



Full wwPDB EM Validation Report ⓘ

Mar 15, 2026 – 08:31 AM UTC

PDB ID : 7TZC / pdb_00007tzc
EMDB ID : EMD-26205
Title : A drug and ATP binding site in type 1 ryanodine receptor
Authors : Melville, Z.; Dridi, H.; Yuan, Q.; Reiken, S.; Anetta, W.; Liu, Y.; Clarke, O.B.; Marks, A.R.
Deposited on : 2022-02-15
Resolution : 2.45 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:

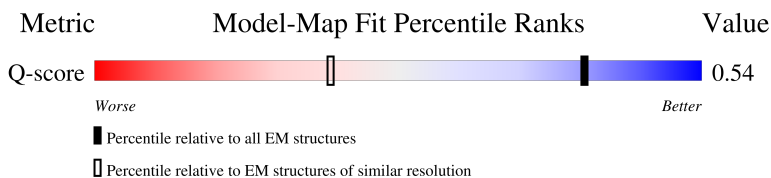
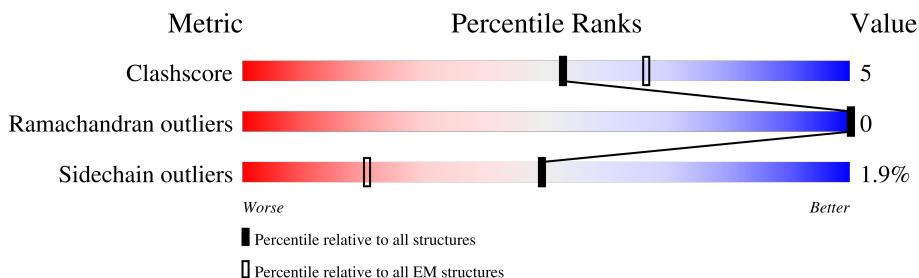
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.45 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.



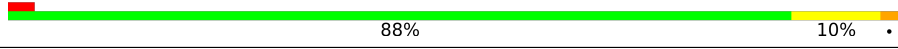
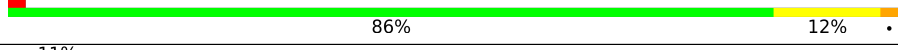
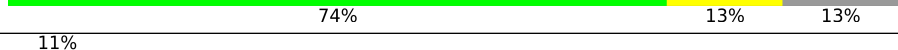
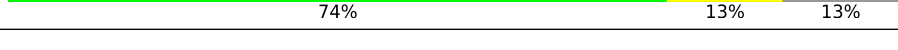
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5931 (1.96 - 2.95)

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	C	150	33% 76% 23% ..
1	D	150	30% 79% 20% ..
1	E	150	33% 78% 21% .
1	K	150	33% 79% 19% ..

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Mol	Chain	Length	Quality of chain
2	F	107	
2	H	107	
2	J	107	
2	O	107	
3	A	5037	
3	B	5037	
3	G	5037	
3	I	5037	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	CFF	I	5105	-	X	-	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 149472 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 Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	149	Total	C	N	O	S	0	0
			1174	719	190	255	10		
1	D	149	Total	C	N	O	S	0	0
			1174	719	190	255	10		
1	E	149	Total	C	N	O	S	0	0
			1174	719	190	255	10		
1	C	149	Total	C	N	O	S	0	0
			1174	719	190	255	10		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-1	HIS	-	expression tag	UNP P0DP23
D	-1	HIS	-	expression tag	UNP P0DP23
E	-1	HIS	-	expression tag	UNP P0DP23
C	-1	HIS	-	expression tag	UNP P0DP23

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	107	Total	C	N	O	S	0	0
			831	527	146	154	4		
2	H	107	Total	C	N	O	S	0	0
			831	527	146	154	4		
2	J	107	Total	C	N	O	S	0	0
			831	527	146	154	4		
2	O	107	Total	C	N	O	S	0	0
			831	527	146	154	4		

- Molecule 3 is a protein called Ryanodine receptor 1.

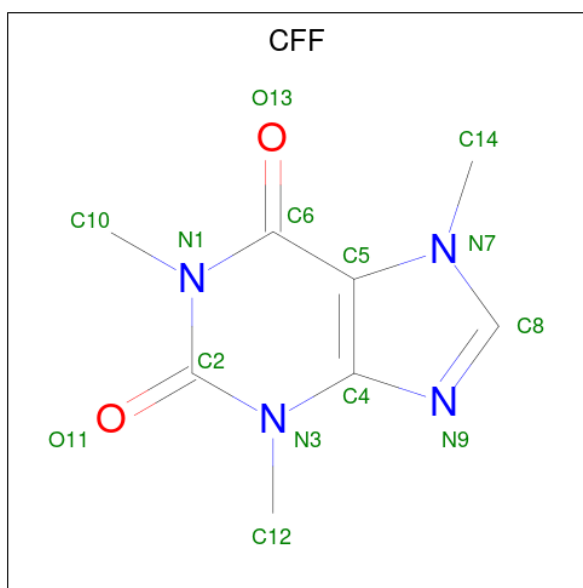
Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		
3	B	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		
3	G	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		
3	I	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
4	K	4	Total	Ca	0
			4	4	
4	D	4	Total	Ca	0
			4	4	
4	E	4	Total	Ca	0
			4	4	
4	C	4	Total	Ca	0
			4	4	
4	A	1	Total	Ca	0
			1	1	
4	B	1	Total	Ca	0
			1	1	
4	G	1	Total	Ca	0
			1	1	
4	I	1	Total	Ca	0
			1	1	

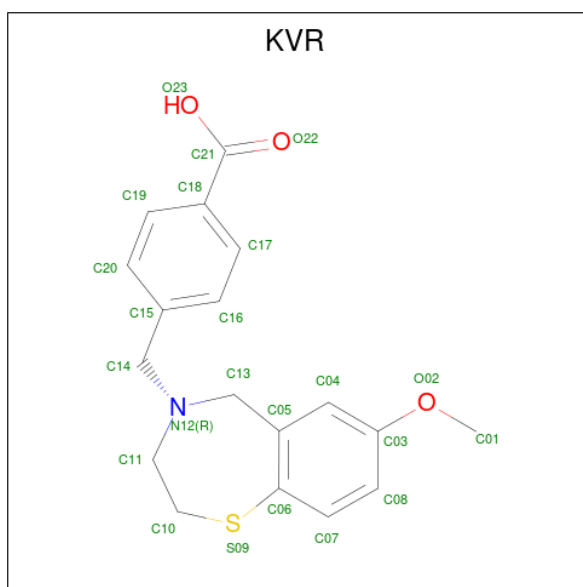
- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

- Molecule 7 is CAFFEINE (CCD ID: CFF) (formula: $C_8H_{10}N_4O_2$).



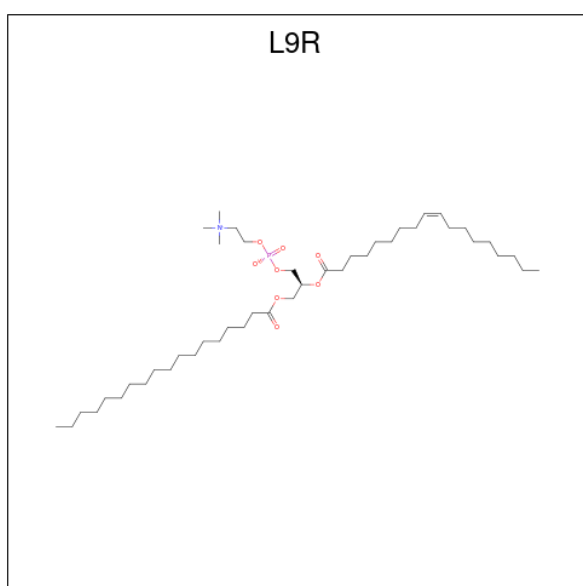
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			14	8	4	2	
7	B	1	Total	C	N	O	0
			14	8	4	2	
7	G	1	Total	C	N	O	0
			14	8	4	2	
7	I	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 8 is 4-[(7-methoxy-2,3-dihydro-1,4-benzothiazepin-4(5H)-yl)methyl]benzoic acid (CCD ID: KVR) (formula: $C_{18}H_{19}NO_3S$).



Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	S	0
			23	18	1	3	1	
8	B	1	Total	C	N	O	S	0
			23	18	1	3	1	
8	G	1	Total	C	N	O	S	0
			23	18	1	3	1	
8	I	1	Total	C	N	O	S	0
			23	18	1	3	1	

- Molecule 9 is (2S)-3-(octadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (CCD ID: L9R) (formula: C₄₄H₈₆NO₈P).

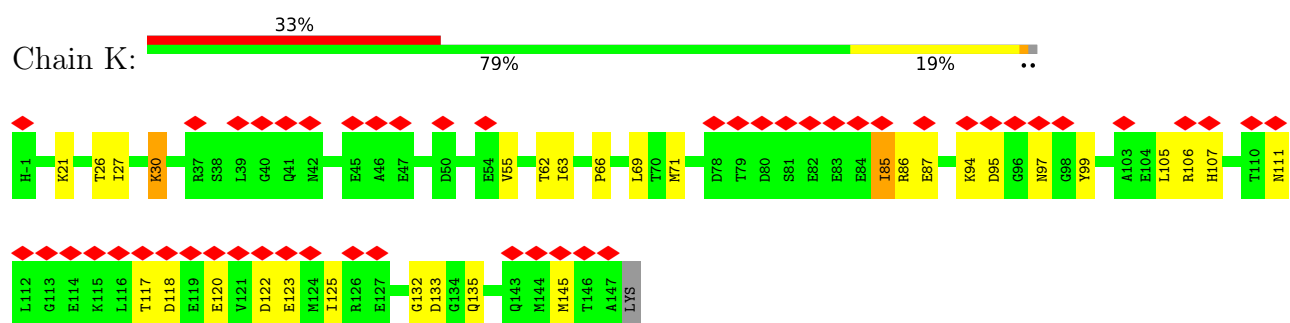


Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	G	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	G	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	I	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	I	1	Total	C	N	O	P	0
			54	44	1	8	1	

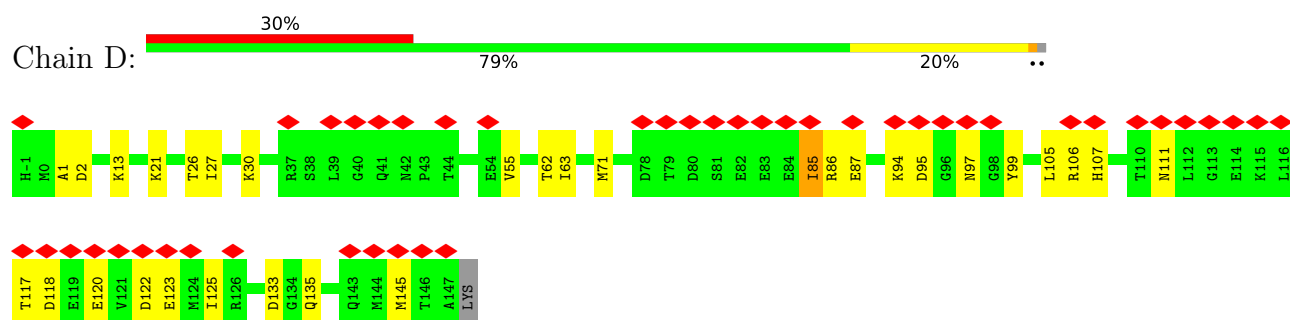
3 Residue-property plots

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

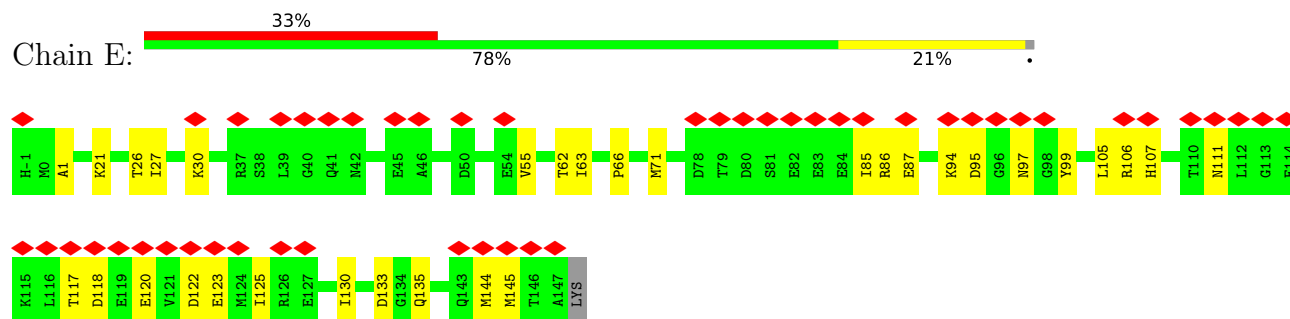
• Molecule 1: Calmodulin-1



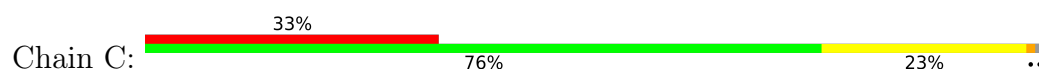
• Molecule 1: Calmodulin-1

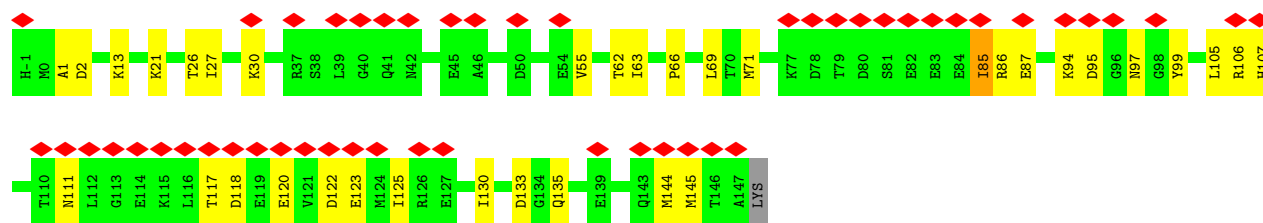


• Molecule 1: Calmodulin-1

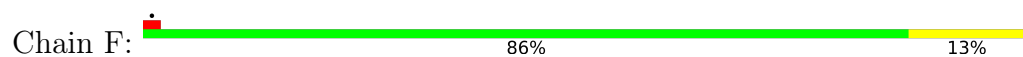


• Molecule 1: Calmodulin-1

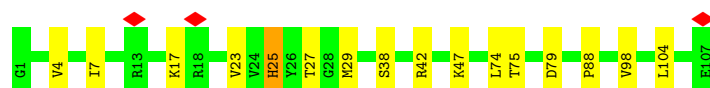
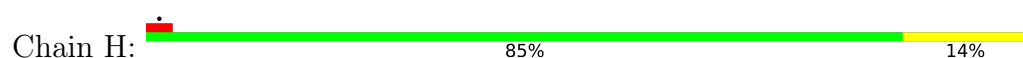




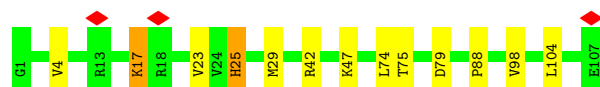
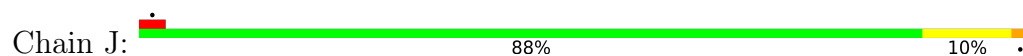
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



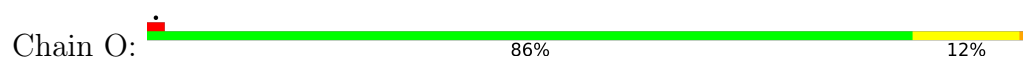
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



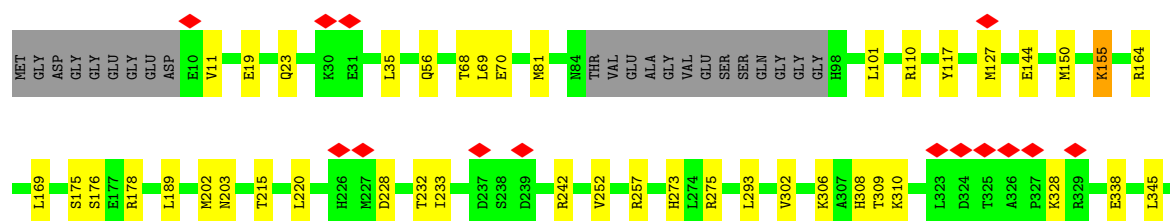
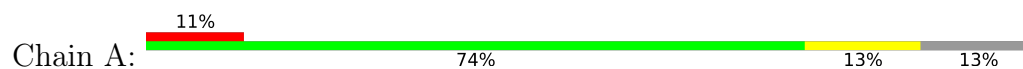
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



- Molecule 3: Ryanodine receptor 1

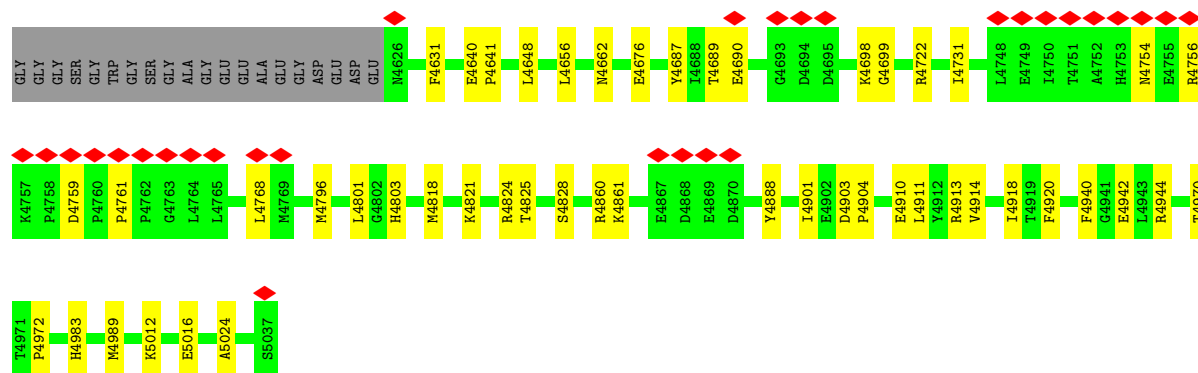




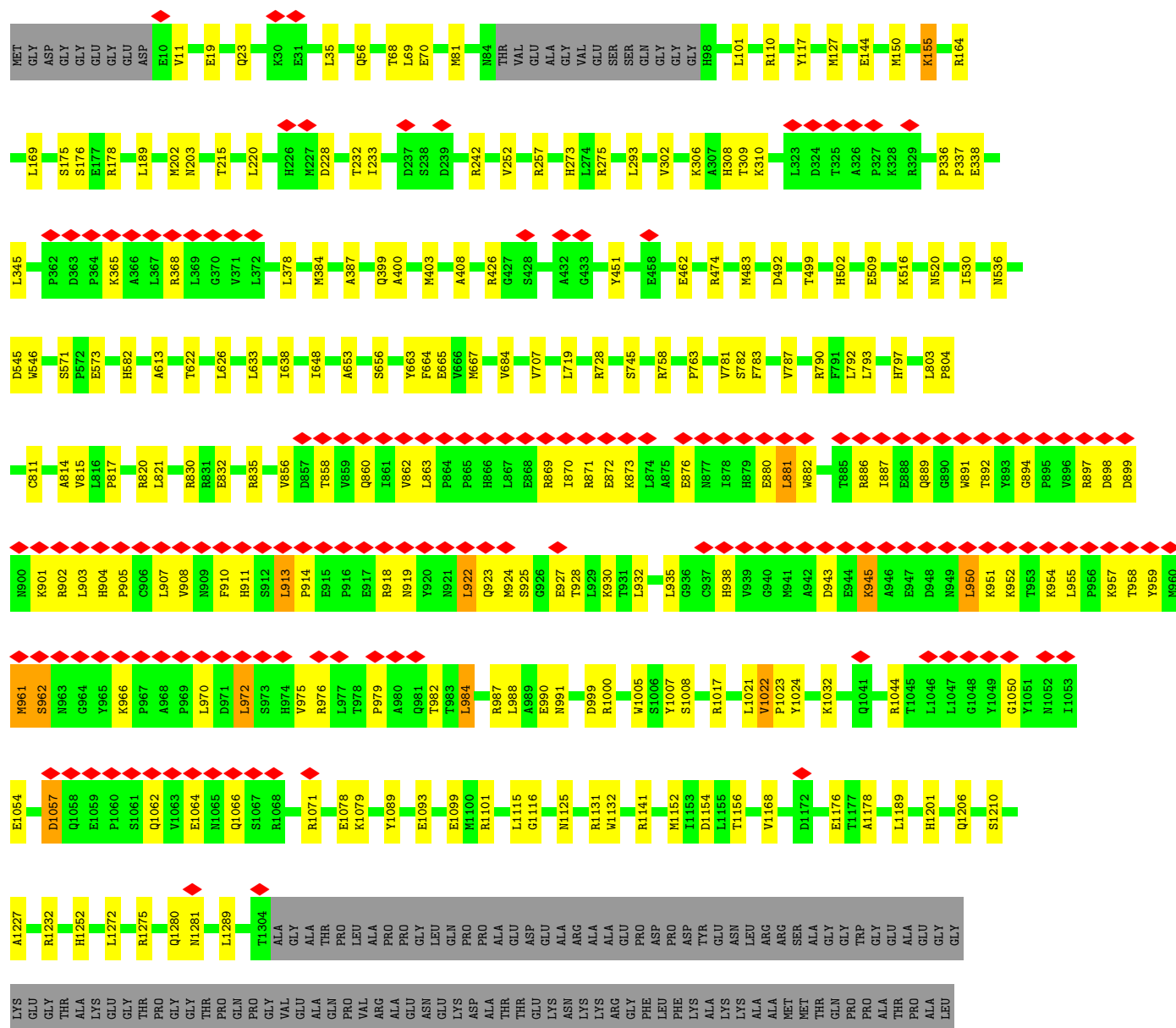
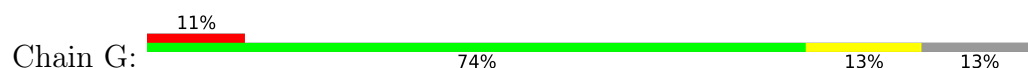
S4074	L3805	T3639	R3414	L3277	THR GLN VAL	F2929	L2867	V2807	12747	R2355
K4090	Q3813	A3680	L3434	W3284	K3123	L2930	S2668	P2808	P2748	E2382
F4093	L3842	E3682	M3437	G3288	G3124	Q2931	R2869	L2809	E2749	R2385
H4097	Q3850	Q3683	F3442	P3293	V3125	W2932	E2870	K2810	K2750	P2390
Q3850	N3851	E3684	W3445	P3294	T3132	Y2935	A2873	L2813	L2751	K2391
K3852	K3852	F3552	S3446	P3295	T3133	A2936	M2874	K2814	D2762	R2392
G3857	G3857	N3556	K3452	P3297	A3135	W2937	A2875	L2815	L2755	V2397
M3858	V3859	L3559	E3455	A3298	L3136	T2938	E2876	M2816	L2756	ARG
V3859	E3564	Q3456	Q3456	G3299	L3137	R2939	Q2877	L2817	K2757	ARG
E3691	V3459	V3460	V3460	A3300	I3147	LEU	L2878	A2818	P2758	ASP
E3692	L3579	V3460	V3460	P3303	F3152	LYS	N2881	W2819	E2759	ARG
K3693	R3582	T3464	T3464	C3304	I3157	ASP	Y2882	E2820	R2650	ARG
K3694	E3583	T3464	T3464	T3305	L3158	MET	H2883	W2821	C2651	GLU
V3695	E3584	A3472	D3472	L3316	D3159	GLU	T2885	T2822	H2661	HIS
D3696	D3585	S3474	S3474	V3324	D3160	L2946	V2886	L2823	F2664	PHE
L3710	D3587	K3475	K3475	V3329	V3161	D2947	G2887	E2824	G2665	GLY
D3717	D3587	K3476	K3476	T3329	L3169	S2970	R2888	K2825	V2666	P2410
K3731	E3590	K3477	K3477	A3332	C3170	E2973	K2889	E2826	P2411	E2412
H3734	V3602	H3478	H3478	M3335	K3179	L2974	K2890	R2827	E2413	N2414
L3735	L3603	L3479	L3479	L3335	L3186	A2975	Q2892	E2830	R2415	R2415
E3736	Y3604	ALA	ALA	F3341	L3186	E2978	E2893	GLU	E2449	E2449
GLU	Q3608	GLY	GLY	A3342	L3194	S2982	L2894	GLU	R2452	R2452
GLY	T3609	ASP	ASP	Q3343	P3208	S2983	E2895	THR	S2720	S2720
GLY	E3610	ALA	ALA	P3344	R3226	G2984	A2896	GLU	S2721	S2721
ASN	GLY	GLN	GLN	T3345	R3227	G2985	K2897	LYS	K2722	K2722
GLY	Y3613	GLY	GLY	V3346	R3228	V2986	G2898	LYS	W2775	W2775
ALA	K3614	GLY	GLY	T3359	R3229	K2987	G2899	LYS	A2723	A2723
ALA	S3615	ASP	ASP	P3360	R3230	K2988	G2900	THR	S2776	S2776
GLU	K3616	GLN	GLN	T3361	L3230	K2988	G2901	ARG	Y2777	Y2777
GLU	K3617	GLU	GLU	A3383	L3230	L3003	T2902	LYS	E2778	E2778
GLU	A3618	ARG	ARG	K3384	P3233	P3004	H2902	LYS	E2779	E2779
THR	V3619	THR	THR	A3385	N3234	F3017	P2903	SER	N2780	N2780
LYS	V3620	LYS	LYS	E3386	S3235	L2904	L2905	GLN	V2781	V2781
LYS	H3621	LYS	LYS	A3387	V3236	T3020	V2906	ALA	D2782	D2782
R3498	K3622	R3498	R3498	E3388	E3236	K3023	P2907	THR	E2783	E2783
R3499	L3623	G3500	G3500	E3389	L3249	K3036	Y2908	TVR	E2784	E2784
D3501	L3624	D3501	D3501	G3390	Y3263	R3036	P2908	ASP	L2785	L2785
S3504	S3625	S3504	S3504	L3392	Y3263	R3036	Y2908	PRD	K2786	K2786
K3626	K3627	K3626	K3626	L3393	Y3263	R3036	Y2908	ARG	T2787	T2787
Q3627	R3628	Q3627	Q3627	L3394	Y3263	R3036	Y2908	GLY	P2737	P2737
R3628	R3629	R3628	R3628	R3395	Y3263	R3036	Y2908	GLY	R2738	R2738
R3630	R3630	R3630	R3630	V3400	Y3263	R3036	Y2908	GLY	P2739	P2739
A3631	A3631	A3631	A3631	R3403	Y3263	R3036	Y2908	GLY	V2740	V2740
V3633	V3633	V3633	V3633	L3412	Y3263	R3036	Y2908	GLY	R2741	R2741
R3637	R3637	R3637	R3637	L3413	Y3263	R3036	Y2908	GLY	T2742	T2742
H3638	H3638	H3638	H3638	L3413	Y3263	R3036	Y2908	GLY	N2743	N2743
									N2744	N2744
									V2745	V2745
									L2746	L2746





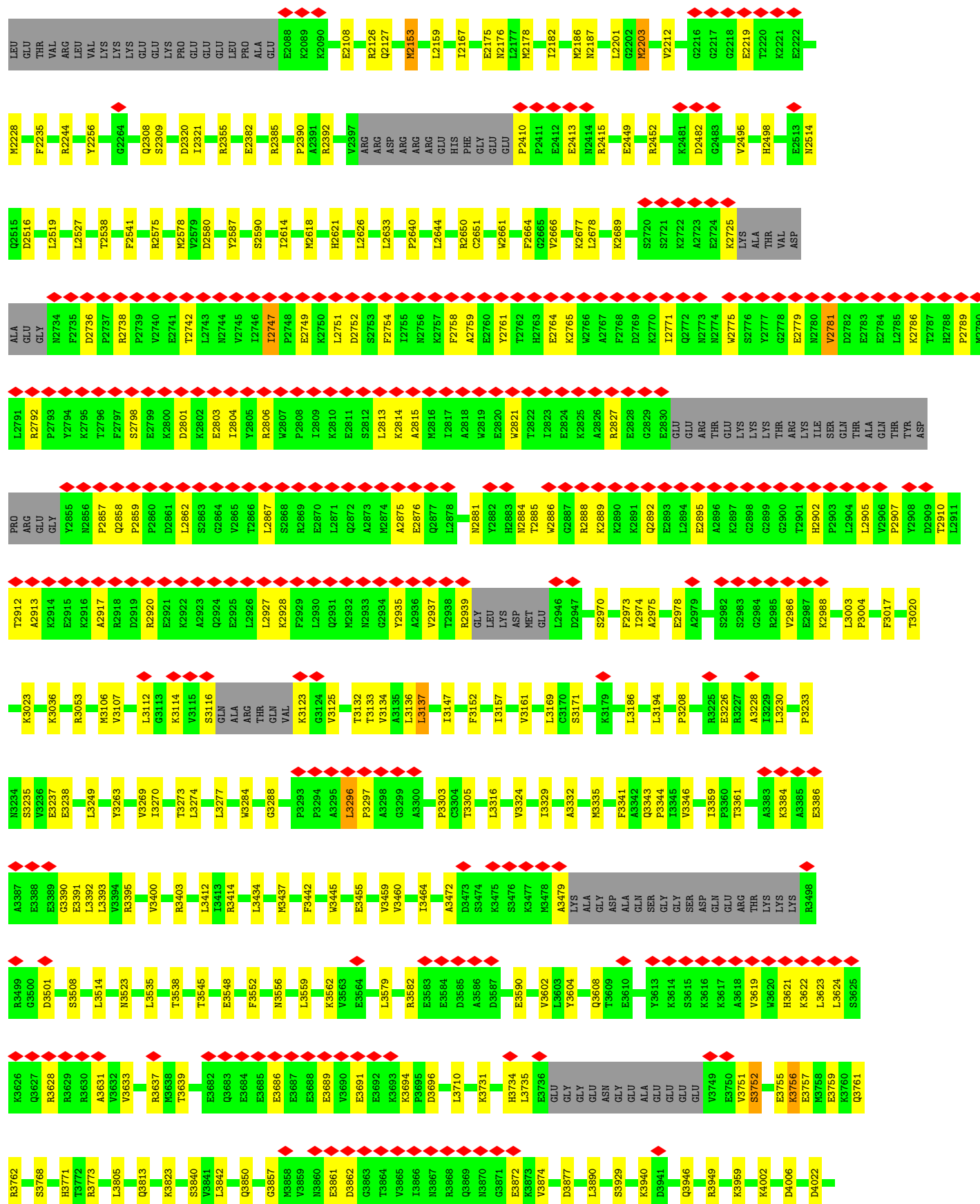


• Molecule 3: Ryanodine receptor 1



E3238	V3107	D3919	Q2858	S2798	Q2738	Y2256	VAL	F1984	T1872	E1622	PRO
L3249	L3112	R2920	P2859	E2799	P2739	G2264	ARG	T1985	T1873	M1636	ARG
Y3263	G3113	E2921	F2860	K2800	V2740	D2282	VAL	M1986	E1874	L1639	LEU
V3269	K3114	K2922	D2861	D2801	E2741	F2541	LYS	S1987	GLU	L1653	HIS
I3270	V3115	A2923	L2862	K2802	T2742	R2576	LYS	A1988	GLU	S1694	ASP
T3273	S3116	Q2924	S2863	E2803	L2743	Q2308	GLU	A1989	GLU	Q1660	VAL
L3274	G1N	E2925	G2864	T2804	N2744	S2309	LYS	A1990	GLU	L1676	VAL
L3277	ALA	L2926	V2865	R2805	V2745	D2320	LYS	T1991	GLU	R1680	PRO
W3284	ARG	K2927	T2866	R2806	I2746	T2321	PRO	R1992	GLU	L1715	ALA
G3288	THR	L2928	L2867	V2807	I2747	V2341	GLU	R1993	GLU	I1716	
	VAL	F2929	S2868	P2808	P2748	R2355	LEU	T1994	GLU	E1721	
	K3123	L2930	R2869	T2809	E2749	E2382	PRO	R1996	GLU	E1733	
	G3124	Q2931	E2870	K2810	K2750	R2390	ALA	S2000	GLU	Q1693	
	V3125	M2932	L2871	E2811	L2751	R2391	GLU	P2001	GLU	L1694	
	T3132	N2933	Q2872	S2812	D2752	R2385	GLU	Q2005	ASP	L1715	
	T3133	G2934	A2873	L2813	S2753	P2390	GLU	A2016	GLU	I1716	
	V3134	Y2935	A2874	K2814	F2754	R2392	ALA	D2017	GLU	E1721	
	A3135	A2936	M2875	A2815	T2755	R2397	GLU	E2018	GLU	E1733	
	L3136	V2937	E2876	M2816	N2756	ARG	E2088	E2019	GLU	G1751	
	L3137	T2938	Q2877	L2817	K2757	ASP	K2089	D2020	GLU	R1752	
	I3147	R2939	L2878	A2818	F2758	ARG	K2090	C2021	GLU	K1753	
	F3152	LEU	N2881	E2820	E2760	ARG	E2108	R2028	GLU	G1754	
	I3157	LYS	H2882	V2821	V2761	ARG	R2126	Q2029	GLU	G1755	
	L3158	ASP	H2883	T2822	H2762	HIS	M2153	D2033	GLU	N1756	
	D3159	MET	N2884	T2823	H2763	GLY	L2159	D2037	GLU	A1757	
	D3160	GLU	T2885	E2824	E2764	GLU	L2167	Q2045	GLU	R1758	
	V3161	L2946	W2886	K2825	K2765	GLU	E2175	L2046	GLU	L1771	
	L3169	D2947	G2887	A2826	T2766	GLU	N2176	GLY	GLU	P1780	
	C3170	S2970	R2888	R2827	A2767	GLU	M2173	GLY	GLU	A1788	
	S3171	K2973	K2889	E2828	K2689	P2410	I2182	GLY	GLU	A1789	
	S3174	T2974	K2890	G2829	D2716	E2412	M2186	GLU	GLU	G1790	
	K3179	A2975	K2891	E2830	K2770	E2413	L2201	GLU	GLU	V1791	
	L3186	E2978	E2893	GLU	I2771	N2414	G2202	GLU	GLU	A1792	
	L3194	S2982	L2894	ARG	Q2772	R2415	M2203	GLU	GLU	E1793	
	L3194	S2983	E2895	THR	N2773	E2449	V2212	PRO	GLY	A1794	
	P3208	G2984	A2896	GLU	N2774	R2452	G2216	GLY	GLY	E1805	
	P3208	R2985	K2897	LYS	W2775	R2452	G2217	THR	GLU	I1572	
	R3225	V2986	G2898	LYS	S2776	V2461	G2218	LEU	GLU	L1576	
	E3226	E2987	G2899	THR	Y2777	D2482	E2219	SER	GLU	M1579	
	A3228	K2988	G2900	ARG	G2778	G2483	K2221	ARG	GLU	R1820	
	I3229	T2901	T2901	LYS	E2779	V2495	T2220	LEU	GLU	Q1824	
	L3230	H2902	H2902	ILE	W2780	H2498	K2223	GLU	GLU	D1828	
	P3004	K2903	P2903	GLN	V2781	V2495	E2222	SER	GLU		
	F3017	L2904	L2904	ALA	D2782	H2498	I2223	ARG	GLU		
	N3234	L2905	L2905	GLN	E2783	E2513	M2228	LEU	GLU		
	S3235	V2906	V2906	THR	E2784	W2514	F2235	SER	GLU		
	V3236	P2907	T2907	TYR	L2785	Q2515	D2235	LEU	GLU		
	E3237	Y2908	Y2908	ASP	K2786	D2516	F2235	GLU	THR		
		D2909	D2909	PRO	T2787						
		T2910	L2911	ARG	H2788						
		T2912	T2912	GLU	P2789						
		A2913	Y2855	GLY	W2790						
		K2914	W2856		L2791						
		E2915	P2857		T2793						
		K2916			Y2794						
		A2917			T2796						
		K2918			F2797						





D4046	D4063	M4064	D4070	S4074	G4086	K4090	K4091	D4092	F4093	M4097	D4098	E4119	I4123	R4137	D4138	M4142	T4148	R4159	E4172	R4175	P4176	Y4177	R4180	L4181	E4182	E4199	W4205	G4226	E4227	C4238	T4241	M4245	P4254	GLY	GLY	PRO									
ALA	ALA	ASP	GLY	MET	GLU	ALA	ALA	ALA	GLY	GLU	GLY	ALA	ALA	GLY	ALA	GLY	VAL	ALA	ALA	ALA	ARG	LEU	ALA	ALA	ALA	ALA	ARG	LEU	GLY	LEU	SER	TYR	ARG	ARG	VAL	GLU	ARG								
LEU	ALA	GLY	THR	GLU	THR	LEU	GLY	GLY	LEU	LEU	ALA	GLY	ALA	GLY	ALA	GLY	GLY	ALA	ALA	GLY	ARG	LEU	LEU	TRP	GLY	SER	GLY	VAL	GLY	GLY	ALA	GLY	VAL	THR	VAL	GLY	ARG								
LEU	GLY	MET	THR	SER	ASP	THR	HIS	GLY	GLN	PRO	GLY	PRO	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ASP	ALA	LEU	ASP	GLY	GLY	GLY	VAL	GLY	HIS	GLY	ALA	GLY	GLY	VAL	VAL	VAL	ALA								
VAL	ASP	GLY	PRO	ARG	GLY	GLY	GLY	THR	GLY	MET	GLY	ASP	PRO	THR	THR	PRO	GLY	SER	ILE	LEU	ARG	LEU	GLY	VAL	ASP	GLY	GLY	VAL	LEU	PRO	GLY	GLY	GLY	PRO	PRO	PRO									
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ASP	GLY	GLY	LYS	ALA	PRO	PRO	ALA	LYS	LYS	ALA	ALA	ALA	GLY	GLY	GLY	GLY	GLY	L4555	VAL	VAL	PRO	GLY	GLY	GLY	GLY	GLY	PRO								
LYS	ALA	ASP	GLY	ASN	GLY	VAL	VAL	PRO	ALA	PRO	GLY	PRO	LYS	PRO	SER	PRO	ALA	LYS	LYS	GLY	GLY	ALA	MET	GLY	GLY	GLY	F4540	L4555	A4570	M4574	S4583	P4587	GLY	GLY	ASP	MET									
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	PRO	GLY	GLY	GLY	GLY	GLY	GLY	GLY	LYS	GLY	GLY	ALA	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ASP	ASP	ASP									
GLY	SER	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	TRP	GLY	GLY	GLY	GLY	GLY	GLY	ASP	GLY	M4626	M4627	F4631	E4640	P4641	L4648	L4656	Y4661	M4662	E4676	Y4687	T4688	T4689	E4690	G4693	D4694	D4695	K4698								
GLY	SER	ALA	GLY	GLY	GLY	SER	SER	GLY	GLY	GLY	TRP	GLY	GLY	GLY	GLY	GLY	GLY	ASP	GLY	M4626	M4627	F4631	E4640	P4641	L4648	L4656	Y4661	M4662	E4676	Y4687	T4688	T4689	E4690	G4693	D4694	D4695	K4698								
G4699	R4722	I4731	L4748	E4749	I4750	T4751	A4752	H4753	M4754	E4755	R4756	K4757	P4758	D4759	P4760	P4761	P4762	G4763	L4764	L4765	L4768	M4769	D4786	M4796	L4801	G4802	H4803	L4813	M4818	G4819	V4820	K4821	R4824	R4860	K4861	E4867	D4868	E4869	D4870	M4880	Y4888	I4901	E4902	D4903	
P4904	E4910	L4911	Y4912	R4913	V4914	D4917	I4918	T4919	F4920	I4931	E4942	L4943	R4944	Y4967	T4970	T4971	P4972	H4983	M4989	K5012	E5016	A5024	E5033	S5037																					

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	153840	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	57.65	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.887	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	426.496, 426.496, 426.496	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.833, 0.833, 0.833	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: L9R, KVR, ATP, CA, CFF, ZN

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	C	0.10	0/1187	0.24	0/1594
1	D	0.09	0/1187	0.24	0/1594
1	E	0.09	0/1187	0.24	0/1594
1	K	0.09	0/1187	0.24	0/1594
2	F	0.33	0/850	0.49	0/1146
2	H	0.33	0/850	0.49	0/1146
2	J	0.33	0/850	0.49	0/1146
2	O	0.33	0/850	0.49	0/1146
3	A	0.15	0/35977	0.30	3/48726 (0.0%)
3	B	0.15	0/35977	0.30	3/48726 (0.0%)
3	G	0.15	0/35977	0.30	3/48726 (0.0%)
3	I	0.15	0/35977	0.30	3/48726 (0.0%)
All	All	0.15	0/152056	0.30	12/205864 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	4920	PHE	N-CA-C	-5.60	105.17	112.23
3	I	4920	PHE	N-CA-C	-5.58	105.20	112.23
3	A	4920	PHE	N-CA-C	-5.58	105.20	112.23
3	B	4920	PHE	N-CA-C	-5.56	105.23	112.23
3	B	4970	THR	CA-C-N	5.08	130.59	120.94
3	B	4970	THR	C-N-CA	5.08	130.59	120.94
3	G	4970	THR	CA-C-N	5.07	130.58	120.94
3	G	4970	THR	C-N-CA	5.07	130.58	120.94
3	I	4970	THR	CA-C-N	5.07	130.57	120.94
3	I	4970	THR	C-N-CA	5.07	130.57	120.94
3	A	4970	THR	CA-C-N	5.07	130.56	120.94
3	A	4970	THR	C-N-CA	5.07	130.56	120.94

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1174	0	1099	22	0
1	D	1174	0	1099	18	0
1	E	1174	0	1099	18	0
1	K	1174	0	1099	19	0
2	F	831	0	831	7	0
2	H	831	0	831	8	0
2	J	831	0	831	7	0
2	O	831	0	831	8	0
3	A	35150	0	34797	374	0
3	B	35150	0	34797	371	0
3	G	35150	0	34797	373	0
3	I	35150	0	34797	378	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
4	E	4	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	K	4	0	0	0	0
5	A	62	0	24	2	0
5	B	62	0	24	2	0
5	G	62	0	24	2	0
5	I	62	0	24	2	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
7	A	14	0	10	0	0
7	B	14	0	10	0	0
7	G	14	0	10	0	0
7	I	14	0	10	0	0
8	A	23	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	23	0	0	0	0
8	G	23	0	0	0	0
8	I	23	0	0	0	0
9	A	108	0	172	9	0
9	B	108	0	172	6	0
9	G	108	0	172	9	0
9	I	108	0	172	8	0
All	All	149472	0	147732	1564	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 5.

All (1564) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:4904:PRO:HB3	3:I:4913:ARG:HG2	1.57	0.86
3:G:4904:PRO:HB3	3:G:4913:ARG:HG2	1.57	0.86
3:A:4904:PRO:HB3	3:A:4913:ARG:HG2	1.57	0.84
3:B:4904:PRO:HB3	3:B:4913:ARG:HG2	1.57	0.83
3:A:2779:GLU:HG3	3:A:2792:ARG:HG2	1.66	0.78
3:G:2779:GLU:HG3	3:G:2792:ARG:HG2	1.66	0.78
3:I:2779:GLU:HG3	3:I:2792:ARG:HG2	1.66	0.77
3:B:2779:GLU:HG3	3:B:2792:ARG:HG2	1.66	0.77
3:A:1505:GLN:HG3	3:G:2771:ILE:HG12	1.67	0.77
3:B:2175:GLU:HG3	3:B:2228:MET:HB2	1.68	0.76
3:I:2175:GLU:HG3	3:I:2228:MET:HB2	1.68	0.76
1:C:106:ARG:HH22	1:C:118:ASP:HA	1.50	0.76
3:A:2175:GLU:HG3	3:A:2228:MET:HB2	1.68	0.76
3:G:2175:GLU:HG3	3:G:2228:MET:HB2	1.68	0.76
1:D:106:ARG:HH22	1:D:118:ASP:HA	1.50	0.75
1:K:106:ARG:HH22	1:K:118:ASP:HA	1.50	0.75
1:E:106:ARG:HH22	1:E:118:ASP:HA	1.50	0.75
3:G:2765:LYS:NZ	3:G:2859:PRO:O	2.22	0.73
3:I:2765:LYS:NZ	3:I:2859:PRO:O	2.22	0.72
1:K:111:ASN:O	3:A:1996:ARG:NH2	2.20	0.72
3:B:2765:LYS:NZ	3:B:2859:PRO:O	2.22	0.72
3:A:2765:LYS:NZ	3:A:2859:PRO:O	2.22	0.71
3:B:2771:ILE:HG12	3:I:1505:GLN:HG3	1.74	0.70
3:G:3114:LYS:HD3	3:G:3116:SER:H	1.58	0.69
3:B:3114:LYS:HD3	3:B:3116:SER:H	1.58	0.68
3:I:3114:LYS:HD3	3:I:3116:SER:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1280:GLN:O	3:A:1281:ASN:ND2	2.27	0.68
3:B:876:GLU:HG2	3:B:918:ARG:HD3	1.76	0.68
3:I:858:THR:HB	3:I:930:LYS:HD2	1.76	0.68
3:A:368:ARG:HE	3:A:2308:GLN:HG3	1.59	0.68
3:A:3114:LYS:HD3	3:A:3116:SER:H	1.58	0.68
3:I:1280:GLN:O	3:I:1281:ASN:ND2	2.27	0.68
3:G:876:GLU:HG2	3:G:918:ARG:HD3	1.76	0.67
3:B:368:ARG:HE	3:B:2308:GLN:HG3	1.59	0.67
3:B:1280:GLN:O	3:B:1281:ASN:ND2	2.27	0.67
3:G:858:THR:HB	3:G:930:LYS:HD2	1.76	0.67
3:A:2771:ILE:HG12	3:B:1505:GLN:HG3	1.77	0.67
3:G:1280:GLN:O	3:G:1281:ASN:ND2	2.27	0.67
3:A:858:THR:HB	3:A:930:LYS:HD2	1.76	0.67
3:G:368:ARG:HE	3:G:2308:GLN:HG3	1.59	0.67
3:I:876:GLU:HG2	3:I:918:ARG:HD3	1.75	0.67
3:A:2781:VAL:HA	3:A:2789:PRO:HB2	1.78	0.66
3:I:368:ARG:HE	3:I:2308:GLN:HG3	1.59	0.66
3:A:1520:VAL:HG12	3:A:1527:MET:HG2	1.78	0.66
3:G:2781:VAL:HA	3:G:2789:PRO:HB2	1.78	0.66
3:A:876:GLU:HG2	3:A:918:ARG:HD3	1.75	0.66
3:I:2781:VAL:HA	3:I:2789:PRO:HB2	1.78	0.66
3:A:3020:THR:HG23	3:A:3023:LYS:H	1.60	0.66
3:B:858:THR:HB	3:B:930:LYS:HD2	1.76	0.66
3:B:2781:VAL:HA	3:B:2789:PRO:HB2	1.78	0.66
3:B:3020:THR:HG23	3:B:3023:LYS:H	1.60	0.66
3:I:3020:THR:HG23	3:I:3023:LYS:H	1.60	0.66
1:K:133:ASP:HA	3:A:3460:VAL:HG11	1.77	0.66
3:B:2792:ARG:NH2	3:B:2798:SER:OG	2.29	0.66
3:I:961:MET:SD	3:I:961:MET:N	2.69	0.65
1:D:133:ASP:HA	3:I:3460:VAL:HG11	1.77	0.65
3:G:1520:VAL:HG12	3:G:1527:MET:HG2	1.78	0.65
3:I:2792:ARG:NH2	3:I:2798:SER:OG	2.29	0.65
3:B:1520:VAL:HG12	3:B:1527:MET:HG2	1.78	0.65
3:I:1520:VAL:HG12	3:I:1527:MET:HG2	1.78	0.65
3:A:2792:ARG:NH2	3:A:2798:SER:OG	2.29	0.65
3:B:972:LEU:HD22	3:B:1044:ARG:HB3	1.79	0.65
3:G:2792:ARG:NH2	3:G:2798:SER:OG	2.29	0.65
3:G:3020:THR:HG23	3:G:3023:LYS:H	1.60	0.65
3:A:972:LEU:HD22	3:A:1044:ARG:HB3	1.79	0.64
3:A:3329:ILE:HD11	3:A:3332:ALA:HB2	1.79	0.64
3:G:972:LEU:HD22	3:G:1044:ARG:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:101:LEU:HB3	3:B:150:MET:HE1	1.80	0.64
3:I:399:GLN:HG2	3:I:403:MET:HE2	1.80	0.64
1:D:1:ALA:HB3	3:I:3861:GLU:HG2	1.79	0.64
3:A:101:LEU:HB3	3:A:150:MET:HE1	1.80	0.64
3:B:399:GLN:HG2	3:B:403:MET:HE2	1.80	0.64
3:A:545:ASP:OD1	3:A:582:HIS:NE2	2.28	0.64
3:B:3329:ILE:HD11	3:B:3332:ALA:HB2	1.79	0.64
3:G:2978:GLU:OE2	3:G:3053:ARG:NH1	2.31	0.64
3:I:2978:GLU:OE2	3:I:3053:ARG:NH1	2.31	0.64
3:G:399:GLN:HG2	3:G:403:MET:HE2	1.80	0.63
3:A:399:GLN:HG2	3:A:403:MET:HE2	1.80	0.63
3:I:972:LEU:HD22	3:I:1044:ARG:HB3	1.79	0.63
3:B:2978:GLU:OE2	3:B:3053:ARG:NH1	2.31	0.63
3:G:638:ILE:HD11	3:G:1636:MET:HE2	1.81	0.63
3:G:961:MET:SD	3:G:961:MET:N	2.69	0.63
3:I:2018:GLU:OE1	3:I:2028:ARG:NH1	2.32	0.63
3:A:638:ILE:HD11	3:A:1636:MET:HE2	1.81	0.63
3:A:961:MET:SD	3:A:961:MET:N	2.69	0.62
3:A:2018:GLU:OE1	3:A:2028:ARG:NH1	2.32	0.62
3:G:3329:ILE:HD11	3:G:3332:ALA:HB2	1.79	0.62
3:I:101:LEU:HB3	3:I:150:MET:HE1	1.80	0.62
3:G:101:LEU:HB3	3:G:150:MET:HE1	1.80	0.62
3:G:2018:GLU:OE1	3:G:2028:ARG:NH1	2.32	0.62
3:A:2309:SER:OG	3:A:2321:ILE:O	2.15	0.62
3:A:3017:PHE:O	3:A:3036:LYS:NZ	2.33	0.62
3:I:3329:ILE:HD11	3:I:3332:ALA:HB2	1.79	0.62
3:I:3959:LYS:NZ	3:I:4022:ASP:OD2	2.32	0.62
3:A:2978:GLU:OE2	3:A:3053:ARG:NH1	2.31	0.62
3:G:3017:PHE:O	3:G:3036:LYS:NZ	2.33	0.62
3:B:3445:TRP:NE1	3:B:3455:GLU:OE1	2.33	0.62
3:G:2614:ILE:HG23	3:G:2618:MET:HE3	1.82	0.62
3:I:3579:LEU:HB2	3:I:3582:ARG:HG2	1.81	0.62
3:G:1116:GLY:HA3	3:G:1132:TRP:HB3	1.81	0.62
3:G:3445:TRP:NE1	3:G:3455:GLU:OE1	2.32	0.62
3:I:2902:HIS:HB3	3:I:2905:LEU:HG	1.82	0.62
3:B:2018:GLU:OE1	3:B:2028:ARG:NH1	2.32	0.62
3:B:2614:ILE:HG23	3:B:2618:MET:HE3	1.82	0.62
3:G:3579:LEU:HB2	3:G:3582:ARG:HG2	1.81	0.62
3:I:2614:ILE:HG23	3:I:2618:MET:HE3	1.82	0.62
3:I:3017:PHE:O	3:I:3036:LYS:NZ	2.33	0.62
3:B:2410:PRO:HB3	3:B:2415:ARG:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2902:HIS:HB3	3:B:2905:LEU:HG	1.82	0.61
3:B:3959:LYS:NZ	3:B:4022:ASP:OD2	2.32	0.61
3:A:2614:ILE:HG23	3:A:2618:MET:HE3	1.82	0.61
3:A:3445:TRP:NE1	3:A:3455:GLU:OE1	2.32	0.61
3:B:1066:GLN:HB2	3:B:1071:ARG:HE	1.65	0.61
3:B:1116:GLY:HA3	3:B:1132:TRP:HB3	1.81	0.61
3:B:3579:LEU:HB2	3:B:3582:ARG:HG2	1.81	0.61
3:I:638:ILE:HD11	3:I:1636:MET:HE2	1.81	0.61
3:I:1116:GLY:HA3	3:I:1132:TRP:HB3	1.81	0.61
3:I:2410:PRO:HB3	3:I:2415:ARG:HB3	1.82	0.61
3:I:3445:TRP:NE1	3:I:3455:GLU:OE1	2.32	0.61
3:B:961:MET:SD	3:B:961:MET:N	2.69	0.61
3:B:3017:PHE:O	3:B:3036:LYS:NZ	2.33	0.61
3:B:622:THR:HG23	3:B:626:LEU:HD12	1.83	0.61
3:G:1066:GLN:HB2	3:G:1071:ARG:HE	1.65	0.61
3:A:2902:HIS:HB3	3:A:2905:LEU:HG	1.82	0.61
3:A:2382:GLU:OE1	3:A:2385:ARG:NH1	2.31	0.61
3:B:638:ILE:HD11	3:B:1636:MET:HE2	1.81	0.61
3:A:622:THR:HG23	3:A:626:LEU:HD12	1.83	0.61
3:A:1116:GLY:HA3	3:A:1132:TRP:HB3	1.81	0.61
3:G:4583:SER:HB3	3:G:4631:PHE:HE2	1.66	0.61
3:G:545:ASP:OD1	3:G:582:HIS:NE2	2.28	0.60
3:A:1066:GLN:HB2	3:A:1071:ARG:HE	1.65	0.60
3:A:2410:PRO:HB3	3:A:2415:ARG:HB3	1.82	0.60
3:G:2902:HIS:HB3	3:G:2905:LEU:HG	1.82	0.60
3:A:228:ASP:OD2	3:B:155:LYS:NZ	2.30	0.60
3:A:3579:LEU:HB2	3:A:3582:ARG:HG2	1.81	0.60
3:G:2410:PRO:HB3	3:G:2415:ARG:HB3	1.82	0.60
3:I:622:THR:HG23	3:I:626:LEU:HD12	1.83	0.60
3:I:2309:SER:OG	3:I:2321:ILE:O	2.15	0.60
3:B:2309:SER:OG	3:B:2321:ILE:O	2.15	0.60
3:G:622:THR:HG23	3:G:626:LEU:HD12	1.83	0.60
3:G:897:ARG:NH2	3:G:899:ASP:OD1	2.35	0.60
3:G:1089:TYR:HD2	3:G:1152:MET:HG2	1.67	0.60
3:I:545:ASP:OD1	3:I:582:HIS:NE2	2.28	0.60
3:I:1066:GLN:HB2	3:I:1071:ARG:HE	1.65	0.60
1:E:99:TYR:HB3	1:E:135:GLN:HB3	1.84	0.60
3:A:4583:SER:HB3	3:A:4631:PHE:HE2	1.66	0.60
1:C:99:TYR:HB3	1:C:135:GLN:HB3	1.84	0.60
1:K:99:TYR:HB3	1:K:135:GLN:HB3	1.84	0.59
3:A:1089:TYR:HD2	3:A:1152:MET:HG2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:633:LEU:HD13	3:B:1639:LEU:HD21	1.84	0.59
3:G:2309:SER:OG	3:G:2321:ILE:O	2.16	0.59
3:G:2382:GLU:OE1	3:G:2385:ARG:NH1	2.31	0.59
3:B:4583:SER:HB3	3:B:4631:PHE:HE2	1.66	0.59
3:G:492:ASP:OD1	3:G:546:TRP:NE1	2.33	0.59
3:I:984:LEU:HD12	3:I:987:ARG:HH12	1.68	0.59
3:A:3959:LYS:NZ	3:A:4022:ASP:OD2	2.32	0.59
3:B:545:ASP:OD1	3:B:582:HIS:NE2	2.28	0.59
3:B:830:ARG:NH2	3:B:832:GLU:OE2	2.36	0.59
3:I:830:ARG:NH2	3:I:832:GLU:OE2	2.36	0.59
3:I:4583:SER:HB3	3:I:4631:PHE:HE2	1.66	0.59
3:A:1448:VAL:HG22	3:A:1554:VAL:HG23	1.85	0.59
3:B:2382:GLU:OE1	3:B:2385:ARG:NH1	2.31	0.59
3:G:633:LEU:HD13	3:G:1639:LEU:HD21	1.84	0.59
3:G:3751:VAL:O	3:G:3756:LYS:NZ	2.35	0.59
1:K:55:VAL:HG21	1:K:71:MET:HB2	1.85	0.59
3:A:894:GLY:HA3	3:A:903:LEU:HB3	1.85	0.59
3:A:897:ARG:NH2	3:A:899:ASP:OD1	2.35	0.59
3:B:894:GLY:HA3	3:B:903:LEU:HB3	1.85	0.59
3:G:830:ARG:NH2	3:G:832:GLU:OE2	2.36	0.59
3:G:3959:LYS:NZ	3:G:4022:ASP:OD2	2.32	0.59
3:A:3751:VAL:O	3:A:3756:LYS:NZ	2.35	0.59
3:G:984:LEU:HD12	3:G:987:ARG:HH12	1.68	0.59
3:B:1089:TYR:HD2	3:B:1152:MET:HG2	1.67	0.59
3:G:155:LYS:NZ	3:I:228:ASP:OD2	2.34	0.59
3:G:1505:GLN:HG3	3:I:2771:ILE:HG12	1.84	0.59
3:B:897:ARG:NH2	3:B:899:ASP:OD1	2.35	0.59
3:B:984:LEU:HD12	3:B:987:ARG:HH12	1.68	0.59
3:I:19:GLU:HG2	3:I:68:THR:HG22	1.85	0.59
3:I:2382:GLU:OE1	3:I:2385:ARG:NH1	2.31	0.59
3:G:516:LYS:O	3:G:520:ASN:ND2	2.31	0.59
3:I:1089:TYR:HD2	3:I:1152:MET:HG2	1.67	0.59
3:B:3751:VAL:O	3:B:3756:LYS:NZ	2.35	0.58
3:B:4138:ASP:O	3:B:4142:ASN:ND2	2.34	0.58
3:I:3751:VAL:O	3:I:3756:LYS:NZ	2.35	0.58
3:B:4570:ALA:O	3:B:4574:ASN:ND2	2.33	0.58
3:G:19:GLU:HG2	3:G:68:THR:HG22	1.85	0.58
3:I:897:ARG:NH2	3:I:899:ASP:OD1	2.35	0.58
3:I:1619:ARG:NH2	3:I:1622:GLU:OE1	2.37	0.58
3:B:19:GLU:HG2	3:B:68:THR:HG22	1.85	0.58
3:B:3132:THR:HG23	3:B:3136:LEU:HD23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:23:VAL:HG22	2:H:47:LYS:HG2	1.86	0.58
3:G:894:GLY:HA3	3:G:903:LEU:HB3	1.85	0.58
3:G:1448:VAL:HG22	3:G:1554:VAL:HG23	1.85	0.58
1:D:99:TYR:HB3	1:D:135:GLN:HB3	1.84	0.58
3:B:1448:VAL:HG22	3:B:1554:VAL:HG23	1.85	0.58
3:I:894:GLY:HA3	3:I:903:LEU:HB3	1.85	0.58
1:C:55:VAL:HG21	1:C:71:MET:HB2	1.85	0.58
3:I:1448:VAL:HG22	3:I:1554:VAL:HG23	1.85	0.58
2:O:23:VAL:HG22	2:O:47:LYS:HG2	1.86	0.58
2:F:23:VAL:HG22	2:F:47:LYS:HG2	1.86	0.58
1:E:55:VAL:HG21	1:E:71:MET:HB2	1.85	0.58
3:A:3579:LEU:HD12	3:A:3582:ARG:HE	1.69	0.58
3:A:633:LEU:HD13	3:A:1639:LEU:HD21	1.84	0.58
3:A:830:ARG:NH2	3:A:832:GLU:OE2	2.36	0.58
3:A:955:LEU:O	3:A:966:LYS:NZ	2.31	0.58
3:A:2650:ARG:NH1	3:A:2651:CYS:SG	2.77	0.58
3:B:516:LYS:O	3:B:520:ASN:ND2	2.31	0.58
3:B:2650:ARG:NH1	3:B:2651:CYS:SG	2.77	0.58
3:G:1619:ARG:NH2	3:G:1622:GLU:OE1	2.36	0.58
3:A:19:GLU:HG2	3:A:68:THR:HG22	1.85	0.58
3:B:1619:ARG:NH2	3:B:1622:GLU:OE1	2.37	0.58
3:G:2650:ARG:NH1	3:G:2651:CYS:SG	2.77	0.58
3:G:3132:THR:HG23	3:G:3136:LEU:HD23	1.85	0.57
3:I:633:LEU:HD13	3:I:1639:LEU:HD21	1.84	0.57
3:I:2650:ARG:NH1	3:I:2651:CYS:SG	2.77	0.57
3:I:56:GLN:O	3:I:309:THR:OG1	2.19	0.57
3:I:70:GLU:OE2	3:I:110:ARG:NE	2.34	0.57
3:I:492:ASP:OD1	3:I:546:TRP:NE1	2.33	0.57
1:D:55:VAL:HG21	1:D:71:MET:HB2	1.85	0.57
3:A:984:LEU:HD12	3:A:987:ARG:HH12	1.68	0.57
3:A:3132:THR:HG23	3:A:3136:LEU:HD23	1.85	0.57
3:I:3579:LEU:HD12	3:I:3582:ARG:HE	1.69	0.57
3:A:1619:ARG:NH2	3:A:1622:GLU:OE1	2.36	0.57
3:I:516:LYS:O	3:I:520:ASN:ND2	2.31	0.57
2:J:23:VAL:HG22	2:J:47:LYS:HG2	1.86	0.57
3:B:1987:SER:HB2	3:B:1994:ARG:HH22	1.70	0.57
3:G:110:ARG:NH2	3:G:117:TYR:OH	2.38	0.57
3:A:4689:THR:OG1	3:A:4690:GLU:OE1	2.23	0.57
3:G:3579:LEU:HD12	3:G:3582:ARG:HE	1.69	0.57
3:I:3132:THR:HG23	3:I:3136:LEU:HD23	1.85	0.57
3:B:127:MET:SD	3:B:127:MET:N	2.78	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:492:ASP:OD1	3:B:546:TRP:NE1	2.33	0.57
3:G:1987:SER:HB2	3:G:1994:ARG:HH22	1.70	0.57
3:A:1792:ALA:O	3:A:2176:ASN:ND2	2.38	0.57
3:G:3759:GLU:OE2	3:G:3762:ARG:NH2	2.38	0.57
3:B:426:ARG:NH2	3:B:509:GLU:OE2	2.38	0.56
3:G:1131:ARG:NH1	3:G:1178:ALA:O	2.38	0.56
3:I:3759:GLU:OE2	3:I:3762:ARG:NH2	2.38	0.56
3:G:384:MET:SD	3:G:384:MET:N	2.77	0.56
3:I:426:ARG:NH2	3:I:509:GLU:OE2	2.38	0.56
3:A:110:ARG:NH2	3:A:117:TYR:OH	2.38	0.56
3:B:1792:ALA:O	3:B:2176:ASN:ND2	2.38	0.56
3:B:2514:ASN:ND2	3:B:2516:ASP:OD1	2.38	0.56
3:B:3324:VAL:HG11	3:B:3361:THR:HG22	1.88	0.56
3:B:3579:LEU:HD12	3:B:3582:ARG:HE	1.69	0.56
3:G:3324:VAL:HG11	3:G:3361:THR:HG22	1.88	0.56
3:I:1131:ARG:NH1	3:I:1178:ALA:O	2.38	0.56
3:I:1454:THR:OG1	3:I:1456:ASP:OD1	2.20	0.56
3:B:3270:ILE:HA	3:B:3274:LEU:HD12	1.88	0.56
3:G:426:ARG:NH2	3:G:509:GLU:OE2	2.38	0.56
3:G:2514:ASN:ND2	3:G:2516:ASP:OD1	2.39	0.56
3:I:110:ARG:NH2	3:I:117:TYR:OH	2.38	0.56
3:I:1792:ALA:O	3:I:2176:ASN:ND2	2.38	0.56
3:I:3324:VAL:HG11	3:I:3361:THR:HG22	1.88	0.56
3:A:127:MET:SD	3:A:127:MET:N	2.78	0.56
3:A:384:MET:SD	3:A:384:MET:N	2.77	0.56
3:A:3455:GLU:OE2	3:A:3508:SER:OG	2.24	0.56
3:B:1131:ARG:NH1	3:B:1178:ALA:O	2.38	0.56
3:B:3759:GLU:OE2	3:B:3762:ARG:NH2	2.38	0.56
3:B:4689:THR:OG1	3:B:4690:GLU:OE1	2.23	0.56
3:G:3270:ILE:HA	3:G:3274:LEU:HD12	1.88	0.56
3:A:3523:ASN:O	3:A:3582:ARG:NH2	2.39	0.56
3:I:1987:SER:HB2	3:I:1994:ARG:HH22	1.70	0.56
3:I:2514:ASN:ND2	3:I:2516:ASP:OD1	2.39	0.56
3:A:3759:GLU:OE2	3:A:3762:ARG:NH2	2.38	0.56
3:B:110:ARG:NH2	3:B:117:TYR:OH	2.38	0.56
3:B:302:VAL:HB	3:B:306:LYS:HE3	1.88	0.56
3:I:127:MET:SD	3:I:127:MET:N	2.78	0.56
3:I:3523:ASN:O	3:I:3582:ARG:NH2	2.39	0.56
3:A:904:HIS:HD1	3:A:905:PRO:HD2	1.71	0.56
3:G:1792:ALA:O	3:G:2176:ASN:ND2	2.38	0.56
3:G:2644:LEU:HD13	3:G:2678:LEU:HD21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:667:MET:SD	3:B:790:ARG:NH2	2.80	0.56
3:G:1676:LEU:HD22	3:G:2167:ILE:HD12	1.88	0.56
3:I:4570:ALA:O	3:I:4574:ASN:ND2	2.33	0.56
3:A:1141:ARG:HB3	3:G:3479:ALA:HA	1.88	0.55
3:A:2514:ASN:ND2	3:A:2516:ASP:OD1	2.39	0.55
3:A:3270:ILE:HA	3:A:3274:LEU:HD12	1.88	0.55
3:A:3324:VAL:HG11	3:A:3361:THR:HG22	1.88	0.55
3:B:3400:VAL:HG23	3:B:3403:ARG:HH21	1.71	0.55
3:G:127:MET:SD	3:G:127:MET:N	2.78	0.55
3:G:4942:GLU:OE1	3:I:4944:ARG:NH1	2.39	0.55
3:I:904:HIS:HD1	3:I:905:PRO:HD2	1.71	0.55
3:A:302:VAL:HB	3:A:306:LYS:HE3	1.88	0.55
3:A:426:ARG:NH2	3:A:509:GLU:OE2	2.38	0.55
3:G:904:HIS:HD1	3:G:905:PRO:HD2	1.71	0.55
1:K:145:MET:SD	1:K:145:MET:N	2.80	0.55
3:A:1131:ARG:NH1	3:A:1178:ALA:O	2.38	0.55
3:G:3400:VAL:HG23	3:G:3403:ARG:HH21	1.71	0.55
3:G:3455:GLU:OE2	3:G:3508:SER:OG	2.24	0.55
3:I:1676:LEU:HD22	3:I:2167:ILE:HD12	1.88	0.55
3:I:3270:ILE:HA	3:I:3274:LEU:HD12	1.88	0.55
1:D:145:MET:SD	1:D:145:MET:N	2.80	0.55
3:A:1676:LEU:HD22	3:A:2167:ILE:HD12	1.88	0.55
3:B:904:HIS:HD1	3:B:905:PRO:HD2	1.71	0.55
3:B:2159:LEU:HD13	3:B:2203:MET:HG3	1.88	0.55
3:B:3169:LEU:HD12	3:B:3194:LEU:HD11	1.89	0.55
3:G:817:PRO:O	3:G:820:ARG:NH2	2.40	0.55
3:I:667:MET:SD	3:I:790:ARG:NH2	2.80	0.55
3:I:2827:ARG:NH2	3:I:2935:TYR:OH	2.40	0.55
2:J:75:THR:HG23	2:J:98:VAL:HG22	1.89	0.55
1:C:145:MET:SD	1:C:145:MET:N	2.80	0.55
3:B:2827:ARG:NH2	3:B:2935:TYR:OH	2.40	0.55
3:G:1057:ASP:OD1	3:G:1057:ASP:N	2.31	0.55
3:I:2159:LEU:HD13	3:I:2203:MET:HG3	1.88	0.55
3:I:2644:LEU:HD13	3:I:2678:LEU:HD21	1.88	0.55
3:I:4901:ILE:HG13	3:I:4913:ARG:NH2	2.21	0.55
2:O:75:THR:HG23	2:O:98:VAL:HG22	1.89	0.55
3:A:667:MET:SD	3:A:790:ARG:NH2	2.80	0.55
3:A:3169:LEU:HD12	3:A:3194:LEU:HD11	1.89	0.55
3:A:4944:ARG:NH1	3:B:4942:GLU:OE1	2.39	0.55
3:G:4689:THR:OG1	3:G:4690:GLU:OE1	2.23	0.55
2:F:75:THR:HG23	2:F:98:VAL:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1987:SER:HB2	3:A:1994:ARG:HH22	1.70	0.55
3:B:3523:ASN:O	3:B:3582:ARG:NH2	2.39	0.55
3:B:3696:ASP:OD2	3:B:3773:ARG:NE	2.38	0.55
3:G:4901:ILE:HG13	3:G:4913:ARG:NH2	2.21	0.55
3:I:3940:LYS:O	3:I:4002:LYS:NZ	2.39	0.55
3:I:4689:THR:OG1	3:I:4690:GLU:OE1	2.23	0.55
1:E:145:MET:N	1:E:145:MET:SD	2.80	0.55
3:A:817:PRO:O	3:A:820:ARG:NH2	2.40	0.55
3:A:2827:ARG:NH2	3:A:2935:TYR:OH	2.40	0.55
3:G:302:VAL:HB	3:G:306:LYS:HE3	1.88	0.55
3:G:2827:ARG:NH2	3:G:2935:TYR:OH	2.40	0.55
3:I:3169:LEU:HD12	3:I:3194:LEU:HD11	1.89	0.55
3:I:4238:CYS:HA	3:I:4989:MET:HE1	1.89	0.55
3:A:2159:LEU:HD13	3:A:2203:MET:HG3	1.88	0.55
3:B:4137:ARG:NH2	3:B:4199:GLU:OE2	2.40	0.55
3:G:3523:ASN:O	3:G:3582:ARG:NH2	2.39	0.55
3:G:3696:ASP:OD2	3:G:3773:ARG:NE	2.38	0.55
3:G:4137:ARG:NH2	3:G:4199:GLU:OE2	2.40	0.55
3:G:4238:CYS:HA	3:G:4989:MET:HE1	1.89	0.55
3:I:384:MET:SD	3:I:384:MET:N	2.77	0.55
3:I:4676:GLU:OE2	3:I:4698:LYS:NZ	2.40	0.55
3:B:4944:ARG:NH1	3:I:4942:GLU:OE1	2.41	0.55
3:G:2159:LEU:HD13	3:G:2203:MET:HG3	1.88	0.55
3:G:2519:LEU:HD13	3:G:2575:ARG:HG3	1.89	0.55
3:I:302:VAL:HB	3:I:306:LYS:HE3	1.88	0.55
2:H:75:THR:HG23	2:H:98:VAL:HG22	1.89	0.55
3:A:1062:GLN:NE2	3:A:1064:GLU:OE1	2.37	0.54
3:A:3400:VAL:HG23	3:A:3403:ARG:HH21	1.71	0.54
3:A:3940:LYS:O	3:A:4002:LYS:NZ	2.39	0.54
3:G:667:MET:SD	3:G:790:ARG:NH2	2.80	0.54
3:G:3169:LEU:HD12	3:G:3194:LEU:HD11	1.89	0.54
3:I:2892:GLN:NE2	3:I:2895:GLU:OE2	2.40	0.54
3:I:3400:VAL:HG23	3:I:3403:ARG:HH21	1.71	0.54
3:A:2892:GLN:NE2	3:A:2895:GLU:OE2	2.40	0.54
3:A:4570:ALA:O	3:A:4574:ASN:ND2	2.33	0.54
3:A:4676:GLU:OE2	3:A:4698:LYS:NZ	2.40	0.54
3:B:4901:ILE:HG13	3:B:4913:ARG:NH2	2.21	0.54
3:I:924:MET:HG3	5:I:5106:ATP:HN61	1.72	0.54
3:A:2644:LEU:HD13	3:A:2678:LEU:HD21	1.88	0.54
3:B:1676:LEU:HD22	3:B:2167:ILE:HD12	1.88	0.54
3:B:1680:ARG:HH12	2:O:88:PRO:HB2	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2644:LEU:HD13	3:B:2678:LEU:HD21	1.88	0.54
3:B:3455:GLU:OE2	3:B:3508:SER:OG	2.24	0.54
3:G:2892:GLN:NE2	3:G:2895:GLU:OE2	2.40	0.54
1:E:95:ASP:OD2	1:E:97:ASN:ND2	2.41	0.54
3:A:70:GLU:OE2	3:A:110:ARG:NE	2.34	0.54
3:A:155:LYS:NZ	3:G:228:ASP:OD2	2.31	0.54
3:A:530:ILE:HG22	3:A:536:ASN:HB3	1.90	0.54
3:A:4137:ARG:NH2	3:A:4199:GLU:OE2	2.40	0.54
3:A:4901:ILE:HG13	3:A:4913:ARG:NH2	2.21	0.54
3:B:530:ILE:HG22	3:B:536:ASN:HB3	1.90	0.54
3:B:4676:GLU:OE2	3:B:4698:LYS:NZ	2.40	0.54
3:G:1062:GLN:NE2	3:G:1064:GLU:OE1	2.37	0.54
3:G:1252:HIS:O	3:G:1275:ARG:NH1	2.41	0.54
3:I:23:GLN:NE2	3:I:203:ASN:OD1	2.41	0.54
3:I:1252:HIS:O	3:I:1275:ARG:NH1	2.41	0.54
3:I:2519:LEU:HD13	3:I:2575:ARG:HG3	1.89	0.54
3:B:23:GLN:NE2	3:B:203:ASN:OD1	2.41	0.54
3:B:1252:HIS:O	3:B:1275:ARG:NH1	2.41	0.54
3:A:492:ASP:OD1	3:A:546:TRP:NE1	2.33	0.54
3:B:2892:GLN:NE2	3:B:2895:GLU:OE2	2.40	0.54
3:G:23:GLN:NE2	3:G:203:ASN:OD1	2.40	0.54
3:I:3233:PRO:HB2	3:I:3238:GLU:HB2	1.90	0.54
3:B:3335:MET:SD	3:B:3403:ARG:NH1	2.81	0.54
3:G:56:GLN:O	3:G:309:THR:OG1	2.19	0.54
3:G:70:GLU:OE2	3:G:110:ARG:NE	2.34	0.54
3:G:530:ILE:HG22	3:G:536:ASN:HB3	1.90	0.54
3:G:4570:ALA:O	3:G:4574:ASN:ND2	2.33	0.54
3:I:817:PRO:O	3:I:820:ARG:NH2	2.40	0.54
3:I:3335:MET:SD	3:I:3403:ARG:NH1	2.81	0.54
3:I:4137:ARG:NH2	3:I:4199:GLU:OE2	2.40	0.54
3:G:924:MET:HG3	5:G:5106:ATP:HN61	1.72	0.54
3:G:2178:MET:HE3	3:G:2182:ILE:HD11	1.90	0.54
3:G:3335:MET:SD	3:G:3403:ARG:NH1	2.81	0.54
3:I:530:ILE:HG22	3:I:536:ASN:HB3	1.90	0.54
3:B:817:PRO:O	3:B:820:ARG:NH2	2.40	0.54
3:B:913:LEU:HD12	3:B:914:PRO:HD2	1.89	0.54
3:G:1454:THR:OG1	3:G:1456:ASP:OD1	2.20	0.54
1:C:95:ASP:OD2	1:C:97:ASN:ND2	2.41	0.54
3:A:2519:LEU:HD13	3:A:2575:ARG:HG3	1.89	0.54
3:A:4942:GLU:OE1	3:G:4944:ARG:NH1	2.41	0.54
3:B:924:MET:HG3	5:B:5305:ATP:HN61	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2519:LEU:HD13	3:B:2575:ARG:HG3	1.89	0.54
3:B:3233:PRO:HB2	3:B:3238:GLU:HB2	1.90	0.54
3:G:293:LEU:HD13	3:G:378:LEU:HD12	1.90	0.54
3:G:4676:GLU:OE2	3:G:4698:LYS:NZ	2.40	0.54
3:I:2970:SER:HA	3:I:2973:PHE:CE2	2.43	0.54
3:I:3455:GLU:OE2	3:I:3508:SER:OG	2.24	0.54
3:A:23:GLN:NE2	3:A:203:ASN:OD1	2.40	0.53
3:G:2970:SER:HA	3:G:2973:PHE:CE2	2.44	0.53
3:A:293:LEU:HD13	3:A:378:LEU:HD12	1.90	0.53
3:B:1454:THR:OG1	3:B:1456:ASP:OD1	2.20	0.53
3:B:3940:LYS:O	3:B:4002:LYS:NZ	2.39	0.53
3:A:1252:HIS:O	3:A:1275:ARG:NH1	2.41	0.53
3:B:4238:CYS:HA	3:B:4989:MET:HE1	1.89	0.53
3:I:293:LEU:HD13	3:I:378:LEU:HD12	1.90	0.53
1:K:95:ASP:OD2	1:K:97:ASN:ND2	2.41	0.53
3:A:3335:MET:SD	3:A:3403:ARG:NH1	2.81	0.53
3:I:913:LEU:HD12	3:I:914:PRO:HD2	1.89	0.53
1:K:27:ILE:HB	1:K:63:ILE:HB	1.91	0.53
1:D:95:ASP:OD2	1:D:97:ASN:ND2	2.41	0.53
3:A:924:MET:HG3	5:A:5305:ATP:HN61	1.72	0.53
3:A:2178:MET:HE3	3:A:2182:ILE:HD11	1.90	0.53
3:G:745:SER:HB2	3:G:758:ARG:HB2	1.91	0.53
3:I:1062:GLN:NE2	3:I:1064:GLU:OE1	2.37	0.53
3:I:2178:MET:HE3	3:I:2182:ILE:HD11	1.90	0.53
3:A:3157:ILE:HA	3:A:3161:VAL:HB	1.91	0.53
3:A:4238:CYS:HA	3:A:4989:MET:HE1	1.89	0.53
3:G:3233:PRO:HB2	3:G:3238:GLU:HB2	1.90	0.53
3:A:913:LEU:HD12	3:A:914:PRO:HD2	1.89	0.53
3:G:3850:GLN:NE2	3:G:3872:GLU:OE1	2.36	0.53
3:G:3940:LYS:O	3:G:4002:LYS:NZ	2.39	0.53
1:D:27:ILE:HB	1:D:63:ILE:HB	1.90	0.53
3:A:3628:ARG:NH1	3:A:3857:GLY:O	2.42	0.53
3:G:400:ALA:HA	3:G:403:MET:HE3	1.91	0.53
3:G:913:LEU:HD12	3:G:914:PRO:HD2	1.89	0.53
3:A:2970:SER:HA	3:A:2973:PHE:CE2	2.43	0.53
3:B:228:ASP:OD2	3:I:155:LYS:NZ	2.34	0.53
3:G:975:VAL:HG12	3:G:1044:ARG:HH11	1.74	0.53
3:G:4138:ASP:O	3:G:4142:ASN:ND2	2.34	0.53
3:I:215:THR:HG22	3:I:273:HIS:HA	1.90	0.53
3:I:975:VAL:HG12	3:I:1044:ARG:HH11	1.74	0.53
3:B:1062:GLN:NE2	3:B:1064:GLU:OE1	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2178:MET:HE3	3:B:2182:ILE:HD11	1.90	0.53
3:B:3850:GLN:NE2	3:B:3872:GLU:OE1	2.36	0.53
3:G:3157:ILE:HA	3:G:3161:VAL:HB	1.91	0.53
3:B:2754:PHE:HE2	3:B:2813:LEU:HD11	1.74	0.52
3:A:215:THR:HG22	3:A:273:HIS:HA	1.90	0.52
3:B:2970:SER:HA	3:B:2973:PHE:CE2	2.43	0.52
3:B:3628:ARG:NH1	3:B:3857:GLY:O	2.42	0.52
3:G:1093:GLU:HB3	3:G:1201:HIS:HB3	1.92	0.52
3:G:3296:LEU:HG	3:G:3297:PRO:HD3	1.92	0.52
3:I:745:SER:HB2	3:I:758:ARG:HB2	1.91	0.52
3:I:4759:ASP:O	3:I:4761:PRO:HD3	2.09	0.52
1:C:1:ALA:HB3	3:B:3861:GLU:HG2	1.90	0.52
3:A:4759:ASP:O	3:A:4761:PRO:HD3	2.09	0.52
3:B:3157:ILE:HA	3:B:3161:VAL:HB	1.91	0.52
3:G:2754:PHE:HE2	3:G:2813:LEU:HD11	1.74	0.52
3:I:400:ALA:HA	3:I:403:MET:HE3	1.91	0.52
1:E:27:ILE:HB	1:E:63:ILE:HB	1.90	0.52
3:A:3296:LEU:HG	3:A:3297:PRO:HD3	1.92	0.52
3:B:70:GLU:OE2	3:B:110:ARG:NE	2.34	0.52
3:B:215:THR:HG22	3:B:273:HIS:HA	1.90	0.52
3:B:293:LEU:HD13	3:B:378:LEU:HD12	1.90	0.52
3:B:499:THR:HG23	3:B:502:HIS:H	1.74	0.52
3:A:3233:PRO:HB2	3:A:3238:GLU:HB2	1.90	0.52
3:I:1093:GLU:HB3	3:I:1201:HIS:HB3	1.92	0.52
3:I:3628:ARG:NH1	3:I:3857:GLY:O	2.42	0.52
1:C:27:ILE:HB	1:C:63:ILE:HB	1.90	0.52
3:A:499:THR:HG23	3:A:502:HIS:H	1.74	0.52
3:I:3813:GLN:NE2	3:I:3890:LEU:O	2.43	0.52
3:A:745:SER:HB2	3:A:758:ARG:HB2	1.91	0.52
3:A:1093:GLU:HB3	3:A:1201:HIS:HB3	1.92	0.52
3:B:2986:VAL:HG22	3:B:2988:LYS:H	1.75	0.52
3:B:3296:LEU:HG	3:B:3297:PRO:HD3	1.92	0.52
3:B:919:ASN:HA	3:B:922:LEU:HB2	1.92	0.52
3:G:215:THR:HG22	3:G:273:HIS:HA	1.90	0.52
3:G:499:THR:HG23	3:G:502:HIS:H	1.74	0.52
3:I:2986:VAL:HG22	3:I:2988:LYS:H	1.75	0.52
3:I:3157:ILE:HA	3:I:3161:VAL:HB	1.91	0.52
3:B:975:VAL:HG12	3:B:1044:ARG:HH11	1.74	0.52
3:B:1156:THR:OG1	3:B:1157:GLU:OE1	2.28	0.52
3:B:3288:GLY:HA2	3:B:3303:PRO:HB3	1.91	0.52
3:G:3288:GLY:HA2	3:G:3303:PRO:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:56:GLN:O	3:B:309:THR:OG1	2.19	0.51
3:B:3446:SER:O	3:B:3452:LYS:NZ	2.42	0.51
3:G:919:ASN:HA	3:G:922:LEU:HB2	1.92	0.51
3:I:3296:LEU:HG	3:I:3297:PRO:HD3	1.92	0.51
3:A:975:VAL:HG12	3:A:1044:ARG:HH11	1.74	0.51
3:A:3696:ASP:OD2	3:A:3773:ARG:NE	2.38	0.51
3:B:1093:GLU:HB3	3:B:1201:HIS:HB3	1.92	0.51
3:I:919:ASN:HA	3:I:922:LEU:HB2	1.92	0.51
3:B:955:LEU:O	3:B:966:LYS:NZ	2.31	0.51
3:G:3813:GLN:NE2	3:G:3890:LEU:O	2.43	0.51
3:G:4759:ASP:O	3:G:4761:PRO:HD3	2.09	0.51
3:A:400:ALA:HA	3:A:403:MET:HE3	1.91	0.51
3:B:400:ALA:HA	3:B:403:MET:HE3	1.91	0.51
3:B:4759:ASP:O	3:B:4761:PRO:HD3	2.09	0.51
3:G:408:ALA:HB2	3:G:483:MET:HE1	1.92	0.51
3:G:891:TRP:HA	3:G:902:ARG:HB3	1.93	0.51
3:I:3414:ARG:HE	3:I:3472:ALA:HB3	1.75	0.51
3:I:3850:GLN:NE2	3:I:3872:GLU:OE1	2.36	0.51
3:A:3288:GLY:HA2	3:A:3303:PRO:HB3	1.91	0.51
3:B:745:SER:HB2	3:B:758:ARG:HB2	1.91	0.51
3:B:3414:ARG:HE	3:B:3472:ALA:HB3	1.75	0.51
3:I:891:TRP:HA	3:I:902:ARG:HB3	1.93	0.51
3:I:3696:ASP:OD2	3:I:3773:ARG:NE	2.38	0.51
3:A:56:GLN:O	3:A:309:THR:OG1	2.19	0.51
3:A:891:TRP:HA	3:A:902:ARG:HB3	1.93	0.51
3:A:3850:GLN:NE2	3:A:3872:GLU:OE1	2.36	0.51
3:B:35:LEU:HD11	3:B:189:LEU:HD13	1.93	0.51
3:G:176:SER:OG	3:G:178:ARG:NH1	2.38	0.51
3:I:2754:PHE:HE2	3:I:2813:LEU:HD11	1.74	0.51
3:A:408:ALA:HB2	3:A:483:MET:HE1	1.92	0.51
3:A:1454:THR:OG1	3:A:1456:ASP:OD1	2.20	0.51
3:A:2754:PHE:HE2	3:A:2813:LEU:HD11	1.74	0.51
3:B:384:MET:SD	3:B:384:MET:N	2.77	0.51
3:I:499:THR:HG23	3:I:502:HIS:H	1.74	0.51
3:A:3414:ARG:HE	3:A:3472:ALA:HB3	1.75	0.51
3:I:3132:THR:HA	3:I:3136:LEU:HB3	1.93	0.51
3:B:3479:ALA:HA	3:I:1141:ARG:HB3	1.93	0.51
3:G:3552:PHE:O	3:G:3556:ASN:ND2	2.35	0.51
3:I:1992:ALA:HA	3:I:1995:THR:HG22	1.93	0.51
3:A:35:LEU:HD11	3:A:189:LEU:HD13	1.93	0.51
3:A:1272:LEU:HD22	3:A:1289:LEU:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3208:PRO:HB2	3:B:3237:GLU:HG3	1.93	0.51
3:I:228:ASP:OD1	3:I:228:ASP:N	2.44	0.51
3:I:955:LEU:O	3:I:966:LYS:NZ	2.31	0.51
1:C:130:ILE:O	3:B:3499:ARG:NH1	2.43	0.50
3:A:1057:ASP:OD1	3:A:1057:ASP:N	2.31	0.50
3:B:3813:GLN:NE2	3:B:3890:LEU:O	2.43	0.50
3:G:1272:LEU:HD22	3:G:1289:LEU:HD11	1.93	0.50
3:I:35:LEU:HD11	3:I:189:LEU:HD13	1.93	0.50
3:I:2736:ASP:OD1	3:I:2736:ASP:N	2.44	0.50
3:I:3288:GLY:HA2	3:I:3303:PRO:HB3	1.91	0.50
3:B:408:ALA:HB2	3:B:483:MET:HE1	1.92	0.50
3:G:3414:ARG:HE	3:G:3472:ALA:HB3	1.75	0.50
1:C:86:ARG:NH2	1:C:87:GLU:OE2	2.45	0.50
3:A:919:ASN:HA	3:A:922:LEU:HB2	1.92	0.50
3:B:891:TRP:HA	3:B:902:ARG:HB3	1.93	0.50
3:G:1289:LEU:HD12	3:G:1562:ILE:HD11	1.93	0.50
3:I:4138:ASP:O	3:I:4142:ASN:ND2	2.34	0.50
3:B:1272:LEU:HD22	3:B:1289:LEU:HD11	1.93	0.50
3:G:35:LEU:HD11	3:G:189:LEU:HD13	1.93	0.50
3:G:2986:VAL:HG22	3:G:2988:LYS:H	1.75	0.50
3:G:3132:THR:HA	3:G:3136:LEU:HB3	1.93	0.50
3:I:408:ALA:HB2	3:I:483:MET:HE1	1.92	0.50
3:I:1272:LEU:HD22	3:I:1289:LEU:HD11	1.93	0.50
2:F:88:PRO:HB2	3:A:1680:ARG:HH12	1.76	0.50
3:A:835:ARG:NH2	3:A:1210:SER:O	2.38	0.50
3:I:892:THR:HA	3:I:961:MET:HB3	1.94	0.50
3:A:892:THR:HA	3:A:961:MET:HB3	1.94	0.50
1:D:86:ARG:NH2	1:D:87:GLU:OE2	2.45	0.50
3:A:2986:VAL:HG22	3:A:2988:LYS:H	1.75	0.50
3:G:3628:ARG:NH1	3:G:3857:GLY:O	2.42	0.50
3:A:4138:ASP:O	3:A:4142:ASN:ND2	2.34	0.50
3:G:4172:GLU:OE1	3:G:4175:ARG:NH1	2.45	0.50
3:A:1992:ALA:HA	3:A:1995:THR:HG22	1.93	0.50
3:G:955:LEU:O	3:G:966:LYS:NZ	2.31	0.50
3:B:1733:GLU:HG2	3:B:2201:LEU:HD23	1.94	0.49
3:B:3132:THR:HA	3:B:3136:LEU:HB3	1.93	0.49
3:B:4172:GLU:OE1	3:B:4175:ARG:NH1	2.45	0.49
3:G:892:THR:HA	3:G:961:MET:HB3	1.94	0.49
3:G:1992:ALA:HA	3:G:1995:THR:HG22	1.93	0.49
3:G:3208:PRO:HB2	3:G:3237:GLU:HG3	1.93	0.49
3:A:1232:ARG:NH2	3:A:1828:ASP:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:4172:GLU:OE1	3:A:4175:ARG:NH1	2.45	0.49
3:I:2867:LEU:HB2	3:I:2928:LYS:HZ3	1.77	0.49
3:I:4801:LEU:HD22	9:I:5101:L9R:H13A	1.92	0.49
1:K:86:ARG:NH2	1:K:87:GLU:OE2	2.45	0.49
1:E:111:ASN:O	3:G:1996:ARG:NH2	2.34	0.49
3:A:1289:LEU:HD12	3:A:1562:ILE:HD11	1.93	0.49
3:A:1733:GLU:HG2	3:A:2201:LEU:HD23	1.94	0.49
1:E:66:PRO:HG3	3:G:2186:MET:HB3	1.94	0.49
3:A:1469:VAL:HG13	3:A:1492:CYS:HB3	1.95	0.49
3:B:892:THR:HA	3:B:961:MET:HB3	1.94	0.49
3:G:889:GLN:HB3	3:G:902:ARG:HH21	1.78	0.49
3:G:3133:THR:HG23	3:G:3134:VAL:HG23	1.94	0.49
3:I:1980:LEU:HD11	3:I:1994:ARG:HB3	1.94	0.49
3:A:3132:THR:HA	3:A:3136:LEU:HB3	1.93	0.49
3:A:4972:PRO:HB3	3:B:5024:ALA:HB3	1.94	0.49
3:B:228:ASP:OD1	3:B:228:ASP:N	2.44	0.49
3:B:1289:LEU:HD12	3:B:1562:ILE:HD11	1.93	0.49
3:G:4182:GLU:OE1	3:G:4983:HIS:NE2	2.46	0.49
3:I:3133:THR:HG23	3:I:3134:VAL:HG23	1.94	0.49
3:I:4172:GLU:OE1	3:I:4175:ARG:NH1	2.45	0.49
3:I:4182:GLU:OE1	3:I:4983:HIS:NE2	2.46	0.49
1:E:86:ARG:NH2	1:E:87:GLU:OE2	2.45	0.49
3:B:1992:ALA:HA	3:B:1995:THR:HG22	1.93	0.49
3:G:1232:ARG:NH2	3:G:1828:ASP:O	2.45	0.49
3:G:2867:LEU:HB2	3:G:2928:LYS:HZ3	1.77	0.49
3:I:1289:LEU:HD12	3:I:1562:ILE:HD11	1.93	0.49
3:I:3208:PRO:HB2	3:I:3237:GLU:HG3	1.93	0.49
3:A:2867:LEU:HB2	3:A:2928:LYS:HZ3	1.78	0.49
3:A:3208:PRO:HB2	3:A:3237:GLU:HG3	1.93	0.49
3:B:2884:ASN:OD1	3:B:2885:THR:N	2.46	0.49
3:A:4182:GLU:OE1	3:A:4983:HIS:NE2	2.46	0.49
3:A:4801:LEU:HD22	9:A:5308:L9R:H13A	1.93	0.49
3:B:1980:LEU:HD11	3:B:1994:ARG:HB3	1.94	0.49
3:B:3633:VAL:HG12	3:B:3637:ARG:HE	1.78	0.49
3:I:1733:GLU:HG2	3:I:2201:LEU:HD23	1.95	0.49
3:I:3459:VAL:HG13	3:I:3464:ILE:HB	1.95	0.49
3:A:3132:THR:HG22	3:A:3137:LEU:HD13	1.95	0.49
3:A:3133:THR:HG23	3:A:3134:VAL:HG23	1.94	0.49
3:A:5012:LYS:NZ	3:A:5016:GLU:OE2	2.41	0.49
3:B:2867:LEU:HB2	3:B:2928:LYS:HZ3	1.77	0.49
3:B:4182:GLU:OE1	3:B:4983:HIS:NE2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:2884:ASN:OD1	3:I:2885:THR:N	2.46	0.49
3:A:3633:VAL:HG12	3:A:3637:ARG:HE	1.78	0.49
3:B:1784:ALA:HA	2:O:55:VAL:HA	1.95	0.49
3:G:3633:VAL:HG12	3:G:3637:ARG:HE	1.78	0.49
3:I:3132:THR:HG22	3:I:3137:LEU:HD13	1.95	0.49
3:A:1447:CYS:HB3	3:A:1555:LEU:HB3	1.95	0.48
3:B:3459:VAL:HG13	3:B:3464:ILE:HB	1.95	0.48
3:G:228:ASP:OD1	3:G:228:ASP:N	2.44	0.48
3:G:1980:LEU:HD11	3:G:1994:ARG:HB3	1.94	0.48
3:G:2884:ASN:OD1	3:G:2885:THR:N	2.46	0.48
3:A:3459:VAL:HG13	3:A:3464:ILE:HB	1.95	0.48
3:B:889:GLN:HB3	3:B:902:ARG:HH21	1.78	0.48
3:B:990:GLU:HG3	3:B:1024:TYR:HB3	1.94	0.48
3:G:1733:GLU:HG2	3:G:2201:LEU:HD23	1.95	0.48
3:G:3514:LEU:HD21	3:G:3602:VAL:HG13	1.95	0.48
3:I:1680:ARG:HH12	2:J:88:PRO:HB2	1.77	0.48
3:I:4983:HIS:O	5:I:5102:ATP:N6	2.46	0.48
1:C:117:THR:OG1	1:C:120:GLU:OE1	2.31	0.48
3:A:4983:HIS:O	5:A:5301:ATP:N6	2.46	0.48
3:B:1232:ARG:NH2	3:B:1828:ASP:O	2.45	0.48
3:B:3514:LEU:HD21	3:B:3602:VAL:HG13	1.95	0.48
3:G:919:ASN:HA	3:G:922:LEU:HD23	1.96	0.48
3:G:990:GLU:HG3	3:G:1024:TYR:HB3	1.94	0.48
3:G:3459:VAL:HG13	3:G:3464:ILE:HB	1.95	0.48
3:G:4731:ILE:O	3:I:4074:SER:OG	2.31	0.48
3:I:2725:LYS:HE2	3:I:2738:ARG:HH22	1.79	0.48
3:A:889:GLN:HB3	3:A:902:ARG:HH21	1.78	0.48
3:B:1575:LEU:HD13	3:B:1579:MET:HE3	1.95	0.48
3:G:3545:THR:HG22	3:G:3548:GLU:HG3	1.95	0.48
3:G:3757:GLU:OE2	3:G:3761:GLN:NE2	2.46	0.48
3:I:919:ASN:HA	3:I:922:LEU:HD23	1.96	0.48
3:I:3633:VAL:HG12	3:I:3637:ARG:HE	1.78	0.48
3:A:228:ASP:OD1	3:A:228:ASP:N	2.44	0.48
3:A:516:LYS:O	3:A:520:ASN:ND2	2.31	0.48
3:A:1575:LEU:HD13	3:A:1579:MET:HE3	1.95	0.48
3:B:1447:CYS:HB3	3:B:1555:LEU:HB3	1.95	0.48
3:B:1469:VAL:HG13	3:B:1492:CYS:HB3	1.95	0.48
3:B:2725:LYS:HE2	3:B:2738:ARG:HH22	1.78	0.48
3:B:3133:THR:HG23	3:B:3134:VAL:HG23	1.94	0.48
3:G:2736:ASP:O	3:G:2738:ARG:NH1	2.47	0.48
3:I:990:GLU:HG3	3:I:1024:TYR:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1447:CYS:HB3	3:I:1555:LEU:HB3	1.95	0.48
3:I:3552:PHE:O	3:I:3556:ASN:ND2	2.35	0.48
9:I:5108:L9R:H6A	9:I:5108:L9R:H4A	1.47	0.48
3:A:1101:ARG:NH1	3:A:1115:LEU:O	2.46	0.48
3:A:3504:SER:HG	3:A:3507:THR:HG1	1.54	0.48
3:B:1101:ARG:NH1	3:B:1115:LEU:O	2.46	0.48
3:G:684:VAL:HG22	3:G:781:VAL:HG12	1.96	0.48
3:G:1780:PRO:HG2	2:H:42:ARG:HD3	1.96	0.48
3:G:2736:ASP:OD1	3:G:2736:ASP:N	2.44	0.48
3:G:3132:THR:HG22	3:G:3137:LEU:HD13	1.94	0.48
3:G:3316:LEU:HD21	3:G:3346:VAL:HG23	1.96	0.48
3:I:1469:VAL:HG13	3:I:1492:CYS:HB3	1.95	0.48
1:D:2:ASP:OD2	3:I:2244:ARG:NH1	2.46	0.48
3:A:919:ASN:HA	3:A:922:LEU:HD23	1.96	0.48
3:A:2884:ASN:OD1	3:A:2885:THR:N	2.46	0.48
3:A:4074:SER:OG	3:B:4731:ILE:O	2.31	0.48
3:B:925:SER:O	3:B:928:THR:OG1	2.32	0.48
3:G:1469:VAL:HG13	3:G:1492:CYS:HB3	1.95	0.48
3:I:728:ARG:NH2	3:I:1489:CYS:SG	2.87	0.48
3:I:1575:LEU:HD13	3:I:1579:MET:HE3	1.95	0.48
3:A:3316:LEU:HD21	3:A:3346:VAL:HG23	1.96	0.48
3:A:4731:ILE:O	3:G:4074:SER:OG	2.31	0.48
3:B:3132:THR:HG22	3:B:3137:LEU:HD13	1.95	0.48
3:B:4983:HIS:O	5:B:5301:ATP:N6	2.46	0.48
3:G:2725:LYS:HE2	3:G:2738:ARG:HH22	1.79	0.48
3:I:3757:GLU:OE2	3:I:3761:GLN:NE2	2.46	0.48
1:E:133:ASP:HA	3:G:3460:VAL:HG11	1.95	0.48
3:A:990:GLU:HG3	3:A:1024:TYR:HB3	1.94	0.48
3:A:2587:TYR:O	3:A:2590:SER:OG	2.31	0.48
3:A:3545:THR:HG22	3:A:3548:GLU:HG3	1.95	0.48
3:B:4555:LEU:HD21	3:B:4656:LEU:HD22	1.96	0.48
3:G:1447:CYS:HB3	3:G:1555:LEU:HB3	1.95	0.48
3:I:3545:THR:HG22	3:I:3548:GLU:HG3	1.95	0.48
3:I:4555:LEU:HD21	3:I:4656:LEU:HD22	1.96	0.48
3:A:793:LEU:HD12	3:A:821:LEU:HD21	1.96	0.48
3:A:3757:GLU:OE2	3:A:3761:GLN:NE2	2.46	0.48
3:B:728:ARG:NH2	3:B:1489:CYS:SG	2.87	0.48
3:B:793:LEU:HD12	3:B:821:LEU:HD21	1.96	0.48
3:B:3768:SER:HA	3:B:3771:HIS:CD2	2.49	0.48
3:G:3768:SER:HA	3:G:3771:HIS:CD2	2.49	0.48
3:I:1078:GLU:OE2	3:I:1654:SER:OG	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1503:PRO:HA	3:A:1508:ARG:HH22	1.79	0.47
3:A:1980:LEU:HD11	3:A:1994:ARG:HB3	1.94	0.47
3:A:2725:LYS:HE2	3:A:2738:ARG:HH22	1.79	0.47
3:A:2736:ASP:O	3:A:2738:ARG:NH1	2.47	0.47
3:B:919:ASN:HA	3:B:922:LEU:HD23	1.96	0.47
3:B:2736:ASP:O	3:B:2738:ARG:NH1	2.47	0.47
3:B:3757:GLU:OE2	3:B:3761:GLN:NE2	2.46	0.47
3:G:728:ARG:NH2	3:G:1489:CYS:SG	2.87	0.47
3:G:3946:GLN:OE1	3:G:3949:ARG:NH2	2.39	0.47
3:A:728:ARG:NH2	3:A:1489:CYS:SG	2.87	0.47
3:A:3263:TYR:HD1	3:A:3270:ILE:HD12	1.79	0.47
3:A:3768:SER:HA	3:A:3771:HIS:CD2	2.49	0.47
3:A:3813:GLN:NE2	3:A:3890:LEU:O	2.43	0.47
3:B:1503:PRO:HA	3:B:1508:ARG:HH22	1.79	0.47
3:B:3263:TYR:HD1	3:B:3270:ILE:HD12	1.79	0.47
3:B:3545:THR:HG22	3:B:3548:GLU:HG3	1.95	0.47
3:G:4983:HIS:O	5:G:5102:ATP:N6	2.46	0.47
3:I:889:GLN:HB3	3:I:902:ARG:HH21	1.78	0.47
3:I:1503:PRO:HA	3:I:1508:ARG:HH22	1.79	0.47
3:I:3514:LEU:HD21	3:I:3602:VAL:HG13	1.95	0.47
1:D:13:LYS:NZ	3:I:2187:ASN:O	2.43	0.47
3:A:176:SER:OG	3:A:178:ARG:NH1	2.38	0.47
3:A:935:LEU:HD23	3:A:987:ARG:HH11	1.80	0.47
3:I:2029:GLN:NE2	3:I:2033:ASP:OD1	2.48	0.47
3:I:2736:ASP:O	3:I:2738:ARG:NH1	2.47	0.47
3:I:3768:SER:HA	3:I:3771:HIS:CD2	2.49	0.47
1:C:13:LYS:NZ	3:B:2187:ASN:O	2.45	0.47
3:B:3552:PHE:O	3:B:3556:ASN:ND2	2.35	0.47
3:B:4006:ASP:OD1	3:B:4006:ASP:N	2.46	0.47
3:G:1575:LEU:HD13	3:G:1579:MET:HE3	1.95	0.47
3:I:2203:MET:HE3	3:I:2235:PHE:HZ	1.80	0.47
3:A:1569:GLN:HB2	3:A:1572:ILE:HD12	1.97	0.47
9:A:5308:L9R:H44	9:A:5308:L9R:H47A	1.52	0.47
3:I:793:LEU:HD12	3:I:821:LEU:HD21	1.96	0.47
3:I:925:SER:O	3:I:928:THR:OG1	2.32	0.47
3:B:935:LEU:HD23	3:B:987:ARG:HH11	1.80	0.47
3:B:4972:PRO:HB3	3:I:5024:ALA:HB3	1.96	0.47
3:G:793:LEU:HD12	3:G:821:LEU:HD21	1.96	0.47
3:G:835:ARG:NH2	3:G:1210:SER:O	2.38	0.47
3:G:3535:LEU:O	3:G:3538:THR:OG1	2.31	0.47
3:G:4006:ASP:OD1	3:G:4006:ASP:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:144:GLU:OE1	3:G:2452:ARG:NH1	2.47	0.47
3:A:2815:ALA:HB1	3:A:2881:ASN:HD22	1.80	0.47
3:A:3479:ALA:HA	3:B:1141:ARG:HB3	1.96	0.47
3:A:3514:LEU:HD21	3:A:3602:VAL:HG13	1.95	0.47
3:B:684:VAL:HG22	3:B:781:VAL:HG12	1.95	0.47
3:B:2020:ASP:OD1	3:B:2020:ASP:N	2.47	0.47
3:B:2029:GLN:NE2	3:B:2033:ASP:OD1	2.47	0.47
3:B:2815:ALA:HB1	3:B:2881:ASN:HD22	1.80	0.47
3:G:943:ASP:HB2	3:G:1050:GLY:HA3	1.97	0.47
3:G:1569:GLN:HB2	3:G:1572:ILE:HD12	1.97	0.47
3:G:2029:GLN:NE2	3:G:2033:ASP:OD1	2.47	0.47
3:G:4148:THR:HG21	3:G:4180:ARG:HH21	1.80	0.47
3:I:684:VAL:HG22	3:I:781:VAL:HG12	1.96	0.47
3:I:1101:ARG:NH1	3:I:1115:LEU:O	2.46	0.47
3:I:3343:GLN:O	3:I:3346:VAL:HG12	2.15	0.47
3:A:684:VAL:HG22	3:A:781:VAL:HG12	1.96	0.47
3:A:2029:GLN:NE2	3:A:2033:ASP:OD1	2.48	0.47
3:A:4006:ASP:N	3:A:4006:ASP:OD1	2.46	0.47
3:B:2626:LEU:HD22	3:B:2640:PRO:HB3	1.97	0.47
3:G:935:LEU:HD23	3:G:987:ARG:HH11	1.80	0.47
3:I:1232:ARG:NH2	3:I:1828:ASP:O	2.45	0.47
3:I:3316:LEU:HD21	3:I:3346:VAL:HG23	1.96	0.47
9:I:5101:L9R:H4A	9:I:5101:L9R:H7B	1.45	0.47
3:A:2538:THR:HG23	3:A:2541:PHE:H	1.80	0.47
3:A:3343:GLN:O	3:A:3346:VAL:HG12	2.15	0.47
9:A:5308:L9R:H7B	9:A:5308:L9R:H4A	1.45	0.47
3:B:872:GLU:HA	3:B:922:LEU:HD11	1.97	0.47
3:B:3343:GLN:O	3:B:3346:VAL:HG12	2.15	0.47
3:B:3862:ASP:OD1	3:B:3862:ASP:N	2.48	0.47
3:G:144:GLU:HG3	3:G:175:SER:HB3	1.96	0.47
3:G:815:VAL:O	3:G:1007:TYR:OH	2.27	0.47
3:G:1653:LEU:O	3:G:1660:GLN:NE2	2.48	0.47
3:G:2626:LEU:HD22	3:G:2640:PRO:HB3	1.97	0.47
3:I:2626:LEU:HD22	3:I:2640:PRO:HB3	1.97	0.47
3:I:2815:ALA:HB1	3:I:2881:ASN:HD22	1.80	0.47
3:I:3263:TYR:HD1	3:I:3270:ILE:HD12	1.79	0.47
1:E:94:LYS:HE3	1:E:107:HIS:HB3	1.97	0.47
3:A:872:GLU:HA	3:A:922:LEU:HD11	1.97	0.47
3:A:2626:LEU:HD22	3:A:2640:PRO:HB3	1.97	0.47
3:A:3862:ASP:OD1	3:A:3862:ASP:N	2.48	0.47
3:B:176:SER:OG	3:B:178:ARG:NH1	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1819:VAL:HG13	3:B:1929:MET:HE1	1.97	0.47
3:I:835:ARG:NH2	3:I:1210:SER:O	2.38	0.47
3:I:935:LEU:HD23	3:I:987:ARG:HH11	1.80	0.47
3:I:943:ASP:HB2	3:I:1050:GLY:HA3	1.97	0.47
3:I:1569:GLN:HB2	3:I:1572:ILE:HD12	1.97	0.47
3:A:2452:ARG:NH1	3:B:144:GLU:OE1	2.49	0.46
3:B:835:ARG:NH2	3:B:1210:SER:O	2.38	0.46
3:B:2203:MET:HE3	3:B:2235:PHE:HZ	1.80	0.46
3:G:2538:THR:HG23	3:G:2541:PHE:H	1.80	0.46
3:G:3343:GLN:O	3:G:3346:VAL:HG12	2.15	0.46
1:D:94:LYS:HE3	1:D:107:HIS:HB3	1.97	0.46
1:C:94:LYS:HE3	1:C:107:HIS:HB3	1.97	0.46
3:A:943:ASP:HB2	3:A:1050:GLY:HA3	1.97	0.46
3:B:1569:GLN:HB2	3:B:1572:ILE:HD12	1.97	0.46
3:B:3944:GLU:OE1	3:B:3946:GLN:N	2.47	0.46
3:G:1503:PRO:HA	3:G:1508:ARG:HH22	1.79	0.46
3:G:1771:LEU:HB3	3:G:2153:MET:HE3	1.98	0.46
3:G:1819:VAL:HG13	3:G:1929:MET:HE1	1.97	0.46
3:G:3263:TYR:HD1	3:G:3270:ILE:HD12	1.79	0.46
3:G:3412:LEU:HD11	3:G:3434:LEU:HD21	1.98	0.46
3:G:5024:ALA:HB3	3:I:4972:PRO:HB3	1.96	0.46
3:I:1819:VAL:HG13	3:I:1929:MET:HE1	1.97	0.46
3:I:2182:ILE:HG22	3:I:2186:MET:HE2	1.97	0.46
3:I:2538:THR:HG23	3:I:2541:PHE:H	1.80	0.46
3:A:1771:LEU:HB3	3:A:2153:MET:HE3	1.98	0.46
3:A:2182:ILE:HG22	3:A:2186:MET:HE2	1.97	0.46
3:A:2203:MET:HE3	3:A:2235:PHE:HZ	1.80	0.46
3:A:3412:LEU:HD11	3:A:3434:LEU:HD21	1.98	0.46
3:B:4074:SER:OG	3:I:4731:ILE:O	2.33	0.46
3:G:1101:ARG:NH1	3:G:1115:LEU:O	2.46	0.46
3:G:2182:ILE:HG22	3:G:2186:MET:HE2	1.97	0.46
3:G:2203:MET:HE3	3:G:2235:PHE:HZ	1.80	0.46
3:G:4555:LEU:HD21	3:G:4656:LEU:HD22	1.96	0.46
3:I:2587:TYR:O	3:I:2590:SER:OG	2.31	0.46
3:A:1819:VAL:HG13	3:A:1929:MET:HE1	1.97	0.46
3:B:3316:LEU:HD21	3:B:3346:VAL:HG23	1.96	0.46
3:G:4801:LEU:HD22	9:G:5101:L9R:H13A	1.97	0.46
3:I:144:GLU:HG3	3:I:175:SER:HB3	1.96	0.46
3:I:4687:TYR:OH	3:I:4699:GLY:O	2.26	0.46
3:A:144:GLU:HG3	3:A:175:SER:HB3	1.96	0.46
3:A:1465:ASP:OD1	3:A:1468:LYS:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1653:LEU:O	3:B:1660:GLN:NE2	2.48	0.46
3:B:3412:LEU:HD11	3:B:3434:LEU:HD21	1.97	0.46
3:G:1996:ARG:HH21	3:G:1999:ARG:HE	1.64	0.46
3:G:2815:ALA:HB1	3:G:2881:ASN:HD22	1.80	0.46
3:G:3604:TYR:O	3:G:3608:GLN:HG2	2.16	0.46
3:I:2020:ASP:OD1	3:I:2020:ASP:N	2.47	0.46
3:I:3946:GLN:OE1	3:I:3949:ARG:NH2	2.39	0.46
3:I:4006:ASP:OD1	3:I:4006:ASP:N	2.46	0.46
3:I:4148:THR:HG21	3:I:4180:ARG:HH21	1.80	0.46
1:K:94:LYS:HE3	1:K:107:HIS:HB3	1.97	0.46
3:A:3552:PHE:O	3:A:3556:ASN:ND2	2.35	0.46
3:G:943:ASP:OD2	3:G:945:LYS:NZ	2.47	0.46
3:A:4148:THR:HG21	3:A:4180:ARG:HH21	1.80	0.46
3:A:4555:LEU:HD21	3:A:4656:LEU:HD22	1.96	0.46
3:B:4801:LEU:HD22	9:B:5308:L9R:H13A	1.97	0.46
3:G:275:ARG:NH1	3:G:338:GLU:OE2	2.49	0.46
3:I:1465:ASP:OD1	3:I:1468:LYS:HG2	2.16	0.46
3:A:1810:LYS:HG2	3:A:1814:MET:HE2	1.98	0.46
3:B:2587:TYR:O	3:B:2590:SER:OG	2.31	0.46
3:B:2736:ASP:OD1	3:B:2736:ASP:N	2.44	0.46
3:G:886:ARG:HB3	3:G:891:TRP:CG	2.51	0.46
3:G:3842:LEU:HB2	3:G:3929:SER:HB2	1.98	0.46
3:I:663:TYR:CD2	3:I:804:PRO:HB3	2.51	0.46
3:I:1653:LEU:O	3:I:1660:GLN:NE2	2.48	0.46
1:K:117:THR:OG1	1:K:120:GLU:OE1	2.31	0.46
3:A:803:LEU:HD12	3:A:804:PRO:HD2	1.98	0.46
3:A:2309:SER:OG	3:A:2320:ASP:OD1	2.34	0.46
3:B:943:ASP:HB2	3:B:1050:GLY:HA3	1.97	0.46
3:B:2538:THR:HG23	3:B:2541:PHE:H	1.80	0.46
3:B:3840:SER:OG	3:B:3877:ASP:OD1	2.29	0.46
3:I:815:VAL:O	3:I:1007:TYR:OH	2.27	0.46
9:I:5108:L9R:H32A	9:I:5108:L9R:H35A	1.75	0.46
3:A:886:ARG:HB3	3:A:891:TRP:CG	2.51	0.46
3:I:2917:ALA:HA	3:I:2920:ARG:HB3	1.98	0.46
1:K:122:ASP:HA	1:K:125:ILE:HG22	1.99	0.45
1:E:117:THR:OG1	1:E:120:GLU:OE1	2.31	0.45
3:B:1024:TYR:CZ	3:B:1032:LYS:HG3	2.51	0.45
3:B:1771:LEU:HB3	3:B:2153:MET:HE3	1.98	0.45
3:B:2309:SER:OG	3:B:2320:ASP:OD1	2.34	0.45
3:B:2355:ARG:NH2	3:B:2449:GLU:OE2	2.49	0.45
3:B:3604:TYR:O	3:B:3608:GLN:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:4754:ASN:HB3	3:B:4756:ARG:HH21	1.81	0.45
3:I:1771:LEU:HB3	3:I:2153:MET:HE3	1.98	0.45
1:K:132:GLY:O	3:A:3456:GLN:NE2	2.43	0.45
3:A:1996:ARG:HH21	3:A:1999:ARG:HE	1.64	0.45
3:A:2917:ALA:HA	3:A:2920:ARG:HB3	1.98	0.45
3:A:3604:TYR:O	3:A:3608:GLN:HG2	2.16	0.45
3:B:144:GLU:HG3	3:B:175:SER:HB3	1.96	0.45
3:B:950:LEU:HD13	3:B:970:LEU:HG	1.99	0.45
3:G:663:TYR:CD2	3:G:804:PRO:HB3	2.51	0.45
9:G:5108:L9R:H6A	9:G:5108:L9R:H4A	1.46	0.45
3:I:943:ASP:OD2	3:I:945:LYS:NZ	2.47	0.45
1:C:2:ASP:OD2	3:B:2244:ARG:NH1	2.49	0.45
3:A:4000:MET:SD	3:A:4020:GLN:NE2	2.73	0.45
3:G:336:PRO:HA	3:G:337:PRO:HD3	1.88	0.45
3:G:803:LEU:HD12	3:G:804:PRO:HD2	1.98	0.45
3:I:872:GLU:HA	3:I:922:LEU:HD11	1.97	0.45
3:I:3412:LEU:HD11	3:I:3434:LEU:HD21	1.97	0.45
3:I:5012:LYS:NZ	3:I:5016:GLU:OE2	2.41	0.45
3:A:233:ILE:O	3:A:257:ARG:NH1	2.49	0.45
3:B:2182:ILE:HG22	3:B:2186:MET:HE2	1.97	0.45
3:B:4148:THR:HG21	3:B:4180:ARG:HH21	1.80	0.45
3:B:5012:LYS:NZ	3:B:5016:GLU:OE2	2.41	0.45
9:B:5307:L9R:H6A	9:B:5307:L9R:H4A	1.46	0.45
3:G:1024:TYR:CZ	3:G:1032:LYS:HG3	2.51	0.45
3:I:886:ARG:HB3	3:I:891:TRP:CG	2.51	0.45
3:A:663:TYR:CD2	3:A:804:PRO:HB3	2.51	0.45
3:B:758:ARG:HG2	3:B:763:PRO:HA	1.99	0.45
3:B:2917:ALA:HA	3:B:2920:ARG:HB3	1.99	0.45
3:G:1810:LYS:HG2	3:G:1814:MET:HE2	1.98	0.45
3:G:2309:SER:OG	3:G:2320:ASP:OD1	2.34	0.45
3:G:3862:ASP:OD1	3:G:3862:ASP:N	2.48	0.45
3:I:665:GLU:HB2	3:I:792:LEU:HB2	1.98	0.45
3:I:2309:SER:OG	3:I:2320:ASP:OD1	2.34	0.45
3:I:3604:TYR:O	3:I:3608:GLN:HG2	2.16	0.45
3:A:2974:ILE:HG13	3:A:2975:ALA:N	2.32	0.45
3:A:4754:ASN:HB3	3:A:4756:ARG:HH21	1.81	0.45
9:A:5307:L9R:H32A	9:A:5307:L9R:H35A	1.75	0.45
3:B:2974:ILE:HG13	3:B:2975:ALA:N	2.32	0.45
3:G:872:GLU:HA	3:G:922:LEU:HD11	1.97	0.45
3:G:2917:ALA:HA	3:G:2920:ARG:HB3	1.99	0.45
9:G:5101:L9R:H4A	9:G:5101:L9R:H7B	1.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1810:LYS:HG2	3:I:1814:MET:HE2	1.98	0.45
3:I:2881:ASN:HA	3:I:2884:ASN:ND2	2.32	0.45
3:I:2907:PRO:O	3:I:2910:THR:OG1	2.35	0.45
3:I:4754:ASN:HB3	3:I:4756:ARG:HH21	1.81	0.45
3:A:665:GLU:HB2	3:A:792:LEU:HB2	1.98	0.45
3:A:950:LEU:HD13	3:A:970:LEU:HG	1.99	0.45
3:A:1008:SER:HB3	3:A:1017:ARG:HB3	1.99	0.45
3:B:665:GLU:HB2	3:B:792:LEU:HB2	1.98	0.45
3:B:803:LEU:HD12	3:B:804:PRO:HD2	1.98	0.45
3:B:1099:GLU:OE2	3:B:1125:ASN:ND2	2.50	0.45
3:B:3842:LEU:HB2	3:B:3929:SER:HB2	1.98	0.45
3:G:1465:ASP:OD1	3:G:1468:LYS:HG2	2.16	0.45
3:I:1996:ARG:HH21	3:I:1999:ARG:HE	1.64	0.45
3:I:2677:LYS:HE2	3:I:2677:LYS:HB3	1.81	0.45
3:I:3840:SER:OG	3:I:3877:ASP:OD1	2.29	0.45
3:A:758:ARG:HG2	3:A:763:PRO:HA	1.99	0.45
3:A:2736:ASP:OD1	3:A:2736:ASP:N	2.44	0.45
3:A:3731:LYS:HA	3:A:3734:HIS:HE1	1.82	0.45
3:B:1008:SER:HB3	3:B:1017:ARG:HB3	1.99	0.45
3:G:2881:ASN:HA	3:G:2884:ASN:ND2	2.32	0.45
3:G:3226:GLU:C	3:G:3228:ALA:H	2.25	0.45
3:G:3731:LYS:HA	3:G:3734:HIS:CE1	2.52	0.45
3:I:803:LEU:HD12	3:I:804:PRO:HD2	1.98	0.45
3:I:3226:GLU:C	3:I:3228:ALA:H	2.25	0.45
3:I:3731:LYS:HA	3:I:3734:HIS:CE1	2.52	0.45
3:I:3842:LEU:HB2	3:I:3929:SER:HB2	1.98	0.45
1:E:122:ASP:HA	1:E:125:ILE:HG22	1.99	0.45
3:A:648:ILE:HG23	3:A:814:ALA:HB3	1.99	0.45
3:A:3731:LYS:HA	3:A:3734:HIS:CE1	2.52	0.45
3:B:663:TYR:CD2	3:B:804:PRO:HB3	2.51	0.45
3:B:2912:THR:OG1	3:B:2913:ALA:N	2.50	0.45
3:G:4648:LEU:HD12	3:G:4803:HIS:HE1	1.82	0.45
3:I:2355:ARG:NH2	3:I:2449:GLU:OE2	2.50	0.45
3:I:2974:ILE:HG13	3:I:2975:ALA:N	2.32	0.45
3:A:856:VAL:H	3:A:991:ASN:ND2	2.15	0.45
3:A:3842:LEU:HB2	3:A:3929:SER:HB2	1.98	0.45
3:A:4152:GLU:OE1	3:A:4194:TYR:OH	2.28	0.45
9:A:5308:L9R:H3A	9:B:5307:L9R:H33A	1.99	0.45
3:B:648:ILE:HG23	3:B:814:ALA:HB3	1.99	0.45
3:B:1465:ASP:OD1	3:B:1468:LYS:HG2	2.16	0.45
3:B:1810:LYS:HG2	3:B:1814:MET:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2452:ARG:NH1	3:I:144:GLU:OE1	2.50	0.45
3:G:2912:THR:OG1	3:G:2913:ALA:N	2.50	0.45
3:G:2974:ILE:HG13	3:G:2975:ALA:N	2.32	0.45
3:I:856:VAL:H	3:I:991:ASN:ND2	2.15	0.45
3:I:1024:TYR:CZ	3:I:1032:LYS:HG3	2.51	0.45
3:I:4661:TYR:OH	3:I:4786:ASP:OD2	2.33	0.45
2:O:4:VAL:HG22	2:O:74:LEU:HD22	1.99	0.45
3:A:275:ARG:NH1	3:A:338:GLU:OE2	2.49	0.44
3:A:4687:TYR:OH	3:A:4699:GLY:O	2.26	0.44
3:B:275:ARG:NH1	3:B:338:GLU:OE2	2.49	0.44
3:G:613:ALA:HB2	3:G:1676:LEU:HD12	1.99	0.44
3:G:3731:LYS:HA	3:G:3734:HIS:HE1	1.82	0.44
3:I:3872:GLU:HG3	3:I:3874:VAL:H	1.83	0.44
2:J:4:VAL:HG22	2:J:74:LEU:HD22	2.00	0.44
3:A:1024:TYR:CZ	3:A:1032:LYS:HG3	2.51	0.44
3:A:3332:ALA:HB3	3:A:3403:ARG:NH1	2.32	0.44
3:A:4640:GLU:HB3	3:A:4641:PRO:HD3	2.00	0.44
9:A:5307:L9R:H33A	9:G:5101:L9R:H3A	2.00	0.44
3:B:886:ARG:HB3	3:B:891:TRP:CG	2.51	0.44
3:B:1996:ARG:HH21	3:B:1999:ARG:HE	1.64	0.44
3:B:3731:LYS:HA	3:B:3734:HIS:HE1	1.82	0.44
3:I:275:ARG:NH1	3:I:338:GLU:OE2	2.49	0.44
3:I:3106:MET:HE2	3:I:3186:LEU:HD13	2.00	0.44
3:A:2020:ASP:OD1	3:A:2020:ASP:N	2.47	0.44
3:A:2821:TRP:HD1	3:A:2939:ARG:HA	1.82	0.44
3:A:3106:MET:HE2	3:A:3186:LEU:HD13	2.00	0.44
3:A:3805:LEU:HB3	3:A:3890:LEU:HB3	1.99	0.44
3:B:943:ASP:OD2	3:B:945:LYS:NZ	2.47	0.44
3:B:2821:TRP:HD1	3:B:2939:ARG:HA	1.82	0.44
3:G:1680:ARG:HH12	2:H:88:PRO:HB2	1.82	0.44
3:G:2355:ARG:NH2	3:G:2449:GLU:OE2	2.49	0.44
3:G:2875:ALA:HB2	3:G:2927:LEU:HD22	2.00	0.44
3:G:3332:ALA:HB3	3:G:3403:ARG:NH1	2.32	0.44
3:G:3872:GLU:HG3	3:G:3874:VAL:H	1.82	0.44
3:I:2912:THR:OG1	3:I:2913:ALA:N	2.50	0.44
1:D:122:ASP:HA	1:D:125:ILE:HG22	1.99	0.44
3:A:2881:ASN:HA	3:A:2884:ASN:ND2	2.32	0.44
3:A:2912:THR:OG1	3:A:2913:ALA:N	2.50	0.44
3:B:2633:LEU:O	3:B:2689:LYS:NZ	2.51	0.44
3:B:3106:MET:HE2	3:B:3186:LEU:HD13	2.00	0.44
3:G:952:LYS:HD3	3:G:970:LEU:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1008:SER:HB3	3:G:1017:ARG:HB3	1.99	0.44
3:G:3171:SER:O	3:G:3174:SER:OG	2.30	0.44
9:G:5108:L9R:H33A	9:I:5101:L9R:H3A	1.99	0.44
3:I:176:SER:OG	3:I:178:ARG:NH1	2.38	0.44
3:I:758:ARG:HG2	3:I:763:PRO:HA	1.99	0.44
3:I:952:LYS:HD3	3:I:970:LEU:HA	2.00	0.44
3:A:923:GLN:O	3:A:927:GLU:HG2	2.18	0.44
3:A:2355:ARG:NH2	3:A:2449:GLU:OE2	2.50	0.44
3:A:3946:GLN:OE1	3:A:3949:ARG:NH2	2.39	0.44
3:B:856:VAL:H	3:B:991:ASN:ND2	2.15	0.44
3:B:4000:MET:SD	3:B:4020:GLN:NE2	2.73	0.44
3:B:4640:GLU:HB3	3:B:4641:PRO:HD3	2.00	0.44
9:B:5308:L9R:H3A	9:I:5108:L9R:H33A	1.99	0.44
3:G:3106:MET:HE2	3:G:3186:LEU:HD13	2.00	0.44
3:G:4177:TYR:CE1	3:G:4199:GLU:HG3	2.53	0.44
3:I:2821:TRP:HD1	3:I:2939:ARG:HA	1.83	0.44
3:I:3442:PHE:CG	3:I:3514:LEU:HD22	2.53	0.44
3:I:3805:LEU:HB3	3:I:3890:LEU:HB3	1.99	0.44
3:I:4640:GLU:HB3	3:I:4641:PRO:HD3	2.00	0.44
3:I:4648:LEU:HD12	3:I:4803:HIS:HE1	1.82	0.44
1:K:85:ILE:H	1:K:85:ILE:HG13	1.57	0.44
3:A:613:ALA:HB2	3:A:1676:LEU:HD12	2.00	0.44
3:A:783:PHE:HB2	3:A:787:VAL:HG21	1.99	0.44
3:A:1694:LEU:HB3	3:A:1715:LEU:HD12	2.00	0.44
3:A:3872:GLU:HG3	3:A:3874:VAL:H	1.82	0.44
3:B:69:LEU:HD13	3:B:101:LEU:HD11	1.99	0.44
3:B:932:LEU:HD21	3:B:988:LEU:HD11	2.00	0.44
3:B:3332:ALA:HB3	3:B:3403:ARG:NH1	2.32	0.44
3:B:4177:TYR:CE1	3:B:4199:GLU:HG3	2.53	0.44
3:G:69:LEU:HD13	3:G:101:LEU:HD11	1.99	0.44
3:G:758:ARG:HG2	3:G:763:PRO:HA	1.99	0.44
3:G:2108:GLU:O	3:G:3694:LYS:NZ	2.51	0.44
3:G:2633:LEU:O	3:G:2689:LYS:NZ	2.51	0.44
3:G:4648:LEU:HD12	3:G:4803:HIS:CE1	2.53	0.44
3:I:1008:SER:HB3	3:I:1017:ARG:HB3	1.99	0.44
3:I:3731:LYS:HA	3:I:3734:HIS:HE1	1.82	0.44
3:I:4177:TYR:CE1	3:I:4199:GLU:HG3	2.53	0.44
1:C:111:ASN:O	3:B:1996:ARG:NH2	2.36	0.44
3:A:4648:LEU:HD12	3:A:4803:HIS:CE1	2.53	0.44
3:B:783:PHE:HB2	3:B:787:VAL:HG21	1.99	0.44
3:B:1820:ARG:O	3:B:1824:GLN:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3731:LYS:HA	3:B:3734:HIS:CE1	2.52	0.44
3:G:4000:MET:SD	3:G:4020:GLN:NE2	2.73	0.44
3:G:4754:ASN:HB3	3:G:4756:ARG:HH21	1.81	0.44
3:G:4818:MET:HA	3:G:4824:ARG:HH11	1.83	0.44
9:G:5101:L9R:H23	9:G:5101:L9R:H20	1.32	0.44
3:I:950:LEU:HD13	3:I:970:LEU:HG	1.99	0.44
2:H:4:VAL:HG22	2:H:74:LEU:HD22	2.00	0.44
3:B:923:GLN:O	3:B:927:GLU:HG2	2.18	0.44
3:B:3872:GLU:HG3	3:B:3874:VAL:H	1.82	0.44
3:G:648:ILE:HG23	3:G:814:ALA:HB3	1.99	0.44
3:G:856:VAL:H	3:G:991:ASN:ND2	2.15	0.44
3:G:950:LEU:HD13	3:G:970:LEU:HG	1.99	0.44
3:G:3752:SER:OG	3:G:3755:GLU:OE1	2.34	0.44
3:I:2633:LEU:O	3:I:2689:LYS:NZ	2.51	0.44
3:I:2875:ALA:HB2	3:I:2927:LEU:HD22	2.00	0.44
1:C:122:ASP:HA	1:C:125:ILE:HG22	1.98	0.44
3:A:664:PHE:HB3	3:A:811:CYS:SG	2.58	0.44
3:A:943:ASP:OD2	3:A:945:LYS:NZ	2.47	0.44
3:A:4648:LEU:HD12	3:A:4803:HIS:HE1	1.82	0.44
3:A:4818:MET:HA	3:A:4824:ARG:HH11	1.83	0.44
3:A:5024:ALA:HB3	3:G:4972:PRO:HB3	1.98	0.44
3:B:1716:ILE:O	3:B:1721:GLU:N	2.51	0.44
3:B:2765:LYS:HA	3:B:2765:LYS:HD3	1.78	0.44
3:B:3226:GLU:C	3:B:3228:ALA:H	2.25	0.44
3:B:4648:LEU:HD12	3:B:4803:HIS:HE1	1.82	0.44
3:G:979:PRO:O	3:G:982:THR:OG1	2.33	0.44
3:G:2821:TRP:HD1	3:G:2939:ARG:HA	1.82	0.44
3:G:4640:GLU:HB3	3:G:4641:PRO:HD3	2.00	0.44
3:I:664:PHE:HB3	3:I:811:CYS:SG	2.58	0.44
3:I:783:PHE:HB2	3:I:787:VAL:HG21	1.99	0.44
3:I:3230:LEU:H	3:I:3230:LEU:HD23	1.83	0.44
1:C:85:ILE:H	1:C:85:ILE:HG13	1.57	0.43
3:A:932:LEU:HD21	3:A:988:LEU:HD11	2.00	0.43
3:A:1653:LEU:O	3:A:1660:GLN:NE2	2.48	0.43
3:A:2633:LEU:O	3:A:2689:LYS:NZ	2.51	0.43
3:A:2875:ALA:HB2	3:A:2927:LEU:HD22	2.00	0.43
3:A:3446:SER:O	3:A:3452:LYS:NZ	2.42	0.43
3:A:3752:SER:OG	3:A:3755:GLU:OE1	2.34	0.43
3:A:4177:TYR:CE1	3:A:4199:GLU:HG3	2.53	0.43
3:A:4205:TRP:HZ3	3:A:4989:MET:HE3	1.83	0.43
3:G:923:GLN:O	3:G:927:GLU:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1141:ARG:HB3	3:I:3479:ALA:HA	2.00	0.43
3:G:4861:LYS:H	3:G:4861:LYS:HG3	1.53	0.43
3:I:2765:LYS:HD3	3:I:2765:LYS:HA	1.78	0.43
3:I:3621:HIS:ND1	3:I:3623:LEU:HD23	2.33	0.43
3:I:3862:ASP:OD1	3:I:3862:ASP:N	2.48	0.43
3:A:815:VAL:O	3:A:1007:TYR:OH	2.27	0.43
3:A:1820:ARG:O	3:A:1824:GLN:HG2	2.18	0.43
3:A:3442:PHE:CG	3:A:3514:LEU:HD22	2.53	0.43
3:A:3556:ASN:HB3	3:A:3559:LEU:HD13	2.00	0.43
3:B:952:LYS:HD3	3:B:970:LEU:HA	2.00	0.43
3:B:3805:LEU:HB3	3:B:3890:LEU:HB3	1.99	0.43
3:G:664:PHE:HB3	3:G:811:CYS:SG	2.58	0.43
3:G:2580:ASP:OD1	3:G:2621:HIS:HB2	2.19	0.43
3:I:451:TYR:CZ	3:I:474:ARG:HD2	2.53	0.43
3:I:1780:PRO:HG2	2:J:42:ARG:HD3	1.99	0.43
2:F:4:VAL:HG22	2:F:74:LEU:HD22	2.00	0.43
3:A:3123:LYS:HG3	3:A:3125:VAL:H	1.83	0.43
3:A:3621:HIS:C	3:A:3622:LYS:HG3	2.43	0.43
3:B:233:ILE:O	3:B:257:ARG:NH1	2.49	0.43
3:B:451:TYR:CZ	3:B:474:ARG:HD2	2.53	0.43
3:B:664:PHE:HB3	3:B:811:CYS:SG	2.58	0.43
3:B:2881:ASN:HA	3:B:2884:ASN:ND2	2.32	0.43
3:B:3852:LYS:HE3	3:B:3852:LYS:HB3	1.89	0.43
3:G:3123:LYS:HG3	3:G:3125:VAL:H	1.83	0.43
3:G:4205:TRP:HZ3	3:G:4989:MET:HE3	1.84	0.43
3:I:1694:LEU:HB3	3:I:1715:LEU:HD12	2.00	0.43
3:I:3332:ALA:HB3	3:I:3403:ARG:NH1	2.32	0.43
3:I:3535:LEU:O	3:I:3538:THR:OG1	2.31	0.43
3:B:1022:VAL:HG22	3:B:1023:PRO:HD2	2.01	0.43
3:B:2764:GLU:HG3	3:B:2857:PRO:HB3	2.01	0.43
3:B:3621:HIS:C	3:B:3622:LYS:HG3	2.43	0.43
3:G:1099:GLU:OE2	3:G:1125:ASN:ND2	2.50	0.43
3:G:3689:GLU:C	3:G:3691:GLU:H	2.26	0.43
3:G:3805:LEU:HB3	3:G:3890:LEU:HB3	1.99	0.43
3:I:1168:VAL:HG11	3:I:1176:GLU:HG2	2.00	0.43
3:I:2888:ARG:O	3:I:2892:GLN:HG2	2.18	0.43
3:I:3752:SER:OG	3:I:3755:GLU:OE1	2.35	0.43
3:I:4205:TRP:HZ3	3:I:4989:MET:HE3	1.83	0.43
9:I:5101:L9R:H47A	9:I:5101:L9R:H44	1.53	0.43
3:A:2108:GLU:O	3:A:3694:LYS:NZ	2.51	0.43
3:A:2580:ASP:OD1	3:A:2621:HIS:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2764:GLU:HG3	3:A:2857:PRO:HB3	2.01	0.43
3:A:3159:ASP:OD1	3:A:3159:ASP:N	2.52	0.43
3:A:3226:GLU:C	3:A:3228:ALA:H	2.25	0.43
3:A:3621:HIS:ND1	3:A:3623:LEU:HD23	2.33	0.43
3:A:3852:LYS:HE3	3:A:3852:LYS:HB3	1.89	0.43
3:A:4967:TYR:OH	3:A:5033:GLU:OE2	2.29	0.43
3:B:1168:VAL:HG11	3:B:1176:GLU:HG2	2.00	0.43
3:B:1694:LEU:HB3	3:B:1715:LEU:HD12	2.00	0.43
3:B:2677:LYS:HB3	3:B:2677:LYS:HE2	1.81	0.43
3:G:665:GLU:HB2	3:G:792:LEU:HB2	1.98	0.43
3:G:3621:HIS:C	3:G:3622:LYS:HG3	2.43	0.43
3:I:328:LYS:HE3	3:I:328:LYS:HB3	1.80	0.43
3:I:2580:ASP:OD1	3:I:2621:HIS:HB2	2.19	0.43
2:J:25:HIS:CD2	2:J:104:LEU:HD11	2.54	0.43
2:F:42:ARG:HD3	3:A:1780:PRO:HG2	2.01	0.43
1:D:117:THR:OG1	1:D:120:GLU:OE1	2.31	0.43
3:A:365:LYS:HB3	3:A:365:LYS:HE3	1.80	0.43
3:A:1099:GLU:OE2	3:A:1125:ASN:ND2	2.50	0.43
3:A:3230:LEU:HD23	3:A:3230:LEU:H	1.83	0.43
3:B:11:VAL:HG11	3:B:164:ARG:HD3	2.01	0.43
3:G:783:PHE:HB2	3:G:787:VAL:HG21	1.99	0.43
3:I:169:LEU:HD22	3:I:202:MET:HG3	2.00	0.43
3:I:613:ALA:HB2	3:I:1676:LEU:HD12	1.99	0.43
3:I:923:GLN:O	3:I:927:GLU:HG2	2.18	0.43
3:I:1022:VAL:HG22	3:I:1023:PRO:HD2	2.01	0.43
3:I:1206:GLN:HA	3:I:1227:ALA:O	2.18	0.43
3:I:1773:PRO:HA	3:I:1774:PRO:HD3	1.90	0.43
3:I:4818:MET:HA	3:I:4824:ARG:HH11	1.83	0.43
2:O:25:HIS:CD2	2:O:104:LEU:HD11	2.54	0.43
3:A:69:LEU:HD13	3:A:101:LEU:HD11	1.99	0.43
3:A:451:TYR:CZ	3:A:474:ARG:HD2	2.53	0.43
3:A:2888:ARG:O	3:A:2892:GLN:HG2	2.18	0.43
3:B:613:ALA:HB2	3:B:1676:LEU:HD12	1.99	0.43
3:B:2580:ASP:OD1	3:B:2621:HIS:HB2	2.19	0.43
3:B:3442:PHE:CG	3:B:3514:LEU:HD22	2.53	0.43
3:B:3556:ASN:HB3	3:B:3559:LEU:HD13	2.00	0.43
3:B:4205:TRP:CZ3	3:B:4989:MET:HE3	2.54	0.43
3:G:11:VAL:HG11	3:G:164:ARG:HD3	2.01	0.43
3:I:69:LEU:HD13	3:I:101:LEU:HD11	1.99	0.43
3:I:648:ILE:HG23	3:I:814:ALA:HB3	1.99	0.43
3:I:932:LEU:HD21	3:I:988:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1057:ASP:OD1	3:I:1057:ASP:N	2.31	0.43
3:I:1753:LYS:HB3	3:I:1758:ARG:HA	2.01	0.43
3:I:2108:GLU:O	3:I:3694:LYS:NZ	2.51	0.43
3:I:3621:HIS:C	3:I:3622:LYS:HG3	2.44	0.43
3:I:4648:LEU:HD12	3:I:4803:HIS:CE1	2.53	0.43
3:A:11:VAL:HG11	3:A:164:ARG:HD3	2.01	0.43
3:A:1022:VAL:HG22	3:A:1023:PRO:HD2	2.01	0.43
3:A:1168:VAL:HG11	3:A:1176:GLU:HG2	2.00	0.43
3:A:4661:TYR:OH	3:A:4786:ASP:OD2	2.33	0.43
3:B:2875:ALA:HB2	3:B:2927:LEU:HD22	2.00	0.43
3:B:3621:HIS:ND1	3:B:3623:LEU:HD23	2.33	0.43
3:I:11:VAL:HG11	3:I:164:ARG:HD3	2.01	0.43
3:I:232:THR:HG21	3:I:252:VAL:HG21	2.01	0.43
3:A:952:LYS:HD3	3:A:970:LEU:HA	2.00	0.43
3:A:1206:GLN:HA	3:A:1227:ALA:O	2.18	0.43
3:A:3391:GLU:HG3	3:A:3395:ARG:HE	1.84	0.43
3:A:3392:LEU:HD13	3:A:3395:ARG:HD2	2.01	0.43
3:A:3944:GLU:OE1	3:A:3946:GLN:N	2.47	0.43
3:A:4205:TRP:CZ3	3:A:4989:MET:HE3	2.54	0.43
9:A:5307:L9R:H6A	9:A:5307:L9R:H4A	1.46	0.43
3:B:169:LEU:HD22	3:B:202:MET:HG3	2.00	0.43
3:B:2108:GLU:O	3:B:3694:LYS:NZ	2.51	0.43
3:B:3123:LYS:HG3	3:B:3125:VAL:H	1.83	0.43
3:B:4648:LEU:HD12	3:B:4803:HIS:CE1	2.53	0.43
3:G:2888:ARG:O	3:G:2892:GLN:HG2	2.18	0.43
3:G:3442:PHE:CG	3:G:3514:LEU:HD22	2.53	0.43
3:G:3556:ASN:HB3	3:G:3559:LEU:HD13	1.99	0.43
3:I:233:ILE:O	3:I:257:ARG:NH1	2.49	0.43
3:I:2801:ASP:HA	3:I:2804:ILE:HG12	2.01	0.43
2:O:17:LYS:HE3	2:O:17:LYS:HB3	1.84	0.43
3:A:925:SER:O	3:A:928:THR:OG1	2.32	0.43
3:B:2021:CYS:O	3:B:2028:ARG:NH2	2.52	0.43
3:G:451:TYR:CZ	3:G:474:ARG:HD2	2.53	0.43
3:G:1022:VAL:HG22	3:G:1023:PRO:HD2	2.01	0.43
3:G:3230:LEU:H	3:G:3230:LEU:HD23	1.82	0.43
3:G:3269:VAL:HA	3:G:3273:THR:HB	2.01	0.43
3:G:3391:GLU:HG3	3:G:3395:ARG:HE	1.84	0.43
3:G:3621:HIS:ND1	3:G:3623:LEU:HD23	2.33	0.43
3:I:3689:GLU:C	3:I:3691:GLU:H	2.26	0.43
1:C:133:ASP:HA	3:B:3460:VAL:HG11	2.01	0.42
3:A:3628:ARG:HG3	3:A:3631:ALA:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3171:SER:O	3:B:3174:SER:OG	2.30	0.42
3:B:3384:LYS:HD2	3:B:3386:GLU:HB3	2.01	0.42
3:B:3392:LEU:HD13	3:B:3395:ARG:HD2	2.01	0.42
3:B:4818:MET:HA	3:B:4824:ARG:HH11	1.83	0.42
3:G:1168:VAL:HG11	3:G:1176:GLU:HG2	2.00	0.42
3:I:1154:ASP:OD1	3:I:1156:THR:OG1	2.37	0.42
3:I:1948:ASP:OD1	3:I:2126:ARG:NH2	2.48	0.42
3:I:4205:TRP:CZ3	3:I:4989:MET:HE3	2.54	0.42
2:F:25:HIS:CD2	2:F:104:LEU:HD11	2.54	0.42
3:A:1716:ILE:O	3:A:1721:GLU:N	2.51	0.42
3:A:2661:TRP:HB3	3:A:2664:PHE:HB2	2.01	0.42
3:B:3230:LEU:H	3:B:3230:LEU:HD23	1.83	0.42
3:B:4910:GLU:O	3:B:4914:VAL:HG13	2.19	0.42
3:G:365:LYS:HE3	3:G:365:LYS:HB3	1.81	0.42
3:G:932:LEU:HD21	3:G:988:LEU:HD11	2.00	0.42
3:G:3392:LEU:HD13	3:G:3395:ARG:HD2	2.01	0.42
3:G:4205:TRP:CZ3	3:G:4989:MET:HE3	2.54	0.42
9:G:5108:L9R:H32A	9:G:5108:L9R:H35A	1.75	0.42
3:I:233:ILE:HD12	3:I:242:ARG:HB3	2.01	0.42
3:I:1716:ILE:O	3:I:1721:GLU:N	2.51	0.42
3:I:1820:ARG:O	3:I:1824:GLN:HG2	2.18	0.42
3:I:3384:LYS:HD2	3:I:3386:GLU:HB3	2.01	0.42
3:I:3556:ASN:HB3	3:I:3559:LEU:HD13	1.99	0.42
3:A:169:LEU:HD22	3:A:202:MET:HG3	2.00	0.42
3:A:1753:LYS:HB3	3:A:1758:ARG:HA	2.01	0.42
3:A:2801:ASP:HA	3:A:2804:ILE:HG12	2.01	0.42
3:A:3414:ARG:HH21	3:A:3472:ALA:H	1.67	0.42
3:B:233:ILE:HD12	3:B:242:ARG:HB3	2.01	0.42
3:B:892:THR:HB	3:B:962:SER:H	1.84	0.42
3:G:719:LEU:HD11	2:H:7:ILE:HA	2.01	0.42
3:G:4152:GLU:OE1	3:G:4194:TYR:OH	2.28	0.42
3:I:2764:GLU:HG3	3:I:2857:PRO:HB3	2.01	0.42
2:H:25:HIS:CD2	2:H:104:LEU:HD11	2.54	0.42
1:K:30:LYS:HE3	1:K:30:LYS:HB3	1.94	0.42
1:E:1:ALA:HB3	3:G:3861:GLU:HG2	2.01	0.42
1:E:26:THR:HB	1:E:62:THR:HB	2.02	0.42
3:A:1690:ASP:OD2	3:A:1693:GLN:NE2	2.52	0.42
3:A:3689:GLU:C	3:A:3691:GLU:H	2.26	0.42
3:B:1000:ARG:HB3	3:B:1005:TRP:HB2	2.01	0.42
3:B:3689:GLU:C	3:B:3691:GLU:H	2.26	0.42
3:G:2661:TRP:HB3	3:G:2664:PHE:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:2751:LEU:HD23	3:G:2751:LEU:H	1.84	0.42
3:I:3123:LYS:HG3	3:I:3125:VAL:H	1.83	0.42
1:C:66:PRO:HG3	3:B:2186:MET:HB3	2.02	0.42
1:C:120:GLU:HA	1:C:123:GLU:HG3	2.02	0.42
3:A:2514:ASN:OD1	3:A:2514:ASN:N	2.53	0.42
3:A:4910:GLU:O	3:A:4914:VAL:HG13	2.19	0.42
3:B:938:HIS:HB3	3:B:1054:GLU:HB3	2.01	0.42
3:B:1947:CYS:SG	3:B:2127:GLN:NE2	2.92	0.42
3:B:2888:ARG:O	3:B:2892:GLN:HG2	2.18	0.42
3:B:3003:LEU:HB2	3:B:3004:PRO:HD3	2.02	0.42
3:G:1154:ASP:OD1	3:G:1156:THR:OG1	2.37	0.42
3:G:2716:ASP:OD1	3:G:2716:ASP:N	2.53	0.42
3:G:2764:GLU:HG3	3:G:2857:PRO:HB3	2.01	0.42
3:I:788:LYS:HE3	3:I:788:LYS:HB2	1.84	0.42
3:I:3414:ARG:HH21	3:I:3472:ALA:H	1.67	0.42
1:D:111:ASN:O	3:I:1996:ARG:NH2	2.40	0.42
3:A:3235:SER:OG	3:A:3237:GLU:OE1	2.37	0.42
3:A:3269:VAL:HA	3:A:3273:THR:HB	2.01	0.42
3:B:1753:LYS:HB3	3:B:1758:ARG:HA	2.01	0.42
3:B:2751:LEU:HD23	3:B:2751:LEU:H	1.84	0.42
3:B:3284:TRP:HB3	3:B:3305:THR:HG21	2.02	0.42
3:G:169:LEU:HD22	3:G:202:MET:HG3	2.00	0.42
3:G:707:VAL:HG23	3:G:782:SER:HB3	2.02	0.42
3:G:1820:ARG:O	3:G:1824:GLN:HG2	2.18	0.42
3:G:2021:CYS:O	3:G:2028:ARG:NH2	2.52	0.42
3:G:3235:SER:OG	3:G:3237:GLU:OE1	2.37	0.42
3:G:3414:ARG:HH21	3:G:3472:ALA:H	1.67	0.42
3:A:2677:LYS:HE2	3:A:2677:LYS:HB3	1.81	0.42
3:G:925:SER:O	3:G:928:THR:OG1	2.32	0.42
3:G:1000:ARG:HB3	3:G:1005:TRP:HB2	2.01	0.42
3:G:1206:GLN:HA	3:G:1227:ALA:O	2.18	0.42
3:G:1690:ASP:OD2	3:G:1693:GLN:NE2	2.52	0.42
3:G:1716:ILE:O	3:G:1721:GLU:N	2.51	0.42
3:I:1099:GLU:OE2	3:I:1125:ASN:ND2	2.50	0.42
3:I:2661:TRP:HB3	3:I:2664:PHE:HB2	2.02	0.42
3:I:3003:LEU:HB2	3:I:3004:PRO:HD3	2.02	0.42
3:I:4910:GLU:O	3:I:4914:VAL:HG13	2.19	0.42
3:I:4967:TYR:OH	3:I:5033:GLU:OE2	2.29	0.42
1:C:26:THR:HB	1:C:62:THR:HB	2.02	0.42
3:A:892:THR:HB	3:A:962:SER:H	1.84	0.42
3:A:2021:CYS:O	3:A:2028:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2390:PRO:C	3:A:2392:ARG:H	2.28	0.42
3:A:3284:TRP:HB3	3:A:3305:THR:HG21	2.02	0.42
3:A:3384:LYS:HD2	3:A:3386:GLU:HB3	2.01	0.42
3:B:232:THR:HG21	3:B:252:VAL:HG21	2.01	0.42
3:B:863:LEU:HD11	3:B:930:LYS:NZ	2.35	0.42
3:B:901:LYS:HG3	3:B:903:LEU:HG	2.02	0.42
3:B:4205:TRP:HZ3	3:B:4989:MET:HE3	1.83	0.42
3:G:233:ILE:HD12	3:G:242:ARG:HB3	2.01	0.42
3:G:901:LYS:HD2	3:G:901:LYS:HA	1.84	0.42
3:G:1753:LYS:HB3	3:G:1758:ARG:HA	2.01	0.42
3:G:3628:ARG:HG3	3:G:3631:ALA:HB3	2.01	0.42
3:G:3944:GLU:OE1	3:G:3946:GLN:N	2.47	0.42
3:G:4091:LYS:HE2	3:G:4091:LYS:HB2	1.89	0.42
3:I:707:VAL:HG23	3:I:782:SER:HB3	2.02	0.42
3:I:2021:CYS:O	3:I:2028:ARG:NH2	2.52	0.42
1:K:120:GLU:HA	1:K:123:GLU:HG3	2.02	0.42
3:A:863:LEU:HD11	3:A:930:LYS:NZ	2.35	0.42
3:B:1948:ASP:OD1	3:B:2126:ARG:NH2	2.48	0.42
3:B:3235:SER:OG	3:B:3237:GLU:OE1	2.37	0.42
3:B:3269:VAL:HA	3:B:3273:THR:HB	2.01	0.42
3:B:3628:ARG:HG3	3:B:3631:ALA:HB3	2.01	0.42
3:B:3946:GLN:OE1	3:B:3949:ARG:NH2	2.39	0.42
3:B:4888:TYR:HE1	3:I:4917:ASP:HB2	1.84	0.42
9:B:5308:L9R:H23	9:B:5308:L9R:H20	1.32	0.42
3:G:4910:GLU:O	3:G:4914:VAL:HG13	2.19	0.42
3:I:892:THR:HB	3:I:962:SER:H	1.84	0.42
3:I:979:PRO:O	3:I:982:THR:OG1	2.33	0.42
3:I:1947:CYS:SG	3:I:2127:GLN:NE2	2.92	0.42
3:I:2514:ASN:OD1	3:I:2514:ASN:N	2.53	0.42
3:I:3390:GLY:HA2	3:I:3393:LEU:HD23	2.02	0.42
1:D:26:THR:HB	1:D:62:THR:HB	2.02	0.42
3:A:2212:VAL:HG11	3:A:2256:TYR:CE2	2.55	0.42
3:A:2263:ILE:HD12	3:A:2263:ILE:HA	1.95	0.42
3:A:2751:LEU:H	3:A:2751:LEU:HD23	1.84	0.42
3:B:1206:GLN:HA	3:B:1227:ALA:O	2.18	0.42
3:B:3390:GLY:HA2	3:B:3393:LEU:HD23	2.02	0.42
3:B:3535:LEU:O	3:B:3538:THR:OG1	2.31	0.42
3:G:870:ILE:HD12	3:G:870:ILE:HA	1.96	0.42
3:G:2519:LEU:HD22	3:G:2578:MET:HE1	2.02	0.42
3:G:2907:PRO:O	3:G:2910:THR:OG1	2.35	0.42
3:I:2858:GLN:HB2	3:I:2859:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3392:LEU:HD13	3:I:3395:ARG:HD2	2.01	0.42
1:D:120:GLU:HA	1:D:123:GLU:HG3	2.02	0.41
1:E:120:GLU:HA	1:E:123:GLU:HG3	2.02	0.41
1:E:144:MET:HE3	1:E:144:MET:HB3	1.94	0.41
3:B:336:PRO:HA	3:B:337:PRO:HD3	1.88	0.41
3:B:707:VAL:HG23	3:B:782:SER:HB3	2.02	0.41
3:B:872:GLU:HG2	3:B:922:LEU:HD21	2.02	0.41
3:B:1057:ASP:OD1	3:B:1057:ASP:N	2.31	0.41
3:B:2661:TRP:HB3	3:B:2664:PHE:HB2	2.01	0.41
3:G:232:THR:HG21	3:G:252:VAL:HG21	2.01	0.41
3:G:345:LEU:HB3	3:G:387:ALA:HB1	2.02	0.41
3:G:938:HIS:HB3	3:G:1054:GLU:HB3	2.01	0.41
3:G:1694:LEU:HB3	3:G:1715:LEU:HD12	2.00	0.41
3:G:2212:VAL:HG11	3:G:2256:TYR:CE2	2.55	0.41
3:G:4093:PHE:O	3:G:4097:MET:HG2	2.20	0.41
3:I:1690:ASP:OD2	3:I:1693:GLN:NE2	2.52	0.41
3:I:3269:VAL:HA	3:I:3273:THR:HB	2.01	0.41
3:A:901:LYS:HG3	3:A:903:LEU:HG	2.02	0.41
3:B:881:LEU:HD13	3:B:881:LEU:HA	1.92	0.41
3:G:892:THR:HB	3:G:962:SER:H	1.84	0.41
3:I:3235:SER:OG	3:I:3237:GLU:OE1	2.37	0.41
3:I:4046:ASP:OD1	3:I:4159:ARG:NH2	2.48	0.41
1:K:66:PRO:HG3	3:A:2192:TYR:OH	2.21	0.41
1:C:144:MET:HE3	1:C:144:MET:HB3	1.94	0.41
3:A:232:THR:HG21	3:A:252:VAL:HG21	2.01	0.41
3:A:233:ILE:HD12	3:A:242:ARG:HB3	2.01	0.41
3:A:4861:LYS:H	3:A:4861:LYS:HG3	1.53	0.41
3:B:2514:ASN:OD1	3:B:2514:ASN:N	2.53	0.41
3:B:2519:LEU:HD22	3:B:2578:MET:HE1	2.02	0.41
3:G:954:LYS:HB3	3:G:966:LYS:HE3	2.03	0.41
3:I:2751:LEU:H	3:I:2751:LEU:HD23	1.84	0.41
3:A:707:VAL:HG23	3:A:782:SER:HB3	2.02	0.41
3:A:1823:GLY:O	3:A:1825:HIS:ND1	2.52	0.41
3:B:1805:GLU:CD	3:B:1805:GLU:H	2.29	0.41
3:G:233:ILE:O	3:G:257:ARG:NH1	2.49	0.41
3:G:3384:LYS:HD2	3:G:3386:GLU:HB3	2.01	0.41
3:G:3852:LYS:HE3	3:G:3852:LYS:HB3	1.89	0.41
3:I:901:LYS:HG3	3:I:903:LEU:HG	2.02	0.41
3:I:3107:VAL:HG21	3:I:3171:SER:HB2	2.03	0.41
3:I:3391:GLU:HG3	3:I:3395:ARG:HE	1.84	0.41
1:C:69:LEU:HD23	1:C:69:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:797:HIS:CG	3:A:821:LEU:HD23	2.56	0.41
3:A:901:LYS:HD2	3:A:901:LYS:HA	1.84	0.41
3:A:938:HIS:HB3	3:A:1054:GLU:HB3	2.01	0.41
3:A:2716:ASP:OD1	3:A:2716:ASP:N	2.53	0.41
3:A:3147:ILE:HG23	3:A:3152:PHE:HB2	2.02	0.41
3:A:4825:THR:O	3:A:4828:SER:OG	2.32	0.41
3:A:4917:ASP:HB2	3:G:4888:TYR:HE1	1.84	0.41
3:B:2749:GLU:HG3	3:B:2752:ASP:HB2	2.03	0.41
3:B:3391:GLU:HG3	3:B:3395:ARG:HE	1.84	0.41
3:B:4093:PHE:O	3:B:4097:MET:HG2	2.20	0.41
3:G:462:GLU:HG3	3:G:3710:LEU:HD13	2.02	0.41
3:G:2514:ASN:OD1	3:G:2514:ASN:N	2.53	0.41
3:G:4060:LYS:HD2	3:G:4060:LYS:HA	1.91	0.41
3:I:938:HIS:HB3	3:I:1054:GLU:HB3	2.02	0.41
3:I:954:LYS:HB3	3:I:966:LYS:HE3	2.03	0.41
3:I:2390:PRO:C	3:I:2392:ARG:H	2.28	0.41
3:I:2775:TRP:CD2	3:I:2786:LYS:HE3	2.56	0.41
3:I:3628:ARG:HG3	3:I:3631:ALA:HB3	2.01	0.41
3:A:1154:ASP:OD1	3:A:1156:THR:OG1	2.37	0.41
3:A:2749:GLU:HG3	3:A:2752:ASP:HB2	2.03	0.41
3:A:2858:GLN:HB2	3:A:2859:PRO:HD3	2.02	0.41
3:A:3003:LEU:HB2	3:A:3004:PRO:HD3	2.02	0.41
3:B:330:ASP:OD1	3:B:330:ASP:N	2.53	0.41
3:B:2858:GLN:HB2	3:B:2859:PRO:HD3	2.02	0.41
3:B:4063:ASP:OD1	3:B:4064:MET:N	2.54	0.41
3:B:4241:THR:HG22	3:B:4245:MET:HE3	2.03	0.41
9:B:5308:L9R:H44	9:B:5308:L9R:H47A	1.52	0.41
3:G:144:GLU:OE1	3:I:2452:ARG:NH1	2.53	0.41
3:G:308:HIS:CE1	3:G:310:LYS:HB3	2.56	0.41
3:G:881:LEU:HD13	3:G:881:LEU:HA	1.92	0.41
3:G:1805:GLU:CD	3:G:1805:GLU:H	2.29	0.41
3:G:2801:ASP:HA	3:G:2804:ILE:HG12	2.01	0.41
3:G:2858:GLN:HB2	3:G:2859:PRO:HD3	2.02	0.41
3:G:3390:GLY:HA2	3:G:3393:LEU:HD23	2.02	0.41
3:G:5012:LYS:NZ	3:G:5016:GLU:OE2	2.41	0.41
3:I:2519:LEU:HD22	3:I:2578:MET:HE1	2.02	0.41
3:I:4063:ASP:OD1	3:I:4064:MET:N	2.54	0.41
2:F:27:THR:HG23	2:F:38:SER:HB2	2.03	0.41
3:A:872:GLU:HG2	3:A:922:LEU:HD21	2.03	0.41
3:A:1000:ARG:HB3	3:A:1005:TRP:HB2	2.01	0.41
3:A:2495:VAL:HG22	3:A:2498:HIS:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3249:LEU:HD23	3:A:3277:LEU:HD21	2.03	0.41
9:A:5308:L9R:H39	9:A:5308:L9R:H42A	1.76	0.41
3:B:2747:ILE:HD13	3:B:2814:LYS:HG2	2.02	0.41
3:B:3107:VAL:HG21	3:B:3171:SER:HB2	2.03	0.41
3:G:797:HIS:CG	3:G:821:LEU:HD23	2.56	0.41
3:G:1078:GLU:OE2	3:G:1654:SER:OG	2.26	0.41
3:G:3159:ASP:OD1	3:G:3159:ASP:N	2.52	0.41
3:G:3501:ASP:OD1	3:G:3501:ASP:N	2.54	0.41
3:G:4839:MET:HE2	3:I:4820:VAL:HG11	2.03	0.41
3:I:1000:ARG:HB3	3:I:1005:TRP:HB2	2.01	0.41
3:I:1805:GLU:CD	3:I:1805:GLU:H	2.29	0.41
3:I:2886:TRP:HA	3:I:2889:LYS:NZ	2.36	0.41
3:I:3284:TRP:HB3	3:I:3305:THR:HG21	2.02	0.41
3:A:880:GLU:CD	3:A:910:PHE:HB3	2.46	0.41
3:A:2519:LEU:HD22	3:A:2578:MET:HE1	2.02	0.41
3:A:2782:ASP:OD1	3:A:2782:ASP:N	2.54	0.41
3:A:3390:GLY:HA2	3:A:3393:LEU:HD23	2.02	0.41
3:A:3680:ALA:HB1	3:A:3683:GLN:NE2	2.36	0.41
3:B:462:GLU:HG3	3:B:3710:LEU:HD13	2.02	0.41
3:B:2886:TRP:HA	3:B:2889:LYS:NZ	2.36	0.41
3:B:2907:PRO:O	3:B:2910:THR:OG1	2.35	0.41
3:B:3590:GLU:CD	3:B:3590:GLU:H	2.29	0.41
3:G:2785:LEU:C	3:G:2786:LYS:HG3	2.46	0.41
3:G:3147:ILE:HG23	3:G:3152:PHE:HB2	2.02	0.41
3:G:3590:GLU:H	3:G:3590:GLU:CD	2.29	0.41
3:G:3680:ALA:HB1	3:G:3683:GLN:NE2	2.36	0.41
3:G:3688:GLU:C	3:G:3690:VAL:H	2.29	0.41
3:I:330:ASP:OD1	3:I:330:ASP:N	2.53	0.41
3:I:653:ALA:HB3	3:I:656:SER:HB2	2.03	0.41
3:I:863:LEU:HD11	3:I:930:LYS:NZ	2.35	0.41
3:I:872:GLU:HG2	3:I:922:LEU:HD21	2.03	0.41
3:I:1804:LEU:HD13	3:I:1853:ILE:HD12	2.03	0.41
3:I:2747:ILE:HD13	3:I:2814:LYS:HG2	2.02	0.41
3:I:3359:ILE:HG23	3:I:3437:MET:HE1	2.02	0.41
3:I:4091:LYS:HB2	3:I:4091:LYS:HE2	1.89	0.41
3:A:1575:LEU:HD23	3:A:1575:LEU:HA	1.90	0.41
3:A:1805:GLU:CD	3:A:1805:GLU:H	2.29	0.41
3:A:1997:GLU:O	3:A:2000:SER:OG	2.37	0.41
3:A:2785:LEU:C	3:A:2786:LYS:HG3	2.46	0.41
3:A:3590:GLU:H	3:A:3590:GLU:CD	2.29	0.41
3:B:275:ARG:HH21	3:B:328:LYS:HG3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:954:LYS:HB3	3:B:966:LYS:HE3	2.03	0.41
3:B:2212:VAL:HG11	3:B:2256:TYR:CE2	2.55	0.41
3:B:2495:VAL:HG22	3:B:2498:HIS:CE1	2.56	0.41
3:B:2801:ASP:HA	3:B:2804:ILE:HG12	2.01	0.41
3:B:3688:GLU:C	3:B:3690:VAL:H	2.29	0.41
3:B:4060:LYS:HD2	3:B:4060:LYS:HA	1.91	0.41
3:B:4687:TYR:OH	3:B:4699:GLY:O	2.26	0.41
3:G:901:LYS:HG3	3:G:903:LEU:HG	2.02	0.41
3:G:1997:GLU:O	3:G:2000:SER:OG	2.37	0.41
3:G:2749:GLU:HG3	3:G:2752:ASP:HB2	2.03	0.41
3:G:3107:VAL:HG21	3:G:3171:SER:HB2	2.03	0.41
3:G:3734:HIS:CG	3:G:3735:LEU:N	2.89	0.41
3:G:4661:TYR:OH	3:G:4786:ASP:OD2	2.33	0.41
3:G:4805:ASN:HD22	9:G:5101:L9R:C31	2.34	0.41
3:I:275:ARG:HH21	3:I:328:LYS:HG3	1.86	0.41
3:I:308:HIS:CE1	3:I:310:LYS:HB3	2.56	0.41
3:I:797:HIS:CG	3:I:821:LEU:HD23	2.56	0.41
3:I:870:ILE:HG12	3:I:1051:TYR:HE2	1.86	0.41
3:I:2212:VAL:HG11	3:I:2256:TYR:CE2	2.55	0.41
3:I:3590:GLU:H	3:I:3590:GLU:CD	2.29	0.41
3:I:4093:PHE:O	3:I:4097:MET:HG2	2.20	0.41
3:I:4880:MET:HE3	3:I:4880:MET:HB2	1.97	0.41
9:I:5101:L9R:H23	9:I:5101:L9R:H20	1.32	0.41
1:K:26:THR:HB	1:K:62:THR:HB	2.02	0.41
3:A:345:LEU:HB3	3:A:387:ALA:HB1	2.02	0.41
3:A:2751:LEU:O	3:A:2755:ILE:HG12	2.21	0.41
3:A:3157:ILE:HG23	3:A:3161:VAL:HG12	2.03	0.41
3:A:4063:ASP:OD1	3:A:4064:MET:N	2.54	0.41
9:A:5308:L9R:H23	9:A:5308:L9R:H20	1.32	0.41
3:B:653:ALA:HB3	3:B:656:SER:HB2	2.03	0.41
3:B:871:ARG:CZ	3:B:922:LEU:HD12	2.51	0.41
3:B:2390:PRO:C	3:B:2392:ARG:H	2.28	0.41
3:B:3147:ILE:HG23	3:B:3152:PHE:HB2	2.02	0.41
3:B:3359:ILE:HG23	3:B:3437:MET:HE1	2.02	0.41
3:B:3414:ARG:HH21	3:B:3472:ALA:H	1.67	0.41
3:B:4152:GLU:OE1	3:B:4194:TYR:OH	2.28	0.41
3:G:2390:PRO:C	3:G:2392:ARG:H	2.28	0.41
3:G:2495:VAL:HG22	3:G:2498:HIS:CE1	2.56	0.41
3:G:3003:LEU:HB2	3:G:3004:PRO:HD3	2.02	0.41
3:G:3284:TRP:HB3	3:G:3305:THR:HG21	2.02	0.41
3:I:462:GLU:HG3	3:I:3710:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3501:ASP:N	3:I:3501:ASP:OD1	2.54	0.41
2:H:27:THR:HG23	2:H:38:SER:HB2	2.03	0.41
1:D:85:ILE:H	1:D:85:ILE:HG13	1.57	0.40
3:A:308:HIS:CE1	3:A:310:LYS:HB3	2.56	0.40
3:A:2282:ASP:HA	3:A:2341:VAL:HG13	2.03	0.40
3:A:2413:GLU:OE2	3:A:2414:ASN:ND2	2.54	0.40
3:A:3359:ILE:HG23	3:A:3437:MET:HE1	2.02	0.40
3:A:3501:ASP:OD1	3:A:3501:ASP:N	2.54	0.40
3:A:4241:THR:HG22	3:A:4245:MET:HE3	2.03	0.40
3:B:979:PRO:O	3:B:982:THR:OG1	2.33	0.40
3:B:1997:GLU:O	3:B:2000:SER:OG	2.37	0.40
3:B:3734:HIS:CG	3:B:3735:LEU:N	2.89	0.40
3:G:871:ARG:CZ	3:G:922:LEU:HD12	2.51	0.40
3:G:4063:ASP:OD1	3:G:4064:MET:N	2.54	0.40
3:G:4754:ASN:OD1	3:G:4755:GLU:N	2.47	0.40
3:I:336:PRO:HA	3:I:337:PRO:HD3	1.88	0.40
3:I:2495:VAL:HG22	3:I:2498:HIS:CE1	2.56	0.40
3:I:2749:GLU:HG3	3:I:2752:ASP:HB2	2.03	0.40
3:I:3823:LYS:HA	3:I:3823:LYS:HD3	1.87	0.40
1:K:69:LEU:HD23	1:K:69:LEU:HA	1.91	0.40
3:A:462:GLU:HG3	3:A:3710:LEU:HD13	2.02	0.40
3:A:871:ARG:CZ	3:A:922:LEU:HD12	2.51	0.40
3:A:954:LYS:HB3	3:A:966:LYS:HE3	2.03	0.40
3:A:2886:TRP:HA	3:A:2889:LYS:NZ	2.36	0.40
3:A:3341:PHE:O	3:A:3344:PRO:HD2	2.21	0.40
3:A:3535:LEU:O	3:A:3538:THR:OG1	2.31	0.40
3:A:4093:PHE:O	3:A:4097:MET:HG2	2.20	0.40
3:A:4154:VAL:HG12	3:A:4157:ASP:HB2	2.03	0.40
3:B:1634:LEU:HD23	3:B:1634:LEU:HA	1.92	0.40
3:B:1690:ASP:OD2	3:B:1693:GLN:NE2	2.52	0.40
3:B:2751:LEU:O	3:B:2755:ILE:HG12	2.21	0.40
3:B:4940:PHE:HZ	3:I:4931:ILE:HG23	1.87	0.40
3:G:863:LEU:HD11	3:G:930:LYS:NZ	2.35	0.40
3:G:2775:TRP:CD2	3:G:2786:LYS:HE3	2.56	0.40
3:G:2881:ASN:HA	3:G:2884:ASN:HD21	1.87	0.40
3:G:3249:LEU:HD23	3:G:3277:LEU:HD21	2.03	0.40
3:G:3341:PHE:O	3:G:3344:PRO:HD2	2.21	0.40
3:I:871:ARG:HB2	3:I:929:LEU:HD12	2.04	0.40
3:I:880:GLU:CD	3:I:910:PHE:HB3	2.46	0.40
3:I:2758:PHE:HA	3:I:2761:TYR:HB2	2.04	0.40
3:I:3341:PHE:O	3:I:3344:PRO:HD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:3562:LYS:HE2	3:I:3562:LYS:HB2	1.91	0.40
2:O:27:THR:HG23	2:O:38:SER:HB2	2.03	0.40
3:A:672:VAL:O	3:A:680:THR:OG1	2.35	0.40
3:A:870:ILE:HG12	3:A:1051:TYR:HE2	1.86	0.40
3:A:1079:LYS:HA	3:A:1189:LEU:HD11	2.04	0.40
3:A:2740:VAL:HG21	3:A:2819:TRP:HE1	1.87	0.40
3:A:2747:ILE:HD13	3:A:2814:LYS:HG2	2.02	0.40
3:A:3971:GLY:N	3:A:3972:PRO:HA	2.37	0.40
3:B:308:HIS:CE1	3:B:310:LYS:HB3	2.56	0.40
3:B:797:HIS:CG	3:B:821:LEU:HD23	2.56	0.40
3:B:2413:GLU:OE2	3:B:2414:ASN:ND2	2.54	0.40
3:B:4825:THR:O	3:B:4828:SER:OG	2.32	0.40
3:G:571:SER:OG	3:G:573:GLU:OE1	2.34	0.40
3:G:880:GLU:CD	3:G:910:PHE:HB3	2.46	0.40
3:G:2001:PRO:O	3:G:2005:GLN:HG3	2.21	0.40
3:G:2282:ASP:HA	3:G:2341:VAL:HG13	2.03	0.40
3:G:2413:GLU:OE2	3:G:2414:ASN:ND2	2.54	0.40
3:G:2759:ALA:HB1	3:G:2806:ARG:HB2	2.04	0.40
3:G:3359:ILE:HG23	3:G:3437:MET:HE1	2.02	0.40
9:G:5101:L9R:H42A	9:G:5101:L9R:H39	1.76	0.40
3:I:345:LEU:HB3	3:I:387:ALA:HB1	2.02	0.40
3:I:871:ARG:CZ	3:I:922:LEU:HD12	2.51	0.40
3:I:2001:PRO:O	3:I:2005:GLN:HG3	2.21	0.40
3:I:2527:LEU:HD12	3:I:2527:LEU:HA	1.92	0.40
3:I:2759:ALA:HB1	3:I:2806:ARG:HB2	2.04	0.40
3:I:3734:HIS:CG	3:I:3735:LEU:N	2.89	0.40
3:I:4241:THR:HG22	3:I:4245:MET:HE3	2.03	0.40
3:A:275:ARG:HE	3:A:328:LYS:HE2	1.87	0.40
3:A:3107:VAL:HG21	3:A:3171:SER:HB2	2.03	0.40
3:B:683:ARG:HG2	3:B:717:ASP:HB3	2.04	0.40
3:B:1488:LYS:HE3	3:B:1488:LYS:HB2	1.86	0.40
3:B:2001:PRO:O	3:B:2005:GLN:HG3	2.22	0.40
3:B:2740:VAL:HG21	3:B:2819:TRP:HE1	1.86	0.40
3:B:2758:PHE:HA	3:B:2761:TYR:HB2	2.04	0.40
3:B:2775:TRP:CD2	3:B:2786:LYS:HE3	2.56	0.40
3:B:3157:ILE:HG23	3:B:3161:VAL:HG12	2.03	0.40
3:G:653:ALA:HB3	3:G:656:SER:HB2	2.03	0.40
3:G:1948:ASP:OD1	3:G:2126:ARG:NH2	2.48	0.40
3:G:4090:LYS:HG2	3:G:4123:ILE:HD11	2.03	0.40
3:G:4967:TYR:OH	3:G:5033:GLU:OE2	2.29	0.40
3:I:1079:LYS:HA	3:I:1189:LEU:HD11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:4090:LYS:HG2	3:I:4123:ILE:HD11	2.04	0.40
3:I:4813:LEU:HD23	3:I:4813:LEU:HA	1.87	0.40
2:J:17:LYS:HE3	2:J:17:LYS:HB3	1.84	0.40
1:E:130:ILE:H	1:E:130:ILE:HG13	1.72	0.40
3:A:1947:CYS:SG	3:A:2127:GLN:NE2	2.92	0.40
3:A:3717:ASP:OD1	3:A:3717:ASP:N	2.55	0.40
3:A:4090:LYS:HG2	3:A:4123:ILE:HD11	2.03	0.40
3:B:1451:GLY:HA3	3:B:1494:MET:HA	2.04	0.40
3:B:3159:ASP:OD1	3:B:3159:ASP:N	2.52	0.40
3:B:3501:ASP:OD1	3:B:3501:ASP:N	2.54	0.40
3:G:1079:LYS:HA	3:G:1189:LEU:HD11	2.04	0.40
3:G:4900:GLU:H	3:G:4900:GLU:HG2	1.70	0.40
3:G:4917:ASP:HB2	3:I:4888:TYR:HE1	1.87	0.40
3:I:1488:LYS:HB2	3:I:1488:LYS:HE3	1.86	0.40
3:I:1823:GLY:O	3:I:1825:HIS:ND1	2.52	0.40
3:I:3147:ILE:HG23	3:I:3152:PHE:HB2	2.02	0.40
3:I:3249:LEU:HD23	3:I:3277:LEU:HD21	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	C	147/150 (98%)	146 (99%)	1 (1%)	0	100	100
1	D	147/150 (98%)	146 (99%)	1 (1%)	0	100	100
1	E	147/150 (98%)	146 (99%)	1 (1%)	0	100	100
1	K	147/150 (98%)	146 (99%)	1 (1%)	0	100	100
2	F	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
2	H	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
2	J	105/107 (98%)	103 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	O	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
3	A	4385/5037 (87%)	4273 (97%)	112 (3%)	0	100	100
3	B	4385/5037 (87%)	4273 (97%)	112 (3%)	0	100	100
3	G	4385/5037 (87%)	4274 (98%)	111 (2%)	0	100	100
3	I	4385/5037 (87%)	4273 (97%)	112 (3%)	0	100	100
All	All	18548/21176 (88%)	18089 (98%)	459 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	C	127/128 (99%)	123 (97%)	4 (3%)	35	50
1	D	127/128 (99%)	123 (97%)	4 (3%)	35	50
1	E	127/128 (99%)	123 (97%)	4 (3%)	35	50
1	K	127/128 (99%)	123 (97%)	4 (3%)	35	50
2	F	89/89 (100%)	85 (96%)	4 (4%)	24	37
2	H	89/89 (100%)	85 (96%)	4 (4%)	24	37
2	J	89/89 (100%)	85 (96%)	4 (4%)	24	37
2	O	89/89 (100%)	85 (96%)	4 (4%)	24	37
3	A	3836/4276 (90%)	3768 (98%)	68 (2%)	51	65
3	B	3836/4276 (90%)	3768 (98%)	68 (2%)	51	65
3	G	3836/4276 (90%)	3768 (98%)	68 (2%)	51	65
3	I	3836/4276 (90%)	3768 (98%)	68 (2%)	51	65
All	All	16208/17972 (90%)	15904 (98%)	304 (2%)	49	64

All (304) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	21	LYS
1	K	30	LYS
1	K	85	ILE
1	K	105	LEU
2	F	17	LYS
2	F	25	HIS
2	F	29	MET
2	F	79	ASP
1	D	21	LYS
1	D	30	LYS
1	D	85	ILE
1	D	105	LEU
1	E	21	LYS
1	E	30	LYS
1	E	85	ILE
1	E	105	LEU
1	C	21	LYS
1	C	30	LYS
1	C	85	ILE
1	C	105	LEU
3	A	81	MET
3	A	155	LYS
3	A	220	LEU
3	A	860	GLN
3	A	862	VAL
3	A	869	ARG
3	A	873	LYS
3	A	881	LEU
3	A	882	TRP
3	A	887	ILE
3	A	898	ASP
3	A	907	LEU
3	A	908	VAL
3	A	911	HIS
3	A	913	LEU
3	A	922	LEU
3	A	945	LYS
3	A	950	LEU
3	A	951	LYS
3	A	957	LYS
3	A	958	THR
3	A	959	TYR
3	A	961	MET

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Mol	Chain	Res	Type
3	A	962	SER
3	A	972	LEU
3	A	976	ARG
3	A	984	LEU
3	A	999	ASP
3	A	1021	LEU
3	A	1022	VAL
3	A	1057	ASP
3	A	1506	GLN
3	A	1872	THR
3	A	1923	GLU
3	A	1990	GLU
3	A	2037	ASP
3	A	2153	MET
3	A	2203	MET
3	A	2219	GLU
3	A	2413	GLU
3	A	2482	ASP
3	A	2666	VAL
3	A	2742	THR
3	A	2747	ILE
3	A	2781	VAL
3	A	2803	GLU
3	A	2862	LEU
3	A	2876	GLU
3	A	2937	VAL
3	A	3112	LEU
3	A	3137	LEU
3	A	3296	LEU
3	A	3619	VAL
3	A	3624	LEU
3	A	3639	THR
3	A	3686	GLU
3	A	3752	SER
3	A	3756	LYS
3	A	4662	ASN
3	A	4722	ARG
3	A	4768	LEU
3	A	4796	MET
3	A	4821	LYS
3	A	4860	ARG
3	A	4861	LYS

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Mol	Chain	Res	Type
3	A	4903	ASP
3	A	4911	LEU
3	A	4918	ILE
3	B	81	MET
3	B	155	LYS
3	B	220	LEU
3	B	860	GLN
3	B	862	VAL
3	B	869	ARG
3	B	873	LYS
3	B	881	LEU
3	B	882	TRP
3	B	887	ILE
3	B	898	ASP
3	B	907	LEU
3	B	908	VAL
3	B	911	HIS
3	B	913	LEU
3	B	922	LEU
3	B	945	LYS
3	B	950	LEU
3	B	951	LYS
3	B	957	LYS
3	B	958	THR
3	B	959	TYR
3	B	961	MET
3	B	962	SER
3	B	972	LEU
3	B	976	ARG
3	B	984	LEU
3	B	999	ASP
3	B	1021	LEU
3	B	1022	VAL
3	B	1057	ASP
3	B	1506	GLN
3	B	1872	THR
3	B	1923	GLU
3	B	1990	GLU
3	B	2037	ASP
3	B	2153	MET
3	B	2203	MET
3	B	2219	GLU

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Mol	Chain	Res	Type
3	B	2413	GLU
3	B	2482	ASP
3	B	2666	VAL
3	B	2742	THR
3	B	2747	ILE
3	B	2781	VAL
3	B	2803	GLU
3	B	2862	LEU
3	B	2876	GLU
3	B	2937	VAL
3	B	3112	LEU
3	B	3137	LEU
3	B	3296	LEU
3	B	3619	VAL
3	B	3624	LEU
3	B	3639	THR
3	B	3686	GLU
3	B	3752	SER
3	B	3756	LYS
3	B	4662	ASN
3	B	4722	ARG
3	B	4768	LEU
3	B	4796	MET
3	B	4821	LYS
3	B	4860	ARG
3	B	4861	LYS
3	B	4903	ASP
3	B	4911	LEU
3	B	4918	ILE
3	G	81	MET
3	G	155	LYS
3	G	220	LEU
3	G	860	GLN
3	G	862	VAL
3	G	869	ARG
3	G	873	LYS
3	G	881	LEU
3	G	882	TRP
3	G	887	ILE
3	G	898	ASP
3	G	907	LEU
3	G	908	VAL

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Mol	Chain	Res	Type
3	G	911	HIS
3	G	913	LEU
3	G	922	LEU
3	G	945	LYS
3	G	950	LEU
3	G	951	LYS
3	G	957	LYS
3	G	958	THR
3	G	959	TYR
3	G	961	MET
3	G	962	SER
3	G	972	LEU
3	G	976	ARG
3	G	984	LEU
3	G	999	ASP
3	G	1021	LEU
3	G	1022	VAL
3	G	1057	ASP
3	G	1506	GLN
3	G	1872	THR
3	G	1923	GLU
3	G	1990	GLU
3	G	2037	ASP
3	G	2153	MET
3	G	2203	MET
3	G	2219	GLU
3	G	2413	GLU
3	G	2482	ASP
3	G	2666	VAL
3	G	2742	THR
3	G	2747	ILE
3	G	2781	VAL
3	G	2803	GLU
3	G	2862	LEU
3	G	2876	GLU
3	G	2937	VAL
3	G	3112	LEU
3	G	3137	LEU
3	G	3296	LEU
3	G	3619	VAL
3	G	3624	LEU
3	G	3639	THR

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Mol	Chain	Res	Type
3	G	3686	GLU
3	G	3752	SER
3	G	3756	LYS
3	G	4662	ASN
3	G	4722	ARG
3	G	4768	LEU
3	G	4796	MET
3	G	4821	LYS
3	G	4860	ARG
3	G	4861	LYS
3	G	4903	ASP
3	G	4911	LEU
3	G	4918	ILE
3	I	81	MET
3	I	155	LYS
3	I	220	LEU
3	I	860	GLN
3	I	862	VAL
3	I	869	ARG
3	I	873	LYS
3	I	881	LEU
3	I	882	TRP
3	I	887	ILE
3	I	898	ASP
3	I	907	LEU
3	I	908	VAL
3	I	911	HIS
3	I	913	LEU
3	I	922	LEU
3	I	945	LYS
3	I	950	LEU
3	I	951	LYS
3	I	957	LYS
3	I	958	THR
3	I	959	TYR
3	I	961	MET
3	I	962	SER
3	I	972	LEU
3	I	976	ARG
3	I	984	LEU
3	I	999	ASP
3	I	1021	LEU

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Mol	Chain	Res	Type
3	I	1022	VAL
3	I	1057	ASP
3	I	1506	GLN
3	I	1872	THR
3	I	1923	GLU
3	I	1990	GLU
3	I	2037	ASP
3	I	2153	MET
3	I	2203	MET
3	I	2219	GLU
3	I	2413	GLU
3	I	2482	ASP
3	I	2666	VAL
3	I	2742	THR
3	I	2747	ILE
3	I	2781	VAL
3	I	2803	GLU
3	I	2862	LEU
3	I	2876	GLU
3	I	2937	VAL
3	I	3112	LEU
3	I	3137	LEU
3	I	3296	LEU
3	I	3619	VAL
3	I	3624	LEU
3	I	3639	THR
3	I	3686	GLU
3	I	3752	SER
3	I	3756	LYS
3	I	4662	ASN
3	I	4722	ARG
3	I	4768	LEU
3	I	4796	MET
3	I	4821	LYS
3	I	4860	ARG
3	I	4861	LYS
3	I	4903	ASP
3	I	4911	LEU
3	I	4918	ILE
2	H	17	LYS
2	H	25	HIS
2	H	29	MET

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Mol	Chain	Res	Type
2	H	79	ASP
2	J	17	LYS
2	J	25	HIS
2	J	29	MET
2	J	79	ASP
2	O	17	LYS
2	O	25	HIS
2	O	29	MET
2	O	79	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (129) such sidechains are listed below:

Mol	Chain	Res	Type
1	K	53	ASN
1	K	107	HIS
1	K	135	GLN
2	F	20	GLN
1	D	53	ASN
1	D	107	HIS
1	D	135	GLN
1	E	-1	HIS
1	E	53	ASN
1	E	135	GLN
1	C	53	ASN
1	C	107	HIS
1	C	135	GLN
3	A	224	HIS
3	A	495	ASN
3	A	838	HIS
3	A	938	HIS
3	A	963	ASN
3	A	991	ASN
3	A	1035	ASN
3	A	1640	HIS
3	A	1660	GLN
3	A	2003	GLN
3	A	2092	GLN
3	A	2180	GLN
3	A	2260	ASN
3	A	2420	HIS
3	A	2441	HIS
3	A	2515	GLN

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Mol	Chain	Res	Type
3	A	2673	HIS
3	A	2772	GLN
3	A	2883	HIS
3	A	2892	GLN
3	A	2933	ASN
3	A	3030	HIS
3	A	3180	ASN
3	A	3449	HIS
3	A	3667	HIS
3	A	3734	HIS
3	A	3761	GLN
3	A	3766	GLN
3	A	4109	GLN
3	A	4547	GLN
3	A	4558	ASN
3	A	4626	ASN
3	B	224	HIS
3	B	495	ASN
3	B	938	HIS
3	B	963	ASN
3	B	991	ASN
3	B	1035	ASN
3	B	1640	HIS
3	B	1660	GLN
3	B	2003	GLN
3	B	2180	GLN
3	B	2260	ASN
3	B	2420	HIS
3	B	2441	HIS
3	B	2515	GLN
3	B	2772	GLN
3	B	2892	GLN
3	B	2933	ASN
3	B	3030	HIS
3	B	3180	ASN
3	B	3449	HIS
3	B	3667	HIS
3	B	3761	GLN
3	B	3766	GLN
3	B	4109	GLN
3	B	4558	ASN
3	B	4626	ASN

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Mol	Chain	Res	Type
3	G	224	HIS
3	G	495	ASN
3	G	838	HIS
3	G	938	HIS
3	G	963	ASN
3	G	991	ASN
3	G	1035	ASN
3	G	1206	GLN
3	G	1420	ASN
3	G	1640	HIS
3	G	1660	GLN
3	G	2003	GLN
3	G	2092	GLN
3	G	2260	ASN
3	G	2441	HIS
3	G	2515	GLN
3	G	2673	HIS
3	G	2892	GLN
3	G	2933	ASN
3	G	3180	ASN
3	G	3667	HIS
3	G	3761	GLN
3	G	3766	GLN
3	G	4109	GLN
3	G	4558	ASN
3	G	4626	ASN
3	I	224	HIS
3	I	495	ASN
3	I	838	HIS
3	I	938	HIS
3	I	963	ASN
3	I	991	ASN
3	I	1035	ASN
3	I	1420	ASN
3	I	1640	HIS
3	I	1660	GLN
3	I	2003	GLN
3	I	2092	GLN
3	I	2180	GLN
3	I	2260	ASN
3	I	2441	HIS
3	I	2515	GLN

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Mol	Chain	Res	Type
3	I	2772	GLN
3	I	2892	GLN
3	I	2933	ASN
3	I	3030	HIS
3	I	3180	ASN
3	I	3449	HIS
3	I	3667	HIS
3	I	3734	HIS
3	I	3761	GLN
3	I	3766	GLN
3	I	4109	GLN
3	I	4558	ASN
3	I	4626	ASN
2	H	20	GLN
2	J	20	GLN
2	O	20	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 48 ligands modelled in this entry, 24 are monoatomic - leaving 24 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ATP	I	5102	-	32,33,33	0.28	0	48,52,52	0.39	0
5	ATP	B	5301	-	32,33,33	0.28	0	48,52,52	0.39	0
8	KVR	G	5107	-	24,25,25	1.41	3 (12%)	31,34,34	1.56	4 (12%)
8	KVR	B	5306	-	24,25,25	1.42	3 (12%)	31,34,34	1.55	4 (12%)
9	L9R	I	5108	-	53,53,53	1.24	5 (9%)	59,61,61	1.12	3 (5%)
5	ATP	A	5305	-	32,33,33	0.25	0	48,52,52	0.29	0
9	L9R	B	5307	-	53,53,53	1.24	5 (9%)	59,61,61	1.12	3 (5%)
9	L9R	I	5101	-	53,53,53	1.21	4 (7%)	59,61,61	1.12	2 (3%)
5	ATP	G	5102	-	32,33,33	0.28	0	48,52,52	0.39	0
9	L9R	G	5108	-	53,53,53	1.24	5 (9%)	59,61,61	1.12	3 (5%)
9	L9R	A	5307	-	53,53,53	1.24	5 (9%)	59,61,61	1.12	3 (5%)
7	CFF	A	5304	-	15,15,15	1.77	4 (26%)	23,23,23	2.95	11 (47%)
5	ATP	I	5106	-	32,33,33	0.26	0	48,52,52	0.29	0
9	L9R	A	5308	-	53,53,53	1.21	4 (7%)	59,61,61	1.12	2 (3%)
7	CFF	I	5105	-	15,15,15	1.77	5 (33%)	23,23,23	2.95	11 (47%)
5	ATP	B	5305	-	32,33,33	0.26	0	48,52,52	0.29	0
5	ATP	A	5301	-	32,33,33	0.28	0	48,52,52	0.39	0
7	CFF	B	5304	-	15,15,15	1.77	4 (26%)	23,23,23	2.96	11 (47%)
5	ATP	G	5106	-	32,33,33	0.25	0	48,52,52	0.29	0
8	KVR	A	5306	-	24,25,25	1.41	3 (12%)	31,34,34	1.55	4 (12%)
9	L9R	B	5308	-	53,53,53	1.21	4 (7%)	59,61,61	1.12	2 (3%)
8	KVR	I	5107	-	24,25,25	1.41	3 (12%)	31,34,34	1.55	4 (12%)
9	L9R	G	5101	-	53,53,53	1.21	4 (7%)	59,61,61	1.12	2 (3%)
7	CFF	G	5105	-	15,15,15	1.76	4 (26%)	23,23,23	2.95	11 (47%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ATP	I	5102	-	-	8/22/38/38	0/3/3/3
5	ATP	B	5301	-	-	8/22/38/38	0/3/3/3
8	KVR	G	5107	-	-	2/10/20/20	0/2/3/3
8	KVR	B	5306	-	-	2/10/20/20	0/2/3/3
9	L9R	I	5108	-	-	30/57/57/57	-
5	ATP	A	5305	-	-	8/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	L9R	B	5307	-	-	30/57/57/57	-
9	L9R	I	5101	-	-	34/57/57/57	-
5	ATP	G	5102	-	-	8/22/38/38	0/3/3/3
9	L9R	G	5108	-	-	30/57/57/57	-
9	L9R	A	5307	-	-	30/57/57/57	-
7	CFF	A	5304	-	-	-	0/2/2/2
5	ATP	I	5106	-	-	8/22/38/38	0/3/3/3
9	L9R	A	5308	-	-	34/57/57/57	-
7	CFF	I	5105	-	-	-	0/2/2/2
5	ATP	B	5305	-	-	8/22/38/38	0/3/3/3
5	ATP	A	5301	-	-	8/22/38/38	0/3/3/3
7	CFF	B	5304	-	-	-	0/2/2/2
5	ATP	G	5106	-	-	8/22/38/38	0/3/3/3
8	KVR	A	5306	-	-	2/10/20/20	0/2/3/3
9	L9R	B	5308	-	-	34/57/57/57	-
8	KVR	I	5107	-	-	2/10/20/20	0/2/3/3
9	L9R	G	5101	-	-	34/57/57/57	-
7	CFF	G	5105	-	-	-	0/2/2/2

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	5306	KVR	C06-S09	4.92	1.82	1.77
8	I	5107	KVR	C06-S09	4.91	1.82	1.77
8	A	5306	KVR	C06-S09	4.88	1.82	1.77
8	G	5107	KVR	C06-S09	4.86	1.82	1.77
7	B	5304	CFF	C6-N1	-3.78	1.32	1.40
7	A	5304	CFF	C6-N1	-3.77	1.32	1.40
7	G	5105	CFF	C6-N1	-3.77	1.32	1.40
7	I	5105	CFF	C6-N1	-3.77	1.32	1.40
9	A	5307	L9R	O2-C31	3.60	1.44	1.34
9	B	5307	L9R	O2-C31	3.60	1.44	1.34
9	G	5108	L9R	O2-C31	3.60	1.44	1.34
9	I	5108	L9R	O2-C31	3.60	1.44	1.34
9	A	5308	L9R	O2-C31	3.55	1.44	1.34
9	I	5101	L9R	O2-C31	3.54	1.44	1.34
9	B	5308	L9R	O2-C31	3.53	1.44	1.34
9	G	5101	L9R	O2-C31	3.53	1.44	1.34
9	G	5108	L9R	O3-C11	3.16	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	5307	L9R	O3-C11	3.14	1.42	1.33
9	I	5108	L9R	O3-C11	3.14	1.42	1.33
9	B	5307	L9R	O3-C11	3.14	1.42	1.33
9	A	5308	L9R	O3-C11	3.03	1.42	1.33
9	B	5308	L9R	O3-C11	3.03	1.42	1.33
9	G	5101	L9R	O3-C11	3.03	1.42	1.33
9	I	5101	L9R	O3-C11	3.03	1.42	1.33
8	G	5107	KVR	C13-C05	2.63	1.55	1.51
8	A	5306	KVR	C13-C05	2.61	1.55	1.51
8	B	5306	KVR	C13-C05	2.58	1.55	1.51
8	I	5107	KVR	C13-C05	2.58	1.55	1.51
9	A	5307	L9R	C32-C31	2.54	1.58	1.50
9	I	5108	L9R	C32-C31	2.54	1.58	1.50
9	B	5307	L9R	C32-C31	2.53	1.58	1.50
9	G	5108	L9R	C32-C31	2.53	1.58	1.50
7	B	5304	CFF	C5-N7	-2.35	1.34	1.38
7	I	5105	CFF	C5-N7	-2.35	1.34	1.38
9	I	5101	L9R	C32-C31	2.34	1.57	1.50
9	A	5308	L9R	C32-C31	2.34	1.57	1.50
9	B	5308	L9R	C32-C31	2.33	1.57	1.50
9	G	5101	L9R	C32-C31	2.33	1.57	1.50
7	A	5304	CFF	C5-N7	-2.32	1.34	1.38
8	A	5306	KVR	C13-N12	-2.30	1.45	1.47
8	I	5107	KVR	C13-N12	-2.30	1.45	1.47
7	G	5105	CFF	C5-N7	-2.30	1.34	1.38
8	B	5306	KVR	C13-N12	-2.30	1.45	1.47
8	G	5107	KVR	C13-N12	-2.29	1.45	1.47
9	I	5101	L9R	O2-C2	-2.28	1.41	1.46
9	B	5308	L9R	O2-C2	-2.25	1.41	1.46
9	G	5101	L9R	O2-C2	-2.25	1.41	1.46
9	A	5308	L9R	O2-C2	-2.24	1.41	1.46
9	A	5307	L9R	O2-C2	-2.14	1.41	1.46
9	B	5307	L9R	O2-C2	-2.13	1.41	1.46
9	G	5108	L9R	O2-C2	-2.13	1.41	1.46
9	I	5108	L9R	O2-C2	-2.11	1.41	1.46
9	I	5108	L9R	P-O3P	2.08	1.67	1.59
9	A	5307	L9R	P-O3P	2.08	1.67	1.59
9	G	5108	L9R	P-O3P	2.08	1.67	1.59
7	G	5105	CFF	O13-C6	-2.08	1.18	1.23
9	B	5307	L9R	P-O3P	2.07	1.67	1.59
7	A	5304	CFF	O13-C6	-2.07	1.18	1.23
7	B	5304	CFF	O13-C6	-2.07	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	5105	CFF	C4-N3	-2.05	1.34	1.38
7	I	5105	CFF	O13-C6	-2.05	1.18	1.23
7	I	5105	CFF	O11-C2	-2.04	1.18	1.22
7	A	5304	CFF	C4-N3	-2.03	1.34	1.38
7	B	5304	CFF	C4-N3	-2.03	1.34	1.38
7	I	5105	CFF	C4-N3	-2.01	1.34	1.38

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	5105	CFF	C14-N7-C8	-8.45	110.47	126.28
7	A	5304	CFF	C14-N7-C8	-8.43	110.51	126.28
7	B	5304	CFF	C14-N7-C8	-8.42	110.52	126.28
7	G	5105	CFF	C14-N7-C8	-8.41	110.54	126.28
7	I	5105	CFF	C14-N7-C5	5.78	141.53	127.77
7	B	5304	CFF	C14-N7-C5	5.77	141.51	127.77
7	A	5304	CFF	C14-N7-C5	5.77	141.50	127.77
7	G	5105	CFF	C14-N7-C5	5.76	141.48	127.77
8	G	5107	KVR	C10-S09-C06	5.26	110.17	102.71
8	A	5306	KVR	C10-S09-C06	5.26	110.16	102.71
8	B	5306	KVR	C10-S09-C06	5.24	110.14	102.71
8	I	5107	KVR	C10-S09-C06	5.24	110.13	102.71
7	I	5105	CFF	C5-C6-N1	4.35	120.02	112.06
7	G	5105	CFF	C5-C6-N1	4.34	120.02	112.06
7	A	5304	CFF	C5-C6-N1	4.33	119.99	112.06
7	B	5304	CFF	C5-C6-N1	4.32	119.98	112.06
9	B	5308	L9R	O2-C31-C32	4.03	120.20	111.48
9	G	5101	L9R	O2-C31-C32	4.03	120.20	111.48
9	A	5308	L9R	O2-C31-C32	4.03	120.20	111.48
9	I	5101	L9R	O2-C31-C32	4.02	120.17	111.48
9	B	5307	L9R	O2-C31-C32	3.92	119.96	111.48
9	A	5307	L9R	O2-C31-C32	3.92	119.95	111.48
9	I	5108	L9R	O2-C31-C32	3.92	119.95	111.48
9	G	5108	L9R	O2-C31-C32	3.89	119.90	111.48
7	B	5304	CFF	N3-C4-N9	3.69	132.07	126.27
7	G	5105	CFF	N3-C4-N9	3.69	132.06	126.27
7	A	5304	CFF	N3-C4-N9	3.67	132.04	126.27
7	I	5105	CFF	N3-C4-N9	3.63	131.98	126.27
8	G	5107	KVR	C11-C10-S09	-3.52	110.15	114.26
8	A	5306	KVR	C11-C10-S09	-3.50	110.16	114.26
8	B	5306	KVR	C11-C10-S09	-3.48	110.18	114.26
8	I	5107	KVR	C11-C10-S09	-3.48	110.19	114.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	5105	CFF	C6-N1-C2	-3.47	120.02	125.66
7	A	5304	CFF	C6-N1-C2	-3.44	120.07	125.66
7	B	5304	CFF	C6-N1-C2	-3.44	120.07	125.66
7	I	5105	CFF	C6-N1-C2	-3.44	120.07	125.66
7	B	5304	CFF	O13-C6-C5	-3.09	120.05	126.38
7	I	5105	CFF	O13-C6-C5	-3.08	120.07	126.38
7	A	5304	CFF	O13-C6-C5	-3.08	120.07	126.38
7	G	5105	CFF	O13-C6-C5	-3.08	120.08	126.38
7	I	5105	CFF	N7-C8-N9	-3.03	108.00	113.48
7	A	5304	CFF	N7-C8-N9	-3.00	108.04	113.48
7	B	5304	CFF	N7-C8-N9	-2.99	108.06	113.48
7	G	5105	CFF	N7-C8-N9	-2.98	108.07	113.48
9	I	5108	L9R	O3-C11-C12	2.86	120.56	111.83
9	B	5307	L9R	O3-C11-C12	2.86	120.56	111.83
9	A	5307	L9R	O3-C11-C12	2.85	120.53	111.83
9	G	5108	L9R	O3-C11-C12	2.83	120.48	111.83
8	I	5107	KVR	C14-N12-C11	-2.79	106.56	111.09
8	G	5107	KVR	C14-N12-C11	-2.78	106.57	111.09
8	A	5306	KVR	C14-N12-C11	-2.76	106.60	111.09
9	A	5308	L9R	O3-C11-C12	2.76	120.24	111.83
9	B	5308	L9R	O3-C11-C12	2.75	120.22	111.83
9	G	5101	L9R	O3-C11-C12	2.75	120.22	111.83
9	I	5101	L9R	O3-C11-C12	2.74	120.18	111.83
8	B	5306	KVR	C14-N12-C11	-2.73	106.66	111.09
7	B	5304	CFF	C6-C5-C4	-2.44	119.85	122.92
7	I	5105	CFF	C6-C5-C4	-2.42	119.87	122.92
7	A	5304	CFF	C6-C5-C4	-2.42	119.87	122.92
7	G	5105	CFF	C6-C5-C4	-2.42	119.88	122.92
9	I	5108	L9R	C4-C5-N	-2.32	108.36	115.82
9	B	5307	L9R	C4-C5-N	-2.32	108.36	115.82
7	B	5304	CFF	N3-C2-N1	2.32	120.04	117.14
9	G	5108	L9R	C4-C5-N	-2.31	108.39	115.82
9	A	5307	L9R	C4-C5-N	-2.31	108.40	115.82
7	A	5304	CFF	N3-C2-N1	2.30	120.01	117.14
7	G	5105	CFF	N3-C2-N1	2.29	120.00	117.14
7	I	5105	CFF	N3-C2-N1	2.28	119.99	117.14
8	A	5306	KVR	O23-C21-C18	2.26	120.64	114.84
8	I	5107	KVR	O23-C21-C18	2.26	120.64	114.84
8	B	5306	KVR	O23-C21-C18	2.26	120.63	114.84
8	G	5107	KVR	O23-C21-C18	2.24	120.57	114.84
7	B	5304	CFF	C8-N9-C4	2.11	108.04	102.98
7	G	5105	CFF	C8-N9-C4	2.10	108.03	102.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	5304	CFF	C8-N9-C4	2.10	108.03	102.98
7	I	5105	CFF	C8-N9-C4	2.10	108.03	102.98
7	B	5304	CFF	C5-C4-N9	-2.07	108.00	112.10
7	G	5105	CFF	C5-C4-N9	-2.07	108.01	112.10
7	A	5304	CFF	C5-C4-N9	-2.05	108.03	112.10
7	I	5105	CFF	C5-C4-N9	-2.04	108.06	112.10

There are no chirality outliers.

All (328) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	5301	ATP	C5'-O5'-PA-O1A
5	A	5301	ATP	C5'-O5'-PA-O2A
5	A	5301	ATP	C5'-O5'-PA-O3A
5	A	5305	ATP	C5'-O5'-PA-O2A
5	A	5305	ATP	C5'-O5'-PA-O3A
5	B	5301	ATP	C5'-O5'-PA-O1A
5	B	5301	ATP	C5'-O5'-PA-O2A
5	B	5301	ATP	C5'-O5'-PA-O3A
5	B	5305	ATP	C5'-O5'-PA-O2A
5	B	5305	ATP	C5'-O5'-PA-O3A
5	G	5102	ATP	C5'-O5'-PA-O1A
5	G	5102	ATP	C5'-O5'-PA-O2A
5	G	5102	ATP	C5'-O5'-PA-O3A
5	G	5106	ATP	C5'-O5'-PA-O2A
5	G	5106	ATP	C5'-O5'-PA-O3A
5	I	5102	ATP	C5'-O5'-PA-O1A
5	I	5102	ATP	C5'-O5'-PA-O2A
5	I	5102	ATP	C5'-O5'-PA-O3A
5	I	5106	ATP	C5'-O5'-PA-O2A
5	I	5106	ATP	C5'-O5'-PA-O3A
8	A	5306	KVR	C15-C14-N12-C11
8	A	5306	KVR	C15-C14-N12-C13
8	B	5306	KVR	C15-C14-N12-C11
8	B	5306	KVR	C15-C14-N12-C13
8	G	5107	KVR	C15-C14-N12-C11
8	G	5107	KVR	C15-C14-N12-C13
8	I	5107	KVR	C15-C14-N12-C11
8	I	5107	KVR	C15-C14-N12-C13
9	A	5308	L9R	C1-O3P-P-O1P
9	A	5308	L9R	C1-O3P-P-O4P
9	A	5308	L9R	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
9	A	5308	L9R	C4-O4P-P-O2P
9	A	5308	L9R	C4-O4P-P-O3P
9	A	5308	L9R	O4P-C4-C5-N
9	B	5308	L9R	C1-O3P-P-O1P
9	B	5308	L9R	C1-O3P-P-O4P
9	B	5308	L9R	C4-O4P-P-O1P
9	B	5308	L9R	C4-O4P-P-O2P
9	B	5308	L9R	C4-O4P-P-O3P
9	B	5308	L9R	O4P-C4-C5-N
9	G	5101	L9R	C1-O3P-P-O1P
9	G	5101	L9R	C1-O3P-P-O4P
9	G	5101	L9R	C4-O4P-P-O1P
9	G	5101	L9R	C4-O4P-P-O2P
9	G	5101	L9R	C4-O4P-P-O3P
9	G	5101	L9R	O4P-C4-C5-N
9	I	5101	L9R	C1-O3P-P-O1P
9	I	5101	L9R	C1-O3P-P-O4P
9	I	5101	L9R	C4-O4P-P-O1P
9	I	5101	L9R	C4-O4P-P-O2P
9	I	5101	L9R	C4-O4P-P-O3P
9	I	5101	L9R	O4P-C4-C5-N
9	A	5307	L9R	C32-C31-O2-C2
9	B	5307	L9R	C32-C31-O2-C2
9	G	5108	L9R	C32-C31-O2-C2
9	I	5108	L9R	C32-C31-O2-C2
9	A	5308	L9R	C20-C21-C22-C23
9	B	5308	L9R	C20-C21-C22-C23
9	G	5101	L9R	C20-C21-C22-C23
9	I	5101	L9R	C20-C21-C22-C23
9	A	5308	L9R	C13-C14-C15-C16
9	B	5308	L9R	C13-C14-C15-C16
9	G	5101	L9R	C13-C14-C15-C16
9	A	5307	L9R	C12-C11-O3-C3
9	B	5307	L9R	C12-C11-O3-C3
9	G	5108	L9R	C12-C11-O3-C3
9	I	5108	L9R	C12-C11-O3-C3
9	I	5101	L9R	C13-C14-C15-C16
9	A	5307	L9R	O11-C11-O3-C3
9	B	5307	L9R	O11-C11-O3-C3
9	G	5108	L9R	O11-C11-O3-C3
9	I	5108	L9R	O11-C11-O3-C3
9	A	5307	L9R	O31-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
9	B	5307	L9R	O31-C31-O2-C2
9	G	5108	L9R	O31-C31-O2-C2
9	I	5108	L9R	O31-C31-O2-C2
9	A	5308	L9R	C11-C12-C13-C14
9	B	5308	L9R	C11-C12-C13-C14
9	G	5101	L9R	C11-C12-C13-C14
9	I	5101	L9R	C11-C12-C13-C14
9	G	5108	L9R	C32-C33-C34-C35
9	I	5108	L9R	C32-C33-C34-C35
9	A	5307	L9R	C32-C33-C34-C35
9	B	5307	L9R	C32-C33-C34-C35
9	A	5308	L9R	C35-C36-C37-C38
9	B	5308	L9R	C35-C36-C37-C38
9	G	5101	L9R	C35-C36-C37-C38
9	I	5101	L9R	C35-C36-C37-C38
9	A	5307	L9R	C33-C34-C35-C36
9	B	5307	L9R	C33-C34-C35-C36
9	G	5108	L9R	C33-C34-C35-C36
9	I	5108	L9R	C33-C34-C35-C36
9	A	5307	L9R	C16-C17-C18-C19
9	A	5308	L9R	C22-C23-C24-C25
9	B	5307	L9R	C16-C17-C18-C19
9	B	5308	L9R	C22-C23-C24-C25
9	G	5101	L9R	C22-C23-C24-C25
9	G	5108	L9R	C16-C17-C18-C19
9	I	5101	L9R	C22-C23-C24-C25
9	I	5108	L9R	C16-C17-C18-C19
9	A	5308	L9R	C15-C16-C17-C18
9	B	5308	L9R	C15-C16-C17-C18
9	G	5101	L9R	C15-C16-C17-C18
9	I	5101	L9R	C15-C16-C17-C18
9	A	5307	L9R	C20-C21-C22-C23
9	B	5307	L9R	C20-C21-C22-C23
9	G	5108	L9R	C20-C21-C22-C23
9	I	5108	L9R	C20-C21-C22-C23
9	A	5308	L9R	C16-C17-C18-C19
9	B	5308	L9R	C16-C17-C18-C19
9	G	5101	L9R	C16-C17-C18-C19
9	I	5101	L9R	C16-C17-C18-C19
9	A	5308	L9R	C42-C43-C44-C45
9	B	5308	L9R	C42-C43-C44-C45
9	G	5101	L9R	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
9	I	5101	L9R	C42-C43-C44-C45
9	A	5307	L9R	C44-C45-C46-C47
9	G	5108	L9R	C44-C45-C46-C47
9	I	5108	L9R	C44-C45-C46-C47
9	A	5307	L9R	C21-C22-C23-C24
9	B	5307	L9R	C21-C22-C23-C24
9	B	5307	L9R	C44-C45-C46-C47
9	G	5108	L9R	C21-C22-C23-C24
9	I	5108	L9R	C21-C22-C23-C24
5	A	5301	ATP	O4'-C4'-C5'-O5'
5	B	5301	ATP	O4'-C4'-C5'-O5'
5	G	5102	ATP	O4'-C4'-C5'-O5'
5	I	5102	ATP	O4'-C4'-C5'-O5'
9	A	5307	L9R	C4-C5-N-C6
9	B	5307	L9R	C4-C5-N-C6
9	G	5108	L9R	C4-C5-N-C6
9	I	5108	L9R	C4-C5-N-C6
9	A	5308	L9R	C12-C13-C14-C15
9	B	5308	L9R	C12-C13-C14-C15
9	G	5101	L9R	C12-C13-C14-C15
9	I	5101	L9R	C12-C13-C14-C15
9	A	5307	L9R	O3P-C1-C2-O2
9	B	5307	L9R	O3P-C1-C2-O2
9	G	5108	L9R	O3P-C1-C2-O2
9	I	5108	L9R	O3P-C1-C2-O2
9	G	5101	L9R	C24-C25-C26-C27
9	I	5101	L9R	C24-C25-C26-C27
9	A	5308	L9R	C24-C25-C26-C27
9	B	5308	L9R	C24-C25-C26-C27
9	A	5307	L9R	C4-C5-N-C8
9	B	5307	L9R	C4-C5-N-C8
9	G	5108	L9R	C4-C5-N-C8
9	I	5108	L9R	C4-C5-N-C8
9	A	5308	L9R	C41-C42-C43-C44
9	B	5308	L9R	C41-C42-C43-C44
9	G	5101	L9R	C41-C42-C43-C44
9	I	5101	L9R	C41-C42-C43-C44
9	A	5308	L9R	C33-C34-C35-C36
9	B	5308	L9R	C33-C34-C35-C36
9	G	5101	L9R	C33-C34-C35-C36
9	I	5101	L9R	C33-C34-C35-C36
9	B	5307	L9R	C4-C5-N-C7

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Mol	Chain	Res	Type	Atoms
9	A	5308	L9R	C32-C33-C34-C35
9	B	5308	L9R	C32-C33-C34-C35
9	G	5101	L9R	C32-C33-C34-C35
9	I	5101	L9R	C32-C33-C34-C35
9	A	5307	L9R	C41-C42-C43-C44
9	B	5307	L9R	C41-C42-C43-C44
9	G	5108	L9R	C41-C42-C43-C44
9	I	5108	L9R	C41-C42-C43-C44
9	A	5308	L9R	C40-C41-C42-C43
9	B	5308	L9R	C40-C41-C42-C43
9	G	5101	L9R	C40-C41-C42-C43
9	I	5101	L9R	C40-C41-C42-C43
5	A	5301	ATP	C3'-C4'-C5'-O5'
5	B	5301	ATP	C3'-C4'-C5'-O5'
5	G	5102	ATP	C3'-C4'-C5'-O5'
5	I	5102	ATP	C3'-C4'-C5'-O5'
9	I	5101	L9R	C17-C18-C19-C20
9	A	5308	L9R	C17-C18-C19-C20
9	B	5308	L9R	C17-C18-C19-C20
9	G	5101	L9R	C17-C18-C19-C20
9	A	5308	L9R	C12-C11-O3-C3
9	B	5308	L9R	C12-C11-O3-C3
9	G	5101	L9R	C12-C11-O3-C3
9	I	5101	L9R	C12-C11-O3-C3
9	A	5307	L9R	C4-C5-N-C7
9	G	5108	L9R	C4-C5-N-C7
9	I	5108	L9R	C4-C5-N-C7
9	A	5307	L9R	C37-C38-C39-C40
9	B	5307	L9R	C37-C38-C39-C40
9	G	5108	L9R	C37-C38-C39-C40
9	I	5108	L9R	C37-C38-C39-C40
9	A	5307	L9R	C35-C36-C37-C38
9	B	5307	L9R	C35-C36-C37-C38
9	G	5108	L9R	C35-C36-C37-C38
9	I	5108	L9R	C35-C36-C37-C38
9	A	5308	L9R	C19-C20-C21-C22
9	B	5308	L9R	C19-C20-C21-C22
9	G	5101	L9R	C19-C20-C21-C22
9	I	5101	L9R	C19-C20-C21-C22
9	B	5308	L9R	C14-C15-C16-C17
9	A	5308	L9R	C14-C15-C16-C17
9	G	5101	L9R	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
9	I	5101	L9R	C14-C15-C16-C17
9	A	5308	L9R	C44-C45-C46-C47
9	B	5308	L9R	C44-C45-C46-C47
9	G	5101	L9R	C44-C45-C46-C47
9	I	5101	L9R	C44-C45-C46-C47
9	A	5308	L9R	C18-C19-C20-C21
9	B	5308	L9R	C18-C19-C20-C21
9	G	5101	L9R	C18-C19-C20-C21
9	I	5101	L9R	C18-C19-C20-C21
9	I	5108	L9R	C24-C25-C26-C27
9	A	5307	L9R	C24-C25-C26-C27
9	B	5307	L9R	C24-C25-C26-C27
9	G	5108	L9R	C24-C25-C26-C27
9	A	5307	L9R	O3P-C1-C2-C3
9	B	5307	L9R	O3P-C1-C2-C3
9	G	5108	L9R	O3P-C1-C2-C3
9	I	5108	L9R	O3P-C1-C2-C3
9	A	5307	L9R	C45-C46-C47-C48
9	G	5108	L9R	C45-C46-C47-C48
9	I	5108	L9R	C45-C46-C47-C48
9	A	5308	L9R	O11-C11-O3-C3
9	G	5101	L9R	O11-C11-O3-C3
9	I	5101	L9R	O11-C11-O3-C3
9	B	5307	L9R	C45-C46-C47-C48
5	A	5305	ATP	O4'-C1'-N9-C4
5	G	5106	ATP	O4'-C1'-N9-C4
9	B	5308	L9R	O11-C11-O3-C3
9	A	5307	L9R	C1-C2-C3-O3
9	B	5307	L9R	C1-C2-C3-O3
9	G	5108	L9R	C1-C2-C3-O3
9	I	5108	L9R	C1-C2-C3-O3
9	A	5307	L9R	O2-C2-C3-O3
9	B	5307	L9R	O2-C2-C3-O3
9	G	5108	L9R	O2-C2-C3-O3
9	I	5108	L9R	O2-C2-C3-O3
9	A	5307	L9R	C13-C14-C15-C16
9	A	5307	L9R	C15-C16-C17-C18
9	B	5307	L9R	C13-C14-C15-C16
9	G	5108	L9R	C13-C14-C15-C16
9	G	5108	L9R	C15-C16-C17-C18
9	I	5108	L9R	C13-C14-C15-C16
9	B	5307	L9R	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
9	I	5108	L9R	C15-C16-C17-C18
5	A	5305	ATP	O4'-C1'-N9-C8
5	B	5305	ATP	O4'-C1'-N9-C8
5	G	5106	ATP	O4'-C1'-N9-C8
5	I	5106	ATP	O4'-C1'-N9-C8
5	B	5305	ATP	O4'-C1'-N9-C4
5	I	5106	ATP	O4'-C1'-N9-C4
9	A	5308	L9R	C39-C40-C41-C42
9	B	5308	L9R	C39-C40-C41-C42
9	G	5101	L9R	C39-C40-C41-C42
9	I	5101	L9R	C39-C40-C41-C42
9	A	5307	L9R	C4-O4P-P-O1P
9	A	5308	L9R	C4-C5-N-C7
9	B	5307	L9R	C4-O4P-P-O1P
9	B	5308	L9R	C4-C5-N-C7
9	G	5101	L9R	C4-C5-N-C7
9	G	5108	L9R	C4-O4P-P-O1P
9	I	5101	L9R	C4-C5-N-C7
9	I	5108	L9R	C4-O4P-P-O1P
5	A	5305	ATP	C3'-C4'-C5'-O5'
5	B	5305	ATP	C3'-C4'-C5'-O5'
5	G	5106	ATP	C3'-C4'-C5'-O5'
5	I	5106	ATP	C3'-C4'-C5'-O5'
9	A	5308	L9R	C4-C5-N-C6
9	B	5308	L9R	C4-C5-N-C6
9	G	5101	L9R	C4-C5-N-C6
9	I	5101	L9R	C4-C5-N-C6
9	A	5308	L9R	C23-C24-C25-C26
9	I	5101	L9R	C23-C24-C25-C26
9	B	5308	L9R	C23-C24-C25-C26
9	G	5101	L9R	C23-C24-C25-C26
5	A	5305	ATP	O4'-C4'-C5'-O5'
5	B	5305	ATP	O4'-C4'-C5'-O5'
5	G	5106	ATP	O4'-C4'-C5'-O5'
5	I	5106	ATP	O4'-C4'-C5'-O5'
5	A	5301	ATP	PG-O3B-PB-O3A
5	G	5102	ATP	PG-O3B-PB-O3A
9	A	5308	L9R	C4-C5-N-C8
9	B	5308	L9R	C4-C5-N-C8
9	G	5101	L9R	C4-C5-N-C8
9	I	5101	L9R	C4-C5-N-C8
9	A	5307	L9R	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
9	B	5307	L9R	C40-C41-C42-C43
9	G	5108	L9R	C40-C41-C42-C43
9	I	5108	L9R	C40-C41-C42-C43
9	G	5101	L9R	C25-C26-C27-C28
9	B	5308	L9R	C25-C26-C27-C28
9	I	5101	L9R	C25-C26-C27-C28
9	A	5308	L9R	C25-C26-C27-C28
5	B	5301	ATP	PG-O3B-PB-O3A
5	I	5102	ATP	PG-O3B-PB-O3A
5	A	5301	ATP	PG-O3B-PB-O1B
5	A	5305	ATP	PG-O3B-PB-O1B
5	A	5305	ATP	PG-O3B-PB-O2B
5	B	5301	ATP	PG-O3B-PB-O1B
5	B	5305	ATP	PG-O3B-PB-O1B
5	B	5305	ATP	PG-O3B-PB-O2B
5	G	5102	ATP	PG-O3B-PB-O1B
5	G	5106	ATP	PG-O3B-PB-O1B
5	G	5106	ATP	PG-O3B-PB-O2B
5	I	5102	ATP	PG-O3B-PB-O1B
5	I	5106	ATP	PG-O3B-PB-O1B
5	I	5106	ATP	PG-O3B-PB-O2B
9	I	5108	L9R	C12-C13-C14-C15
9	G	5108	L9R	C12-C13-C14-C15
9	A	5307	L9R	C12-C13-C14-C15
9	B	5307	L9R	C12-C13-C14-C15
9	A	5307	L9R	O2-C31-C32-C33
9	B	5307	L9R	O2-C31-C32-C33
9	G	5108	L9R	O2-C31-C32-C33
9	I	5108	L9R	O2-C31-C32-C33
9	B	5307	L9R	C43-C44-C45-C46
9	A	5307	L9R	C43-C44-C45-C46
9	G	5108	L9R	C43-C44-C45-C46
9	I	5108	L9R	C43-C44-C45-C46
5	A	5301	ATP	C4'-C5'-O5'-PA
5	B	5301	ATP	C4'-C5'-O5'-PA
5	G	5102	ATP	C4'-C5'-O5'-PA
5	I	5102	ATP	C4'-C5'-O5'-PA
9	A	5308	L9R	C45-C46-C47-C48
9	I	5101	L9R	C45-C46-C47-C48
9	G	5101	L9R	C45-C46-C47-C48
9	B	5308	L9R	C45-C46-C47-C48
9	B	5307	L9R	O31-C31-C32-C33

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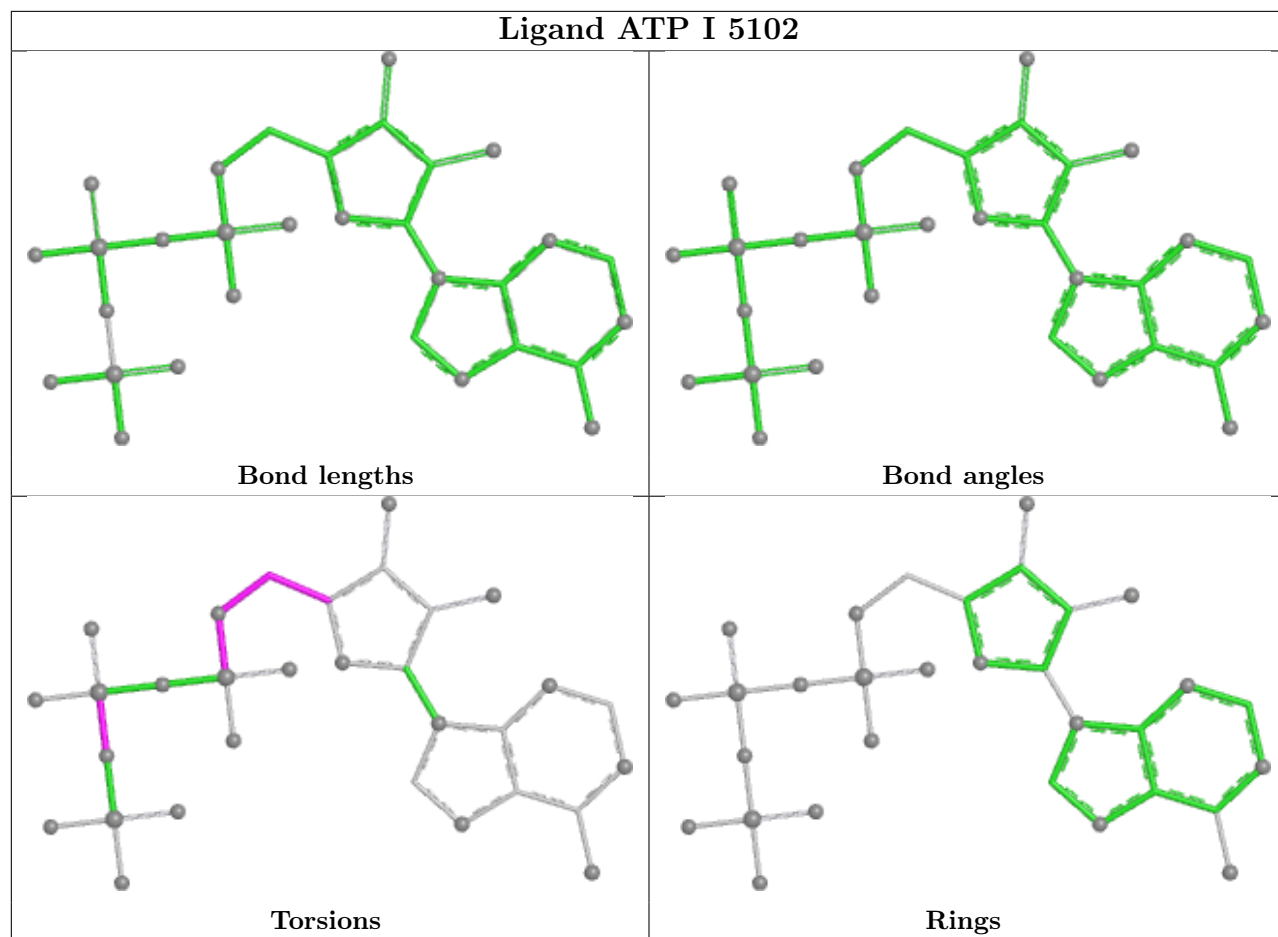
Mol	Chain	Res	Type	Atoms
9	I	5108	L9R	O31-C31-C32-C33
9	A	5307	L9R	O31-C31-C32-C33
9	G	5108	L9R	O31-C31-C32-C33

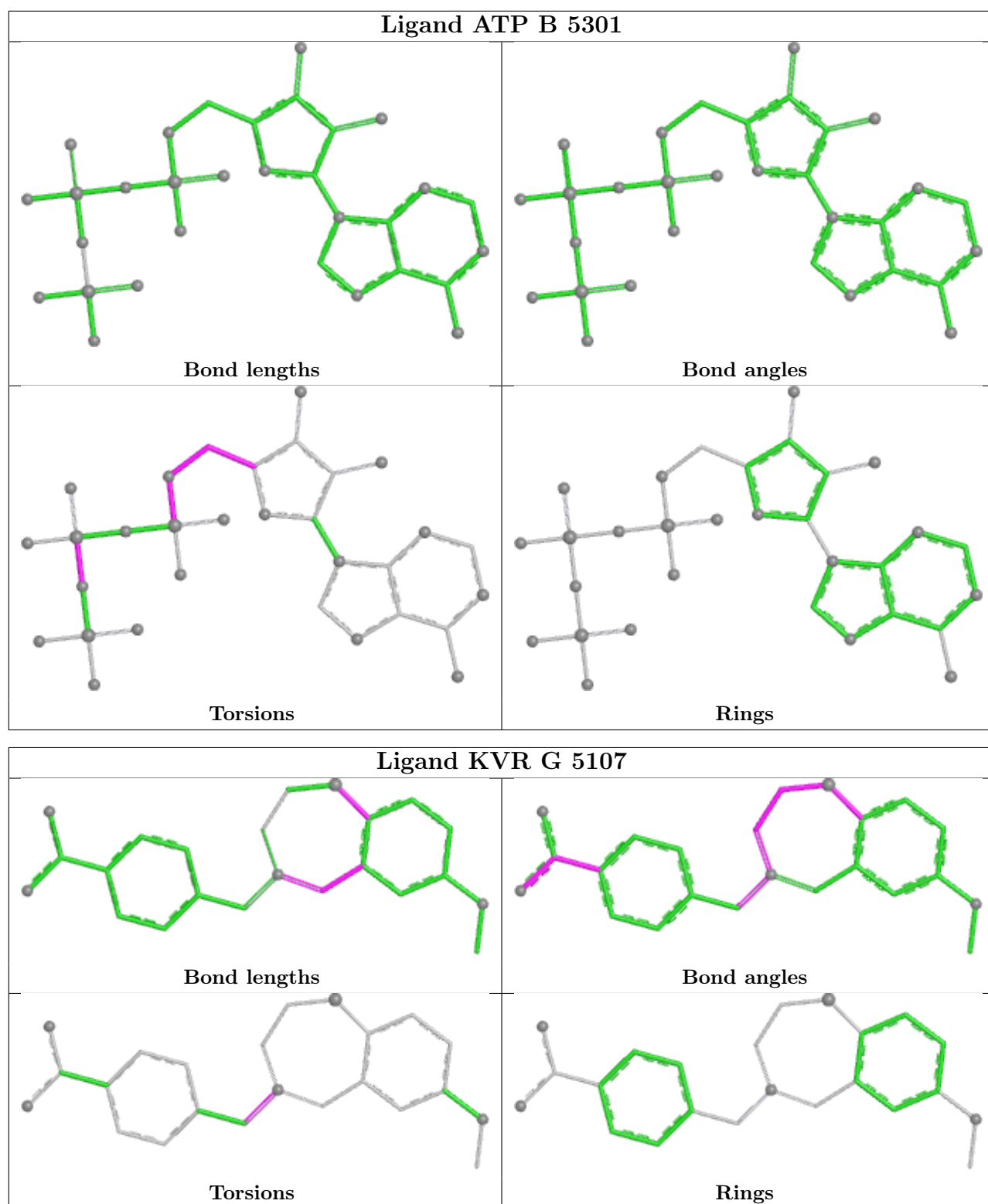
There are no ring outliers.

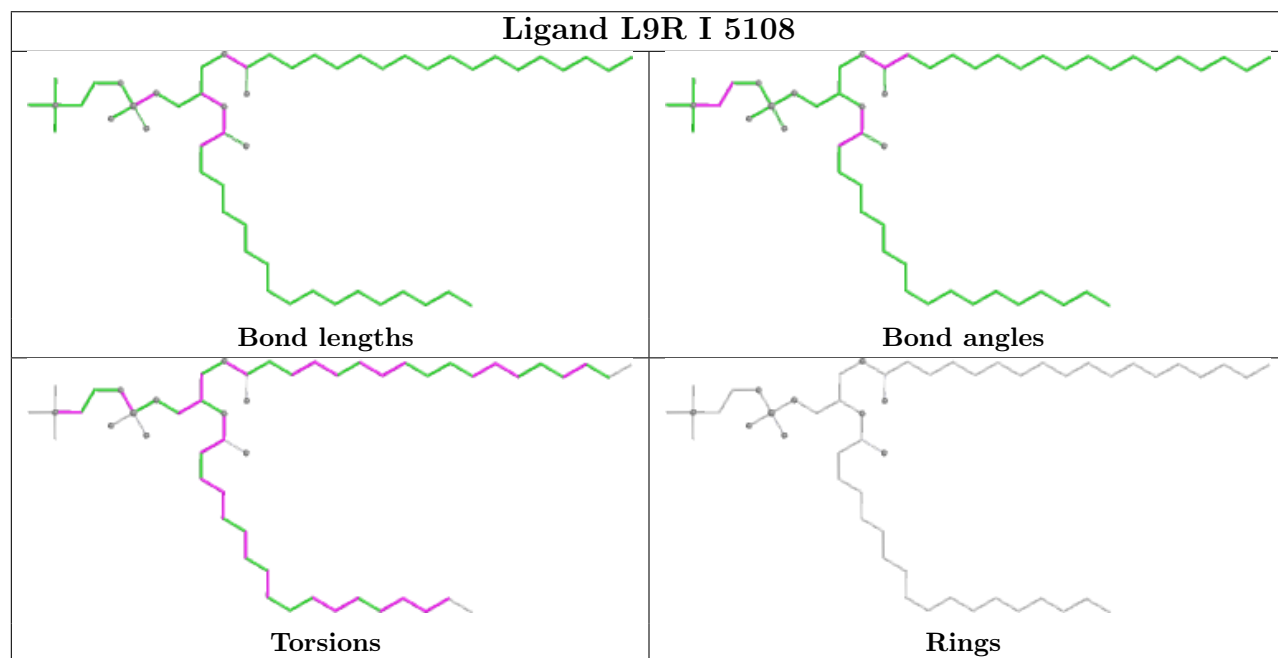
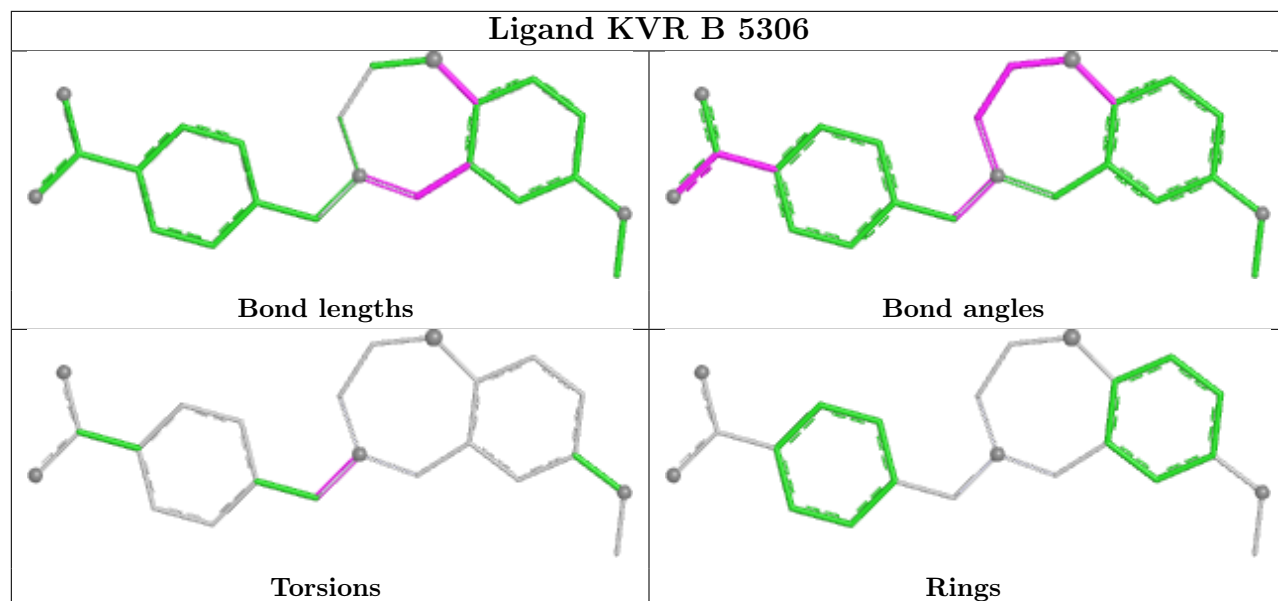
16 monomers are involved in 36 short contacts:

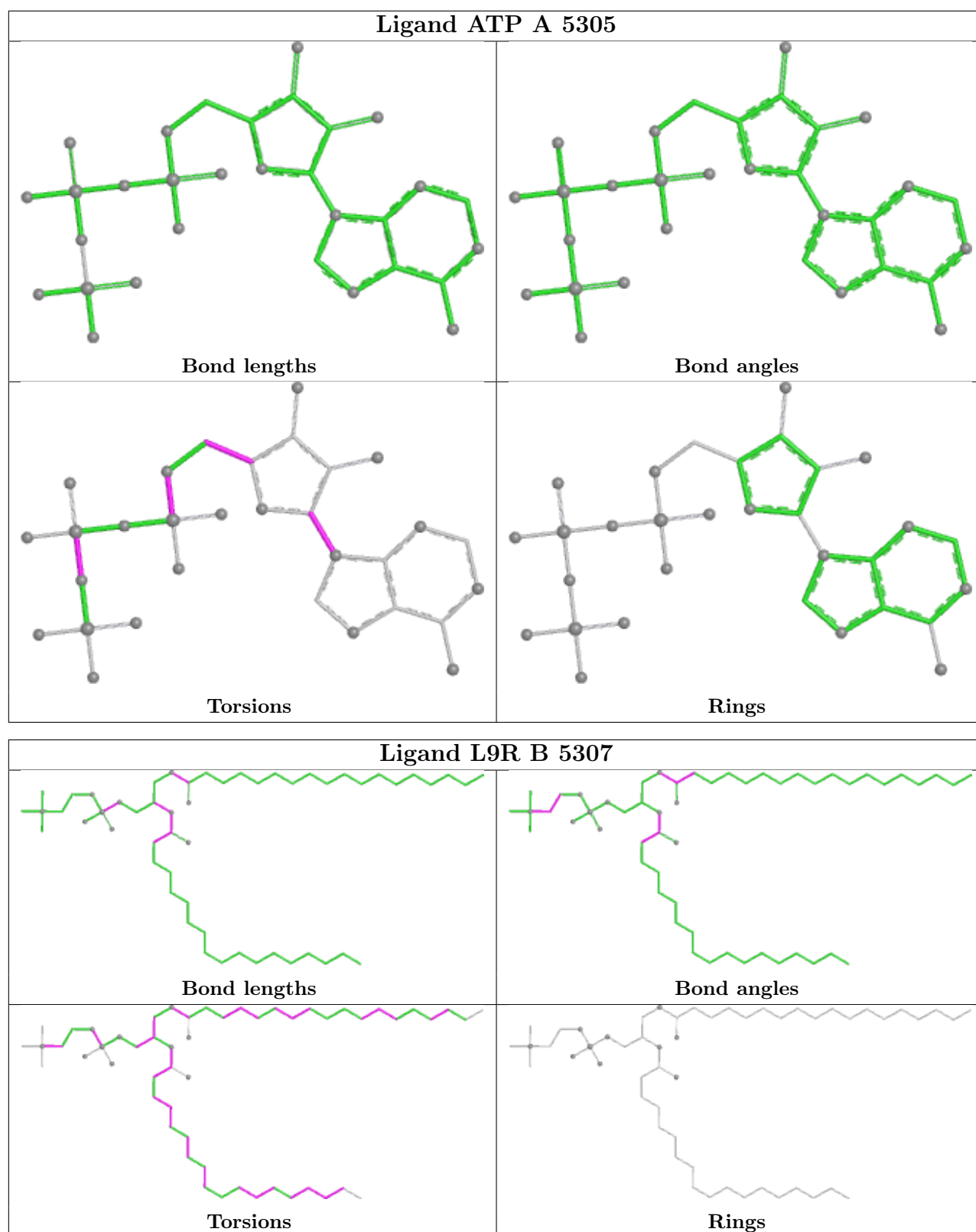
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	5102	ATP	1	0
5	B	5301	ATP	1	0
9	I	5108	L9R	3	0
5	A	5305	ATP	1	0
9	B	5307	L9R	2	0
9	I	5101	L9R	5	0
5	G	5102	ATP	1	0
9	G	5108	L9R	3	0
9	A	5307	L9R	3	0
5	I	5106	ATP	1	0
9	A	5308	L9R	6	0
5	B	5305	ATP	1	0
5	A	5301	ATP	1	0
5	G	5106	ATP	1	0
9	B	5308	L9R	4	0
9	G	5101	L9R	6	0

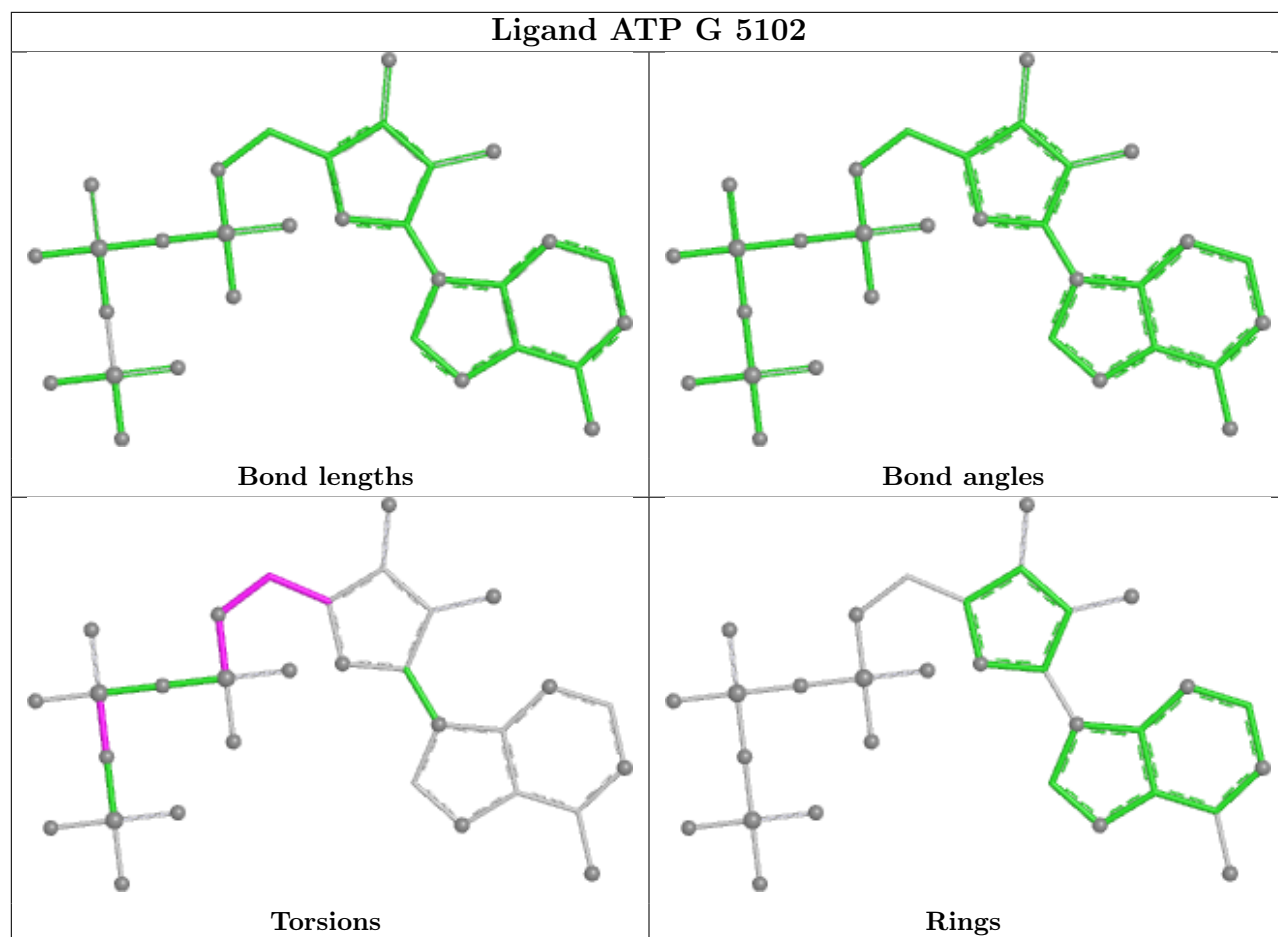
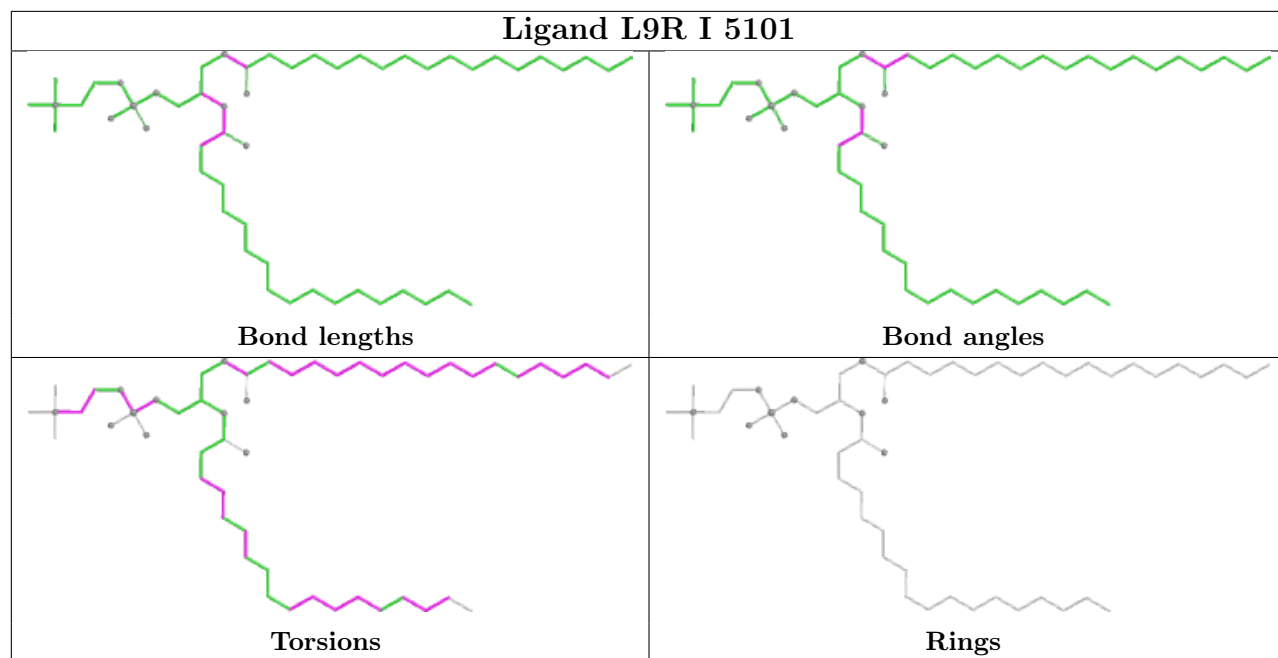
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

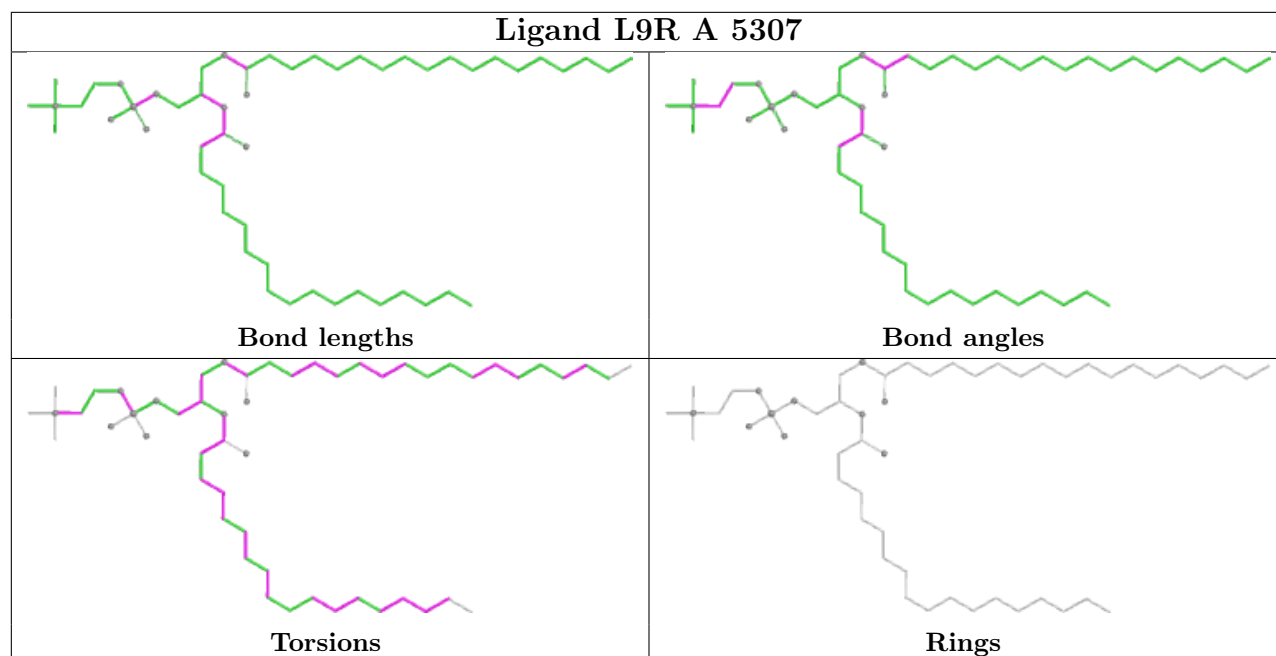
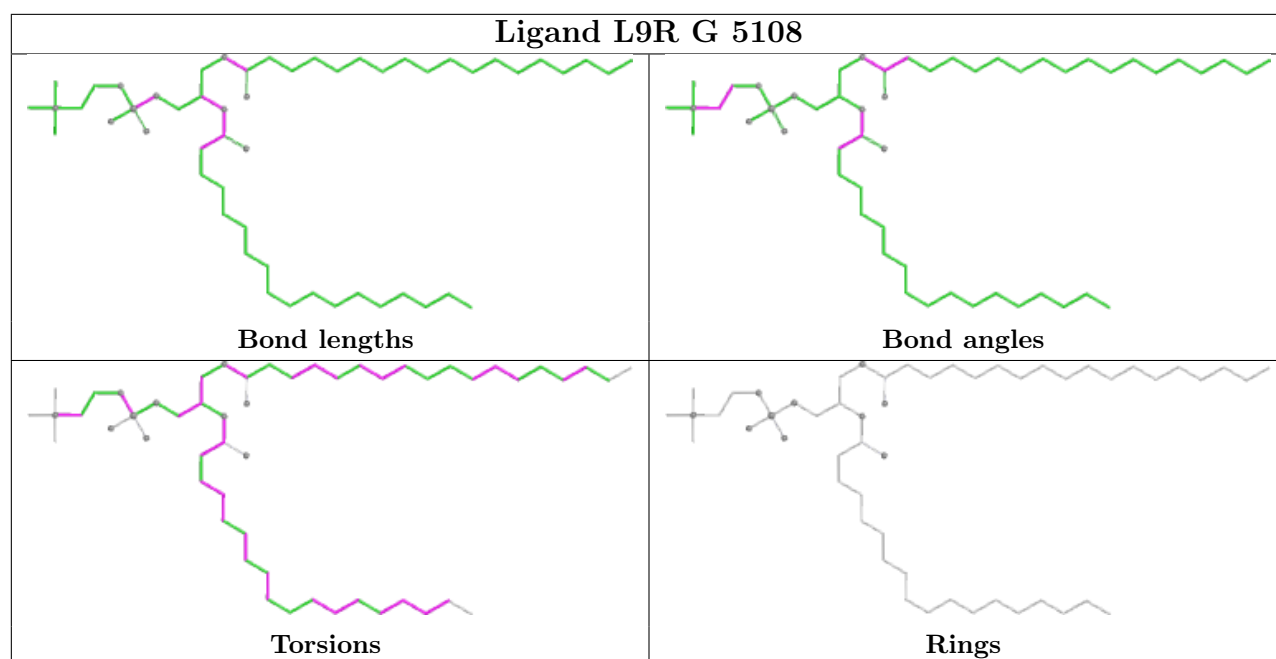


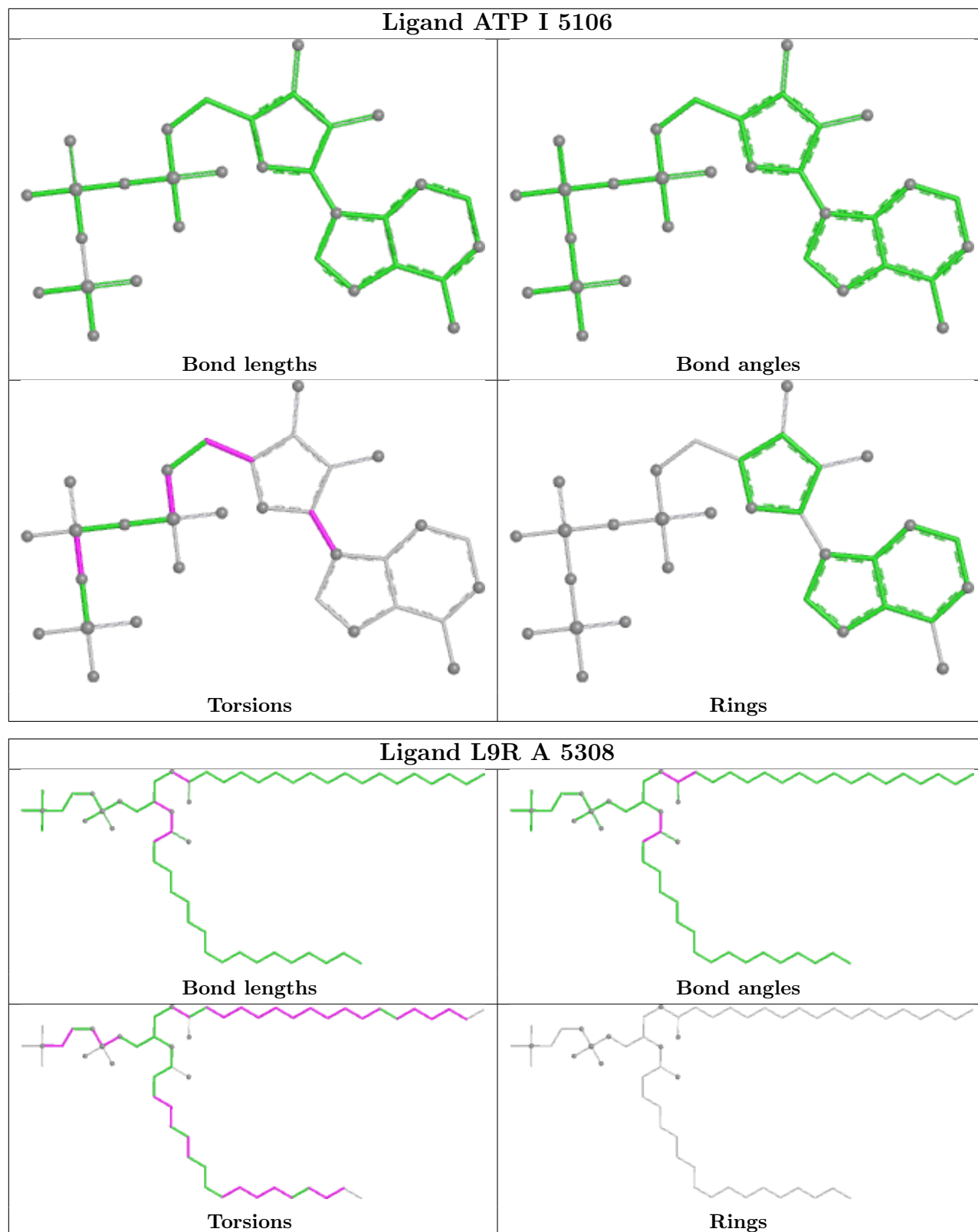


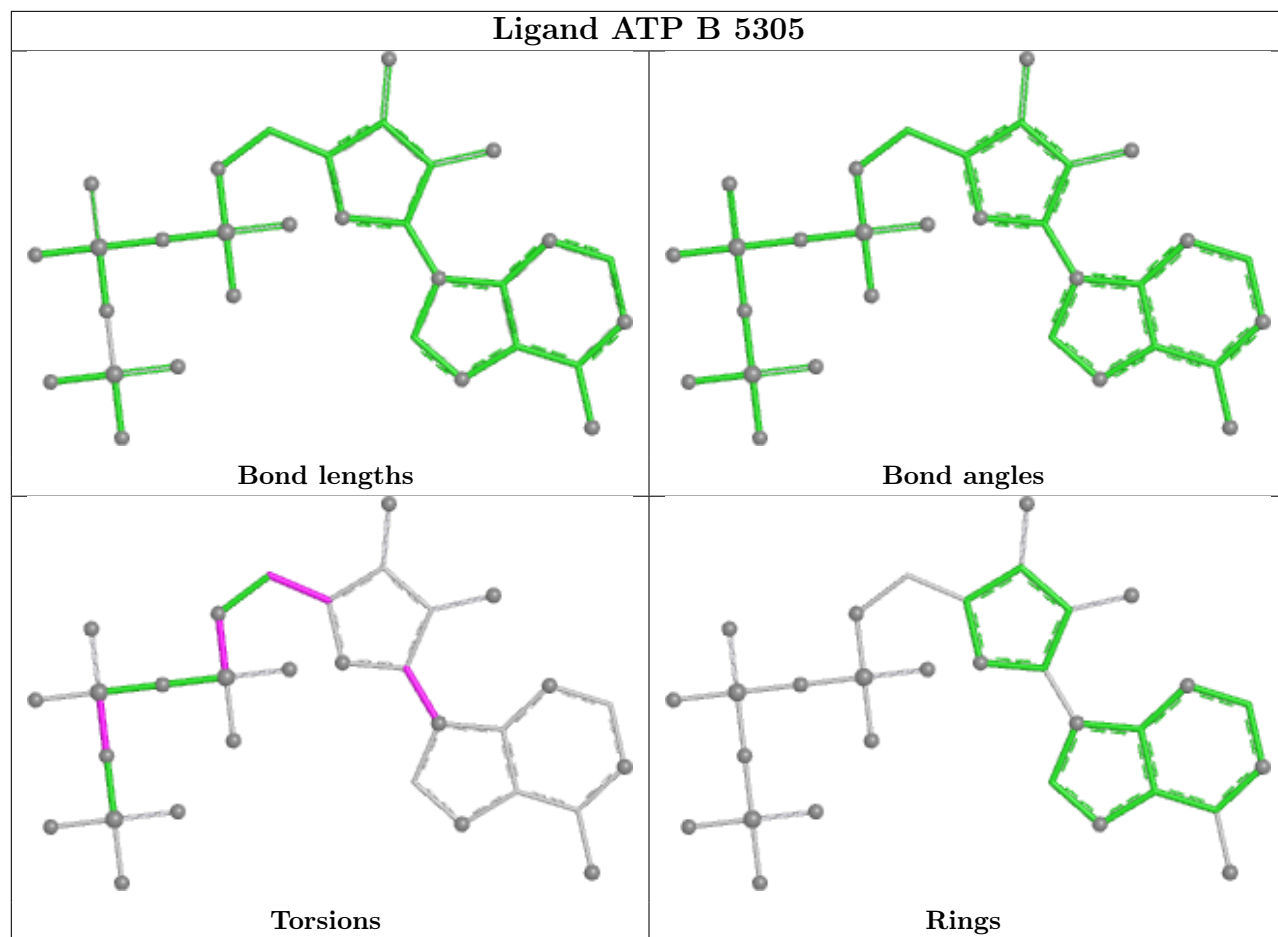


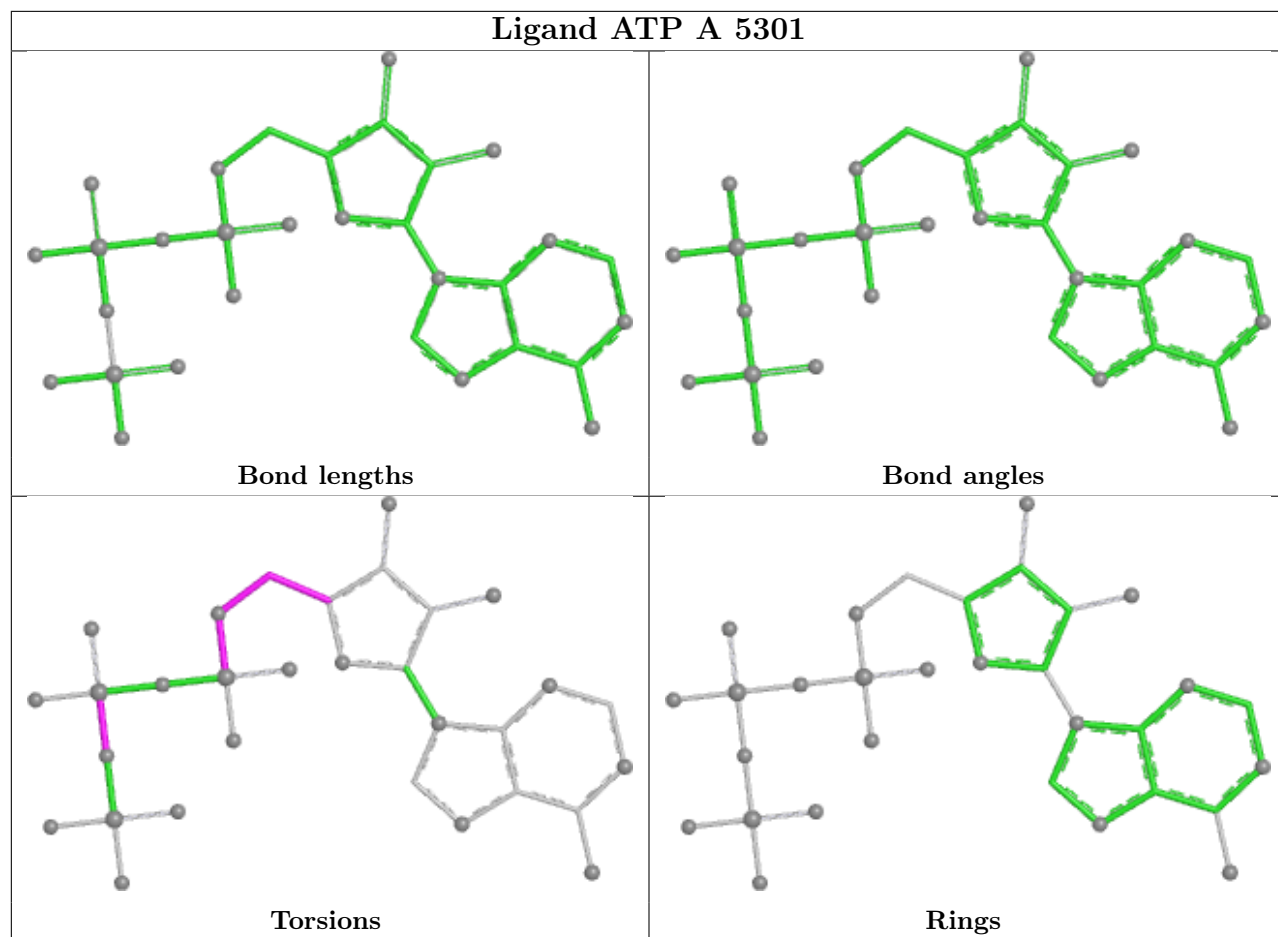


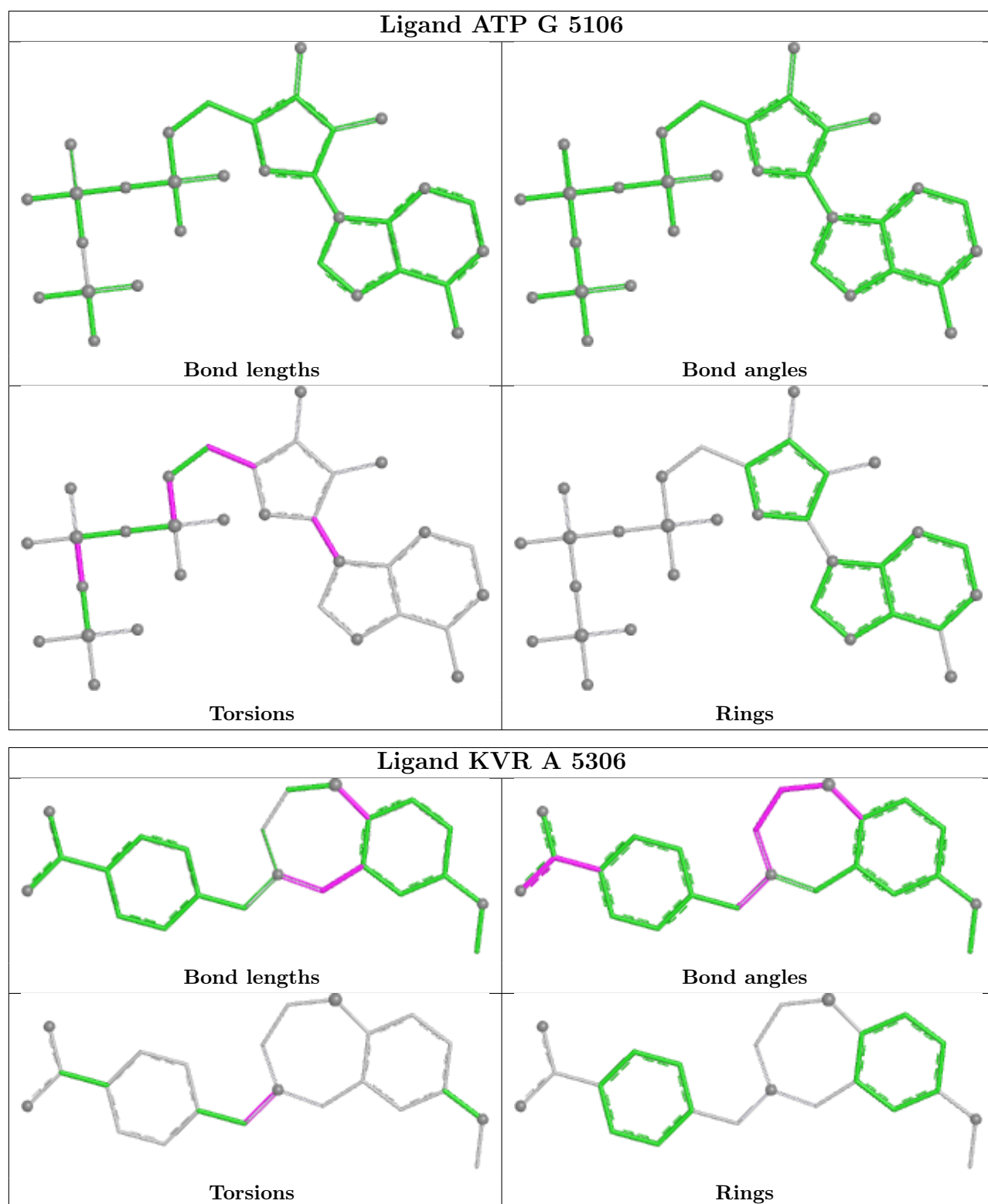


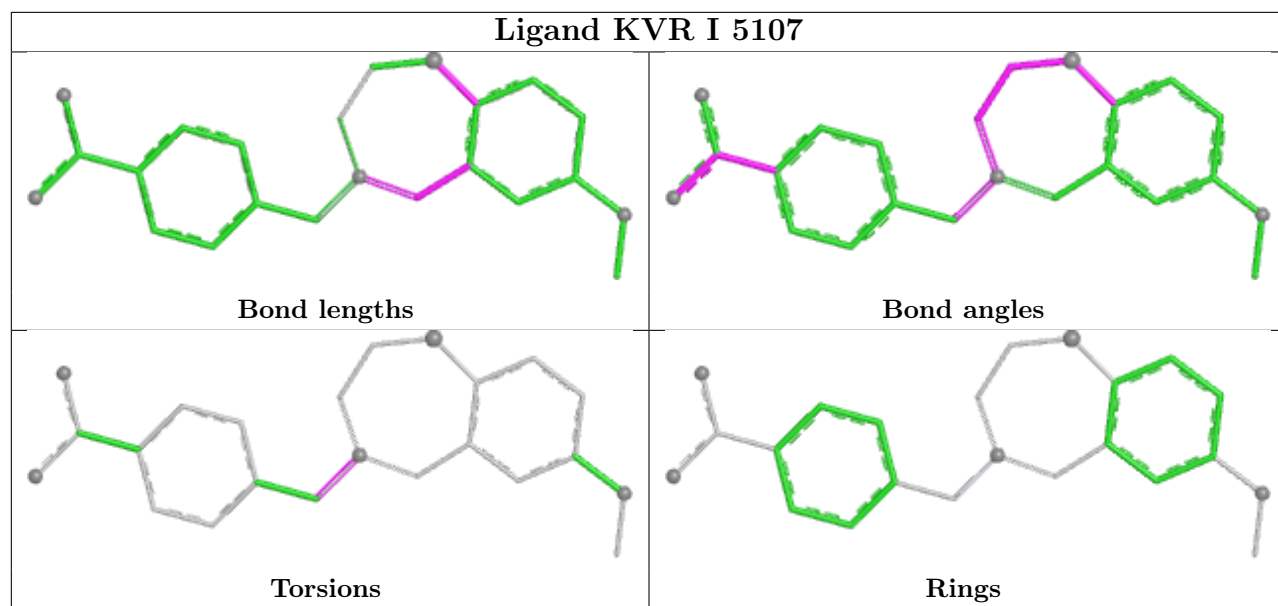
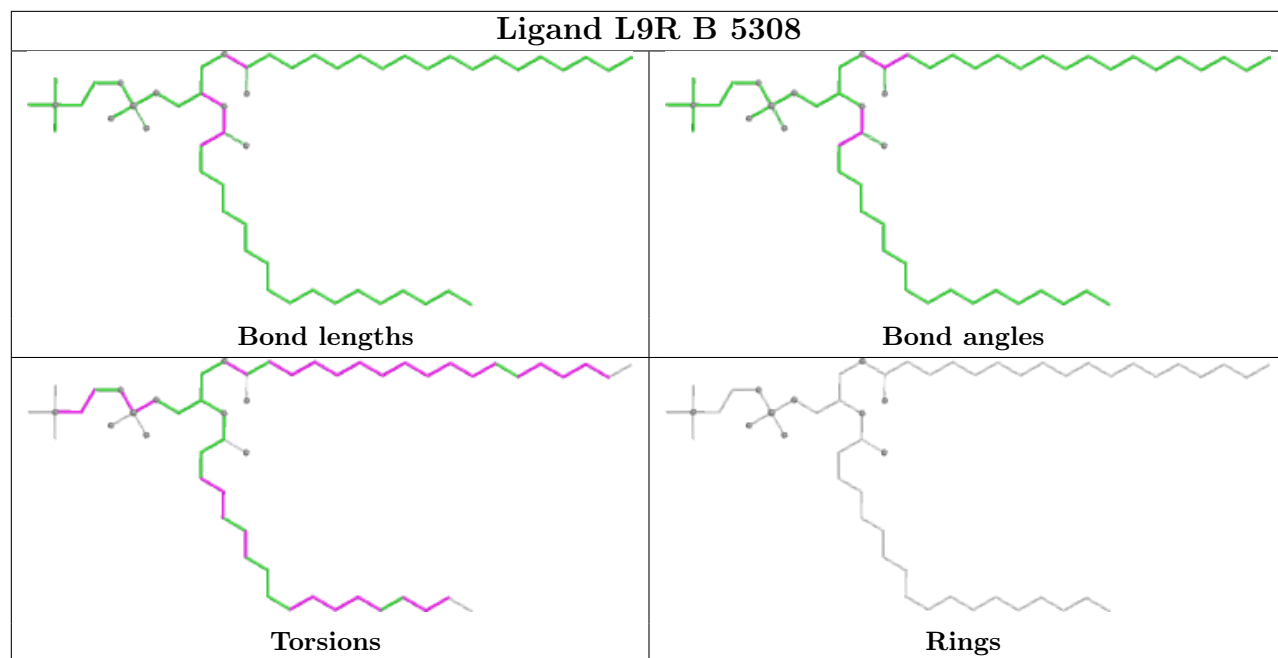


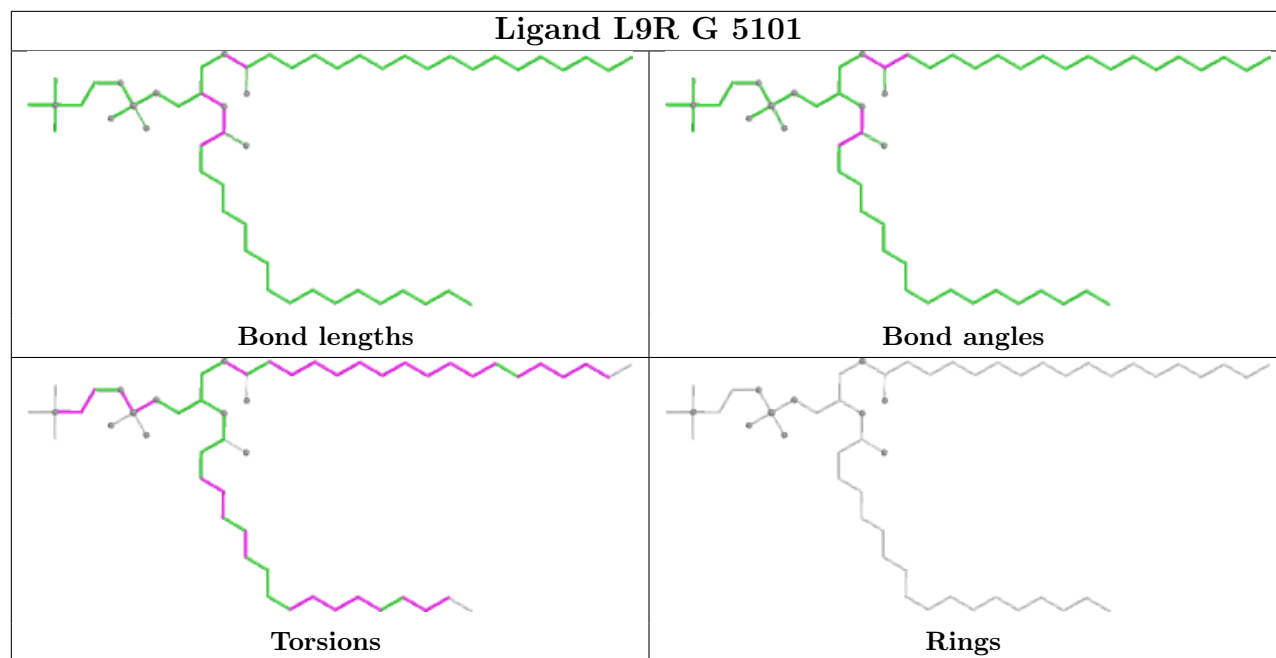












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

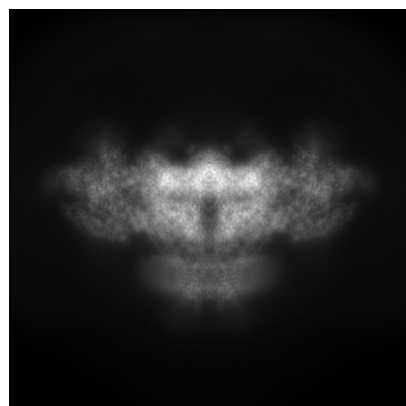
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26205. These allow visual inspection of the internal detail of the map and identification of artifacts.

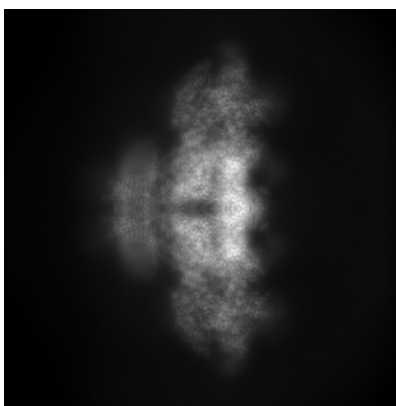
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

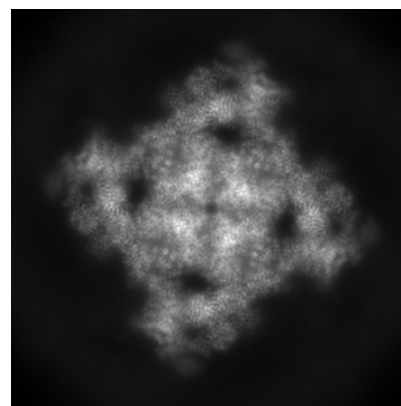
6.1.1 Primary map



X

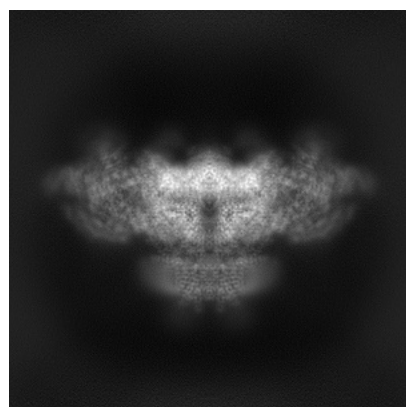


Y

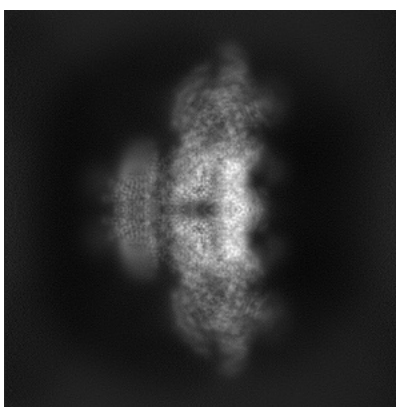


Z

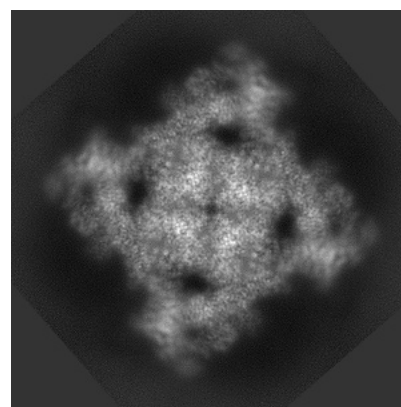
6.1.2 Raw map



X



Y



Z

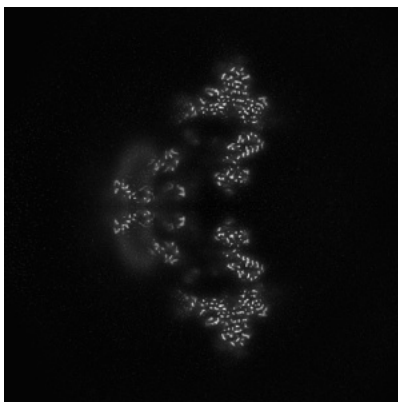
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

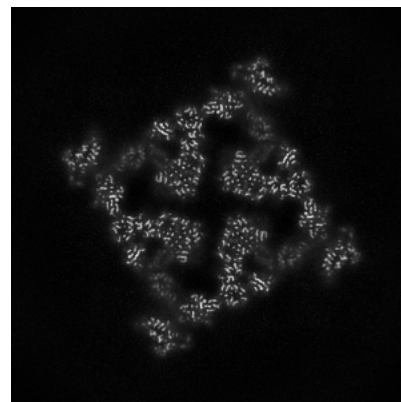
6.2.1 Primary map



X Index: 256

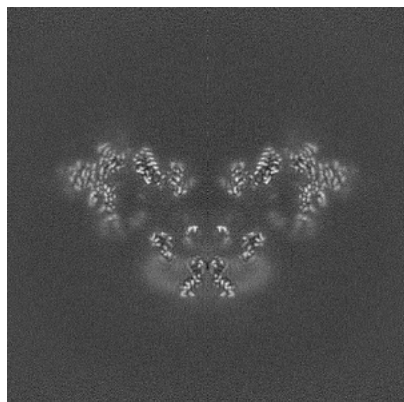


Y Index: 256

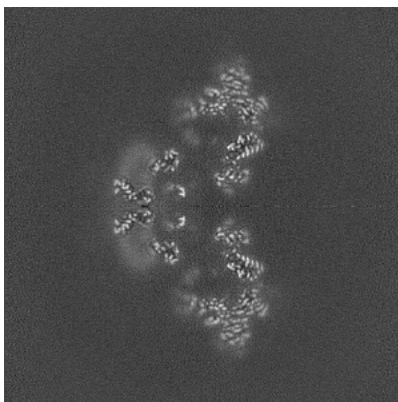


Z Index: 256

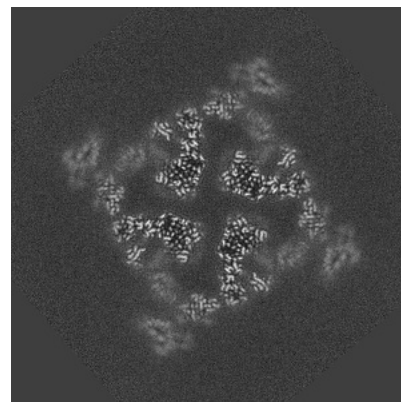
6.2.2 Raw map



X Index: 256



Y Index: 256

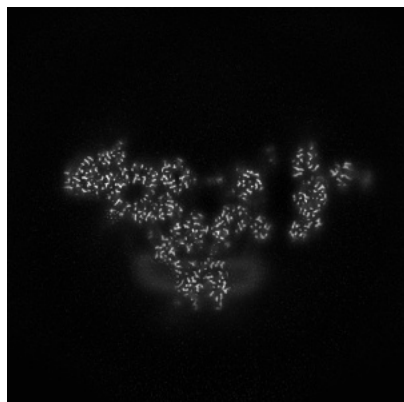


Z Index: 256

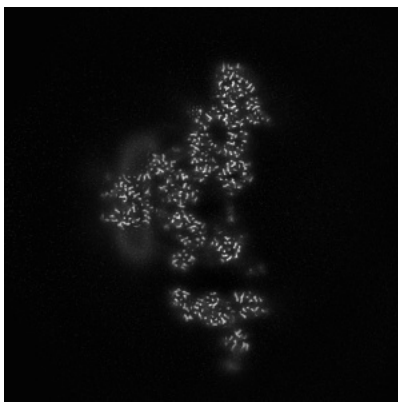
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

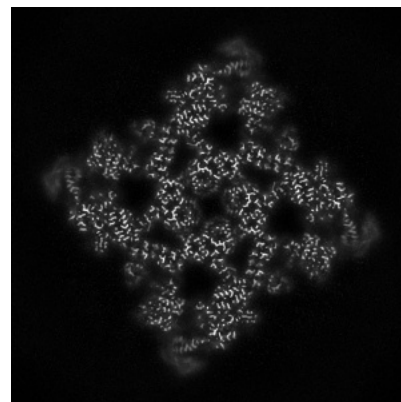
6.3.1 Primary map



X Index: 272

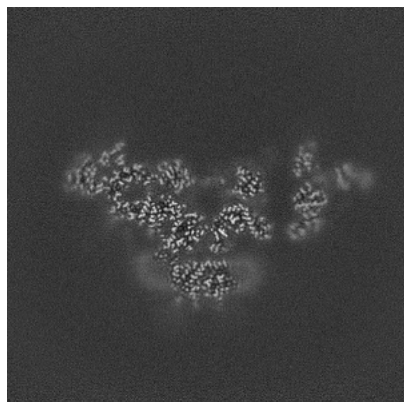


Y Index: 272

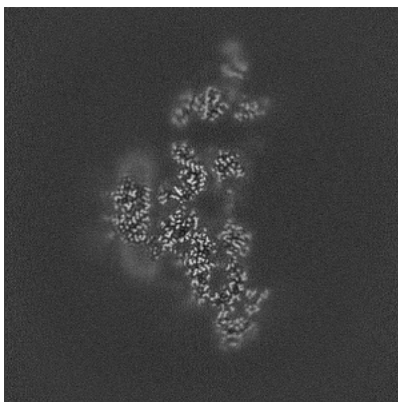


Z Index: 286

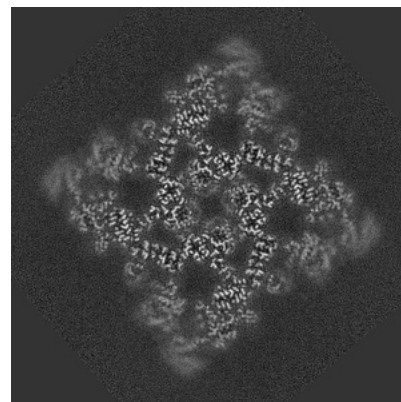
6.3.2 Raw map



X Index: 275



Y Index: 237

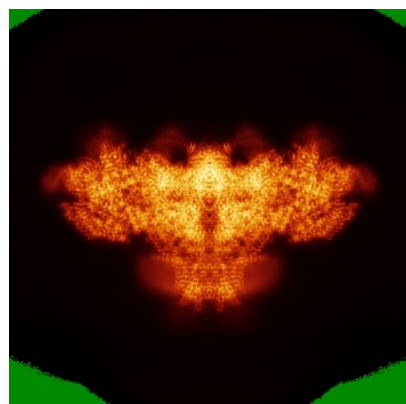


Z Index: 286

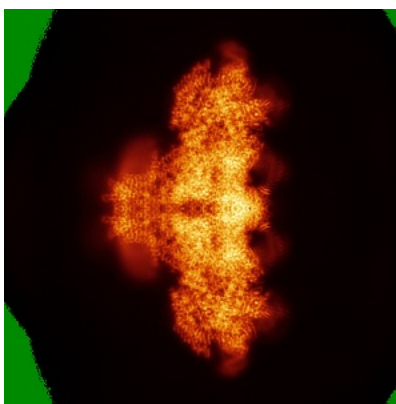
The images above show the largest variance slices of the map in three orthogonal directions.

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

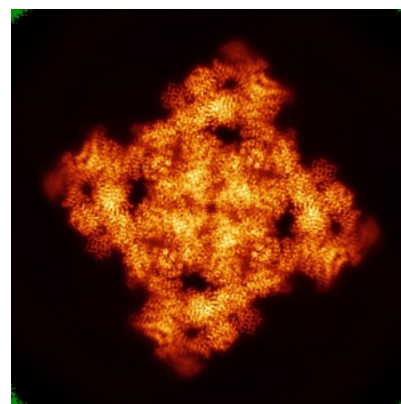
6.4.1 Primary map



X



Y

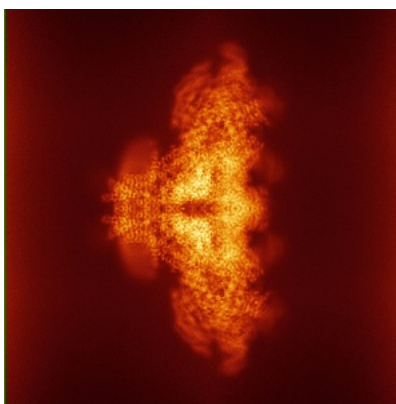


Z

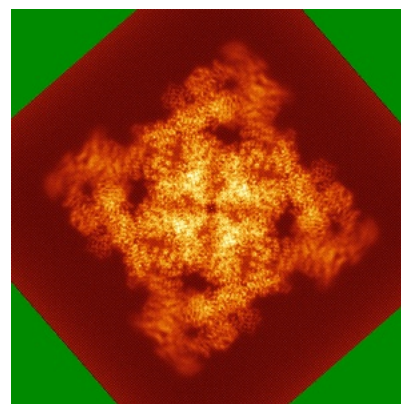
6.4.2 Raw map



X



Y

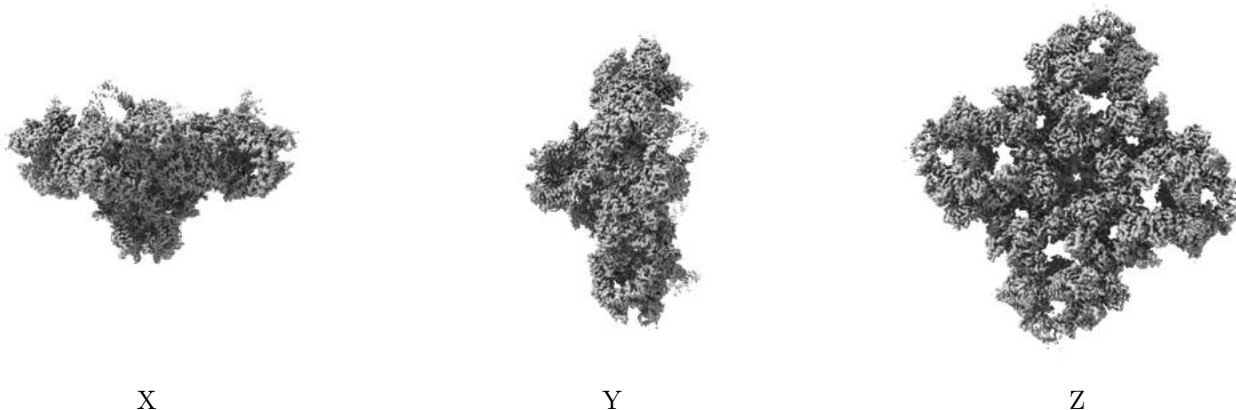


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

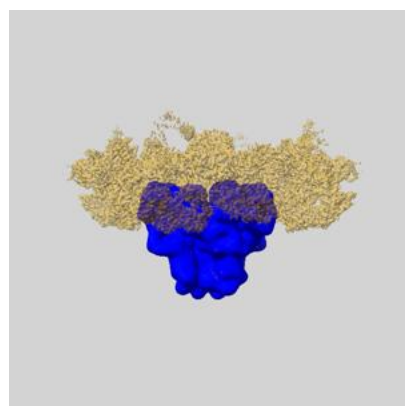
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

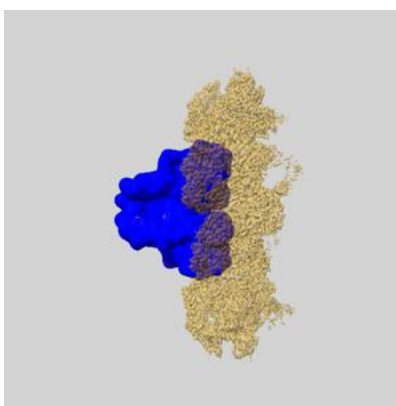
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

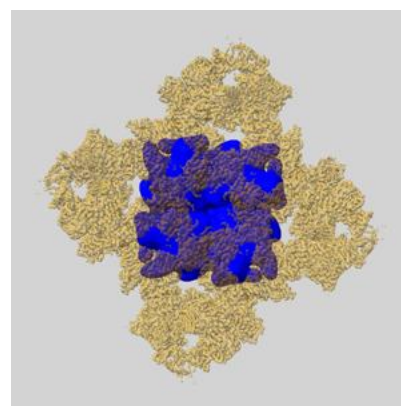
6.6.1 emd_26205_msk_1.map [i](#)



X

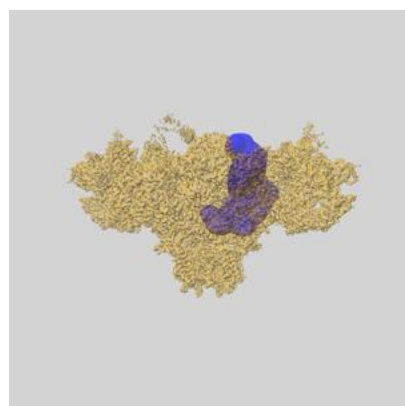


Y

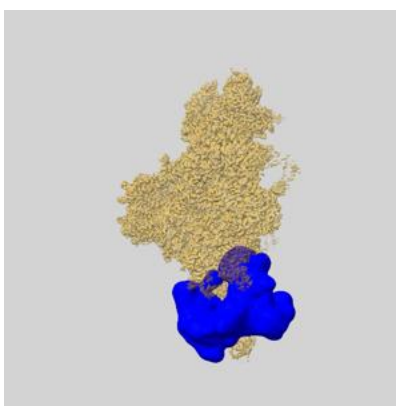


Z

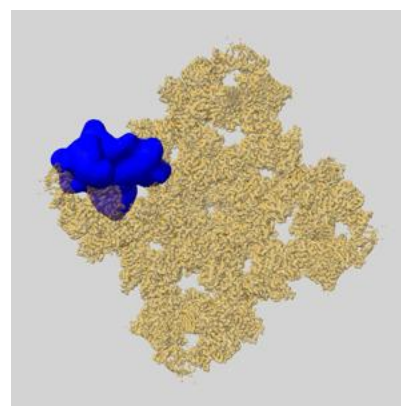
6.6.2 emd_26205_msk_2.map [i](#)



X

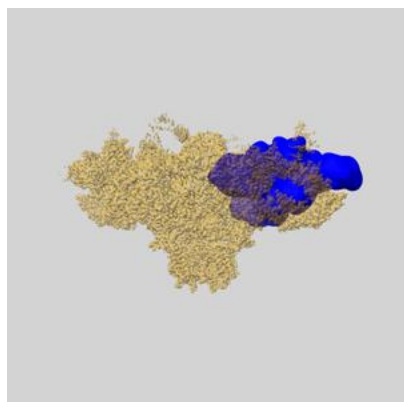


Y

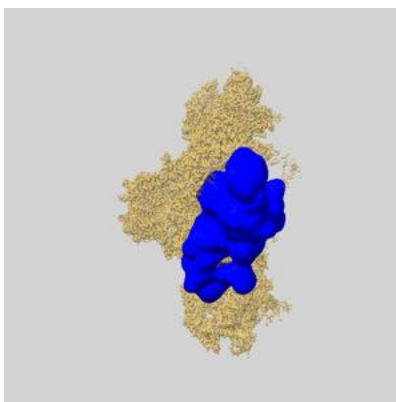


Z

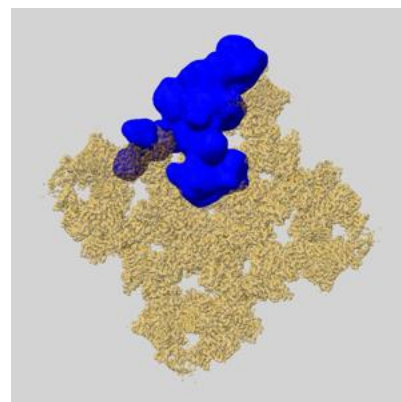
6.6.3 emd_26205_msk_3.map [i](#)



X



Y

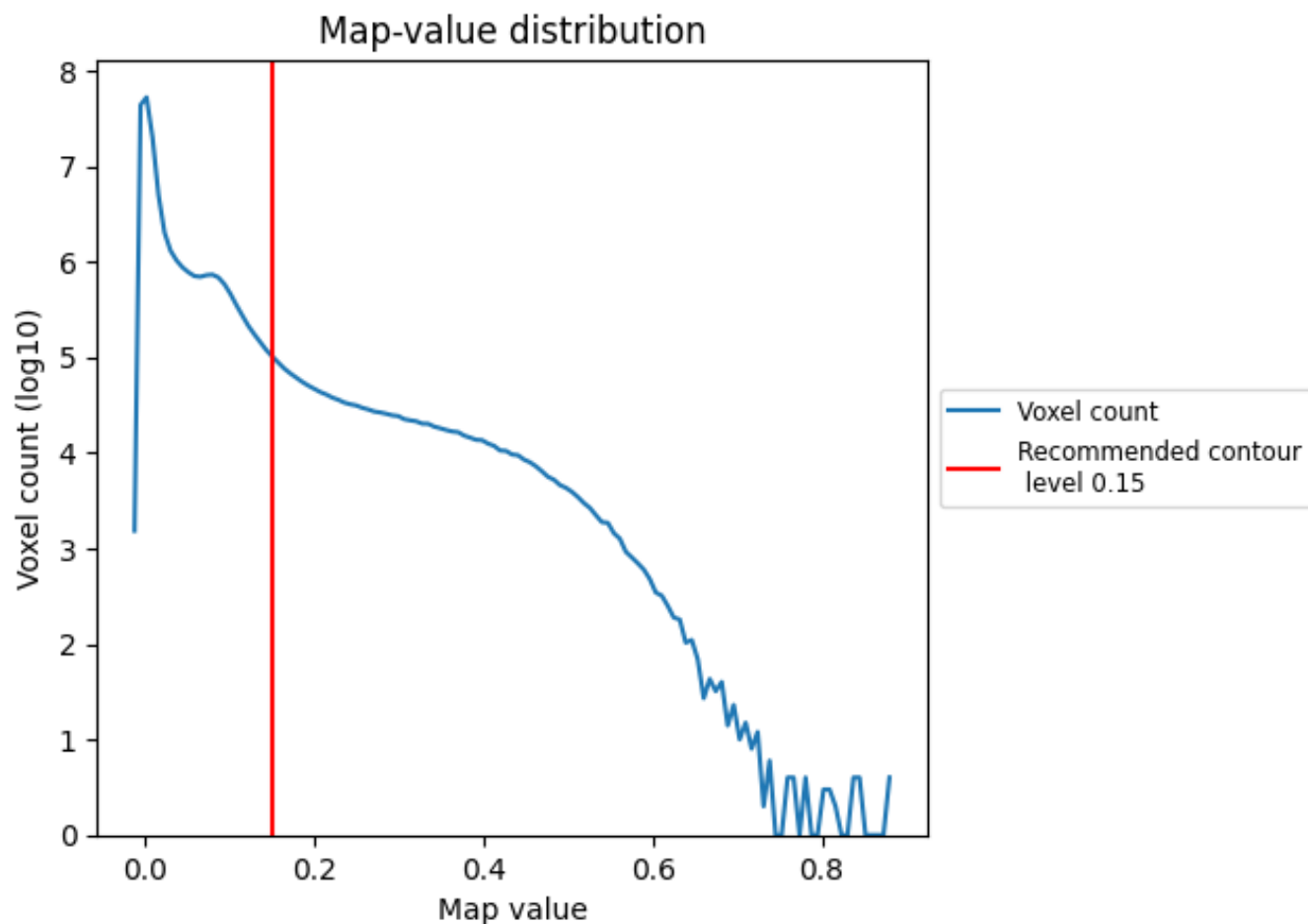


Z

7 Map analysis [i](#)

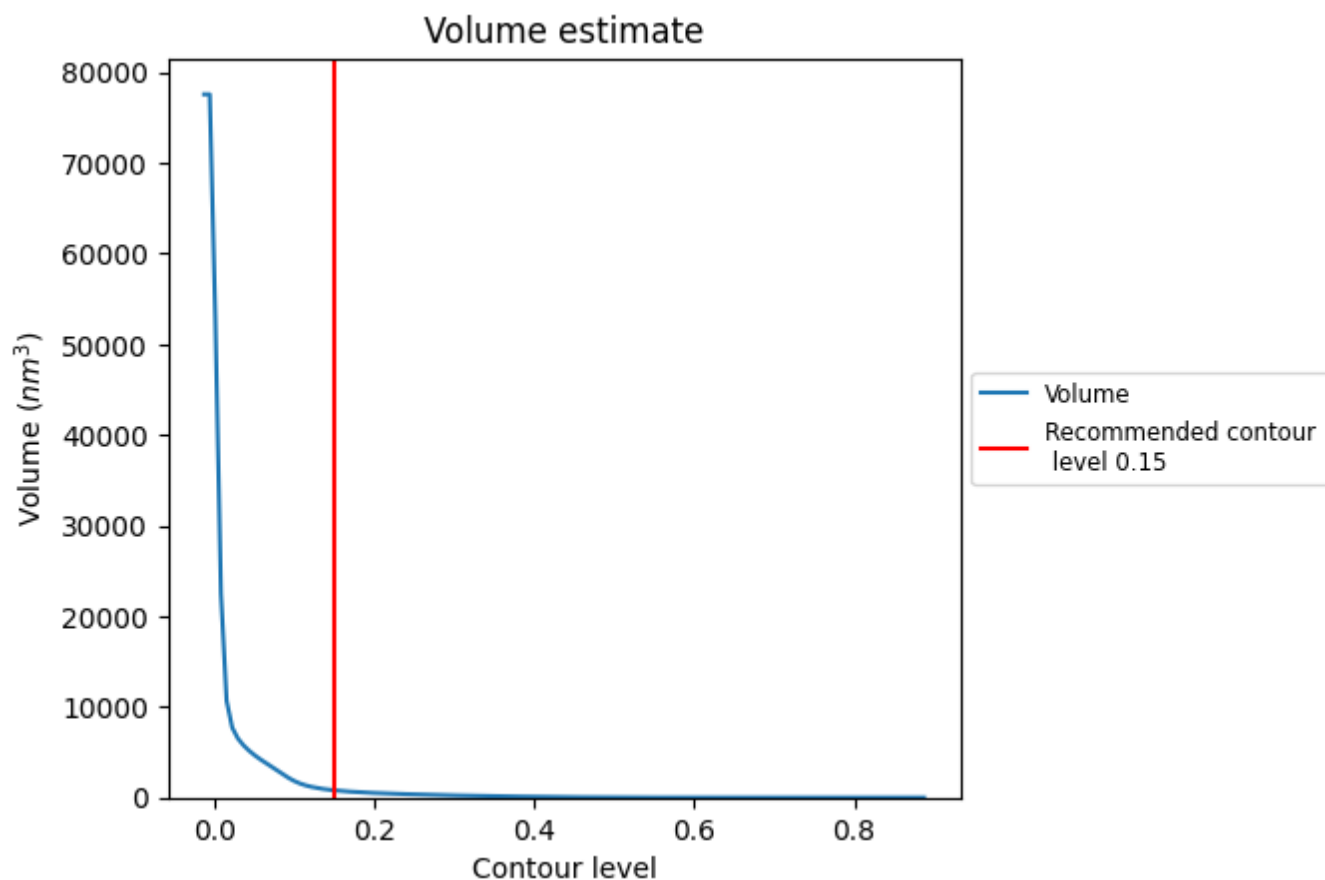
This section contains the results of statistical analysis of the map.

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.

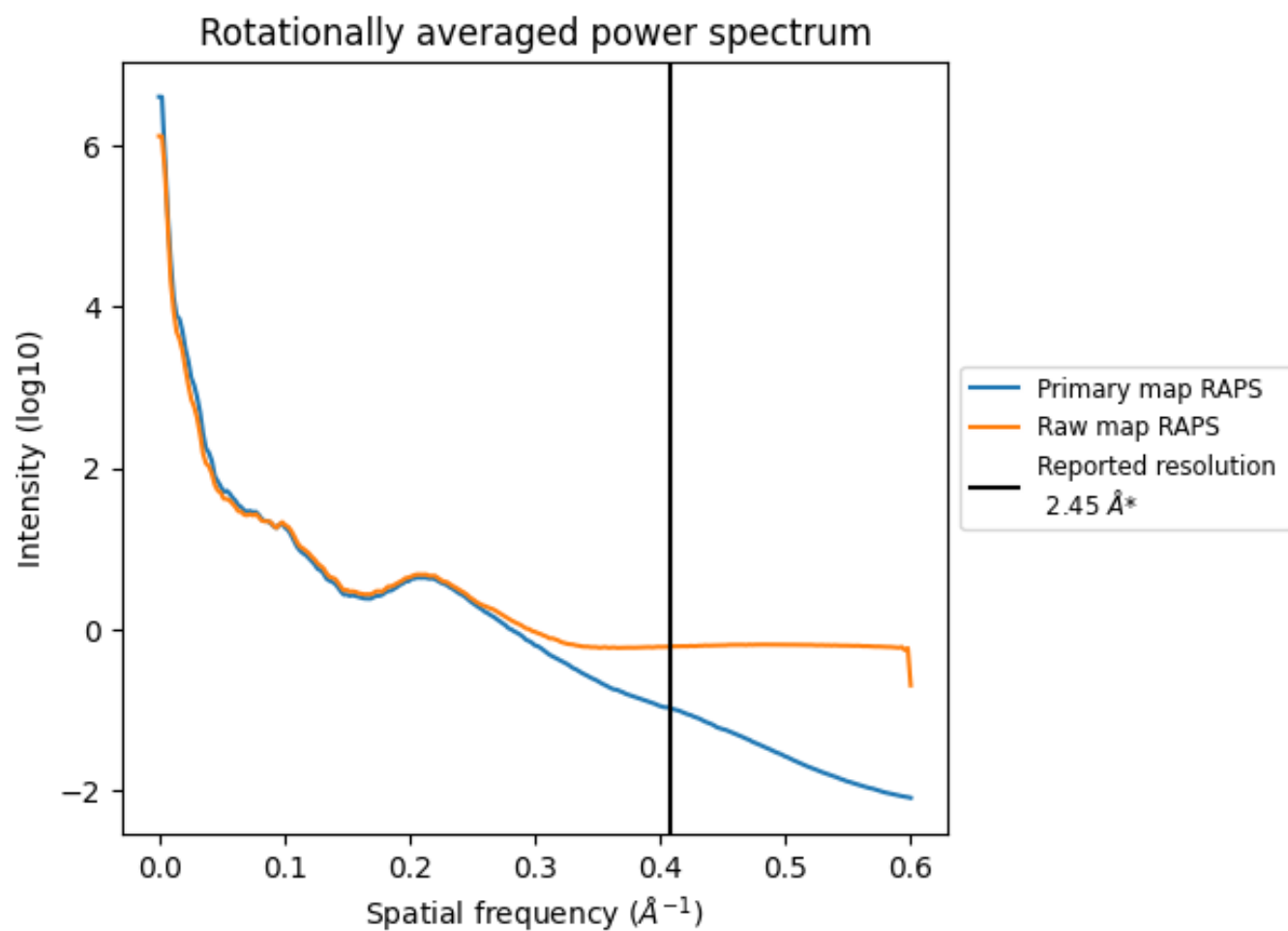
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 800 nm³; this corresponds to an approximate mass of 723 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 ⓘ

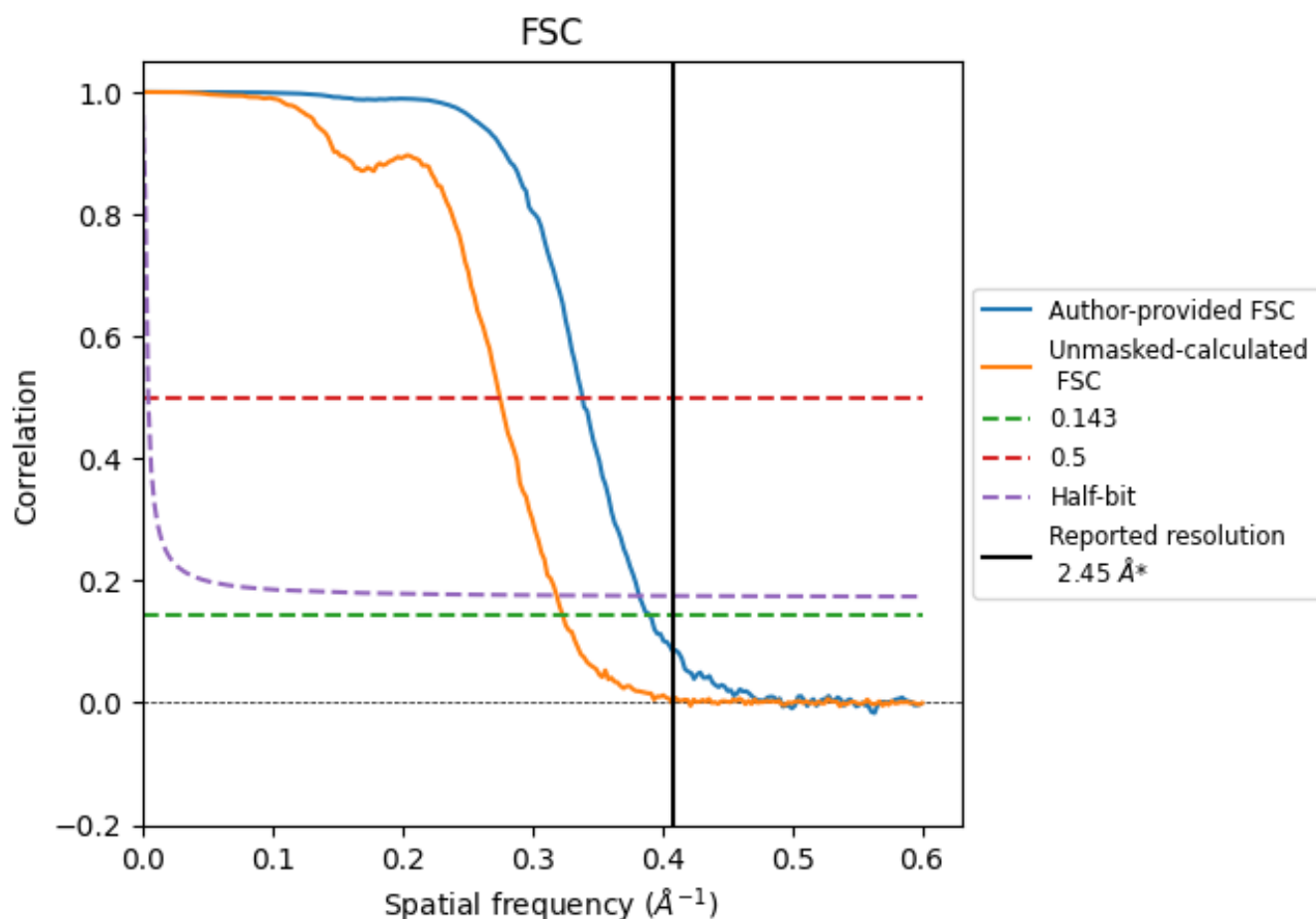


*Reported resolution corresponds to spatial frequency of 0.408 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.408 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

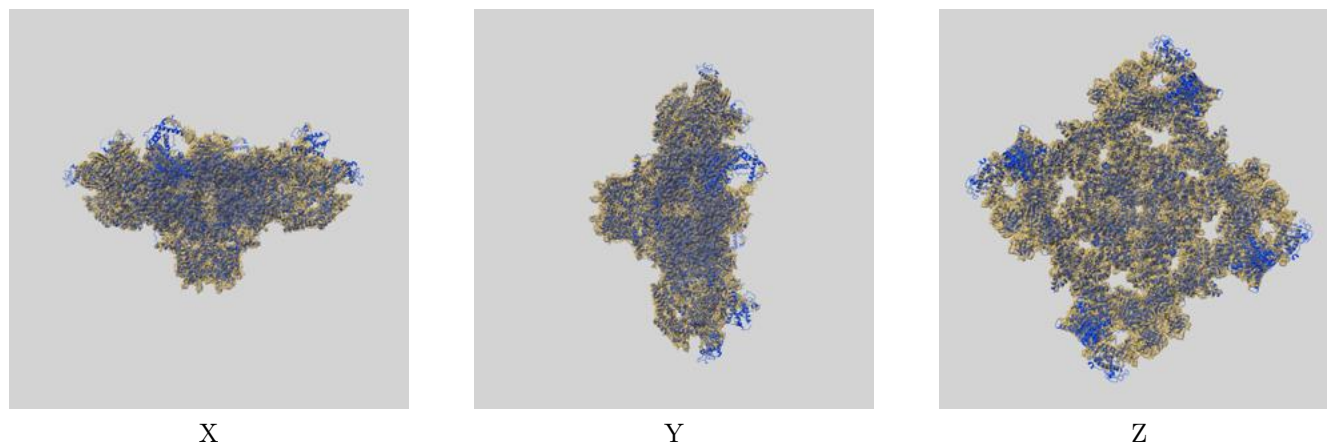
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.45	-	-
Author-provided FSC curve	2.56	2.95	2.62
Unmasked-calculated*	3.09	3.63	3.14

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.09 differs from the reported value 2.45 by more than 10 %

9 Map-model fit [i](#)

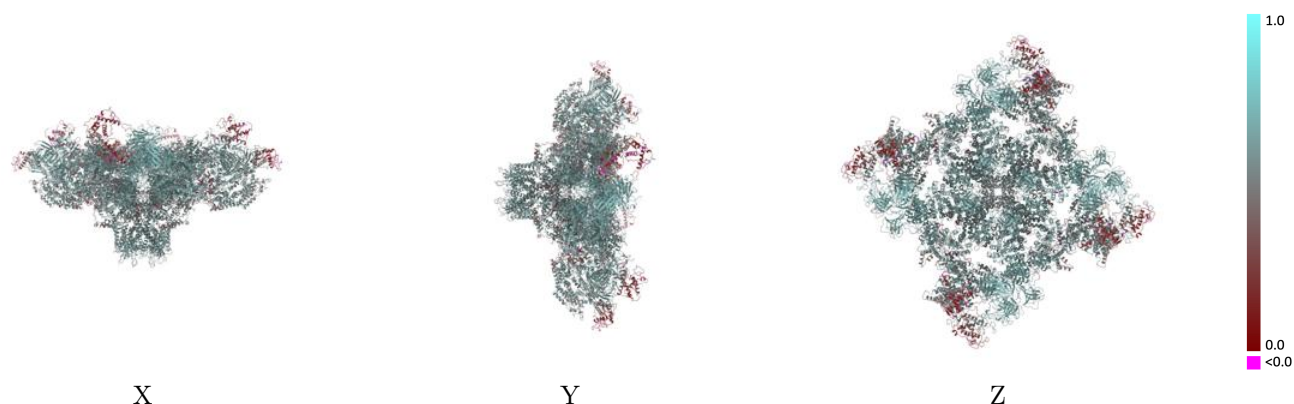
This section contains information regarding the fit between EMDB map EMD-26205 and PDB model 7TZC. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



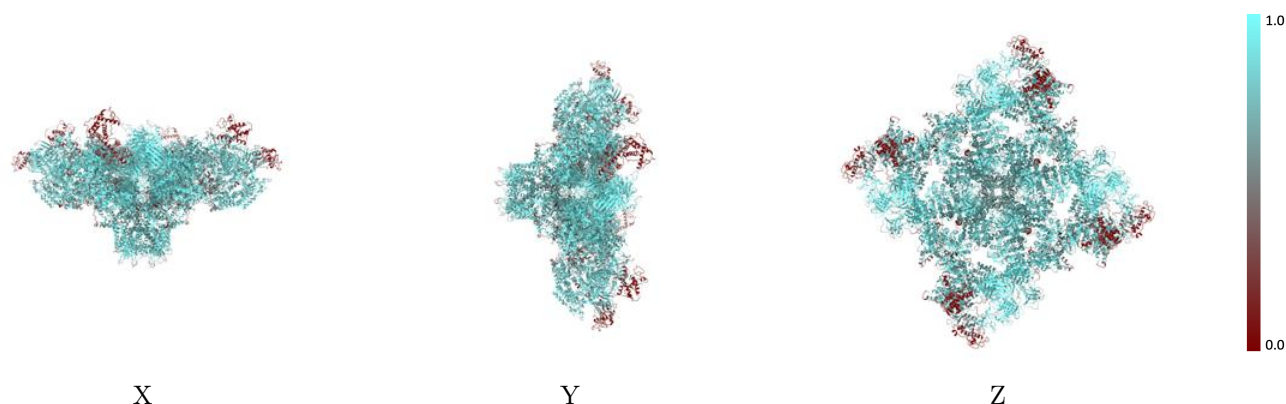
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



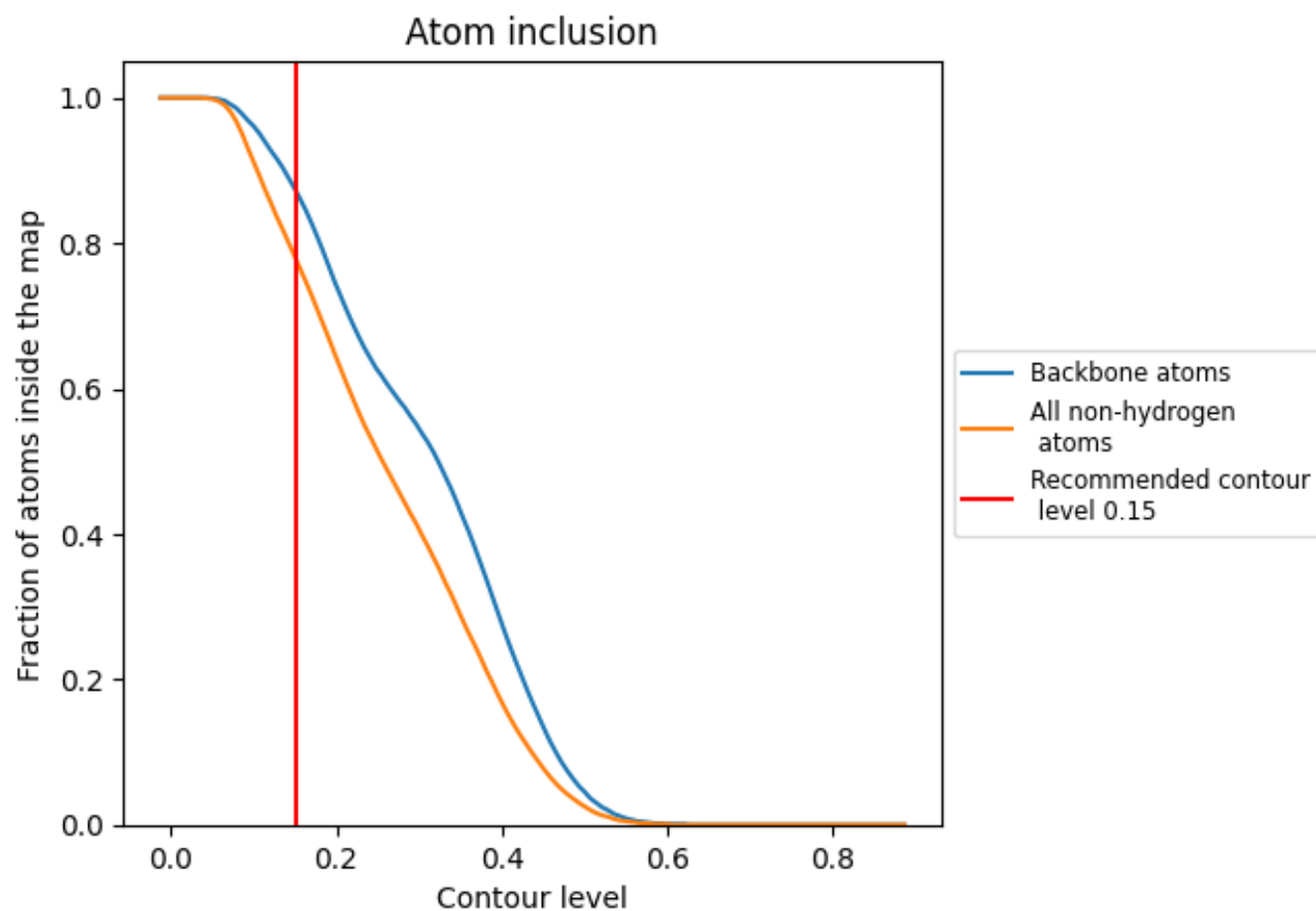
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 78% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7810	0.5400
A	0.7900	0.5430
B	0.7890	0.5400
C	0.5240	0.4370
D	0.5310	0.4320
E	0.5310	0.4390
F	0.8040	0.6020
G	0.7890	0.5410
H	0.7930	0.6020
I	0.7890	0.5420
J	0.7890	0.6020
K	0.5280	0.4400
O	0.8020	0.6030

