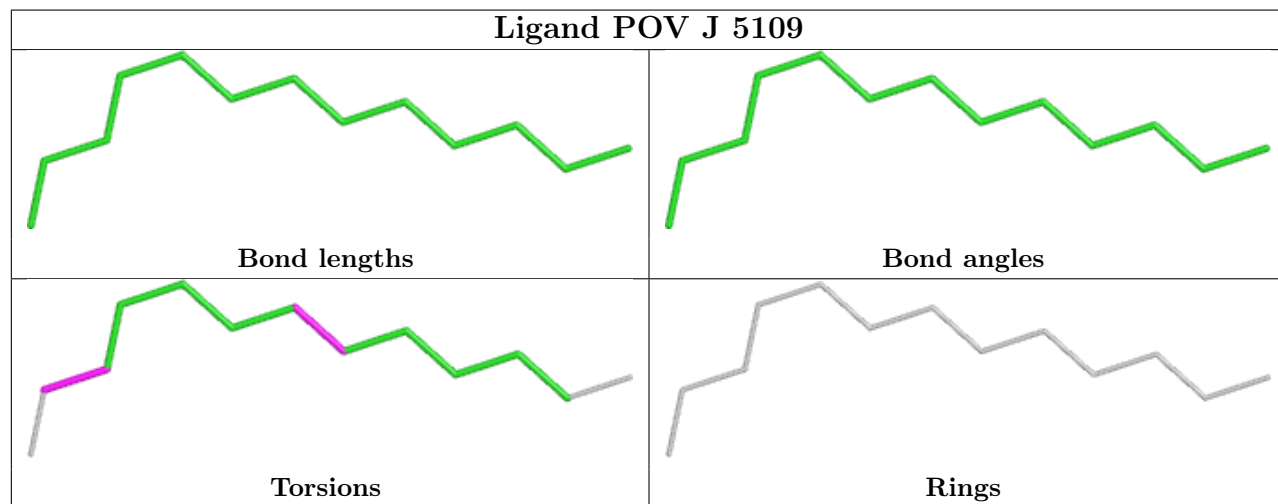
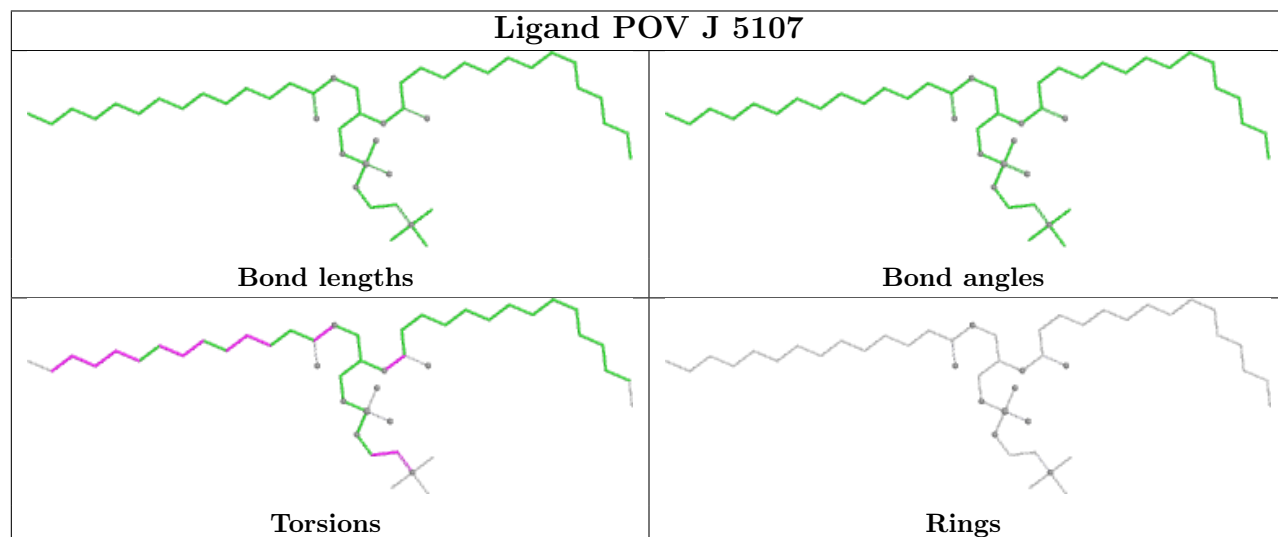
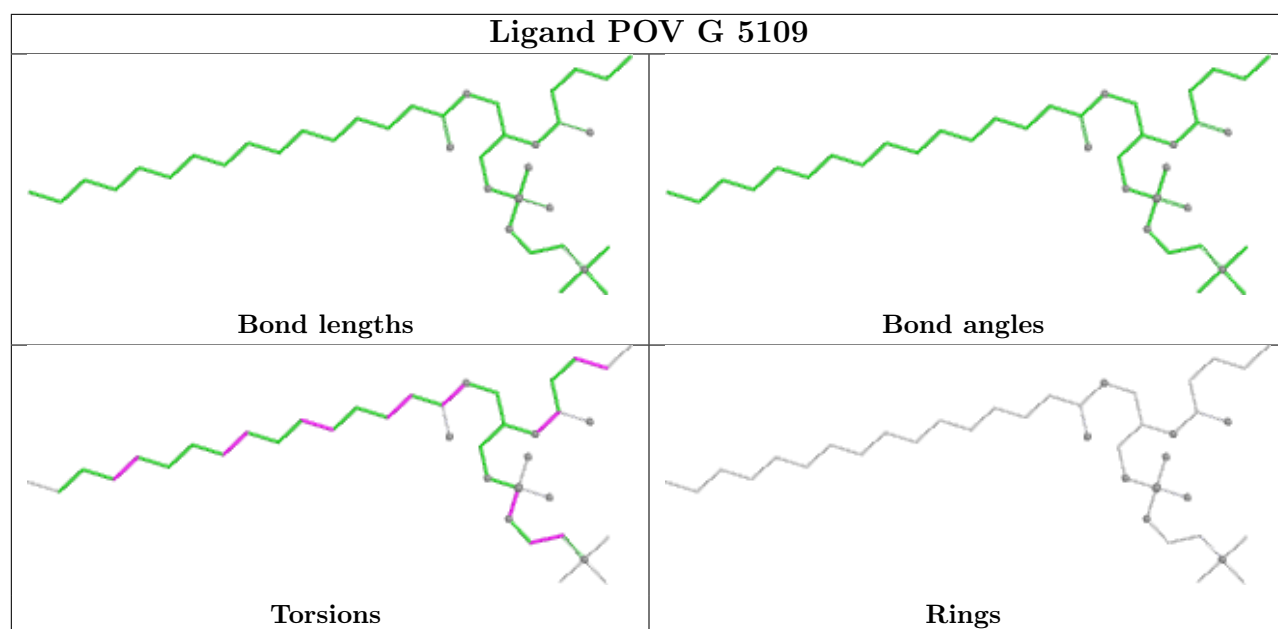


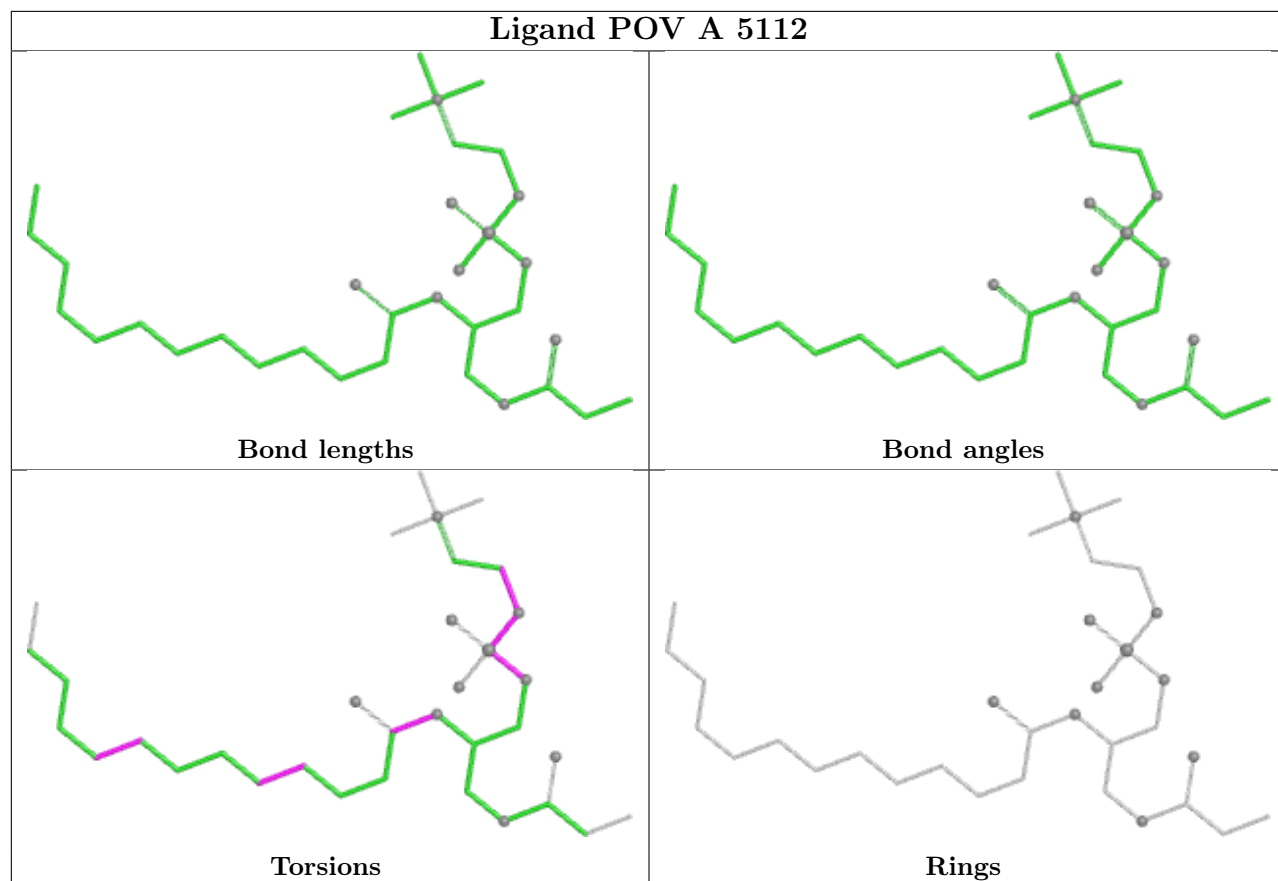


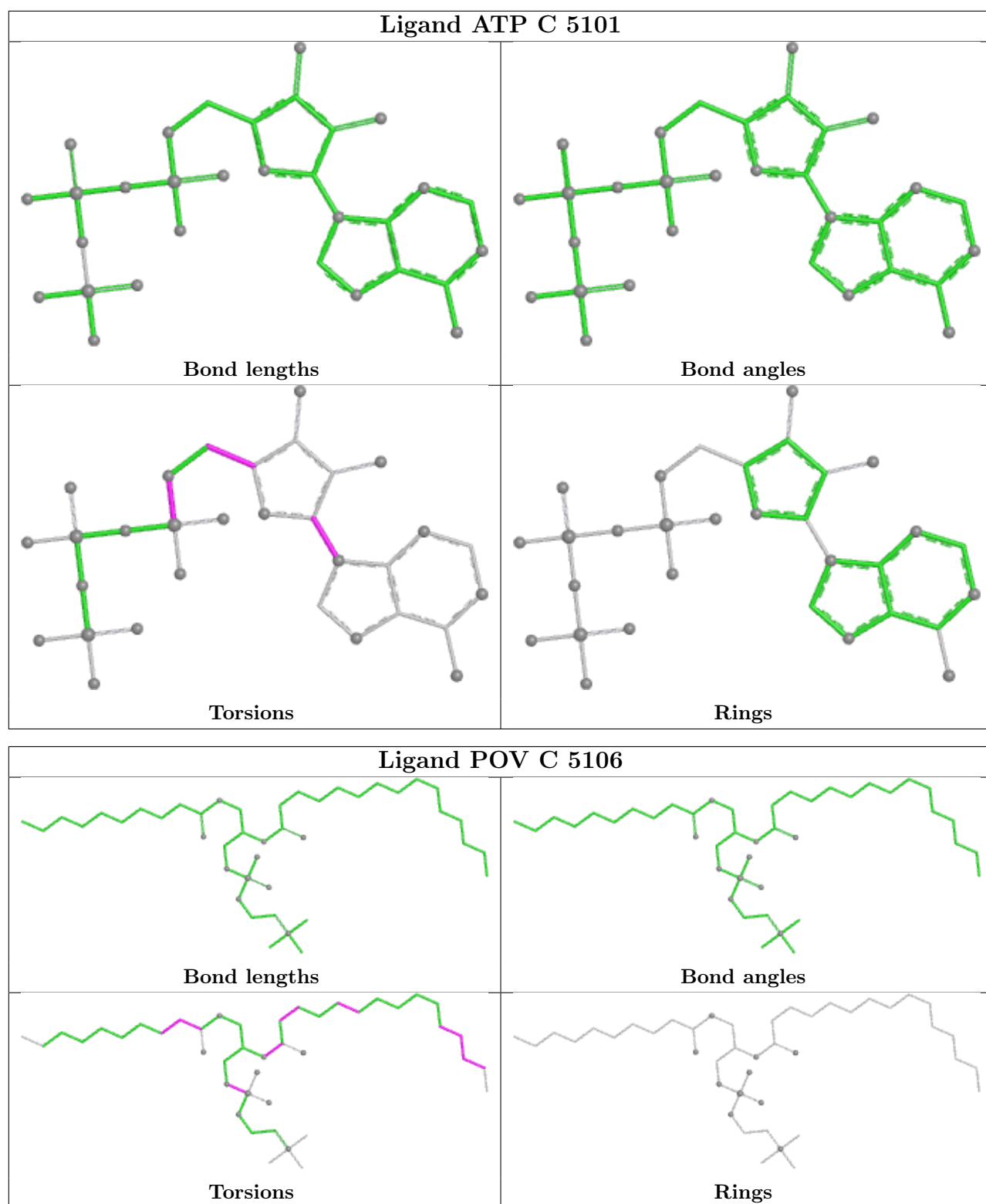


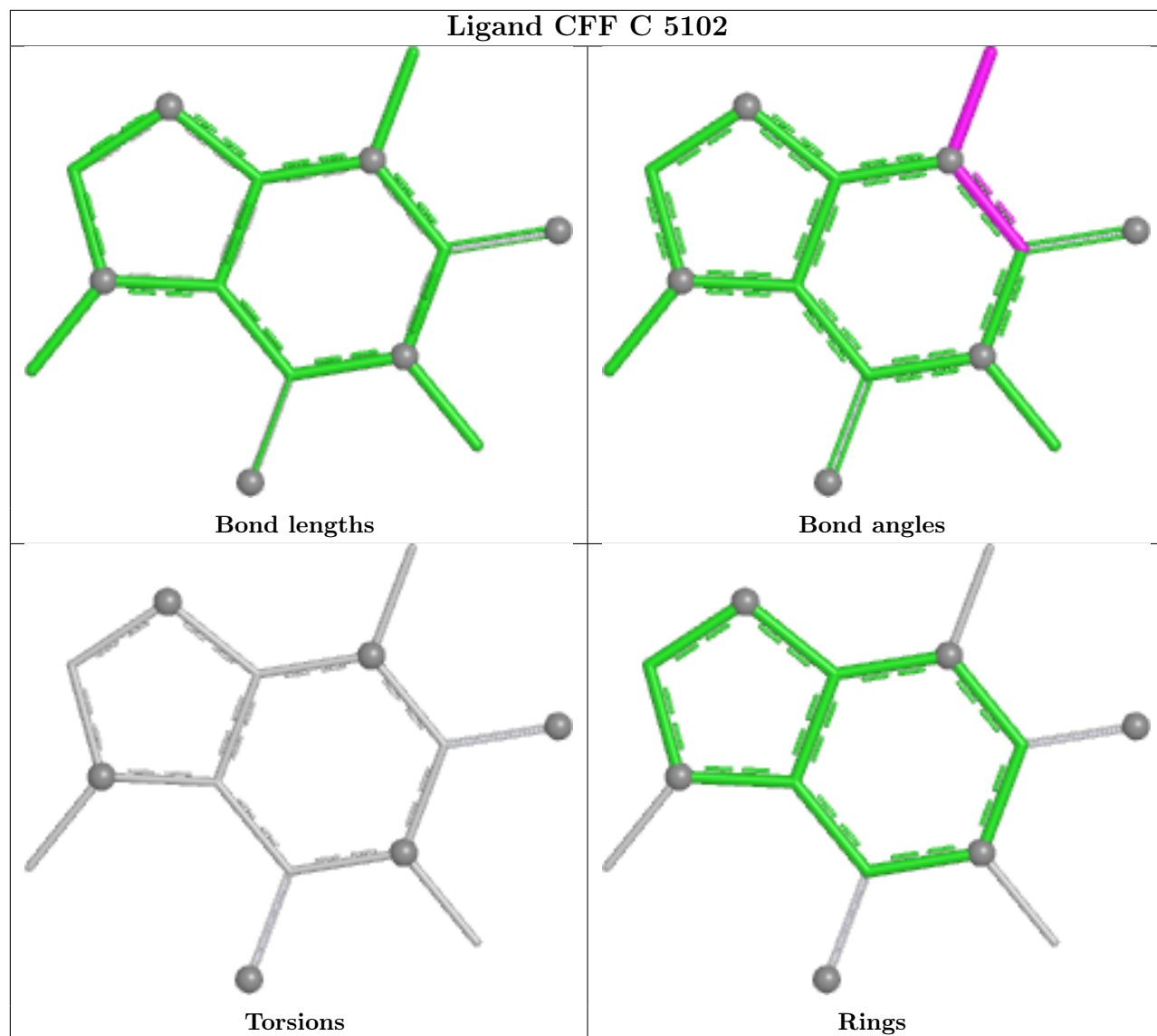


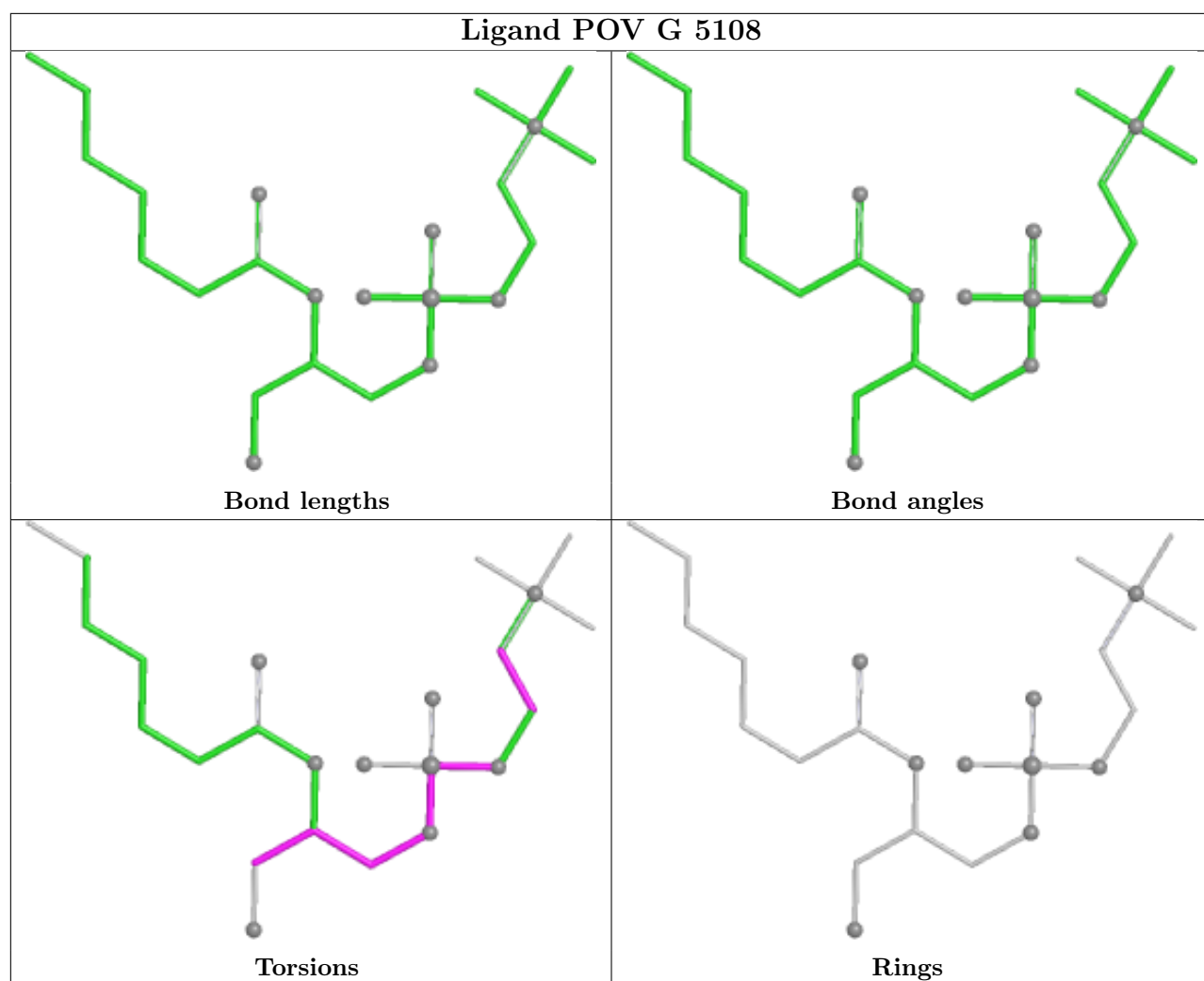


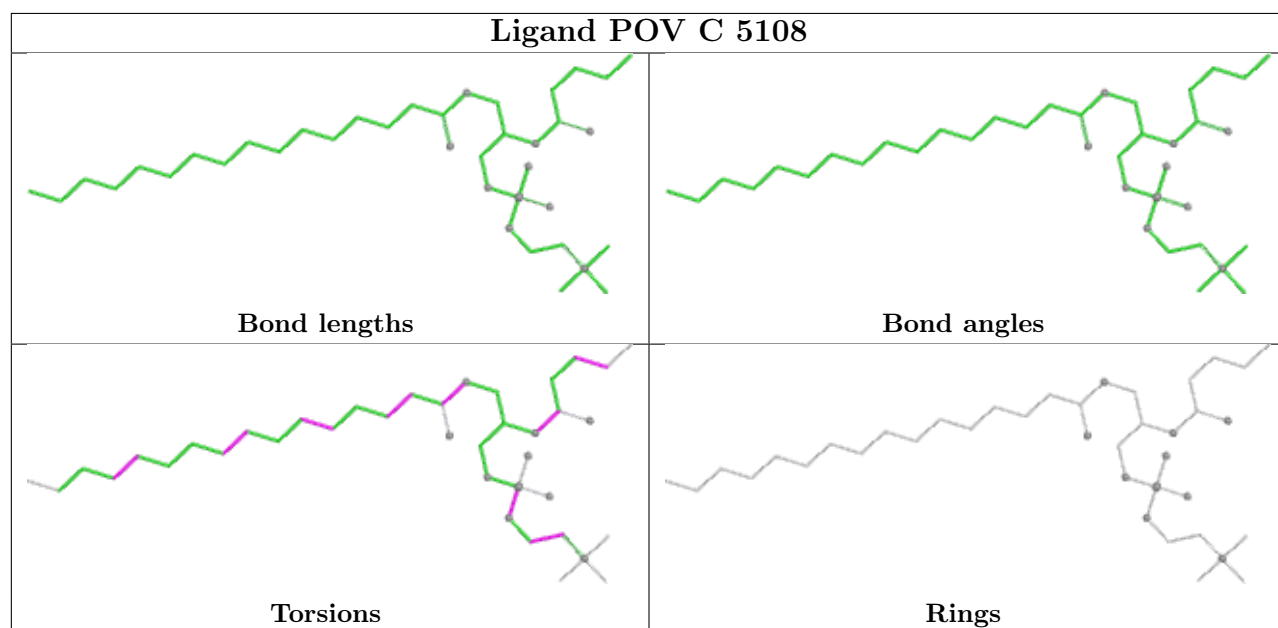
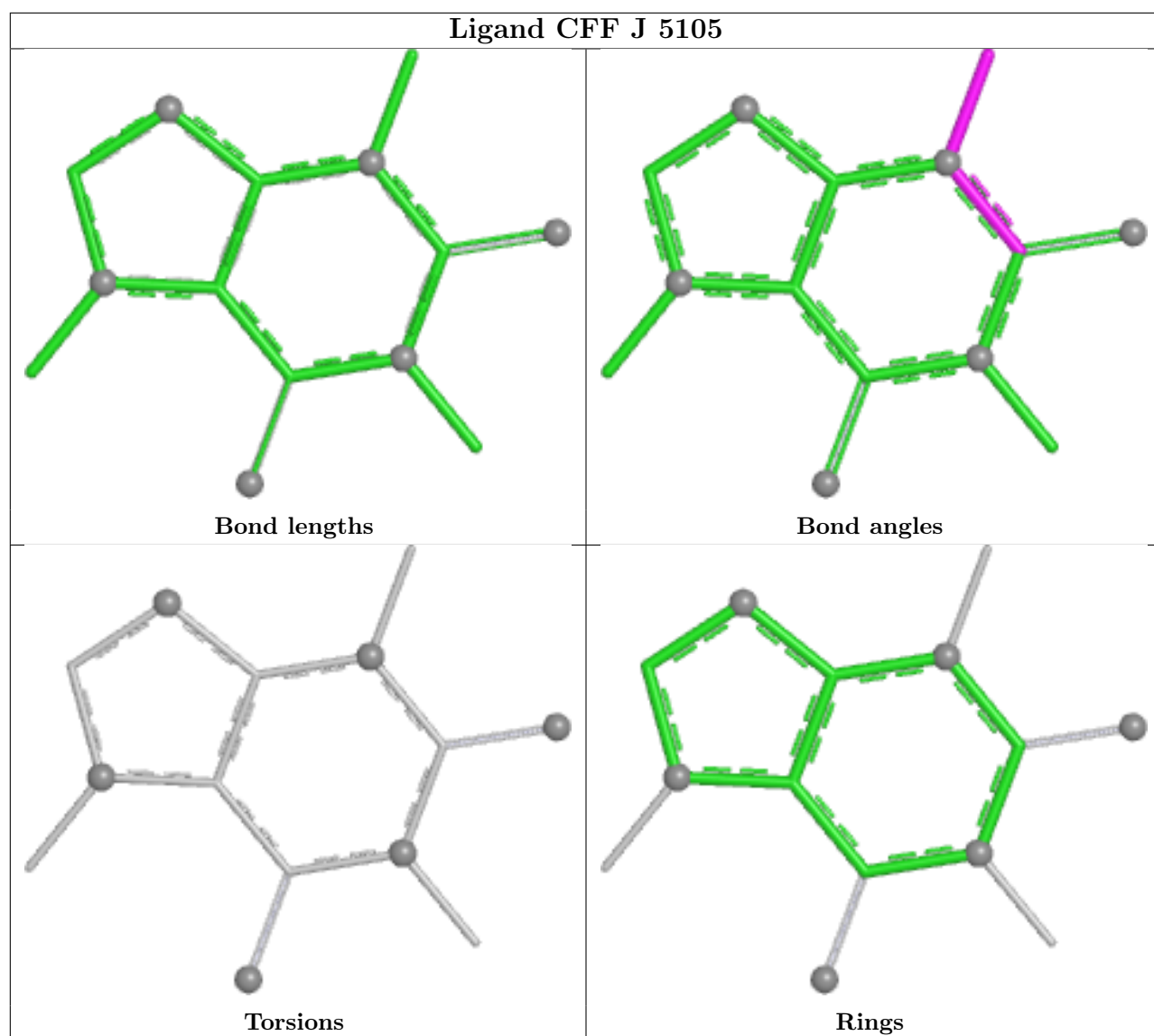


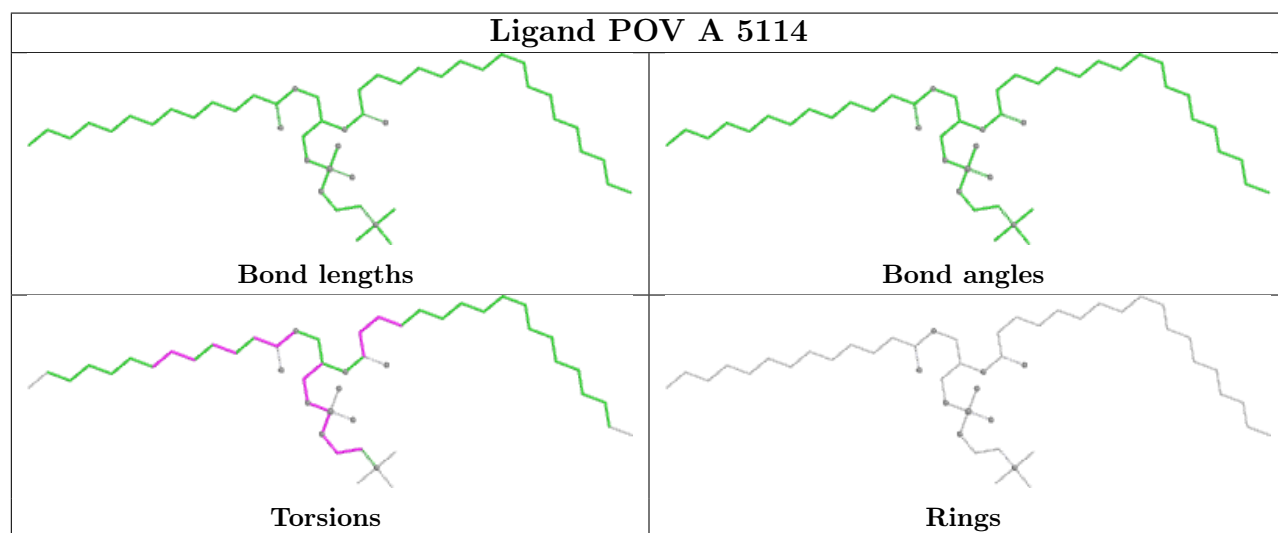
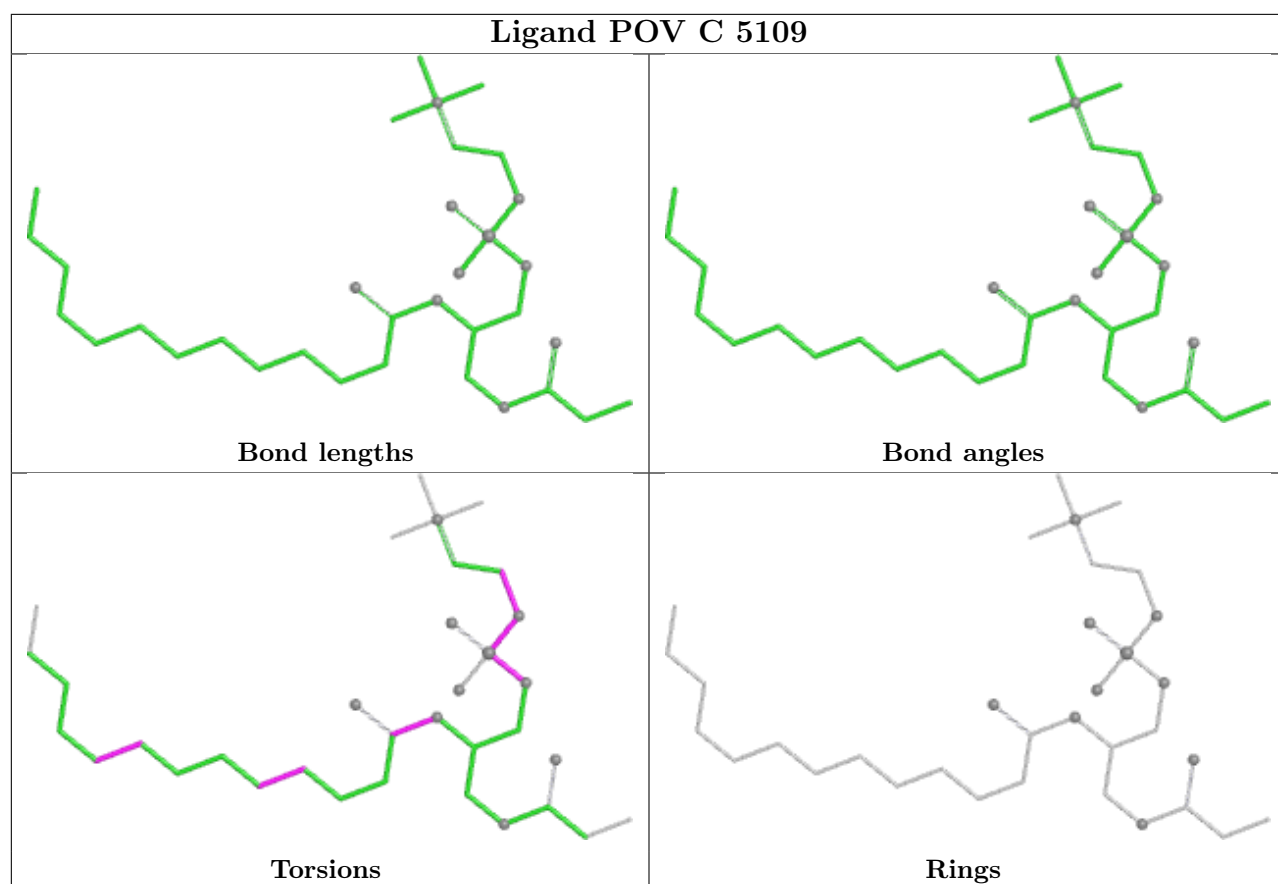


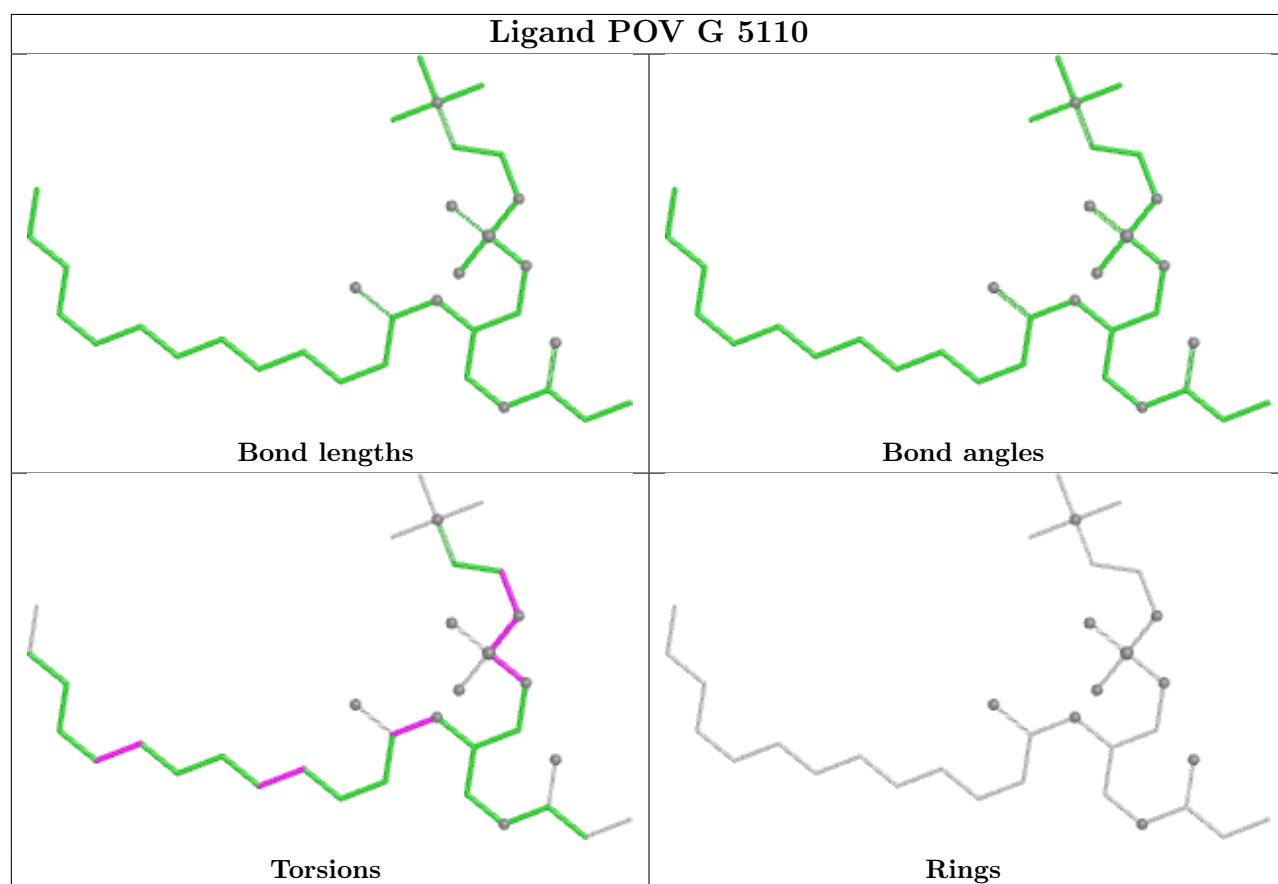
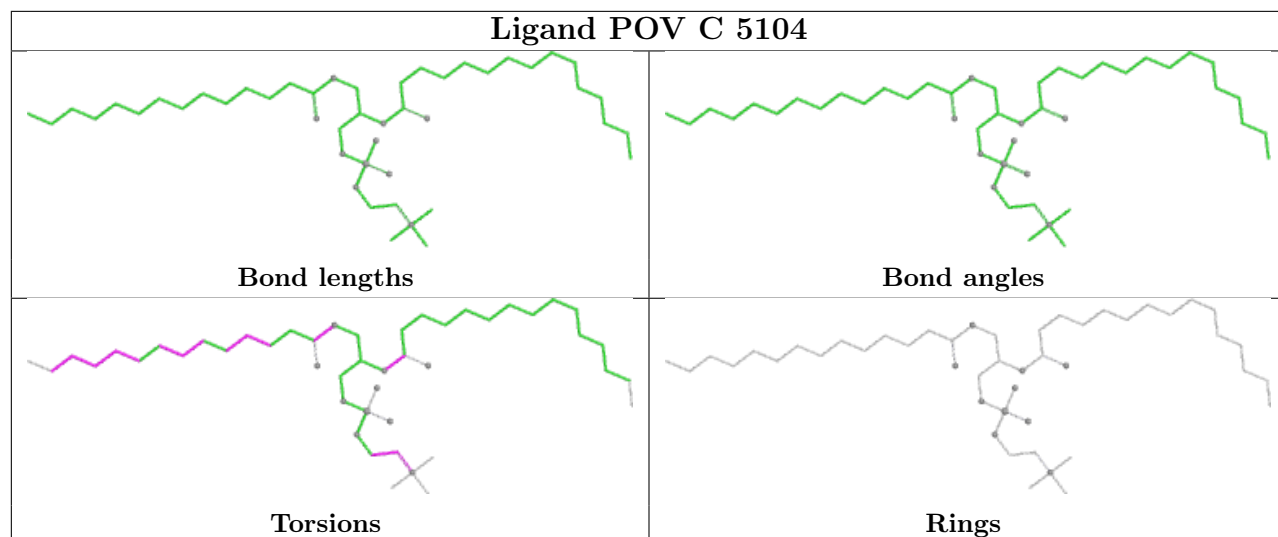


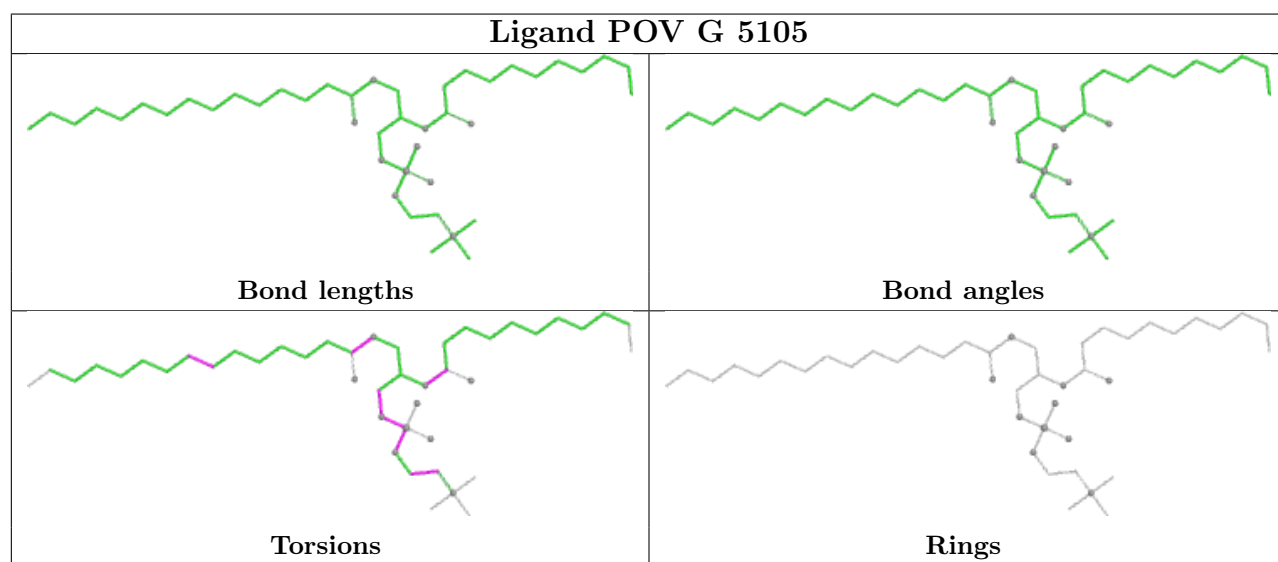
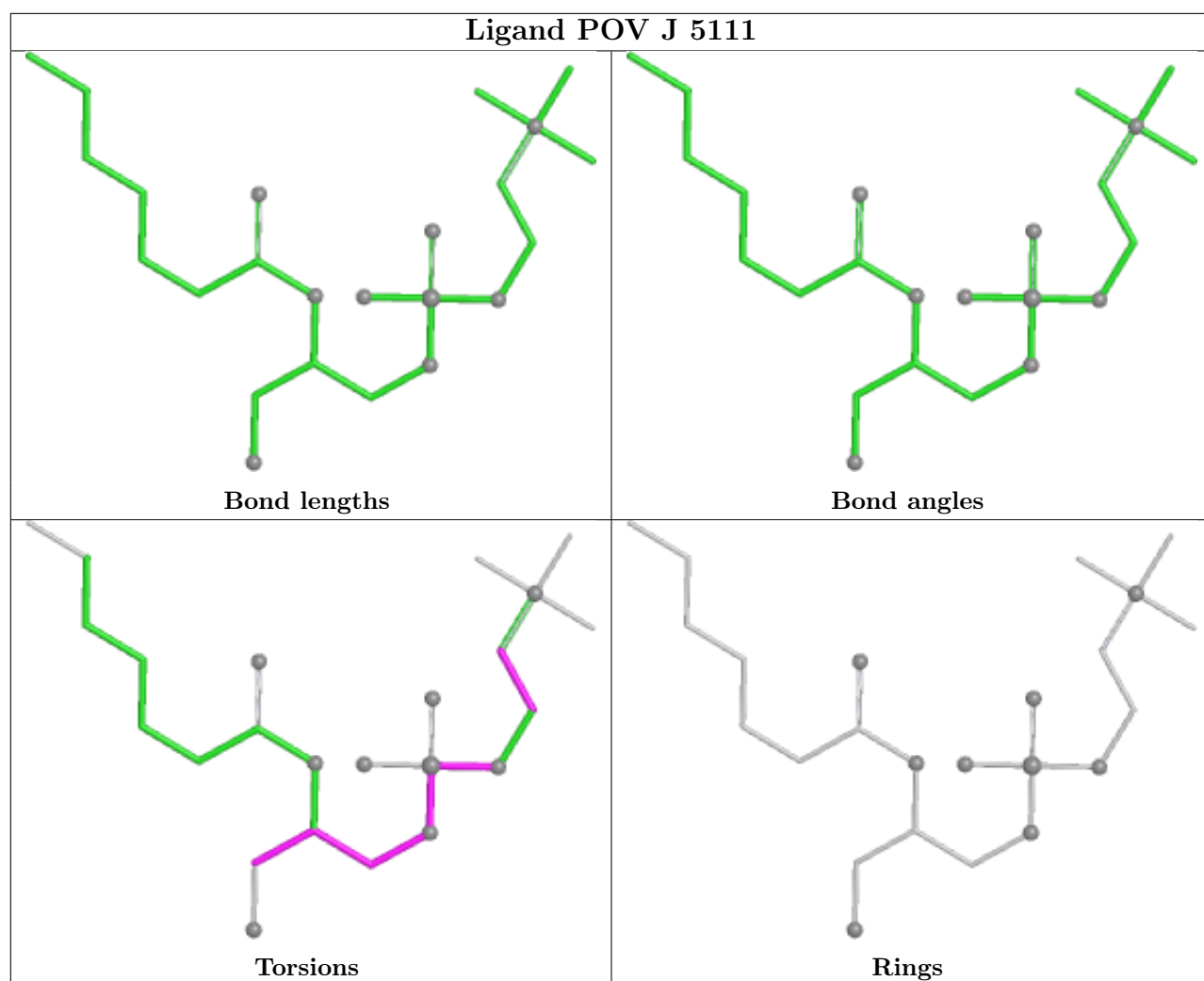


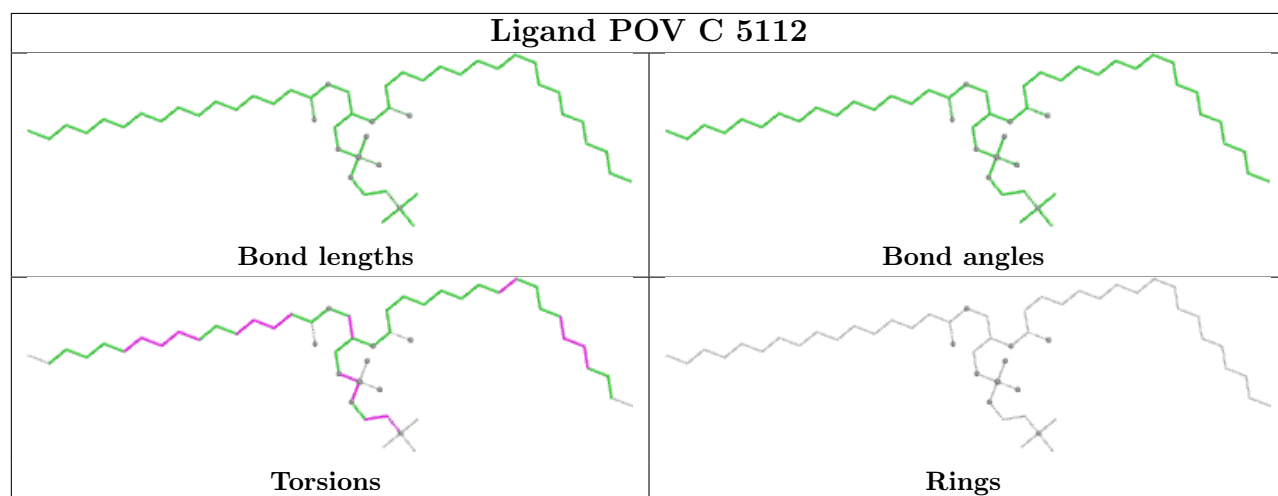
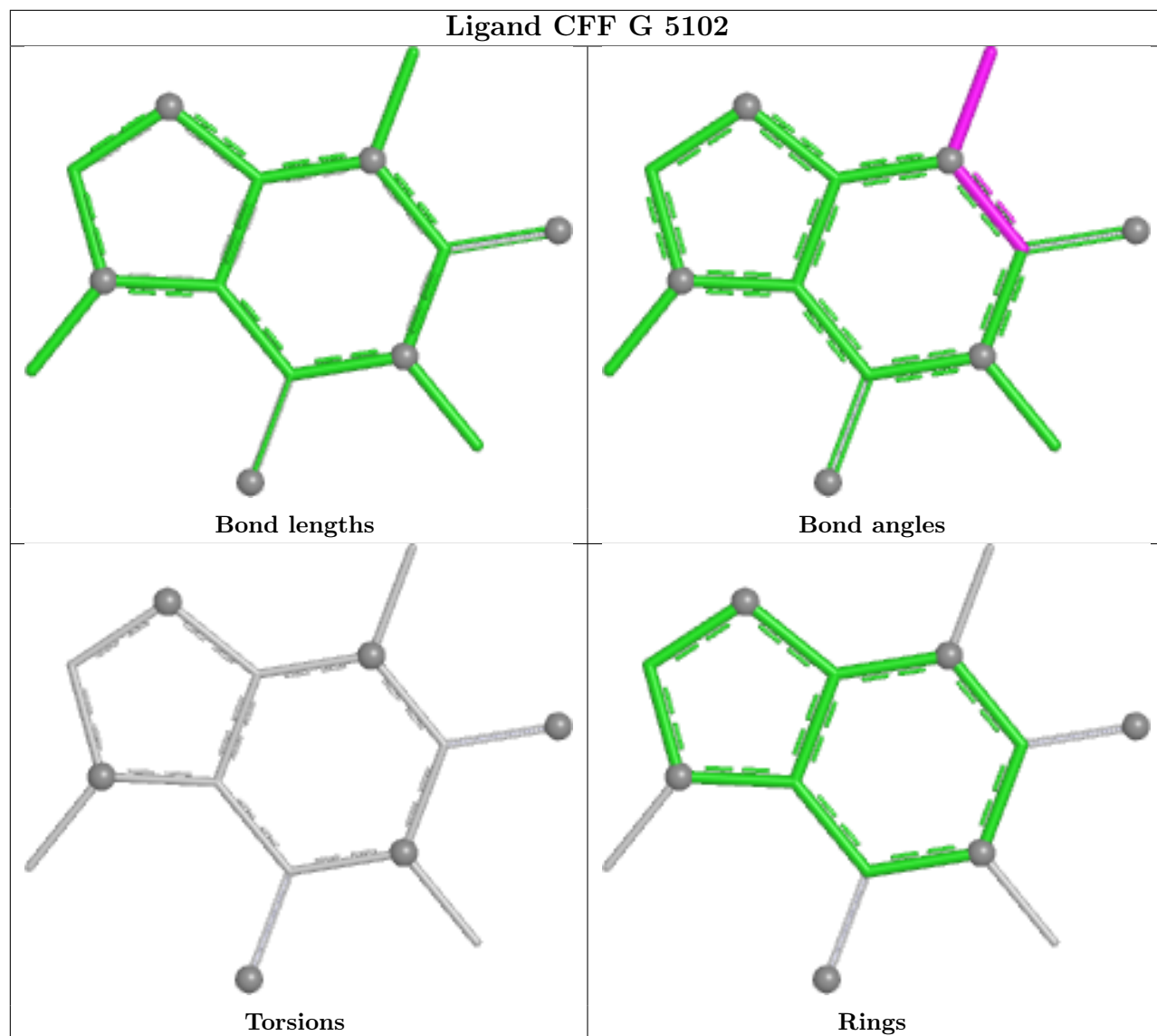


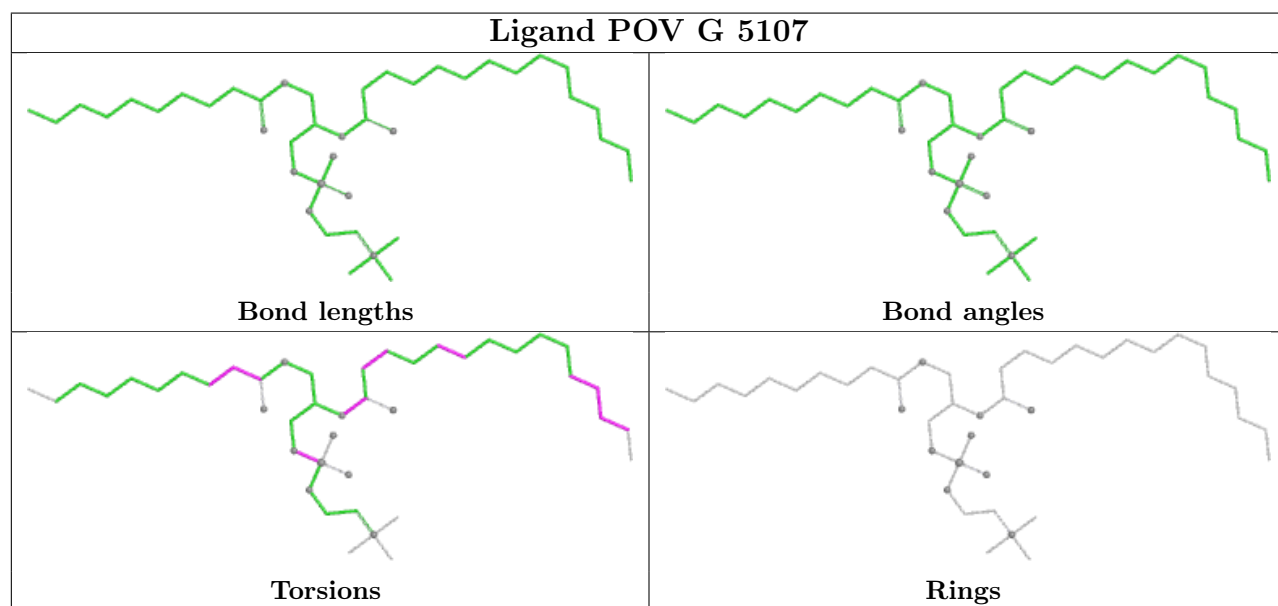
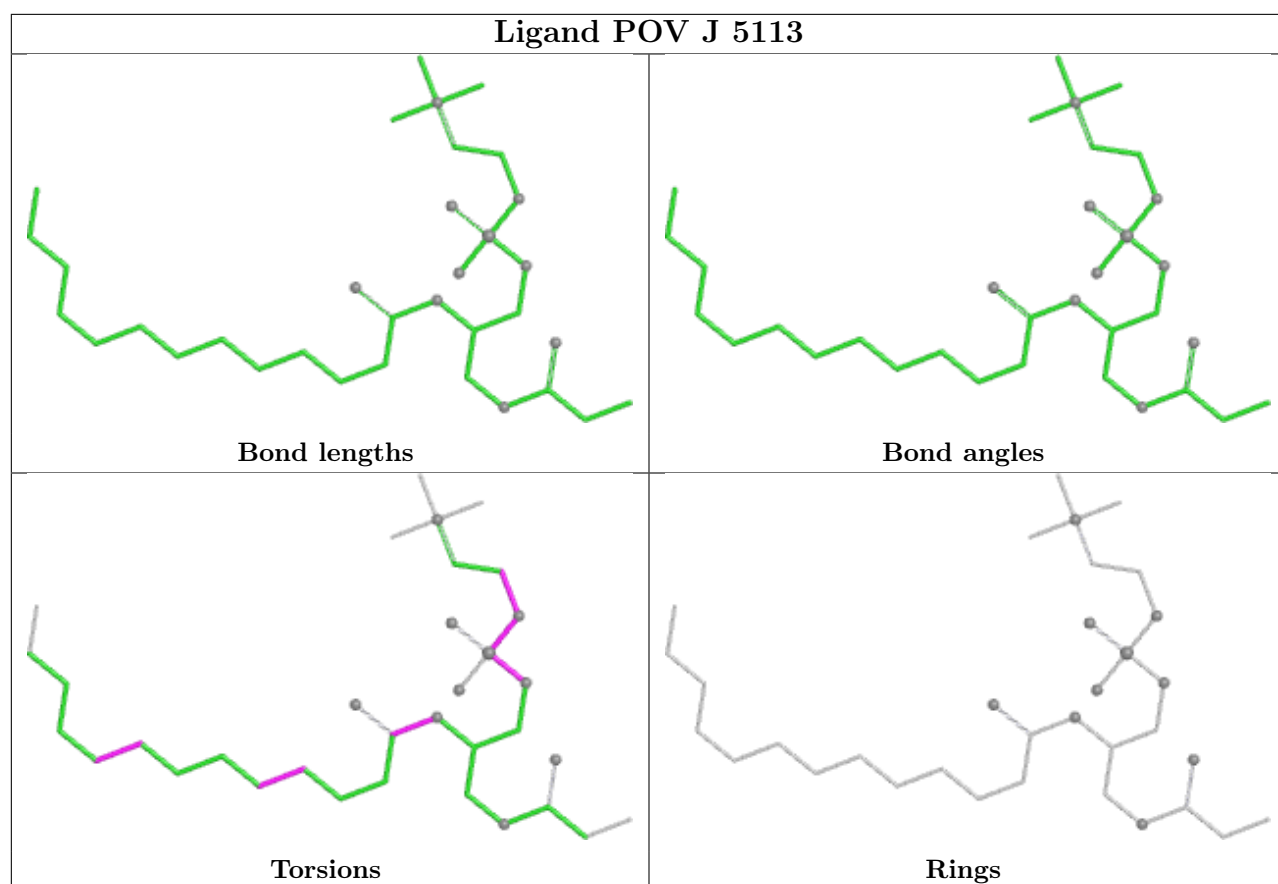


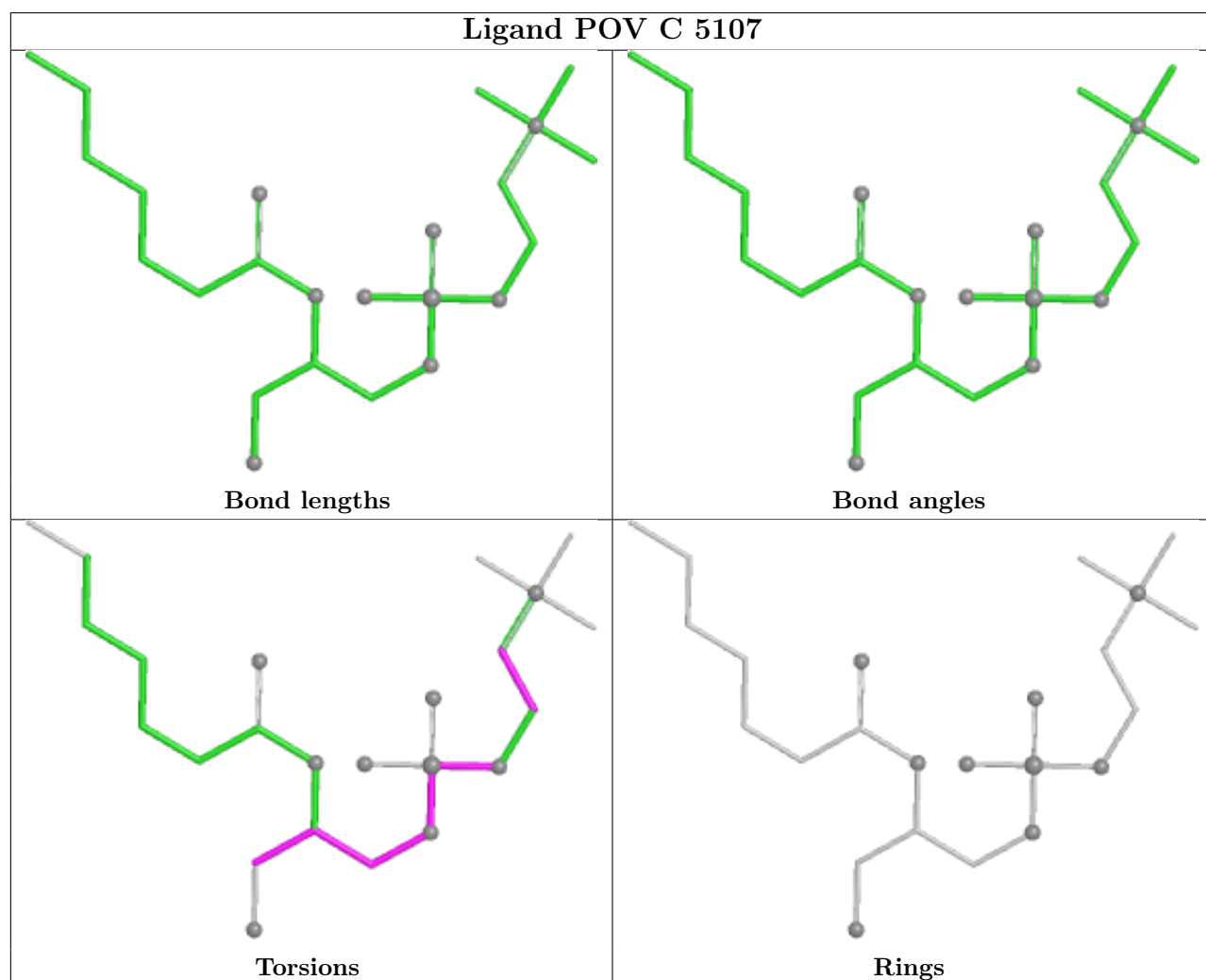
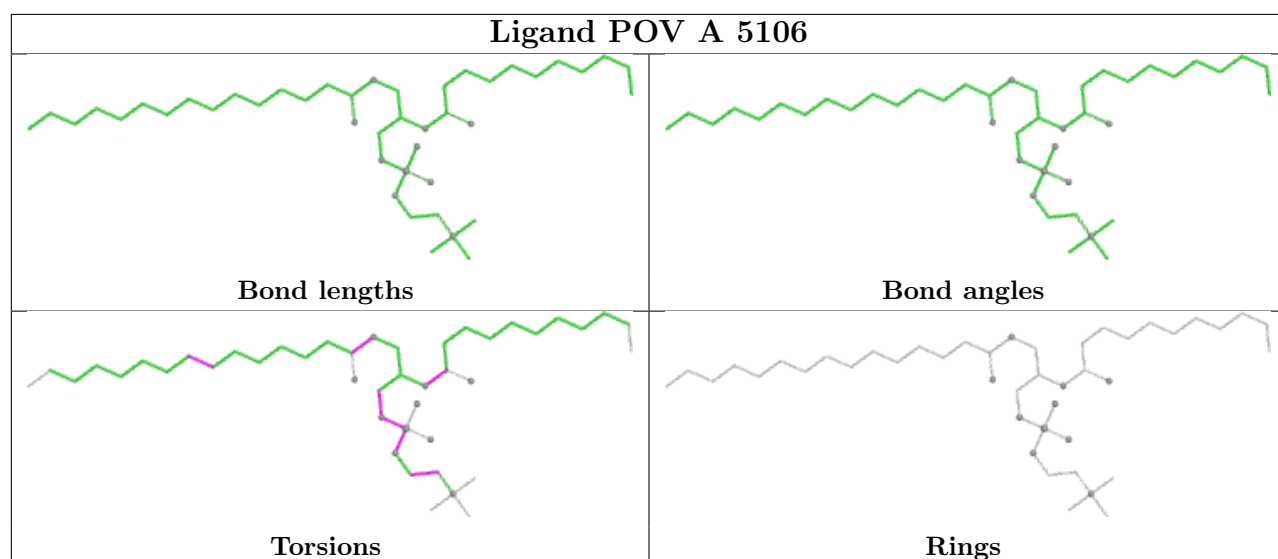


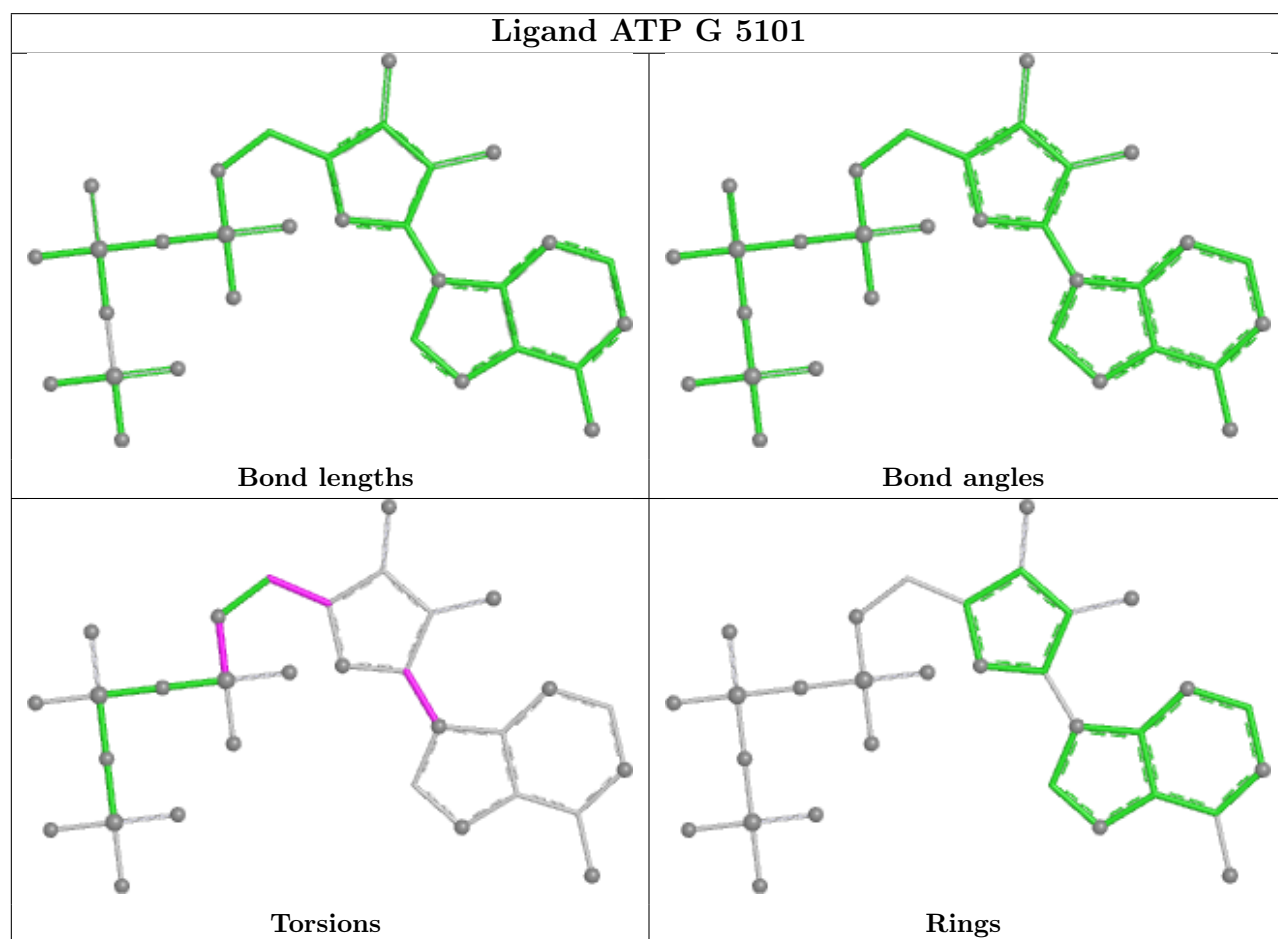
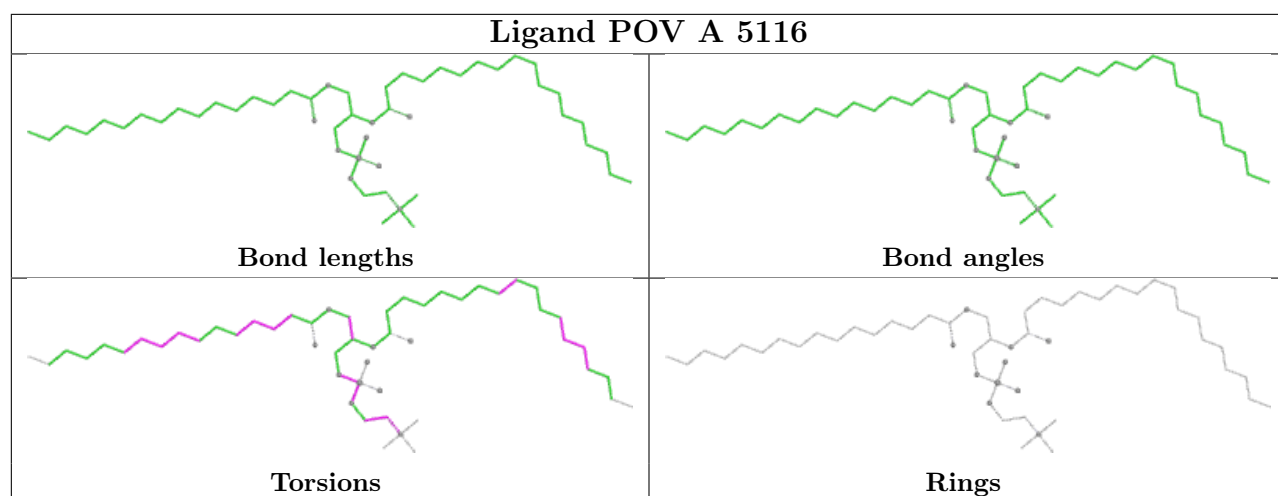


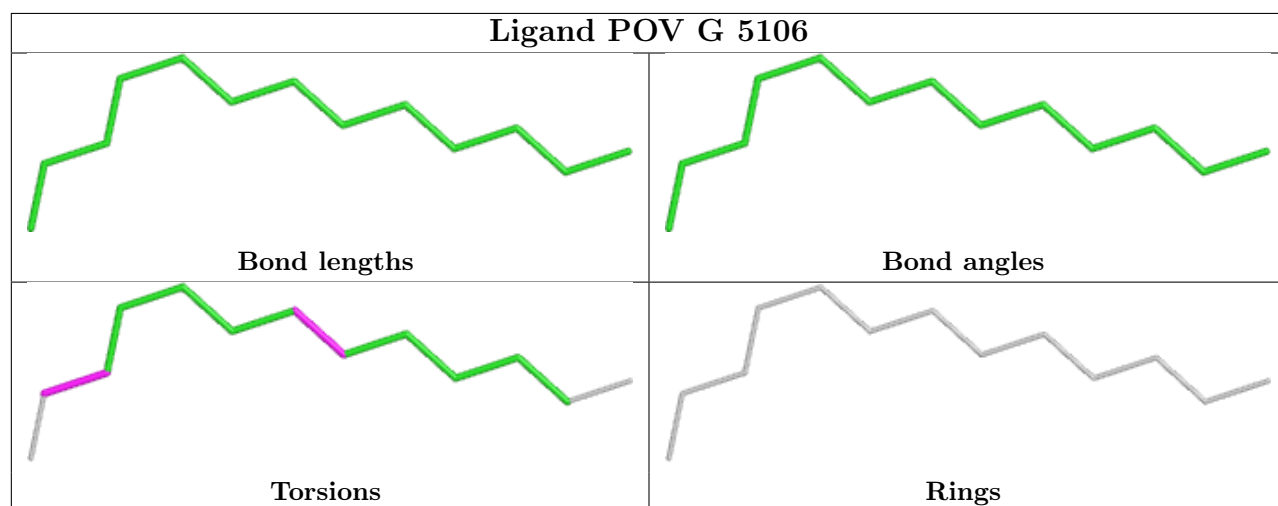
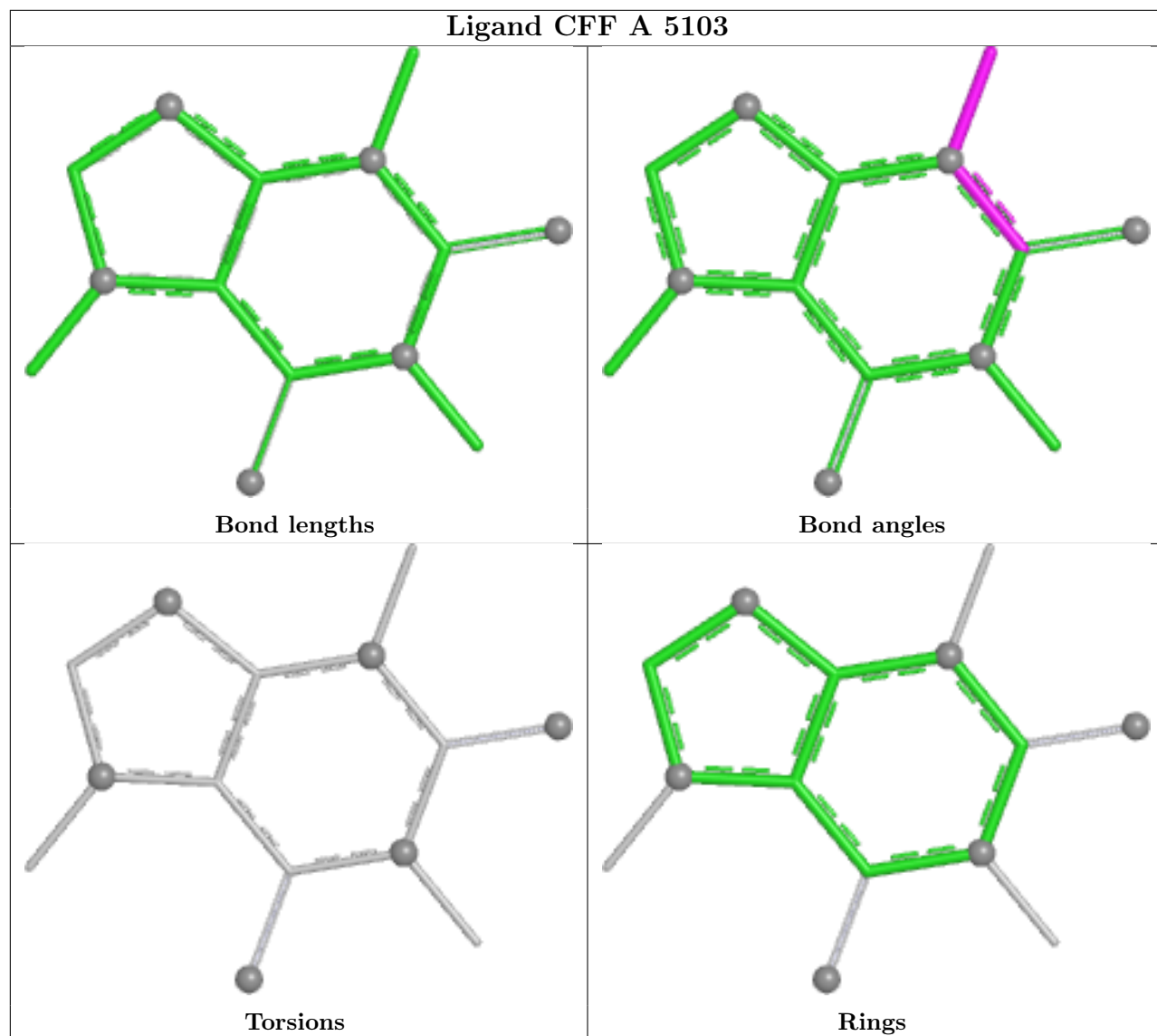


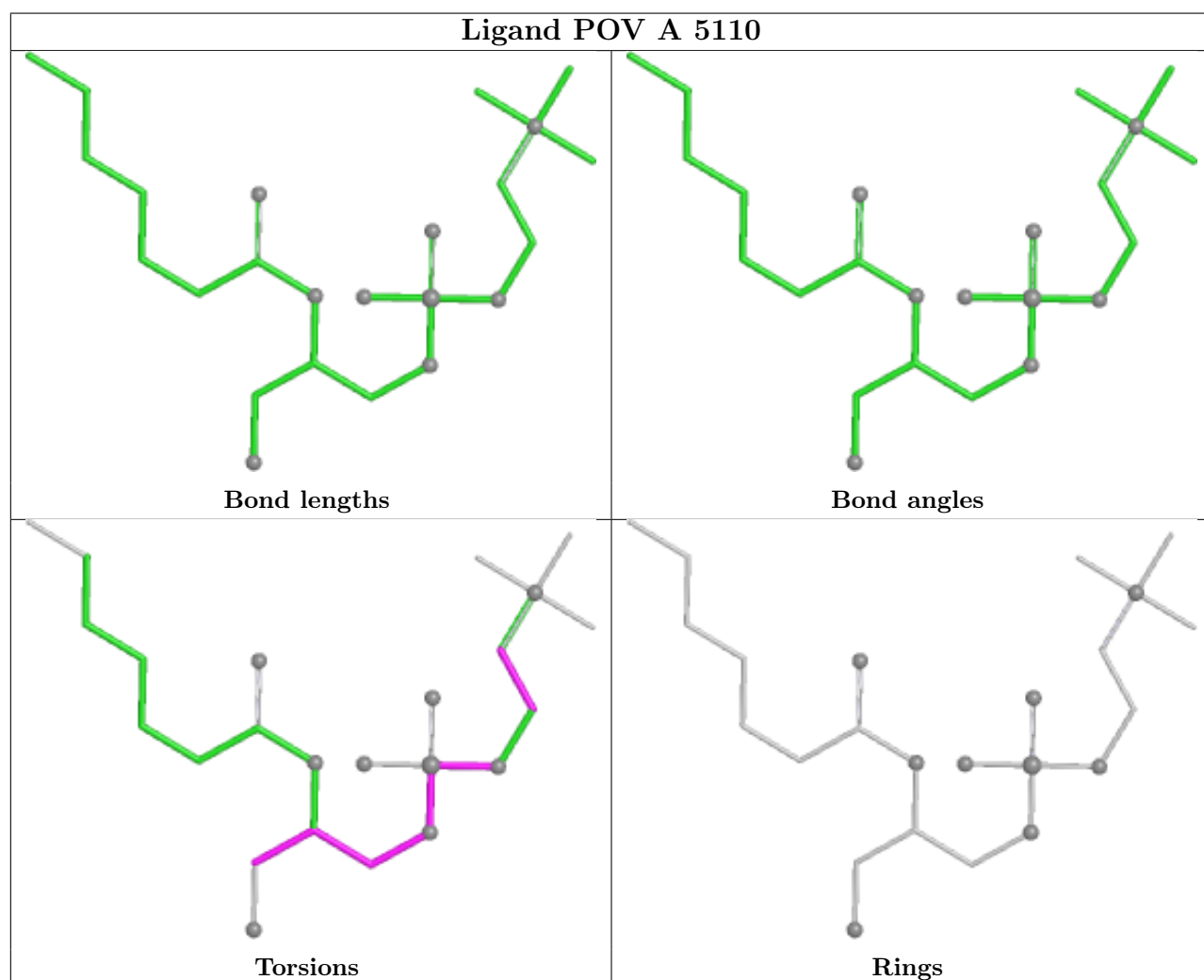
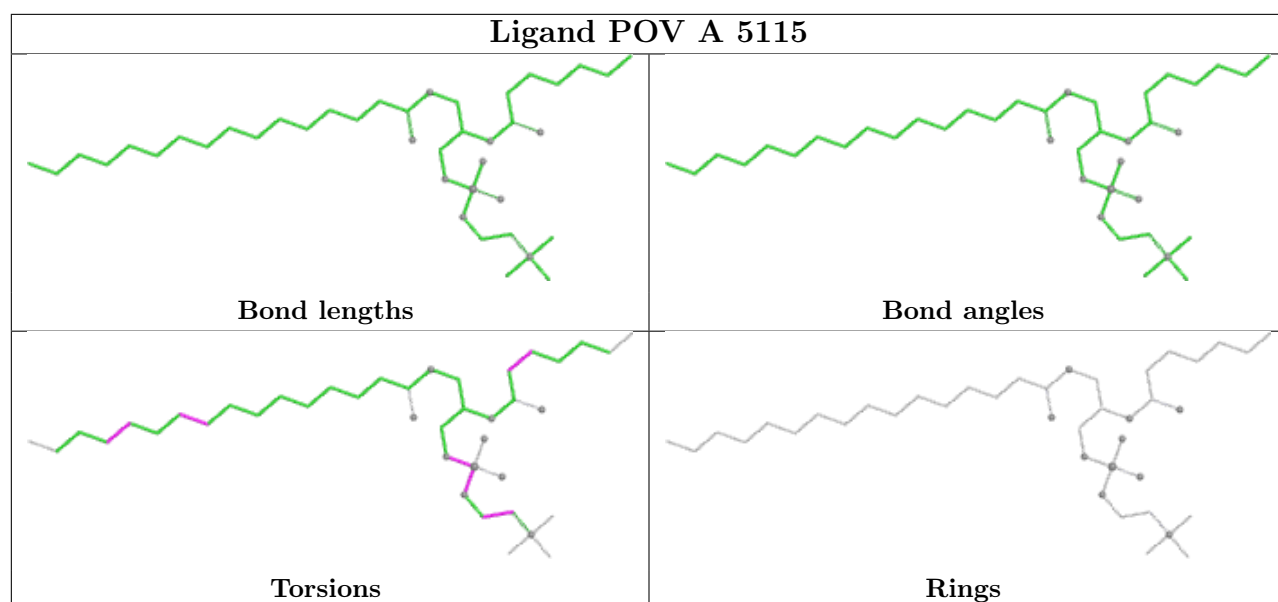












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

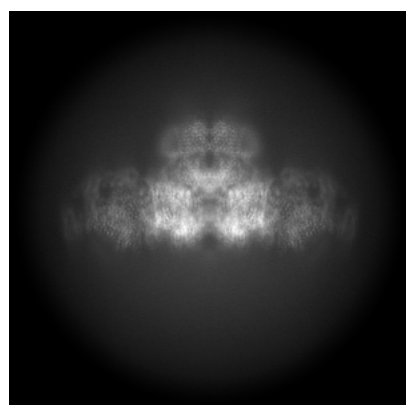
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52091. These allow visual inspection of the internal detail of the map and identification of artifacts.

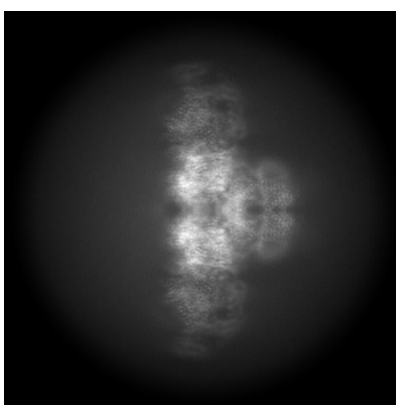
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

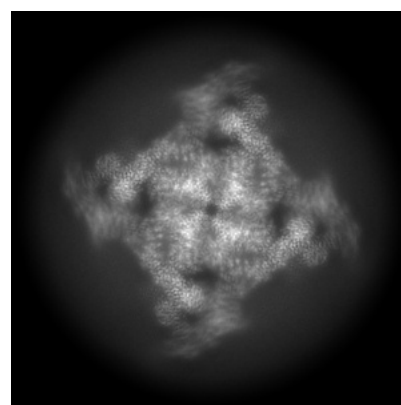
6.1.1 Primary map



X



Y

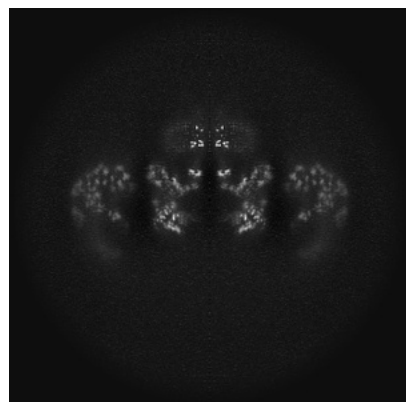


Z

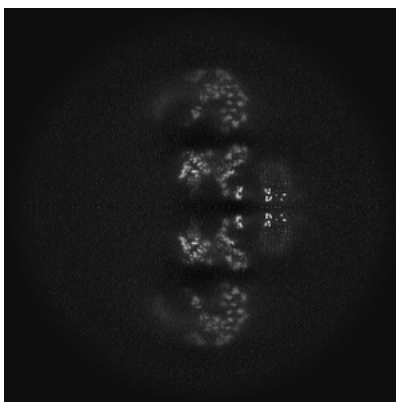
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

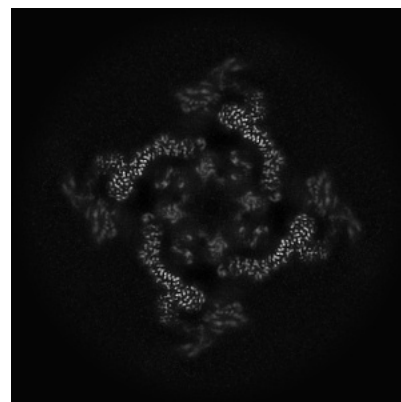
6.2.1 Primary map



X Index: 168



Y Index: 168

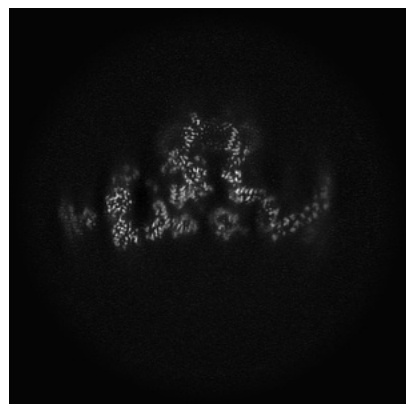


Z Index: 168

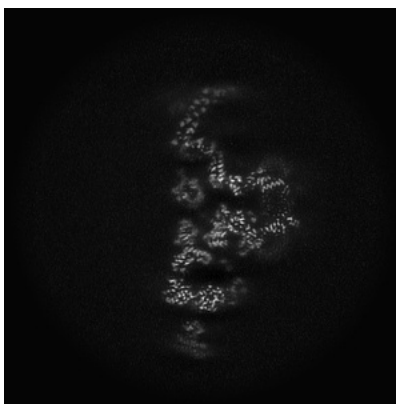
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

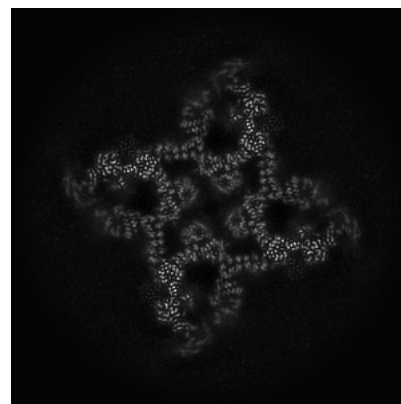
6.3.1 Primary map



X Index: 149



Y Index: 187

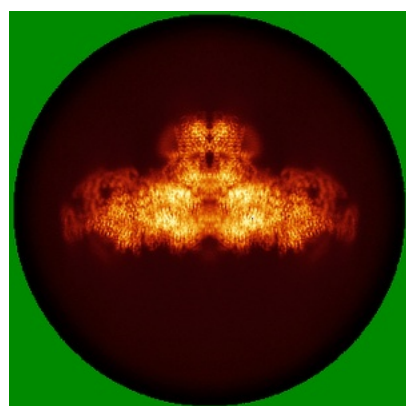


Z Index: 159

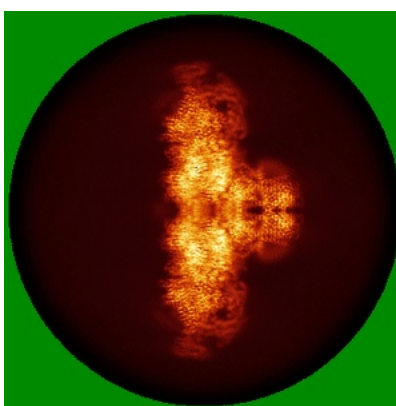
The images above show the largest variance slices of the map in three orthogonal directions.

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

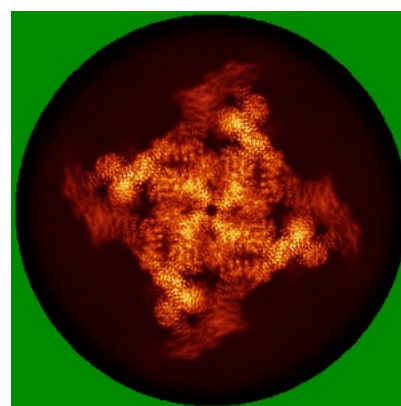
6.4.1 Primary map



X



Y

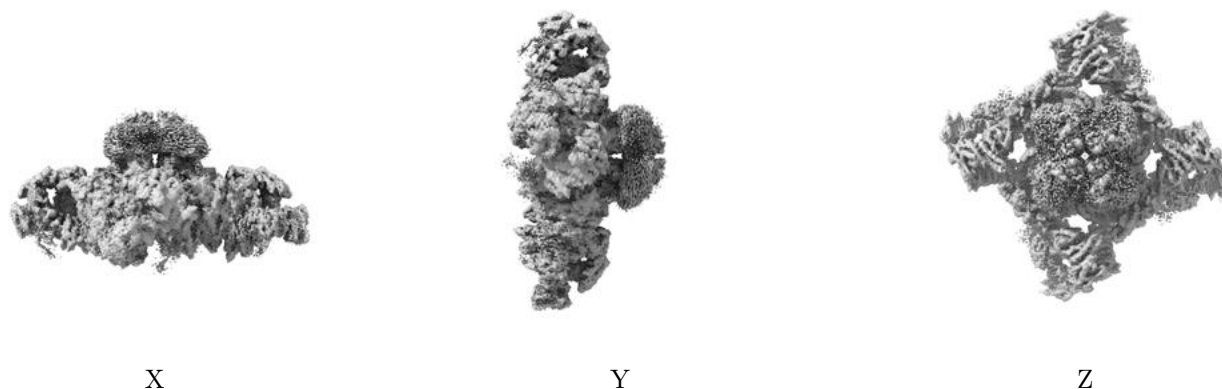


Z

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



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.

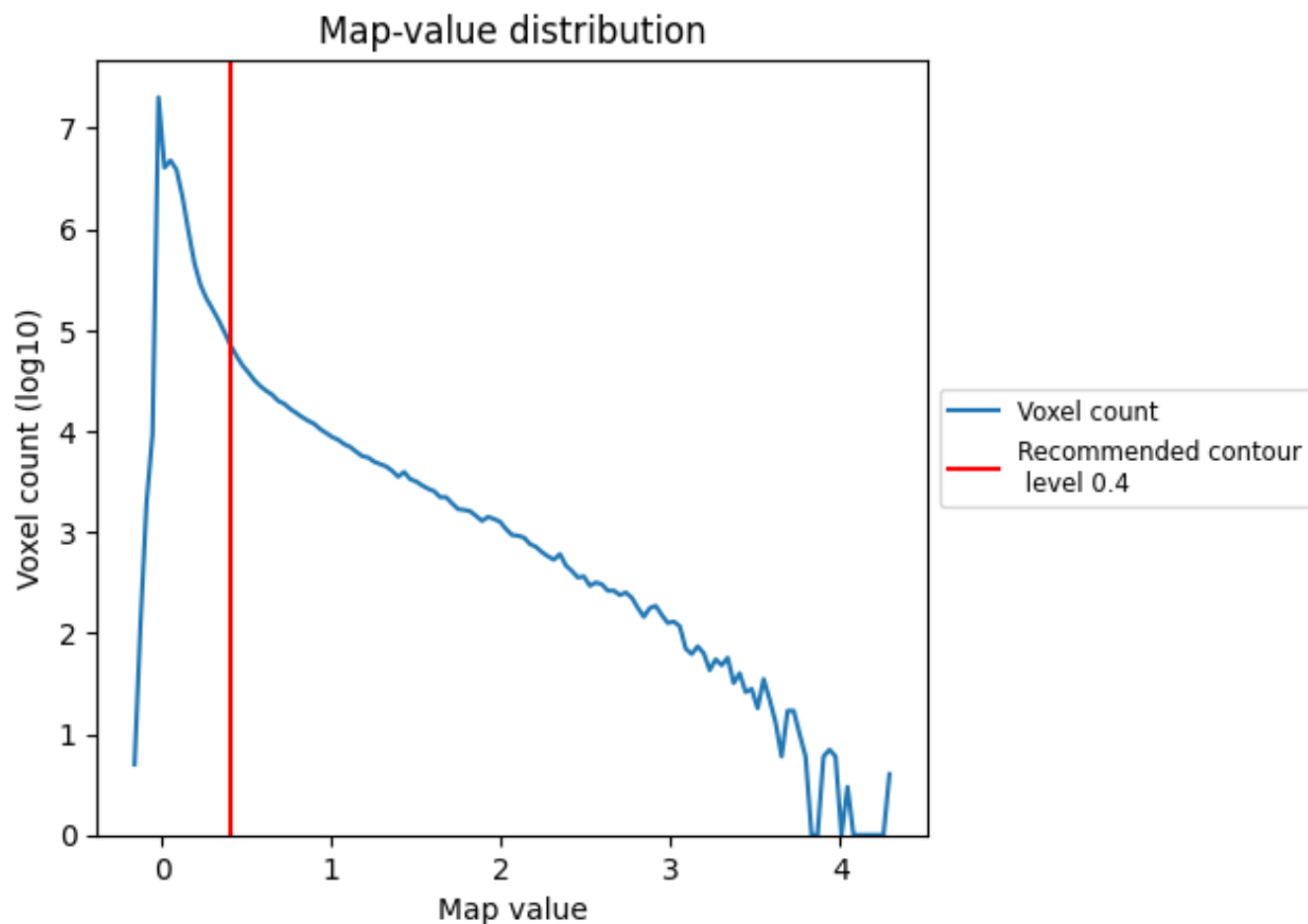
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

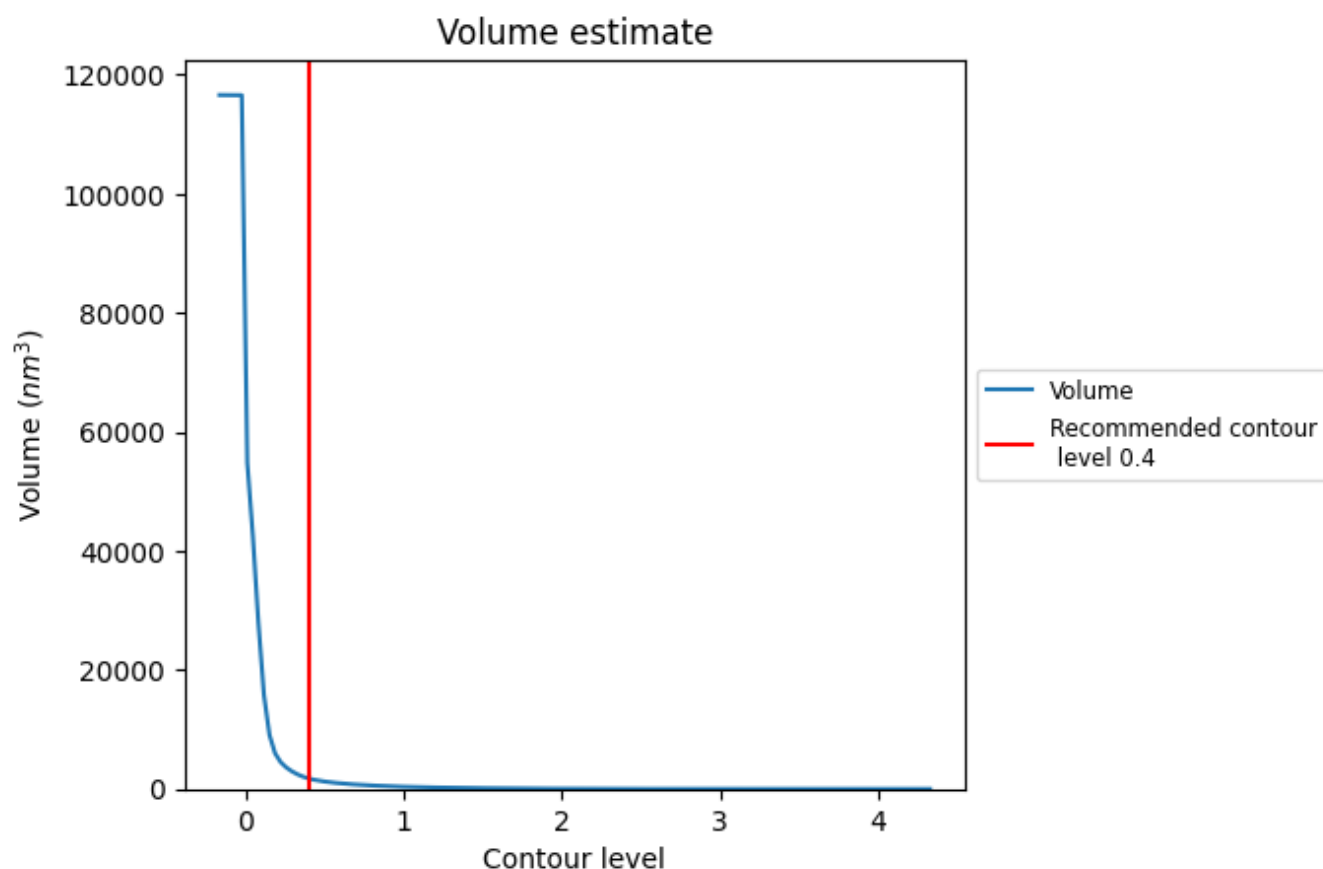
This section contains the results of statistical analysis of the map.

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.

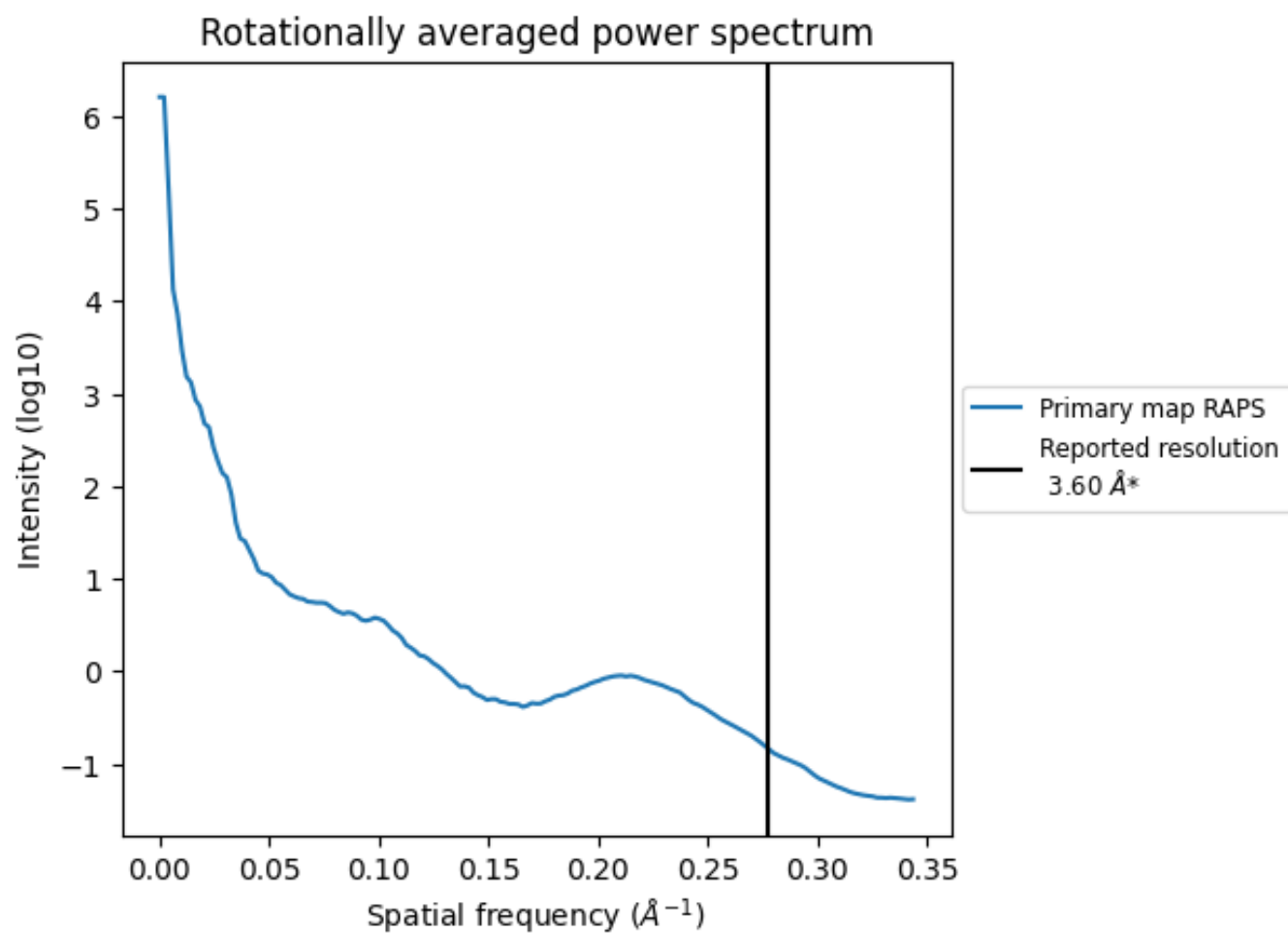
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1771 nm³; this corresponds to an approximate mass of 1600 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 0.278 Å⁻¹

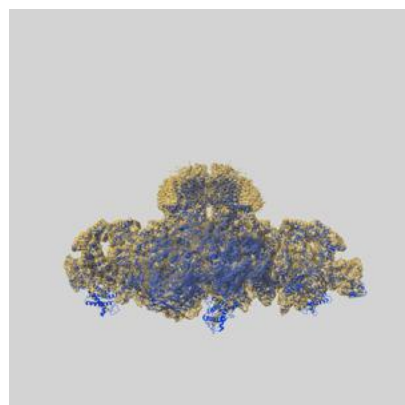
8 Fourier-Shell correlation

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

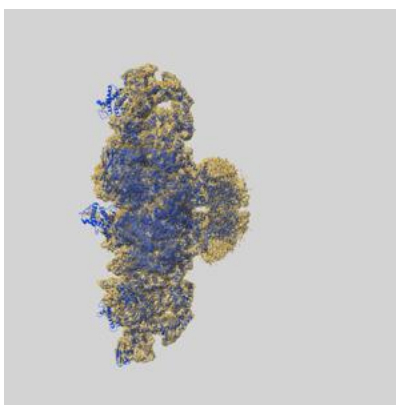
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52091 and PDB model 9HEQ. Per-residue inclusion information can be found in section [3](#) on page [10](#).

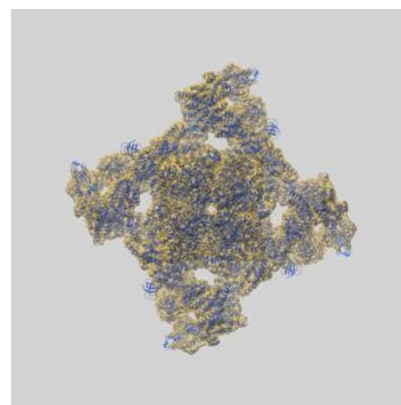
9.1 Map-model overlay [i](#)



X



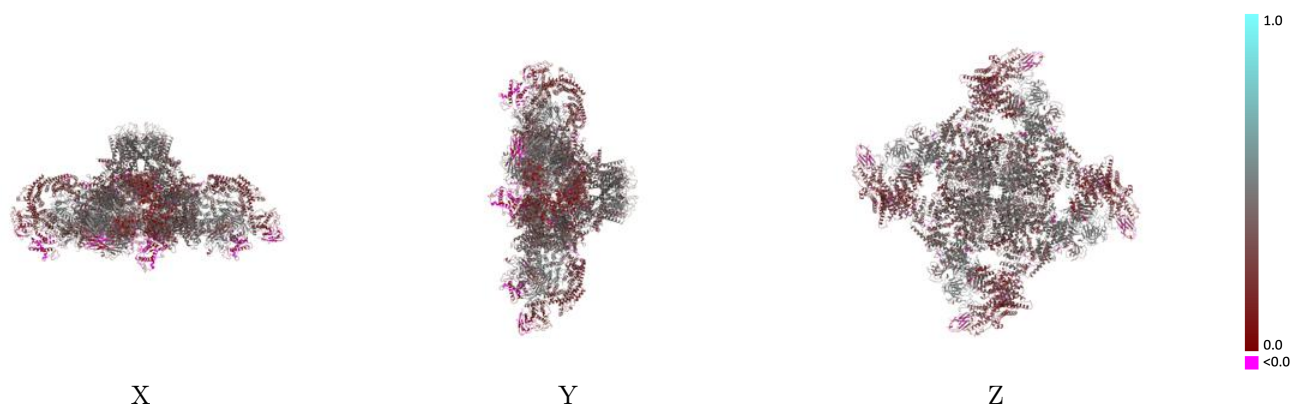
Y



Z

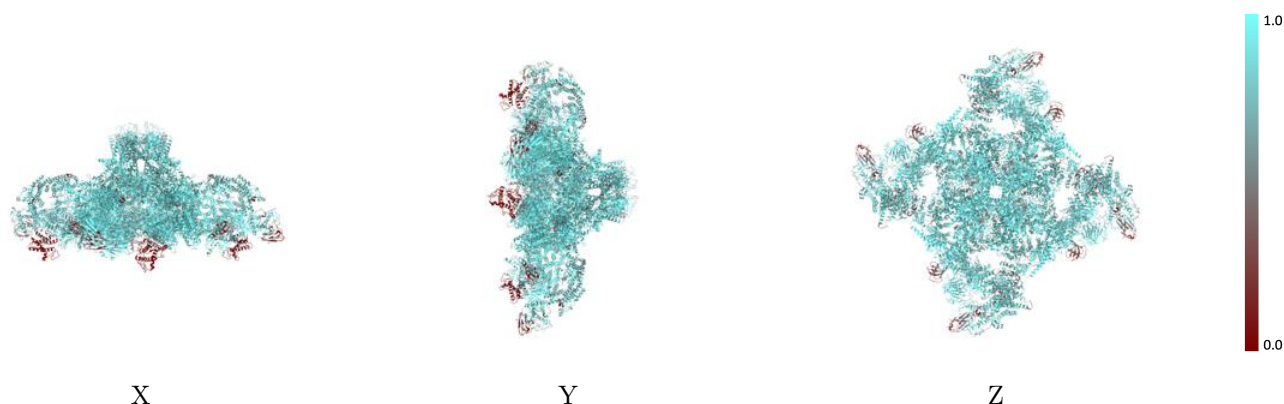
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



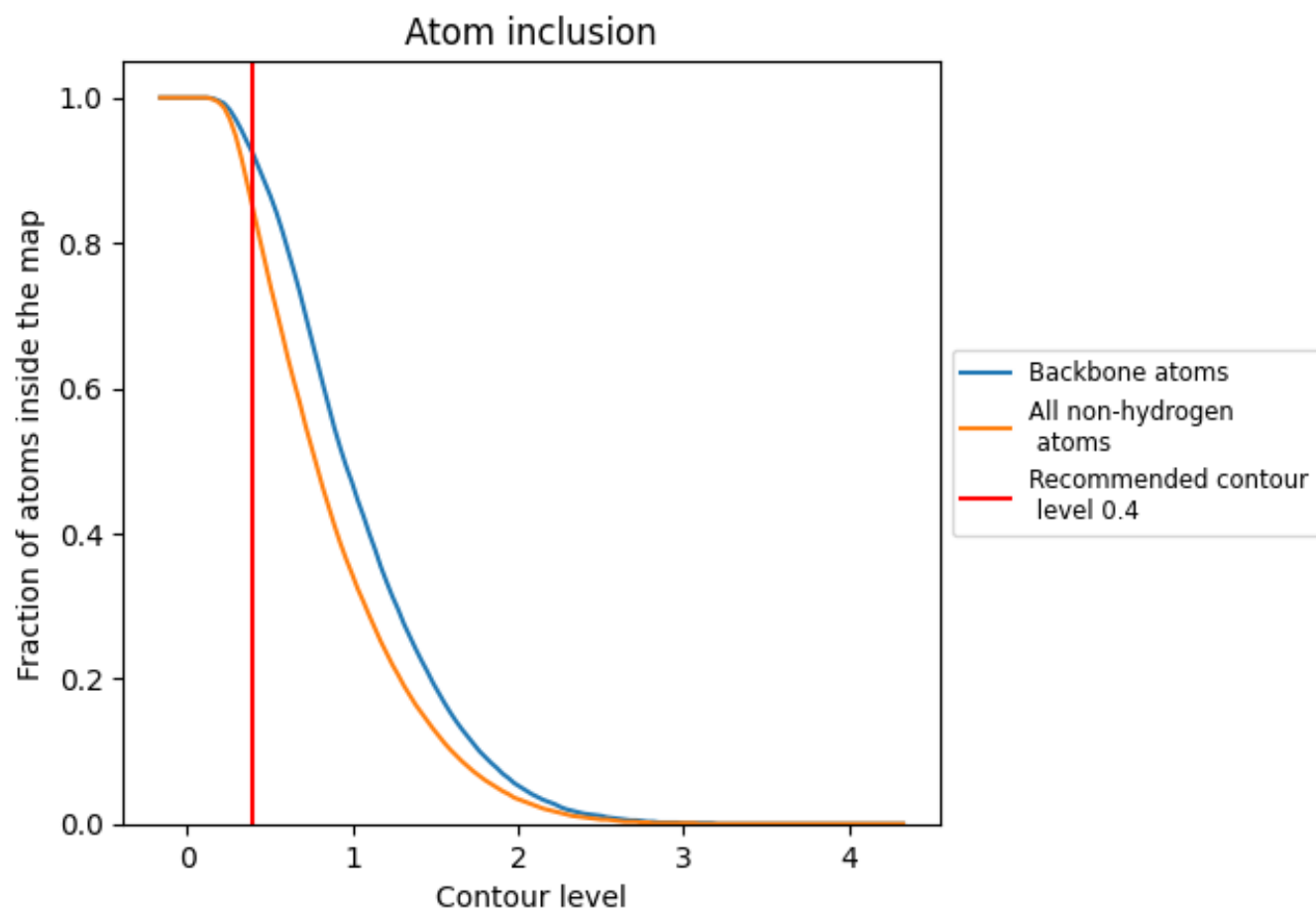
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 84% 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	<div></div> 0.8450	<div></div> 0.3410
A	<div></div> 0.8670	<div></div> 0.3470
B	<div></div> 0.4180	<div></div> 0.1050
C	<div></div> 0.8660	<div></div> 0.3460
D	<div></div> 0.4210	<div></div> 0.1080
E	<div></div> 0.3950	<div></div> 0.3530
F	<div></div> 0.4000	<div></div> 0.3520
G	<div></div> 0.8680	<div></div> 0.3470
H	<div></div> 0.4240	<div></div> 0.1080
I	<div></div> 0.4030	<div></div> 0.3580
J	<div></div> 0.8680	<div></div> 0.3470
K	<div></div> 0.4190	<div></div> 0.1100
L	<div></div> 0.3970	<div></div> 0.3560

