



## Full wwPDB EM Validation Report ⓘ

Nov 4, 2024 – 05:45 AM EST

PDB ID : 7TZC  
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](mailto: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>.

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

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

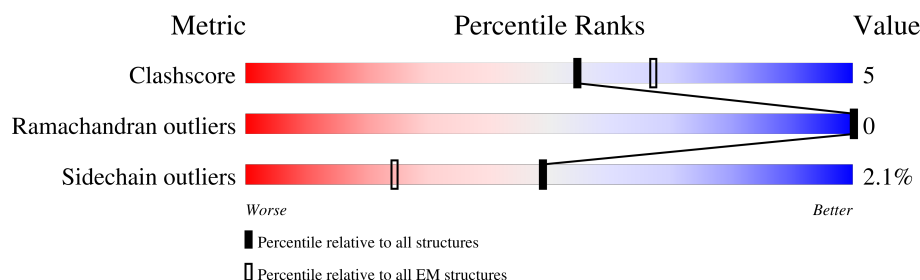
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>33%</div> <div>77%</div> <div>22%</div> <div>..</div> </div>
1	D	150	<div> <div>30%</div> <div>79%</div> <div>20%</div> <div>..</div> </div>
1	E	150	<div> <div>33%</div> <div>79%</div> <div>20%</div> <div>..</div> </div>
1	K	150	<div> <div>33%</div> <div>78%</div> <div>20%</div> <div>..</div> </div>
2	F	107	<div> <div>86%</div> <div>14%</div> </div>
2	H	107	<div> <div>85%</div> <div>15%</div> </div>
2	J	107	<div> <div>88%</div> <div>11%</div> <div>.</div> </div>
2	O	107	<div> <div>86%</div> <div>13%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	A	5037	<div><div>11%</div><div>75%</div><div>12%</div><div>13%</div></div>
3	B	5037	<div><div>11%</div><div>75%</div><div>12%</div><div>13%</div></div>
3	G	5037	<div><div>11%</div><div>75%</div><div>12%</div><div>13%</div></div>
3	I	5037	<div><div>11%</div><div>75%</div><div>12%</div><div>13%</div></div>

## 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 (three-letter code: 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 (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).

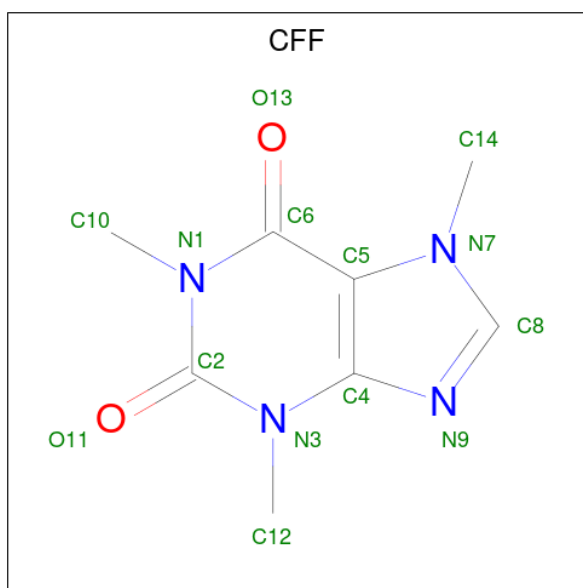


Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total 31	C 10	N 5	O 13	P 3	0
5	A	1	Total 31	C 10	N 5	O 13	P 3	0
5	B	1	Total 31	C 10	N 5	O 13	P 3	0
5	B	1	Total 31	C 10	N 5	O 13	P 3	0
5	G	1	Total 31	C 10	N 5	O 13	P 3	0
5	G	1	Total 31	C 10	N 5	O 13	P 3	0
5	I	1	Total 31	C 10	N 5	O 13	P 3	0
5	I	1	Total 31	C 10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

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

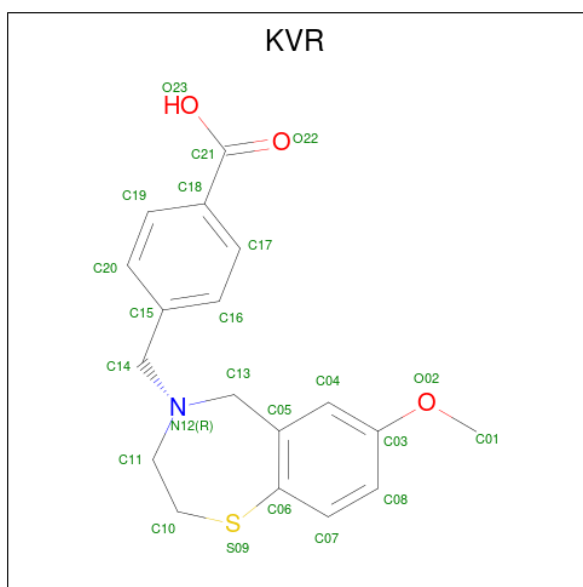
Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total Zn 1 1	0
6	B	1	Total Zn 1 1	0
6	G	1	Total Zn 1 1	0
6	I	1	Total Zn 1 1	0

- Molecule 7 is CAFFEINE (three-letter code: CFF) (formula:  $C_8H_{10}N_4O_2$ ).



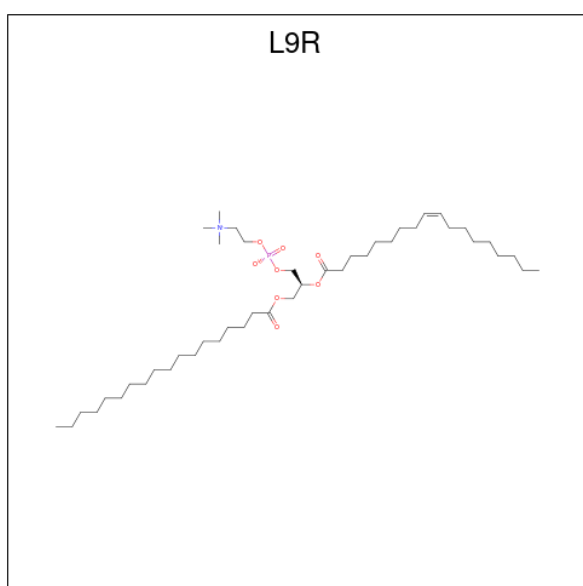
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			14	8	4	2	
7	B	1	Total	C	N	O	0
			14	8	4	2	
7	G	1	Total	C	N	O	0
			14	8	4	2	
7	I	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 8 is 4-[(7-methoxy-2,3-dihydro-1,4-benzothiazepin-4(5H)-yl)methyl]benzoic acid (three-letter code: 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 (three-letter code: L9R) (formula: C<sub>44</sub>H<sub>86</sub>NO<sub>8</sub>P).



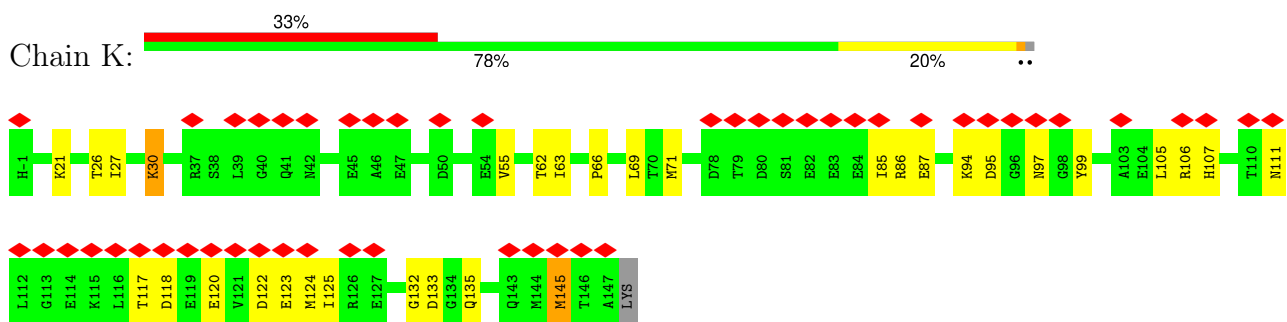


Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	G	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	G	1	Total	C	N	O	P	0
			54	44	1	8	1	
9	I	1	Total	C	N	O	P	0
			54	44	1	8	1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

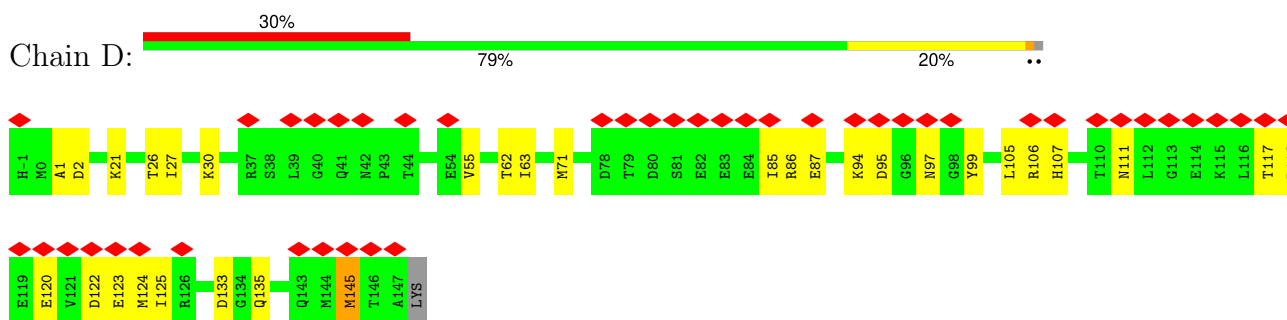
### 3 Residue-property plots

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.

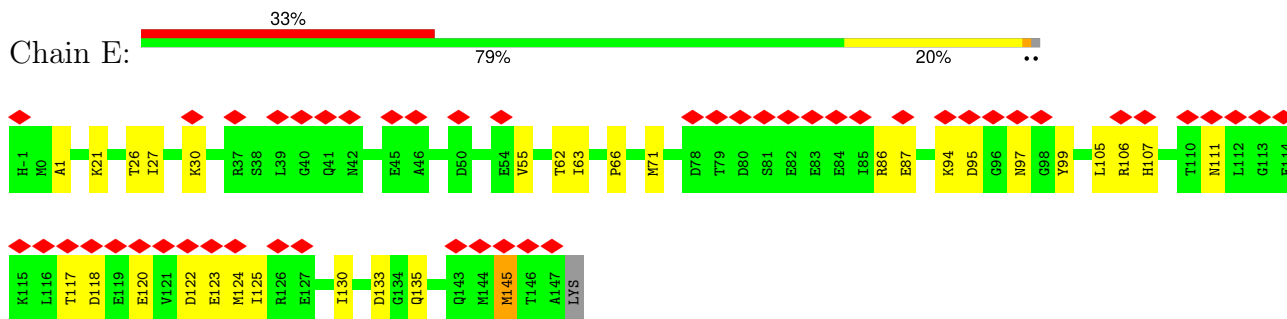
#### • Molecule 1: Calmodulin-1



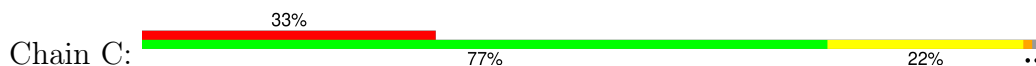
#### • Molecule 1: Calmodulin-1

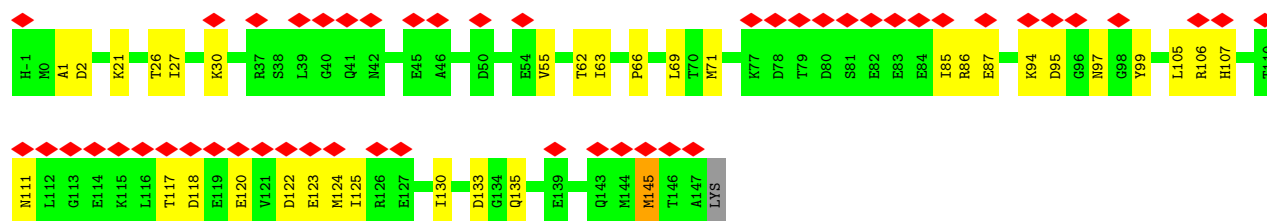


#### • Molecule 1: Calmodulin-1

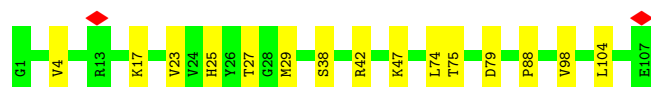
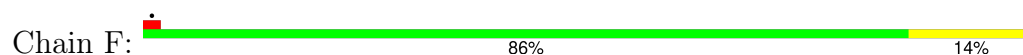


#### • Molecule 1: Calmodulin-1

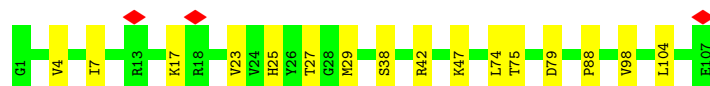
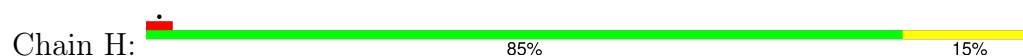




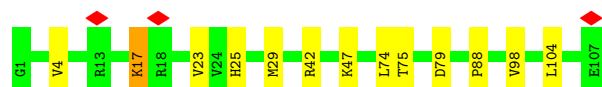
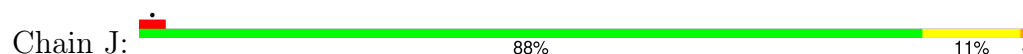
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



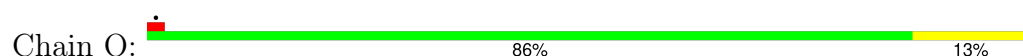
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



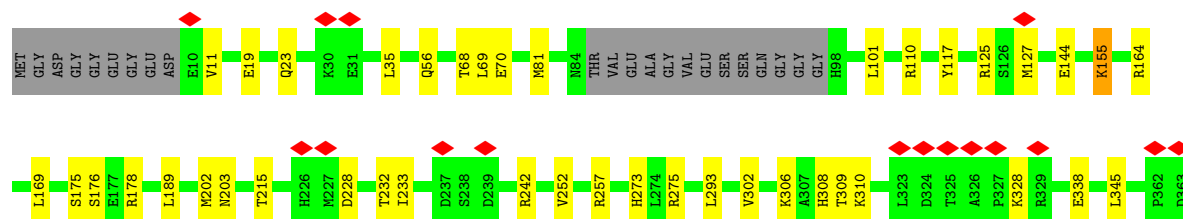
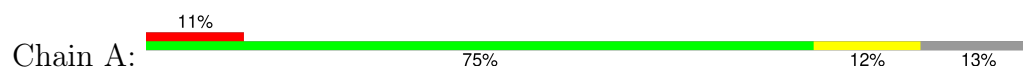
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

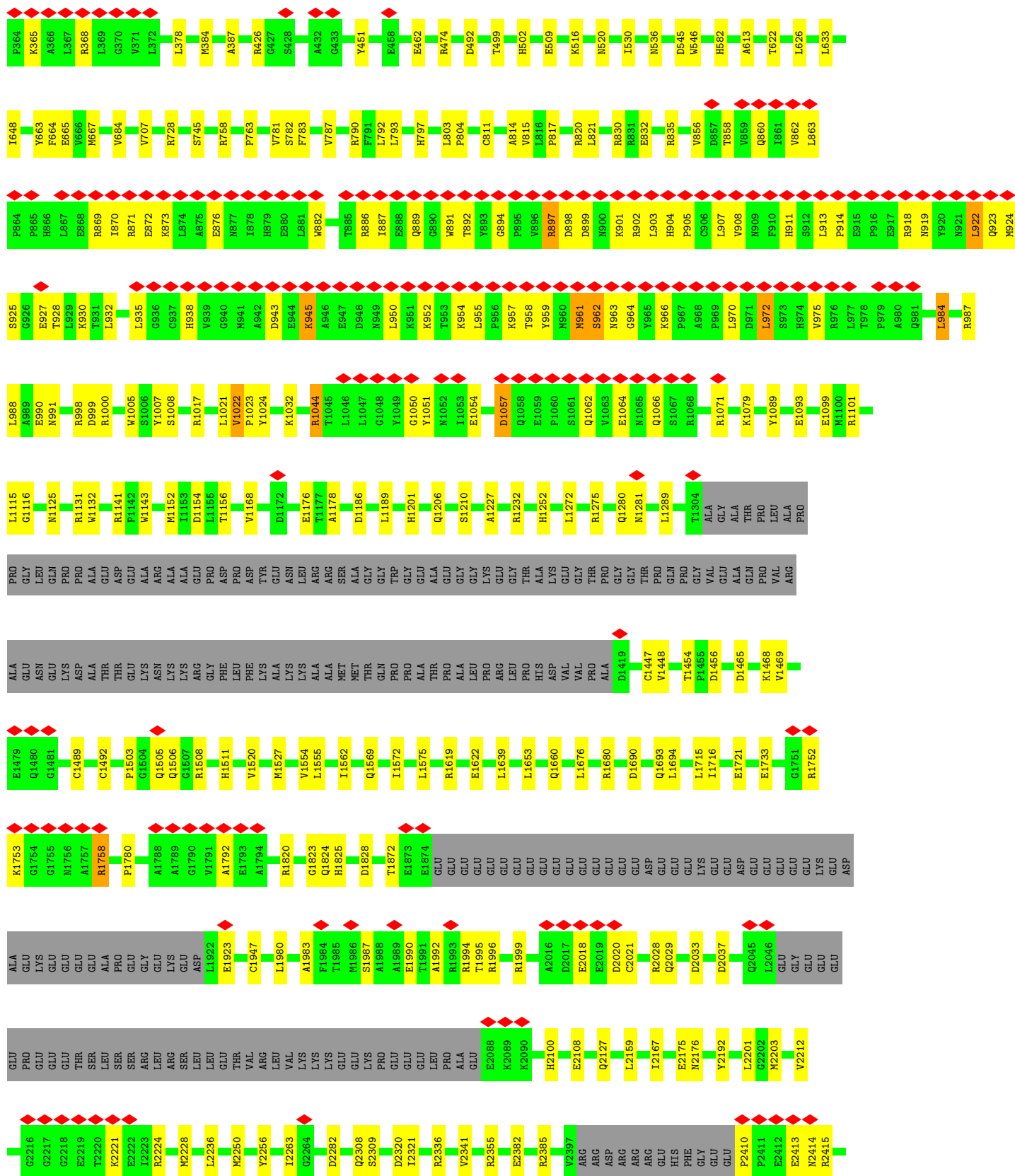


- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

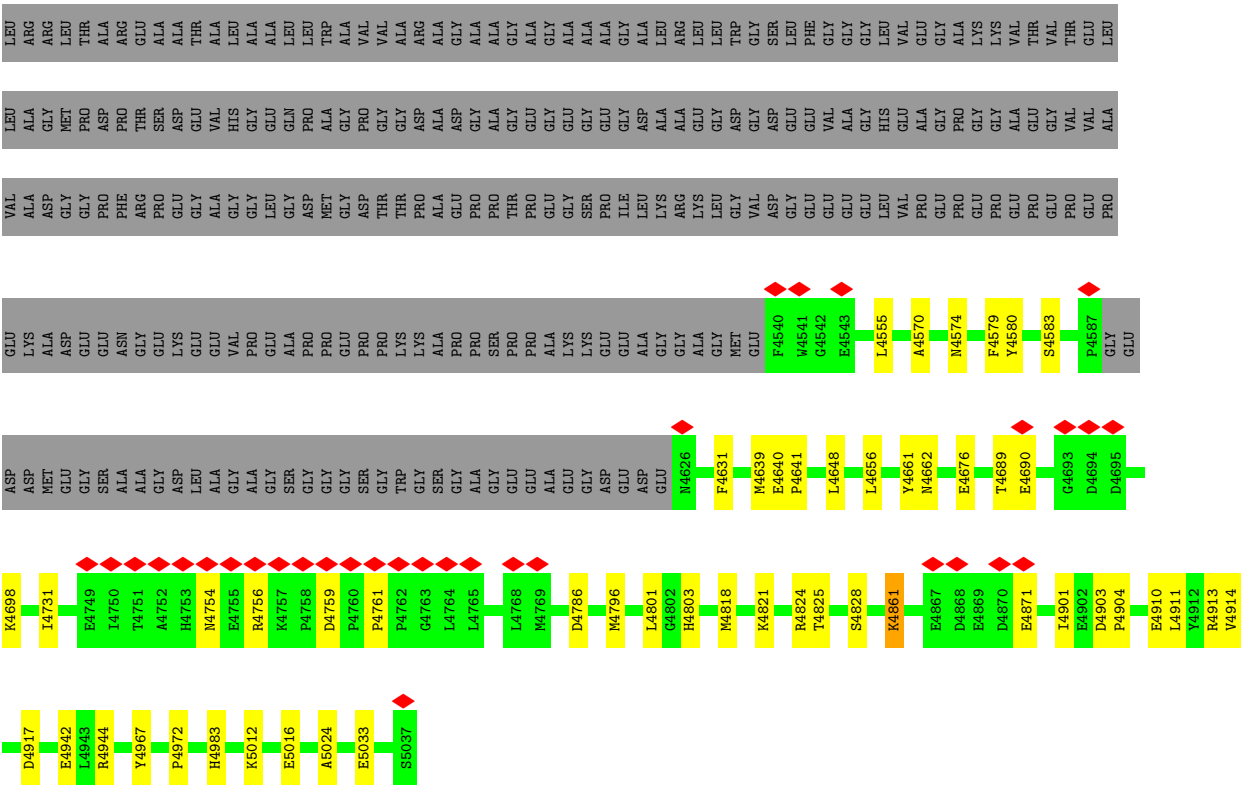


- Molecule 3: Ryanodine receptor 1

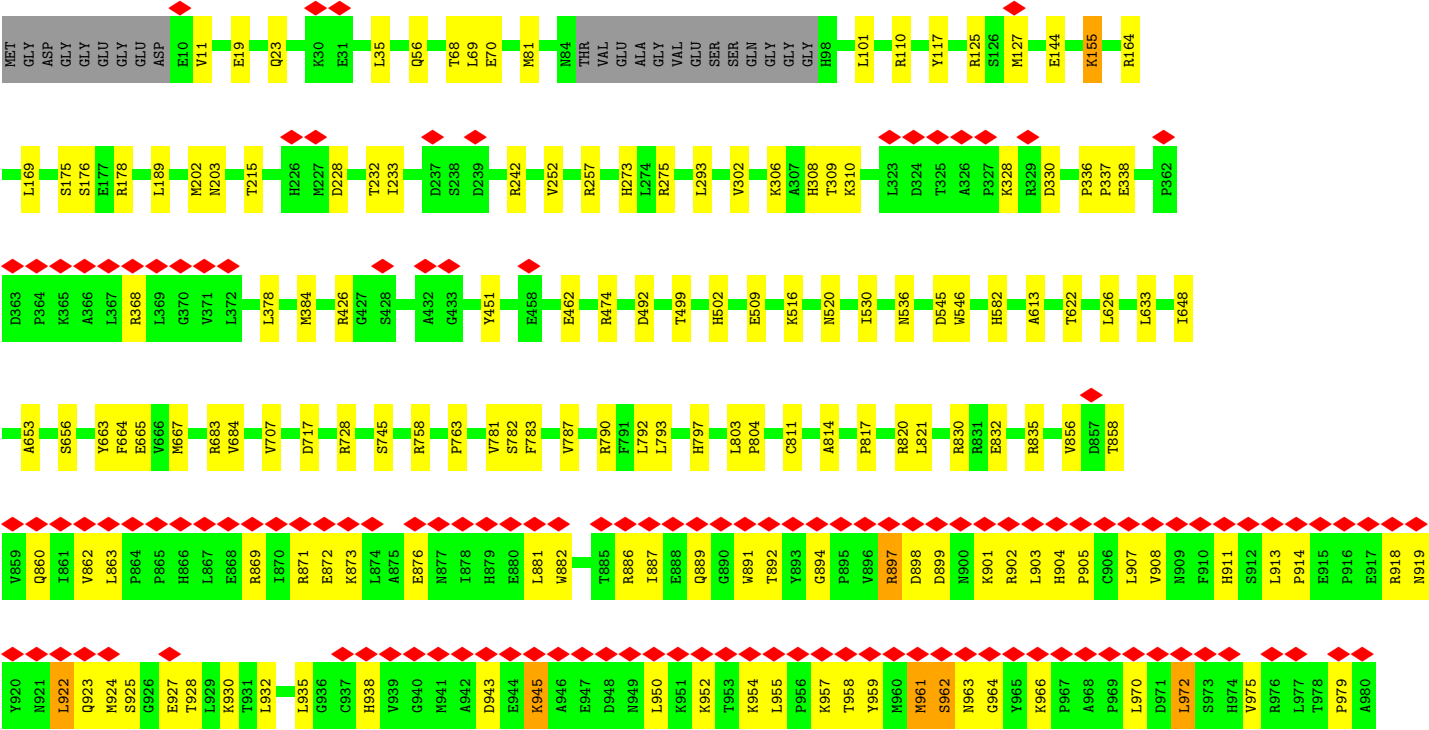








● Molecule 3: Ryanodine receptor 1

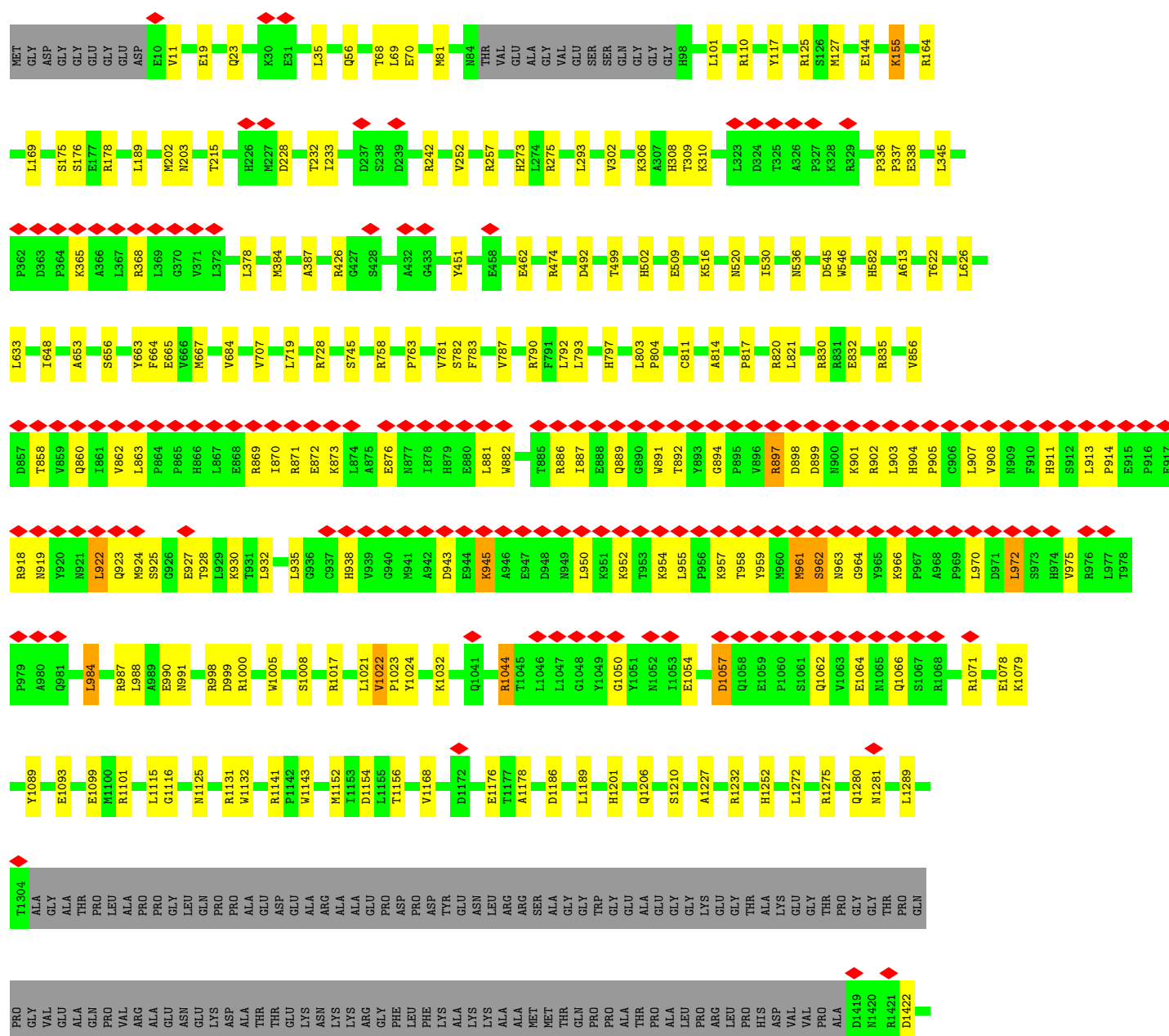
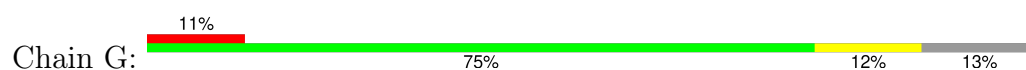


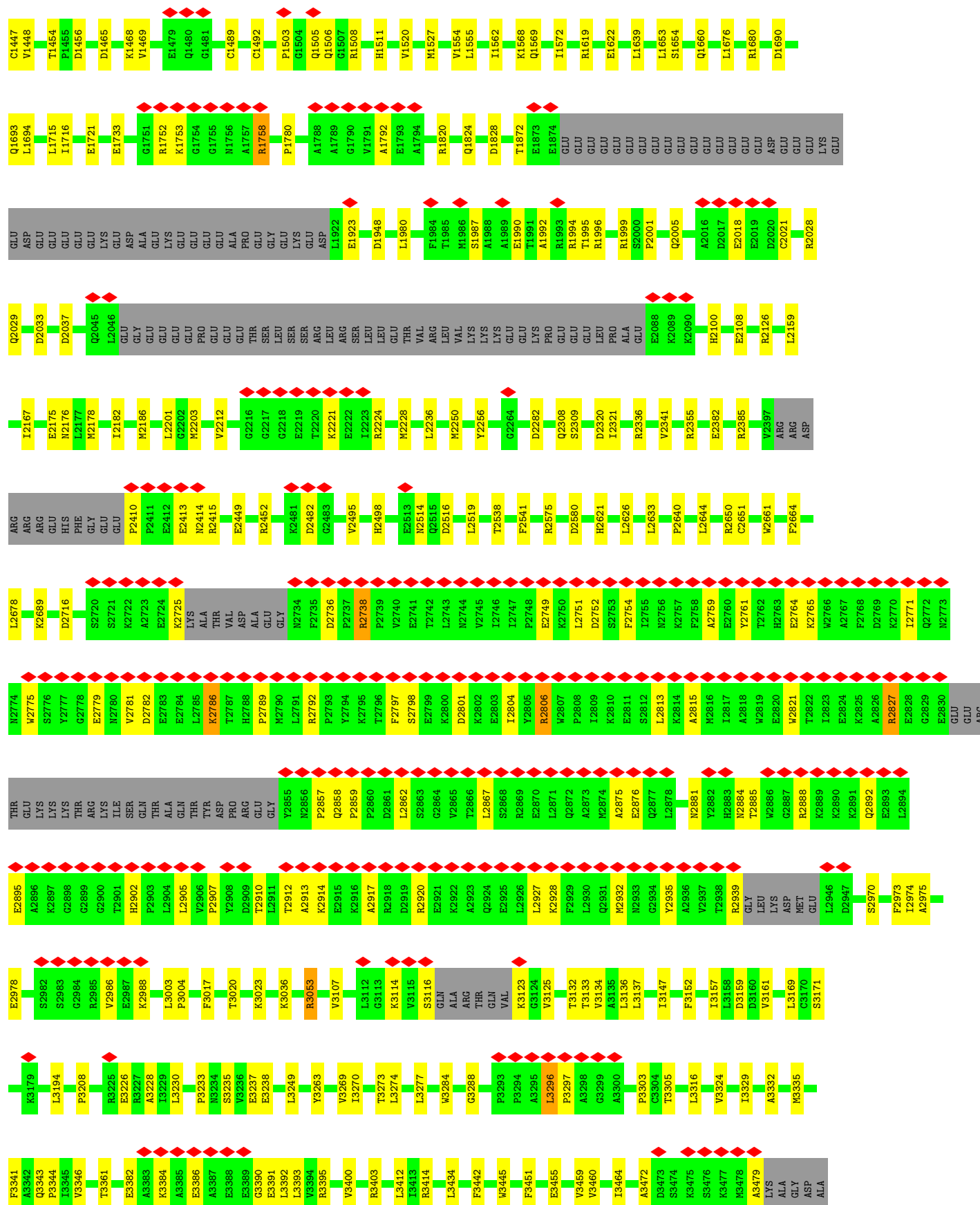


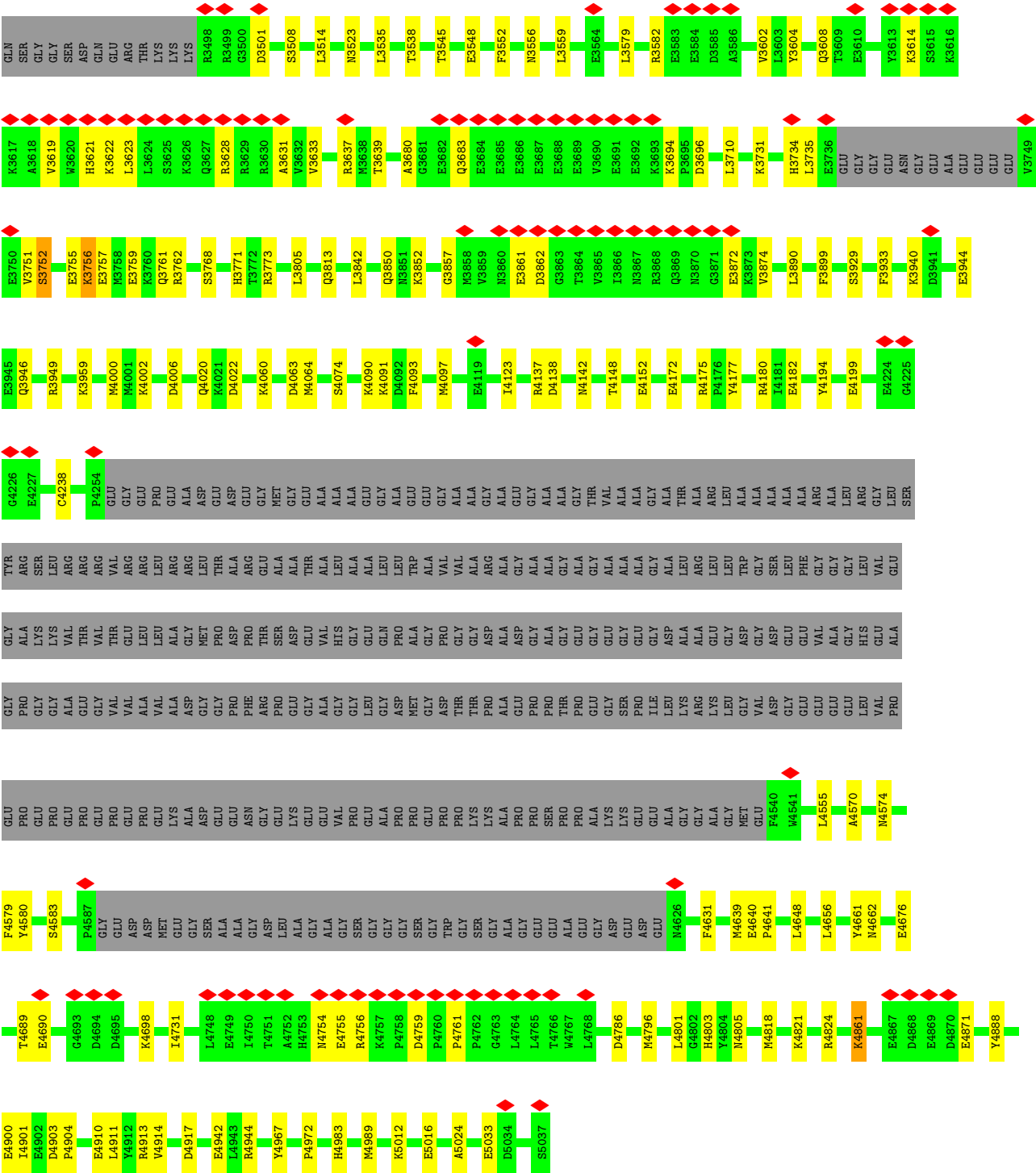
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GLY	LYS	PRO	SER	ALA	GLU	K4060	Q3813	T3638	L3514	V3394	P3233	P3004	L2904
VAL	GLU	GLY	ALA	ALA	THR	D4063	S3840	T3639	N3523	R3395	N3234	F3017	V2906
PRO	PRO	GLY	GLY	ALA	GLU	M4064	L3842	E3682	L3536	V3400	V3235	T3020	P2907
ALA	ALA	LEU	GLY	ALA	GLY	D4070	Q3850	Q3683	T3538	R3403	E3237	K3023	Y2908
GLY	PRO	GLY	GLY	ALA	GLU	S4074	N3851	E3684	T3545	L3412	E3238	K3036	Y2909
PRO	PRO	GLY	GLY	ALA	GLU	S4075	K3852	E3685	E3548	L3413	Y3263	R3053	T2912
PRO	PRO	GLY	GLY	ALA	GLU	F4093	G3857	E3686	F3552	R3414	V3269	K2913	A2913
LYS	LYS	THR	GLY	VAL	ALA	M4097	M3858	E3687	E3564	L3434	I3270	V3107	K2914
ALA	ALA	VAL	GLY	VAL	ALA	N4097	V3859	E3688	L3579	F3442	L3274	V3112	E2915
ALA	ALA	VAL	GLY	VAL	ALA	E4116	N3860	E3689	R3582	L3445	W3284	G3113	K2916
ALA	ALA	VAL	GLY	VAL	ALA	S4119	E3861	E3690	E3583	S3446	Q3288	G3114	A2917
ALA	ALA	VAL	GLY	VAL	ALA	R4137	D3862	E3691	E3584	F3451	P3293	V3115	R2918
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ALA	ALA	VAL	GLY	VAL	ALA	T4148	I3866	E3694	L3579	V3459	L3296	K3123	E2921
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ALA	ALA	VAL	GLY	VAL	ALA	E4172	Q3868	E3696	E3564	I3464	A3298	V3125	A2923
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ALA	ALA	VAL	GLY	VAL	ALA	Y4177	E3872	E3699	E3564	S3474	G3298	V3125	L2926
ALA	ALA	VAL	GLY	VAL	ALA	R4180	K3873	E3700	E3564	K3603	P3303	T3132	F2929
ALA	ALA	VAL	GLY	VAL	ALA	E4182	V3874	E3701	E3564	K3604	C3304	T3133	L2930
ALA	ALA	VAL	GLY	VAL	ALA	Y4194	D3877	E3702	E3564	S3476	T3305	V3134	Q2931
ALA	ALA	VAL	GLY	VAL	ALA	E4199	L3890	E3703	E3564	K3477	L3316	L3137	M2932
ALA	ALA	VAL	GLY	VAL	ALA	F4224	F3899	E3704	E3564	M3478	V3324	L3137	N2933
ALA	ALA	VAL	GLY	VAL	ALA	G4225	S3929	E3705	E3564	A3479	L3329	T3147	K2934
ALA	ALA	VAL	GLY	VAL	ALA	G4226	F3933	E3706	E3564	ALA	A3332	F3152	Y2935
ALA	ALA	VAL	GLY	VAL	ALA	E4227	K3941	E3707	E3564	ALA	M3335	L3157	T2938
ALA	ALA	VAL	GLY	VAL	ALA	P4254	E3944	E3708	E3564	ALA	Q3343	L3158	R2939
ALA	ALA	VAL	GLY	VAL	ALA	GLU	E3945	E3709	E3564	ALA	V3346	D3160	GLY
ALA	ALA	VAL	GLY	VAL	ALA	GLY	Q3946	E3710	E3564	ALA	T3361	V3161	LEU
ALA	ALA	VAL	GLY	VAL	ALA	GLY	R3949	E3711	E3564	ALA	E3382	C3170	LYS
ALA	ALA	VAL	GLY	VAL	ALA	GLY	K3959	E3712	E3564	ALA	A3383	S3171	ASP
ALA	ALA	VAL	GLY	VAL	ALA	GLY	M4000	E3713	E3564	ALA	K3384	K3179	MET
ALA	ALA	VAL	GLY	VAL	ALA	GLY	M4001	E3714	E3564	ALA	A3385	L3194	GLU
ALA	ALA	VAL	GLY	VAL	ALA	GLY	K4002	E3715	E3564	ALA	E3386	P3208	L2946
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ALA	ALA	VAL	GLY	VAL	ALA	GLY	Q4020	E3717	E3564	ALA	E3388	L3194	S2970
ALA	ALA	VAL	GLY	VAL	ALA	GLY	K4021	E3718	E3564	ALA	E3389	P3208	F2973
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ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3721	E3564	ALA	E3391	R3295	E2978
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3722	E3564	ALA	E3391	L3194	S2982
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3723	E3564	ALA	E3391	P3208	S2983
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3724	E3564	ALA	E3391	R3295	Q2984
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3725	E3564	ALA	E3391	L3194	R2985
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3726	E3564	ALA	E3391	P3208	V2986
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3727	E3564	ALA	E3391	R3295	E2987
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3728	E3564	ALA	E3391	L3194	K2988
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3729	E3564	ALA	E3391	P3208	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3730	E3564	ALA	E3391	R3295	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3731	E3564	ALA	E3391	L3194	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3732	E3564	ALA	E3391	P3208	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3733	E3564	ALA	E3391	R3295	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3734	E3564	ALA	E3391	L3194	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3735	E3564	ALA	E3391	P3208	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3736	E3564	ALA	E3391	R3295	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3737	E3564	ALA	E3391	L3194	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3738	E3564	ALA	E3391	P3208	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3739	E3564	ALA	E3391	R3295	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3740	E3564	ALA	E3391	L3194	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3741	E3564	ALA	E3391	P3208	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3742	E3564	ALA	E3391	R3295	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3743	E3564	ALA	E3391	L3194	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3744	E3564	ALA	E3391	P3208	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3745	E3564	ALA	E3391	R3295	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3746	E3564	ALA	E3391	L3194	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3747	E3564	ALA	E3391	P3208	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3748	E3564	ALA	E3391	R3295	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3749	E3564	ALA	E3391	L3194	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3750	E3564	ALA	E3391	P3208	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3751	E3564	ALA	E3391	R3295	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3752	E3564	ALA	E3391	L3194	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3753	E3564	ALA	E3391	P3208	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3754	E3564	ALA	E3391	R3295	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3755	E3564	ALA	E3391	L3194	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3756	E3564	ALA	E3391	P3208	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3757	E3564	ALA	E3391	R3295	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3758	E3564	ALA	E3391	L3194	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3759	E3564	ALA	E3391	P3208	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3760	E3564	ALA	E3391	R3295	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3761	E3564	ALA	E3391	L3194	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3762	E3564	ALA	E3391	P3208	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3763	E3564	ALA	E3391	R3295	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3764	E3564	ALA	E3391	L3194	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3765	E3564	ALA	E3391	P3208	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3766	E3564	ALA	E3391	R3295	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3767	E3564	ALA	E3391	L3194	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3768	E3564	ALA	E3391	P3208	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3769	E3564	ALA	E3391	R3295	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3770	E3564	ALA	E3391	L3194	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3771	E3564	ALA	E3391	P3208	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3772	E3564	ALA	E3391	R3295	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3773	E3564	ALA	E3391	L3194	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3774	E3564	ALA	E3391	P3208	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3775	E3564	ALA	E3391	R3295	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3776	E3564	ALA	E3391	L3194	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3777	E3564	ALA	E3391	P3208	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3778	E3564	ALA	E3391	R3295	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3779	E3564	ALA	E3391	L3194	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3780	E3564	ALA	E3391	P3208	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3781	E3564	ALA	E3391	R3295	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3782	E3564	ALA	E3391	L3194	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3783	E3564	ALA	E3391	P3208	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3784	E3564	ALA	E3391	R3295	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3785	E3564	ALA	E3391	L3194	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3786	E3564	ALA	E3391	P3208	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3787	E3564	ALA	E3391	R3295	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3788	E3564	ALA	E3391	L3194	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3789	E3564	ALA	E3391	P3208	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3790	E3564	ALA	E3391	R3295	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3791	E3564	ALA	E3391	L3194	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3792	E3564	ALA	E3391	P3208	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3793	E3564	ALA	E3391	R3295	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3794	E3564	ALA	E3391	L3194	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3795	E3564	ALA	E3391	P3208	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3796	E3564	ALA	E3391	R3295	
ALA	ALA	VAL	GLY	VAL	ALA	GLY		E3797	E3564	ALA			



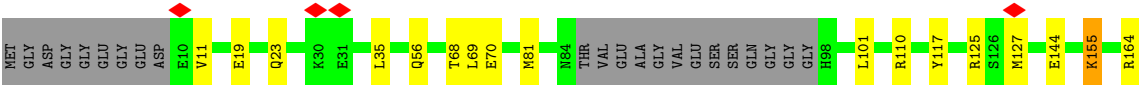
- Molecule 3: Ryanodine receptor 1







● Molecule 3: Ryanodine receptor 1









## 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.24	0/1187	0.44	0/1594
1	D	0.24	0/1187	0.44	0/1594
1	E	0.24	0/1187	0.44	0/1594
1	K	0.24	0/1187	0.44	0/1594
2	F	0.32	0/850	0.52	0/1146
2	H	0.32	0/850	0.52	0/1146
2	J	0.32	0/850	0.52	0/1146
2	O	0.32	0/850	0.52	0/1146
3	A	0.25	0/35977	0.46	0/48726
3	B	0.25	0/35977	0.46	0/48726
3	G	0.25	0/35977	0.46	0/48726
3	I	0.25	0/35977	0.46	0/48726
All	All	0.25	0/152056	0.46	0/205864

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1174	0	1099	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1174	0	1099	17	0
1	E	1174	0	1099	17	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	347	0
3	B	35150	0	34797	347	0
3	G	35150	0	34797	347	0
3	I	35150	0	34797	353	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
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	1461	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 (1461) 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
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:I:2765:LYS:NZ	3:I: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:1:ALA:HB3	3:I:3861:GLU:HG2	1.79	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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:G:3579:LEU:HB2	3:G:3582:ARG:HG2	1.81	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
3:B:2902:HIS:HB3	3:B:2905:LEU:HG	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:3959:LYS:NZ	3:I:4022:ASP:OD2	2.32	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:3959:LYS:NZ	3:B:4022:ASP:OD2	2.32	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:56:GLN:O	3:B:309:THR:OG1	2.19	0.55
3:B:2827:ARG:NH2	3:B:2935:TYR:OH	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:2765:LYS:HZ3	3:B:2857:PRO:HB2	1.71	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
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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:913:LEU:HD12	3:B:914:PRO:HD2	1.89	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
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:A:1252:HIS:O	3:A:1275:ARG:NH1	2.41	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:A:3940:LYS:O	3:A:4002:LYS:NZ	2.39	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: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:A:3157:ILE:HA	3:A:3161:VAL:HB	1.91	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: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: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
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:B:1422:ASP:OD2	3:B:1568:LYS:NZ	2.37	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:I:961:MET:HE2	3:I:964:GLY:H	1.75	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: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:I:3940:LYS:O	3:I:4002:LYS:NZ	2.39	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:G:961:MET:HE2	3:G:964:GLY:H	1.75	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:961:MET:HE2	3:A:964:GLY:H	1.75	0.51
3:B:4759:ASP:O	3:B:4761:PRO:HD3	2.09	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:155:LYS:NZ	3:I:228:ASP:OD2	2.34	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: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
3:A:4172:GLU:OE1	3:A:4175:ARG:NH1	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:4182:GLU:OE1	3:B:4983:HIS:NE2	2.46	0.49
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:A:2867:LEU:HB2	3:A:2928:LYS:HZ3	1.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:961:MET:HE1	3:B:964:GLY:H	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:3940:LYS:O	3:B:4002:LYS:NZ	2.39	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:3316:LEU:HD21	3:A:3346:VAL:HG23	1.96	0.48
3:B:2867:LEU:HB2	3:B:2928:LYS:HZ3	1.78	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:2867:LEU:HB2	3:I:2928:LYS:HZ3	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:3545:THR:HG22	3:A:3548:GLU:HG3	1.95	0.48
3:A:4731:ILE:O	3:G:4074:SER:OG	2.31	0.48
3:B:4555:LEU:HD21	3:B:4656:LEU:HD22	1.96	0.48
3:G:925:SER:O	3:G:928:THR:OG1	2.32	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2867:LEU:HB2	3:G:2928:LYS:HZ3	1.80	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
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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1454:THR:OG1	3:A:1456:ASP:OD1	2.20	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: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
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:G:943:ASP:OD2	3:G:945:LYS:NZ	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:2538:THR:HG23	3:I:2541:PHE:H	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:4555:LEU:HD21	3:G:4656:LEU:HD22	1.96	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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
3:B:4754:ASN:HB3	3:B:4756:ARG:HH21	1.81	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:B:4579:PHE:CD1	3:B:4639:MET:HE1	2.51	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: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:G:3862:ASP:OD1	3:G:3862:ASP:N	2.48	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:2309:SER:OG	3:G:2320:ASP:OD1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:I:2881:ASN:HA	3:I:2884:ASN:ND2	2.32	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: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:B:3752:SER:OG	3:B:3755:GLU:OE1	2.35	0.45
3:G:2881:ASN:HA	3:G:2884:ASN:ND2	2.32	0.45
3:G:2974:ILE:HG13	3:G:2975:ALA:N	2.32	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:952:LYS:HD3	3:G:970:LEU:HA	2.00	0.44
3:G:1008:SER:HB3	3:G:1017:ARG:HB3	1.99	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: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
3:B:3731:LYS:HA	3:B:3734:HIS:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:4648:LEU:HD12	3:B:4803:HIS:HE1	1.82	0.44
3:G:2821:TRP:HD1	3:G:2939:ARG:HA	1.82	0.44
3:G:4579:PHE:CD1	3:G:4639:MET:HE1	2.53	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:G:923:GLN:O	3:G:927:GLU:HG2	2.18	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:4579:PHE:CD1	3:A:4639:MET:HE1	2.52	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:1454:THR:OG1	3:G:1456:ASP:OD1	2.20	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: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: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:3446:SER:O	3:B:3452:LYS:NZ	2.42	0.43
3:G:1099:GLU:OE2	3:G:1125:ASN:ND2	2.50	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
9:I:5101:L9R:H47A	9:I:5101:L9R:H44	1.53	0.43
3:A:2580:ASP:OD1	3:A:2621:HIS:HB2	2.19	0.43
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:2765:LYS:HZ3	3:A:2857:PRO:HB2	1.84	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:2236:LEU:HD13	3:A:2250:MET:HE1	2.01	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2587:TYR:O	3:A:2590:SER:OG	2.31	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
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
3:I:4579:PHE:CD1	3:I:4639:MET:HE1	2.54	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:2765:LYS:HZ3	3:I:2857:PRO:HB2	1.84	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
3:B:2236:LEU:HD13	3:B:2250:MET:HE1	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1422:ASP:OD2	3:G:1568:LYS:NZ	2.37	0.42
3:G:3392:LEU:HD13	3:G:3395:ARG:HD2	2.01	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:2108:GLU:O	3:A:3694:LYS:NZ	2.51	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:B:1000:ARG:HB3	3:B:1005:TRP:HB2	2.01	0.42
3:G:2661:TRP:HB3	3:G:2664:PHE:HB2	2.01	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:2236:LEU:HD13	3:I:2250:MET:HE1	2.01	0.42
3:A:2677:LYS:HE2	3:A:2677:LYS:HB3	1.81	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
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: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:2236:LEU:HD13	3:G:2250:MET:HE1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
3:I:4712:PRO:O	3:I:4718:LYS:NZ	2.40	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: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
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
3:A:1983:ALA:O	3:A:1987:SER:OG	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:979:PRO:O	3:I:982:THR:OG1	2.33	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
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:G:954:LYS:HB3	3:G:966:LYS:HE3	2.03	0.41
3:G:4238:CYS:HA	3:G:4989:MET:HE1	2.02	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:2178:MET:HE3	3:G:2182:ILE:HD11	2.03	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: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
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:I:1000:ARG:HB3	3:I:1005:TRP:HB2	2.01	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2886:TRP:HA	3:B:2889:LYS:NZ	2.36	0.41
3:G:3147:ILE:HG23	3:G:3152:PHE:HB2	2.02	0.41
3:G:3680:ALA:HB1	3:G:3683:GLN:NE2	2.36	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: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:B:275:ARG:HH21	3:B:328:LYS:HG3	1.86	0.41
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:3501:ASP:OD1	3:B:3501:ASP:N	2.54	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: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:1997:GLU:O	3:I:2000:SER:OG	2.37	0.41
3:I:2212:VAL:HG11	3:I:2256:TYR:CE2	2.55	0.41
3:I:2587:TYR:O	3:I:2590:SER:OG	2.31	0.41
3:I:4093:PHE:O	3:I:4097:MET:HG2	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:871:ARG:CZ	3:B:922:LEU:HD12	2.51	0.41
3:B:3147:ILE:HG23	3:B:3152:PHE:HB2	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: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
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:3501:ASP:OD1	3:A:3501:ASP:N	2.54	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:2782:ASP:N	3:G:2782:ASP:OD1	2.54	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:2782:ASP:N	3:I:2782:ASP:OD1	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
3:I:3562:LYS:HE2	3:I:3562:LYS:HB2	1.91	0.40
3:I:4651:THR:HG23	3:I:4796:MET:HE1	2.03	0.40
2:O:27:THR:HG23	2:O:38:SER:HB2	2.03	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:961:MET:HE2	3:B:961:MET:HB2	1.93	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:B:4967:TYR:OH	3:B:5033:GLU:OE2	2.29	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:979:PRO:O	3:B:982:THR:OG1	2.33	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:G:1079:LYS:HA	3:G:1189:LEU:HD11	2.04	0.40
3:G:3226:GLU:C	3:G:3228:ALA:H	2.25	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:3226:GLU:C	3:I:3228:ALA:H	2.25	0.40
3:I:3249:LEU:HD23	3:I:3277:LEU:HD21	2.03	0.40
3:I:3717:ASP:N	3:I:3717:ASP:OD1	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	147/150 (98%)	146 (99%)	1 (1%)	0	100	100
1	D	147/150 (98%)	146 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	122 (96%)	5 (4%)	27	41
1	D	127/128 (99%)	122 (96%)	5 (4%)	27	41
1	E	127/128 (99%)	122 (96%)	5 (4%)	27	41
1	K	127/128 (99%)	122 (96%)	5 (4%)	27	41
2	F	89/89 (100%)	86 (97%)	3 (3%)	32	46
2	H	89/89 (100%)	86 (97%)	3 (3%)	32	46
2	J	89/89 (100%)	86 (97%)	3 (3%)	32	46
2	O	89/89 (100%)	86 (97%)	3 (3%)	32	46
3	A	3836/4276 (90%)	3760 (98%)	76 (2%)	50	65
3	B	3836/4276 (90%)	3760 (98%)	76 (2%)	50	65
3	G	3836/4276 (90%)	3760 (98%)	76 (2%)	50	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	I	3836/4276 (90%)	3760 (98%)	76 (2%)	50	65
All	All	16208/17972 (90%)	15872 (98%)	336 (2%)	49	64

All (336) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	21	LYS
1	K	30	LYS
1	K	105	LEU
1	K	124	MET
1	K	145	MET
2	F	17	LYS
2	F	29	MET
2	F	79	ASP
1	D	21	LYS
1	D	30	LYS
1	D	105	LEU
1	D	124	MET
1	D	145	MET
1	E	21	LYS
1	E	30	LYS
1	E	105	LEU
1	E	124	MET
1	E	145	MET
1	C	21	LYS
1	C	30	LYS
1	C	105	LEU
1	C	124	MET
1	C	145	MET
3	A	81	MET
3	A	125	ARG
3	A	155	LYS
3	A	860	GLN
3	A	862	VAL
3	A	869	ARG
3	A	873	LYS
3	A	882	TRP
3	A	887	ILE
3	A	897	ARG
3	A	898	ASP
3	A	907	LEU
3	A	908	VAL

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Mol	Chain	Res	Type
3	A	911	HIS
3	A	922	LEU
3	A	945	LYS
3	A	957	LYS
3	A	958	THR
3	A	959	TYR
3	A	961	MET
3	A	962	SER
3	A	963	ASN
3	A	972	LEU
3	A	984	LEU
3	A	998	ARG
3	A	999	ASP
3	A	1021	LEU
3	A	1022	VAL
3	A	1044	ARG
3	A	1057	ASP
3	A	1143	TRP
3	A	1186	ASP
3	A	1506	GLN
3	A	1511	HIS
3	A	1752	ARG
3	A	1758	ARG
3	A	1872	THR
3	A	1923	GLU
3	A	1990	GLU
3	A	2037	ASP
3	A	2100[A]	HIS
3	A	2100[B]	HIS
3	A	2221	LYS
3	A	2224	ARG
3	A	2336	ARG
3	A	2482	ASP
3	A	2738	ARG
3	A	2761	TYR
3	A	2786	LYS
3	A	2797	PHE
3	A	2806	ARG
3	A	2827	ARG
3	A	2862	LEU
3	A	2876	GLU
3	A	2914	LYS

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Mol	Chain	Res	Type
3	A	2932	MET
3	A	3053	ARG
3	A	3296	LEU
3	A	3382	GLU
3	A	3451	PHE
3	A	3614	LYS
3	A	3619	VAL
3	A	3622	LYS
3	A	3639	THR
3	A	3752	SER
3	A	3756	LYS
3	A	3899	PHE
3	A	3933	PHE
3	A	4580	TYR
3	A	4662	ASN
3	A	4796	MET
3	A	4821	LYS
3	A	4861	LYS
3	A	4871	GLU
3	A	4903	ASP
3	A	4911	LEU
3	B	81	MET
3	B	125	ARG
3	B	155	LYS
3	B	860	GLN
3	B	862	VAL
3	B	869	ARG
3	B	873	LYS
3	B	882	TRP
3	B	887	ILE
3	B	897	ARG
3	B	898	ASP
3	B	907	LEU
3	B	908	VAL
3	B	911	HIS
3	B	922	LEU
3	B	945	LYS
3	B	957	LYS
3	B	958	THR
3	B	959	TYR
3	B	961	MET
3	B	962	SER

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Mol	Chain	Res	Type
3	B	963	ASN
3	B	972	LEU
3	B	984	LEU
3	B	998	ARG
3	B	999	ASP
3	B	1021	LEU
3	B	1022	VAL
3	B	1044	ARG
3	B	1057	ASP
3	B	1143	TRP
3	B	1186	ASP
3	B	1506	GLN
3	B	1511	HIS
3	B	1752	ARG
3	B	1758	ARG
3	B	1872	THR
3	B	1923	GLU
3	B	1990	GLU
3	B	2037	ASP
3	B	2100[A]	HIS
3	B	2100[B]	HIS
3	B	2221	LYS
3	B	2224	ARG
3	B	2336	ARG
3	B	2482	ASP
3	B	2738	ARG
3	B	2761	TYR
3	B	2786	LYS
3	B	2797	PHE
3	B	2806	ARG
3	B	2827	ARG
3	B	2862	LEU
3	B	2876	GLU
3	B	2914	LYS
3	B	2932	MET
3	B	3053	ARG
3	B	3296	LEU
3	B	3382	GLU
3	B	3451	PHE
3	B	3614	LYS
3	B	3619	VAL
3	B	3622	LYS

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Mol	Chain	Res	Type
3	B	3639	THR
3	B	3752	SER
3	B	3756	LYS
3	B	3899	PHE
3	B	3933	PHE
3	B	4580	TYR
3	B	4662	ASN
3	B	4796	MET
3	B	4821	LYS
3	B	4861	LYS
3	B	4871	GLU
3	B	4903	ASP
3	B	4911	LEU
3	G	81	MET
3	G	125	ARG
3	G	155	LYS
3	G	860	GLN
3	G	862	VAL
3	G	869	ARG
3	G	873	LYS
3	G	882	TRP
3	G	887	ILE
3	G	897	ARG
3	G	898	ASP
3	G	907	LEU
3	G	908	VAL
3	G	911	HIS
3	G	922	LEU
3	G	945	LYS
3	G	957	LYS
3	G	958	THR
3	G	959	TYR
3	G	961	MET
3	G	962	SER
3	G	963	ASN
3	G	972	LEU
3	G	984	LEU
3	G	998	ARG
3	G	999	ASP
3	G	1021	LEU
3	G	1022	VAL
3	G	1044	ARG

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Mol	Chain	Res	Type
3	G	1057	ASP
3	G	1143	TRP
3	G	1186	ASP
3	G	1506	GLN
3	G	1511	HIS
3	G	1752	ARG
3	G	1758	ARG
3	G	1872	THR
3	G	1923	GLU
3	G	1990	GLU
3	G	2037	ASP
3	G	2100[A]	HIS
3	G	2100[B]	HIS
3	G	2221	LYS
3	G	2224	ARG
3	G	2336	ARG
3	G	2482	ASP
3	G	2738	ARG
3	G	2761	TYR
3	G	2786	LYS
3	G	2797	PHE
3	G	2806	ARG
3	G	2827	ARG
3	G	2862	LEU
3	G	2876	GLU
3	G	2914	LYS
3	G	2932	MET
3	G	3053	ARG
3	G	3296	LEU
3	G	3382	GLU
3	G	3451	PHE
3	G	3614	LYS
3	G	3619	VAL
3	G	3622	LYS
3	G	3639	THR
3	G	3752	SER
3	G	3756	LYS
3	G	3899	PHE
3	G	3933	PHE
3	G	4580	TYR
3	G	4662	ASN
3	G	4796	MET

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Mol	Chain	Res	Type
3	G	4821	LYS
3	G	4861	LYS
3	G	4871	GLU
3	G	4903	ASP
3	G	4911	LEU
3	I	81	MET
3	I	125	ARG
3	I	155	LYS
3	I	860	GLN
3	I	862	VAL
3	I	869	ARG
3	I	873	LYS
3	I	882	TRP
3	I	887	ILE
3	I	897	ARG
3	I	898	ASP
3	I	907	LEU
3	I	908	VAL
3	I	911	HIS
3	I	922	LEU
3	I	945	LYS
3	I	957	LYS
3	I	958	THR
3	I	959	TYR
3	I	961	MET
3	I	962	SER
3	I	963	ASN
3	I	972	LEU
3	I	984	LEU
3	I	998	ARG
3	I	999	ASP
3	I	1021	LEU
3	I	1022	VAL
3	I	1044	ARG
3	I	1057	ASP
3	I	1143	TRP
3	I	1186	ASP
3	I	1506	GLN
3	I	1511	HIS
3	I	1752	ARG
3	I	1758	ARG
3	I	1872	THR

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Mol	Chain	Res	Type
3	I	1923	GLU
3	I	1990	GLU
3	I	2037	ASP
3	I	2100[A]	HIS
3	I	2100[B]	HIS
3	I	2221	LYS
3	I	2224	ARG
3	I	2336	ARG
3	I	2482	ASP
3	I	2738	ARG
3	I	2761	TYR
3	I	2786	LYS
3	I	2797	PHE
3	I	2806	ARG
3	I	2827	ARG
3	I	2862	LEU
3	I	2876	GLU
3	I	2914	LYS
3	I	2932	MET
3	I	3053	ARG
3	I	3296	LEU
3	I	3382	GLU
3	I	3451	PHE
3	I	3614	LYS
3	I	3619	VAL
3	I	3622	LYS
3	I	3639	THR
3	I	3752	SER
3	I	3756	LYS
3	I	3899	PHE
3	I	3933	PHE
3	I	4580	TYR
3	I	4662	ASN
3	I	4796	MET
3	I	4821	LYS
3	I	4861	LYS
3	I	4871	GLU
3	I	4903	ASP
3	I	4911	LEU
2	H	17	LYS
2	H	29	MET
2	H	79	ASP

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	991	ASN
3	A	2180	GLN
3	A	2881	ASN
3	B	991	ASN
3	B	2180	GLN
3	B	2881	ASN
3	B	3734	HIS
3	B	3761	GLN
3	G	991	ASN
3	G	2881	ASN
3	I	991	ASN
3	I	2180	GLN
3	I	2881	ASN

### 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$
7	CFF	G	5105	-	8,15,15	2.03	3 (37%)	8,23,23	1.45	1 (12%)
7	CFF	I	5105	-	8,15,15	2.03	3 (37%)	8,23,23	1.46	1 (12%)
8	KVR	B	5306	-	24,25,25	1.42	3 (12%)	31,34,34	1.55	4 (12%)
5	ATP	I	5102	-	28,33,33	0.63	0	34,52,52	0.85	2 (5%)
7	CFF	B	5304	-	8,15,15	2.02	3 (37%)	8,23,23	1.45	1 (12%)
7	CFF	A	5304	-	8,15,15	2.02	3 (37%)	8,23,23	1.45	1 (12%)
9	L9R	G	5108	-	53,53,53	1.24	5 (9%)	59,61,61	1.12	3 (5%)
9	L9R	B	5307	-	53,53,53	1.24	5 (9%)	59,61,61	1.12	3 (5%)
5	ATP	G	5102	-	28,33,33	0.61	0	34,52,52	0.85	2 (5%)
9	L9R	A	5307	-	53,53,53	1.24	5 (9%)	59,61,61	1.12	3 (5%)
5	ATP	B	5301	-	28,33,33	0.62	0	34,52,52	0.85	2 (5%)
8	KVR	G	5107	-	24,25,25	1.41	3 (12%)	31,34,34	1.56	4 (12%)
9	L9R	A	5308	-	53,53,53	1.21	4 (7%)	59,61,61	1.12	2 (3%)
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%)
5	ATP	G	5106	-	28,33,33	0.62	0	34,52,52	0.59	1 (2%)
5	ATP	I	5106	-	28,33,33	0.62	0	34,52,52	0.59	1 (2%)
5	ATP	B	5305	-	28,33,33	0.62	0	34,52,52	0.59	1 (2%)
9	L9R	I	5101	-	53,53,53	1.21	4 (7%)	59,61,61	1.12	2 (3%)
5	ATP	A	5305	-	28,33,33	0.62	0	34,52,52	0.59	1 (2%)
9	L9R	I	5108	-	53,53,53	1.24	5 (9%)	59,61,61	1.12	3 (5%)
5	ATP	A	5301	-	28,33,33	0.62	0	34,52,52	0.85	2 (5%)
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%)

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



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	CFF	G	5105	-	-	-	0/2/2/2
7	CFF	I	5105	-	-	-	0/2/2/2
8	KVR	B	5306	-	-	2/10/20/20	0/2/3/3
5	ATP	I	5102	-	-	8/18/38/38	0/3/3/3
7	CFF	B	5304	-	-	-	0/2/2/2
7	CFF	A	5304	-	-	-	0/2/2/2
9	L9R	G	5108	-	-	30/57/57/57	-
9	L9R	B	5307	-	-	30/57/57/57	-
5	ATP	G	5102	-	-	8/18/38/38	0/3/3/3
9	L9R	A	5307	-	-	30/57/57/57	-
5	ATP	B	5301	-	-	8/18/38/38	0/3/3/3
8	KVR	G	5107	-	-	2/10/20/20	0/2/3/3
9	L9R	A	5308	-	-	34/57/57/57	-
8	KVR	A	5306	-	-	2/10/20/20	0/2/3/3
9	L9R	B	5308	-	-	34/57/57/57	-
5	ATP	G	5106	-	-	6/18/38/38	0/3/3/3
5	ATP	I	5106	-	-	6/18/38/38	0/3/3/3
5	ATP	B	5305	-	-	6/18/38/38	0/3/3/3
9	L9R	I	5101	-	-	34/57/57/57	-
5	ATP	A	5305	-	-	6/18/38/38	0/3/3/3
9	L9R	I	5108	-	-	30/57/57/57	-
5	ATP	A	5301	-	-	8/18/38/38	0/3/3/3
8	KVR	I	5107	-	-	2/10/20/20	0/2/3/3
9	L9R	G	5101	-	-	34/57/57/57	-

All (60) 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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	G	5101	L9R	O2-C31	3.53	1.44	1.34
7	B	5304	CFF	C6-N1	-3.32	1.32	1.38
7	A	5304	CFF	C6-N1	-3.30	1.32	1.38
7	G	5105	CFF	C6-N1	-3.30	1.32	1.38
7	I	5105	CFF	C6-N1	-3.30	1.32	1.38
7	G	5105	CFF	C5-C4	-3.24	1.33	1.39
7	I	5105	CFF	C5-C4	-3.24	1.33	1.39
7	A	5304	CFF	C5-C4	-3.23	1.33	1.39
7	B	5304	CFF	C5-C4	-3.23	1.33	1.39
9	G	5108	L9R	O3-C11	3.16	1.42	1.33
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	G	5105	CFF	O13-C6	-2.43	1.18	1.24
7	A	5304	CFF	O13-C6	-2.42	1.18	1.24
7	B	5304	CFF	O13-C6	-2.42	1.18	1.24
7	I	5105	CFF	O13-C6	-2.40	1.18	1.24
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
8	A	5306	KVR	C13-N12	-2.30	1.45	1.47
8	I	5107	KVR	C13-N12	-2.30	1.45	1.47
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
9	B	5307	L9R	P-O3P	2.07	1.67	1.59

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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
5	I	5102	ATP	C4'-O4'-C1'	-3.55	106.67	109.92
5	B	5301	ATP	C4'-O4'-C1'	-3.53	106.69	109.92
5	A	5301	ATP	C4'-O4'-C1'	-3.53	106.69	109.92
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
5	G	5102	ATP	C4'-O4'-C1'	-3.49	106.73	109.92
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
7	I	5105	CFF	C14-N7-C8	-3.11	110.47	125.43
7	A	5304	CFF	C14-N7-C8	-3.10	110.51	125.43
7	B	5304	CFF	C14-N7-C8	-3.10	110.52	125.43
7	G	5105	CFF	C14-N7-C8	-3.09	110.54	125.43
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
5	I	5102	ATP	C5-C6-N6	2.34	123.88	120.31
5	A	5301	ATP	C5-C6-N6	2.34	123.87	120.31
5	G	5102	ATP	C5-C6-N6	2.34	123.87	120.31
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
5	G	5106	ATP	C5-C6-N6	2.32	123.84	120.31
9	G	5108	L9R	C4-C5-N	-2.31	108.39	115.82
5	B	5301	ATP	C5-C6-N6	2.31	123.84	120.31
9	A	5307	L9R	C4-C5-N	-2.31	108.40	115.82
5	A	5305	ATP	C5-C6-N6	2.31	123.83	120.31
5	I	5106	ATP	C5-C6-N6	2.30	123.81	120.31
5	B	5305	ATP	C5-C6-N6	2.28	123.79	120.31
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

There are no chirality outliers.

All (320) 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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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
9	B	5308	L9R	O11-C11-O3-C3
9	A	5307	L9R	C1-C2-C3-O3
9	B	5307	L9R	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
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
9	I	5108	L9R	C15-C16-C17-C18
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'

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Mol	Chain	Res	Type	Atoms
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
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

*Continued on next page...*

*Continued from previous page...*

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

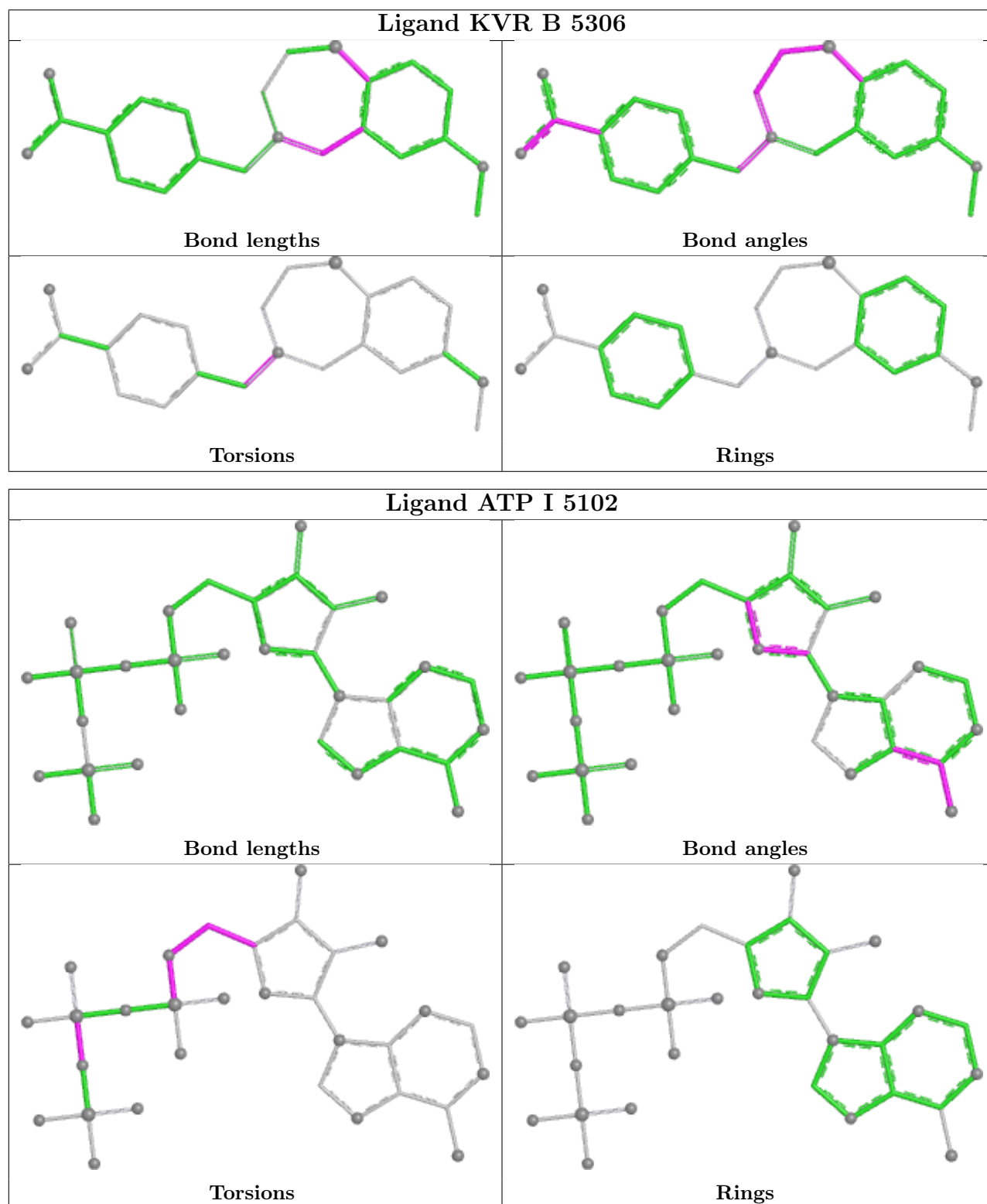
There are no ring outliers.

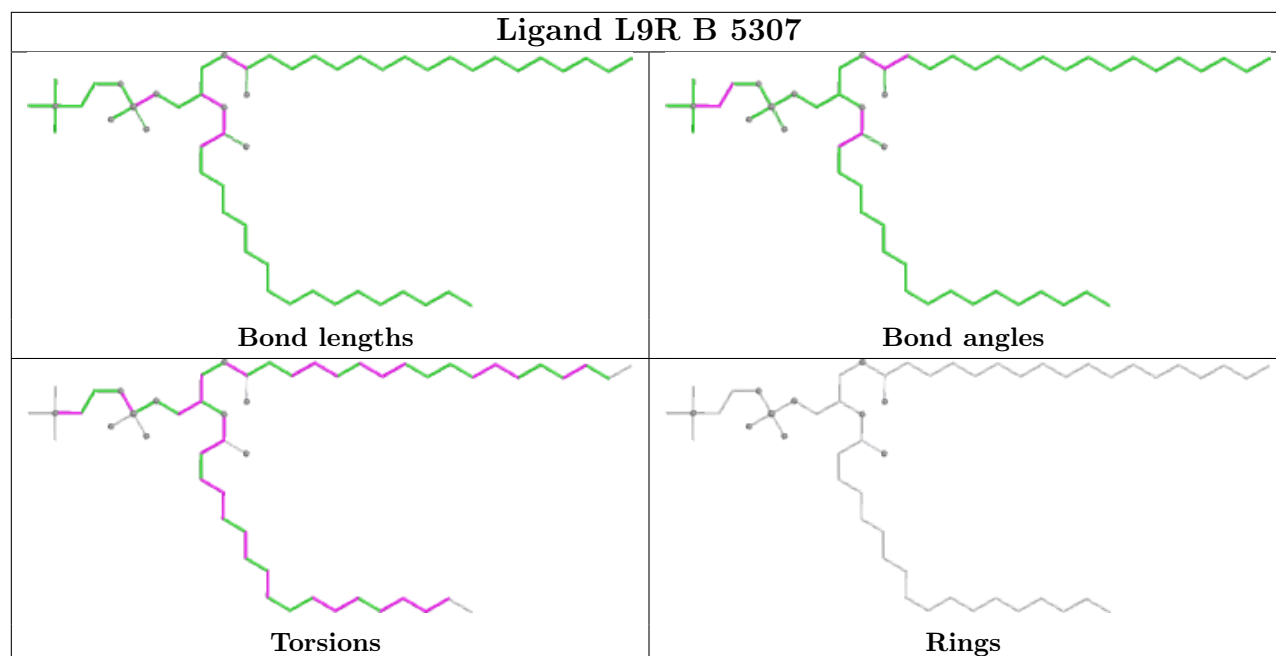
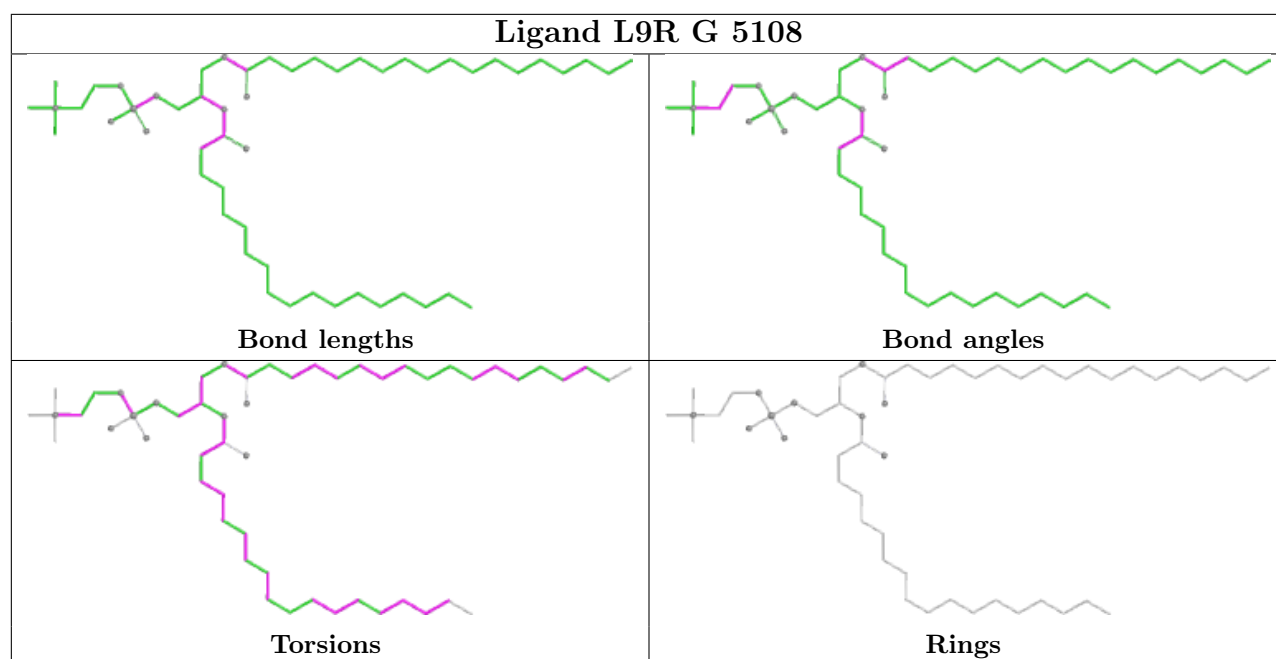
16 monomers are involved in 36 short contacts:

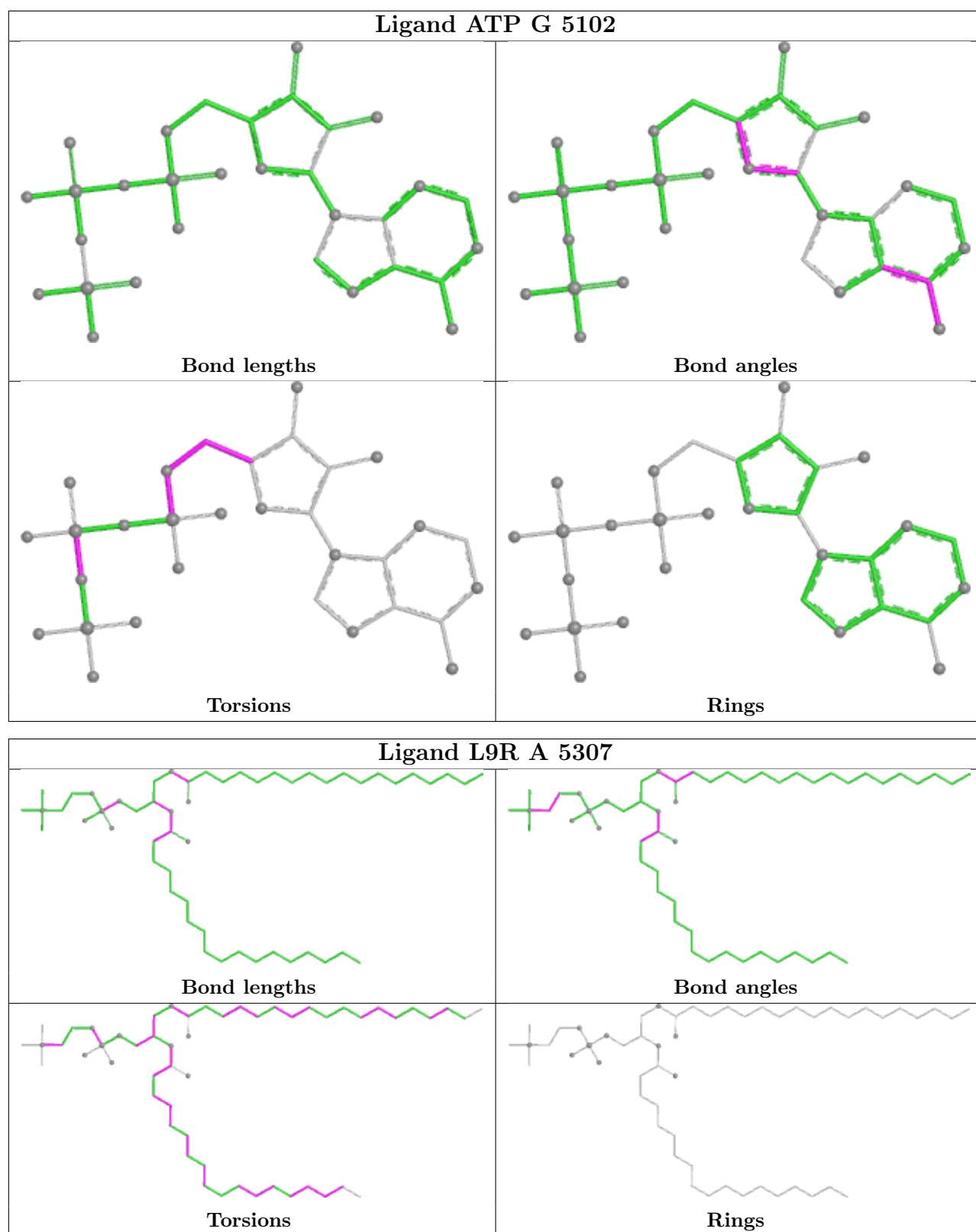
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	5102	ATP	1	0
9	G	5108	L9R	3	0
9	B	5307	L9R	2	0
5	G	5102	ATP	1	0
9	A	5307	L9R	3	0
5	B	5301	ATP	1	0
9	A	5308	L9R	6	0
9	B	5308	L9R	4	0
5	G	5106	ATP	1	0
5	I	5106	ATP	1	0
5	B	5305	ATP	1	0
9	I	5101	L9R	5	0
5	A	5305	ATP	1	0
9	I	5108	L9R	3	0
5	A	5301	ATP	1	0
9	G	5101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

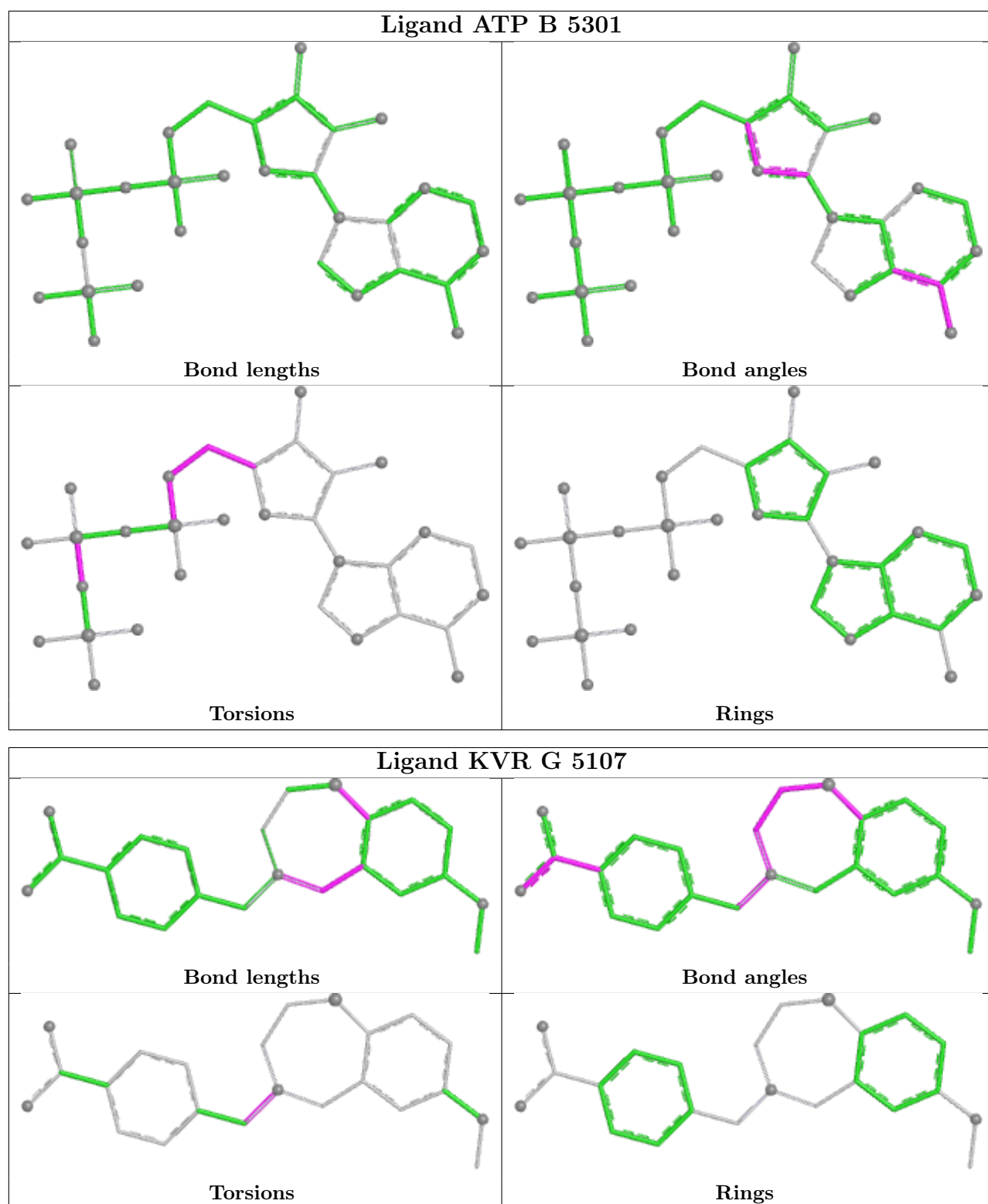
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

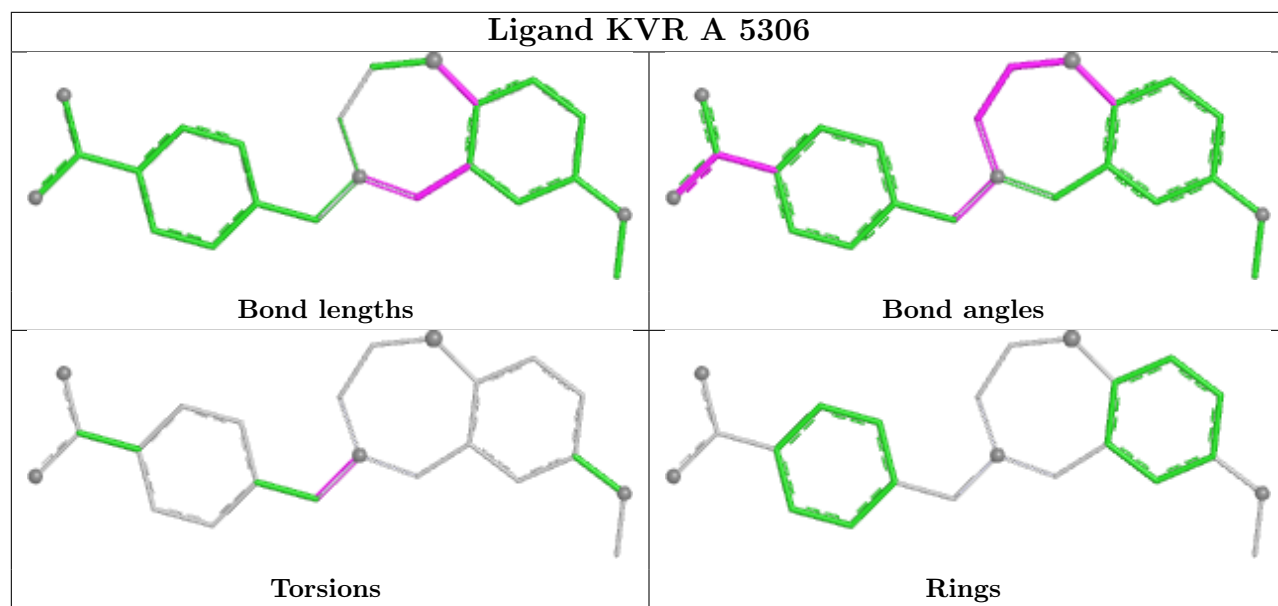
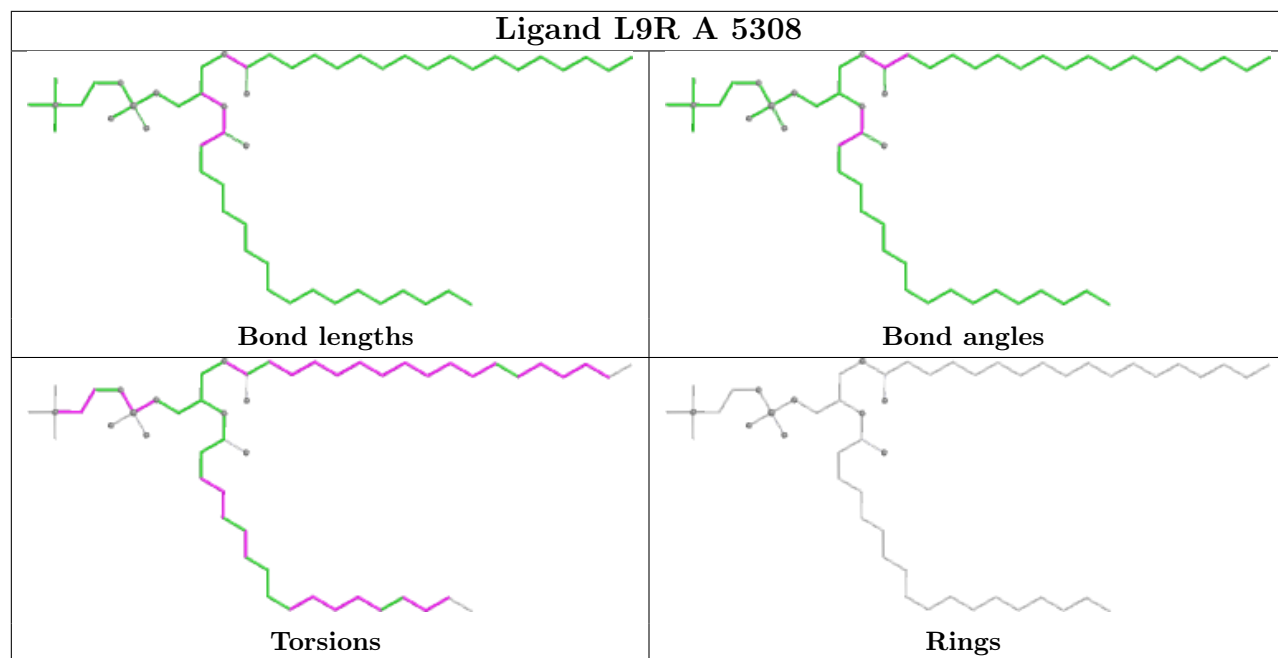


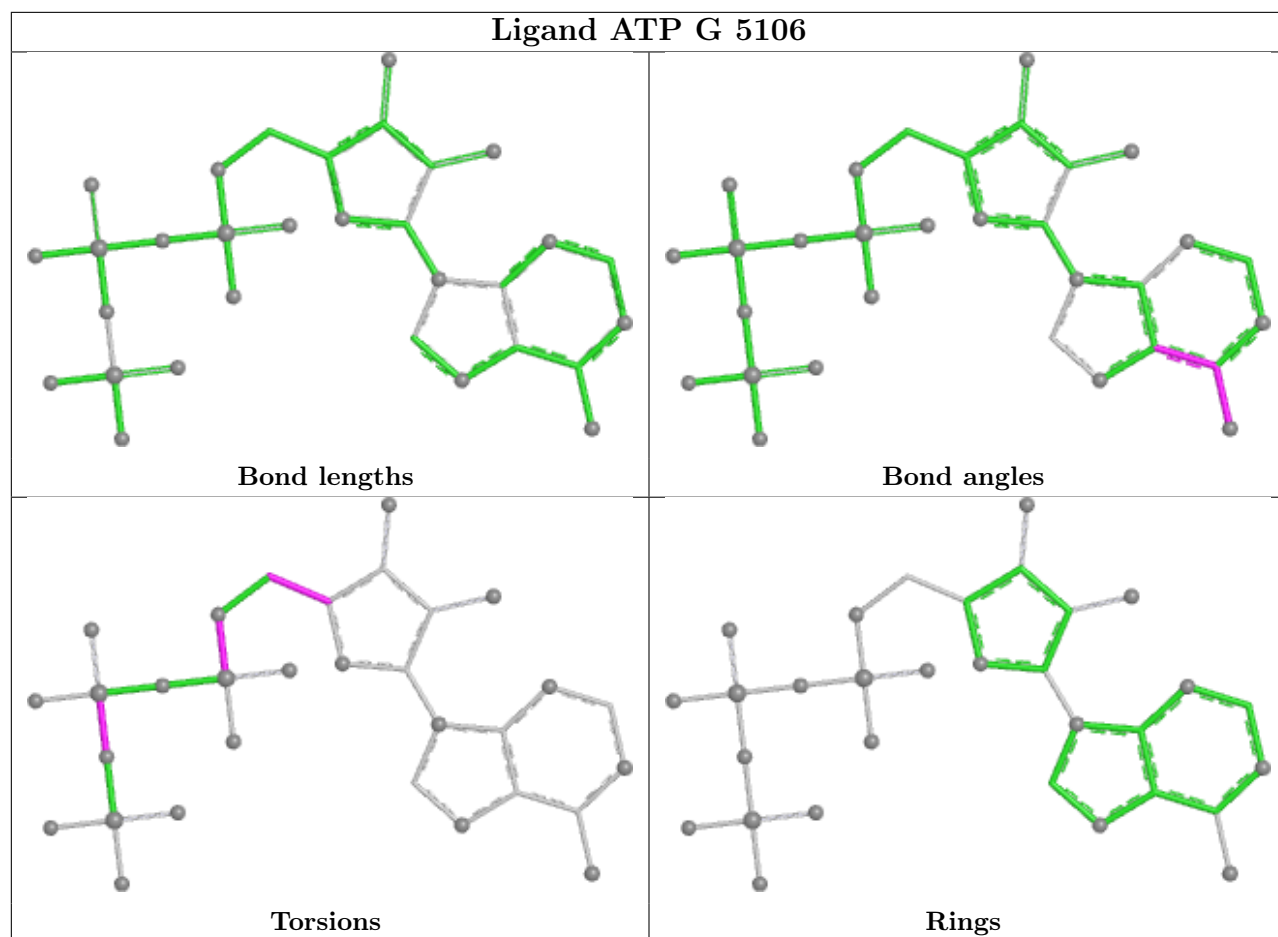
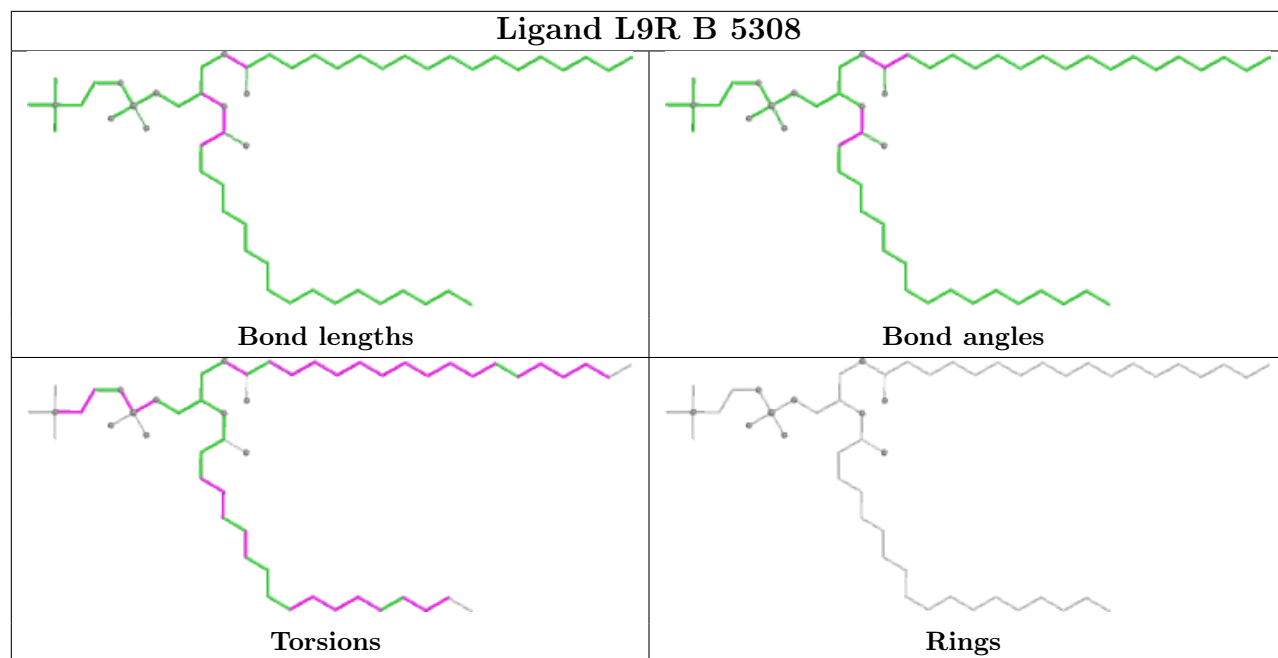


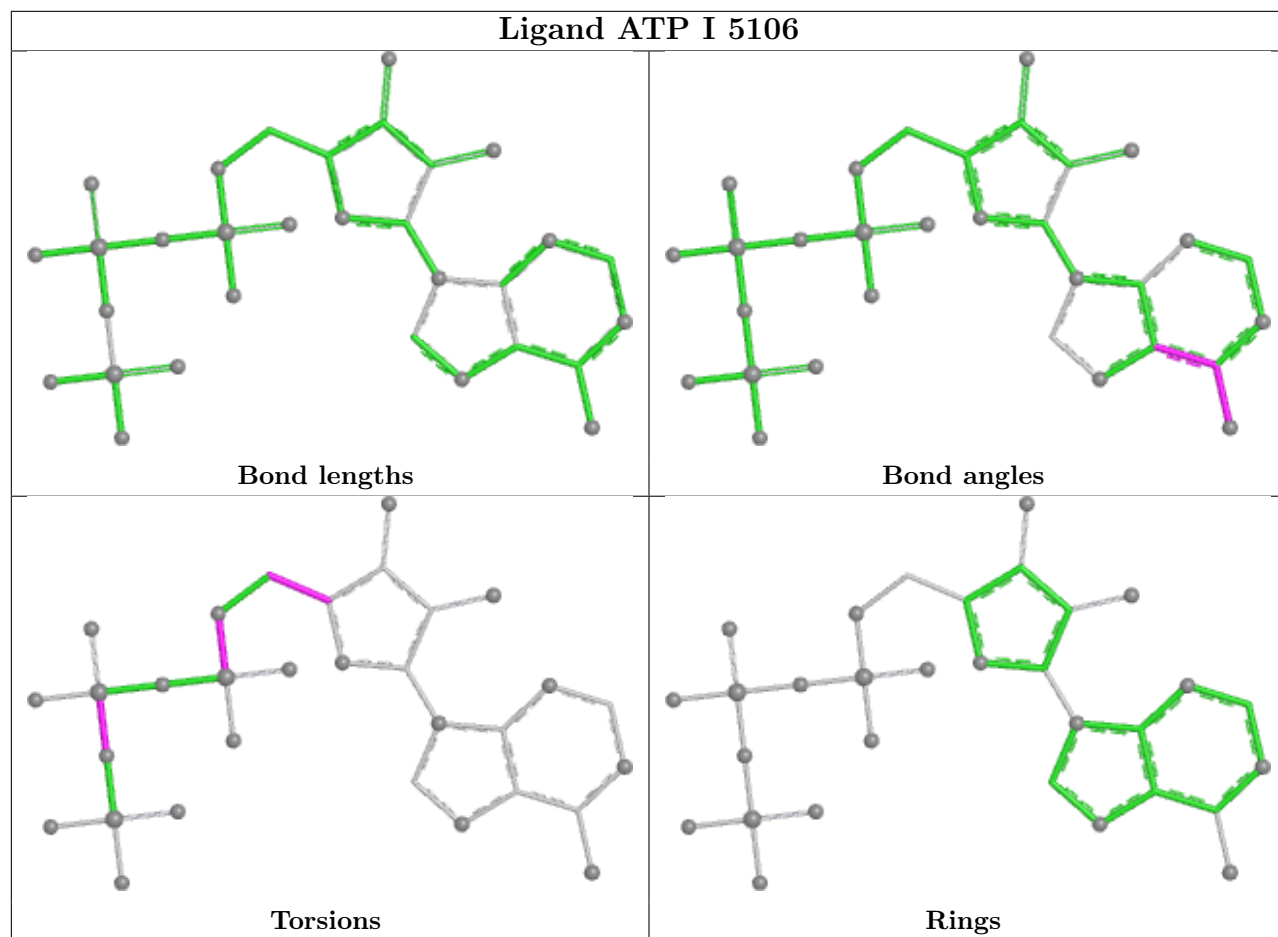


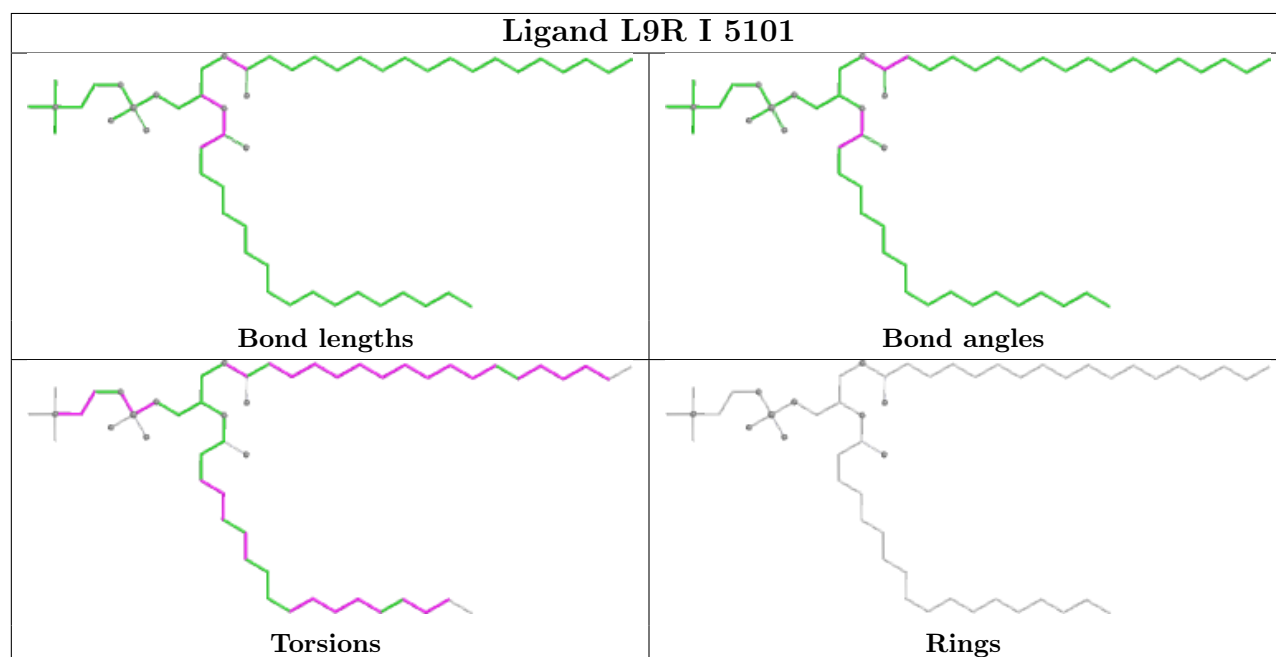
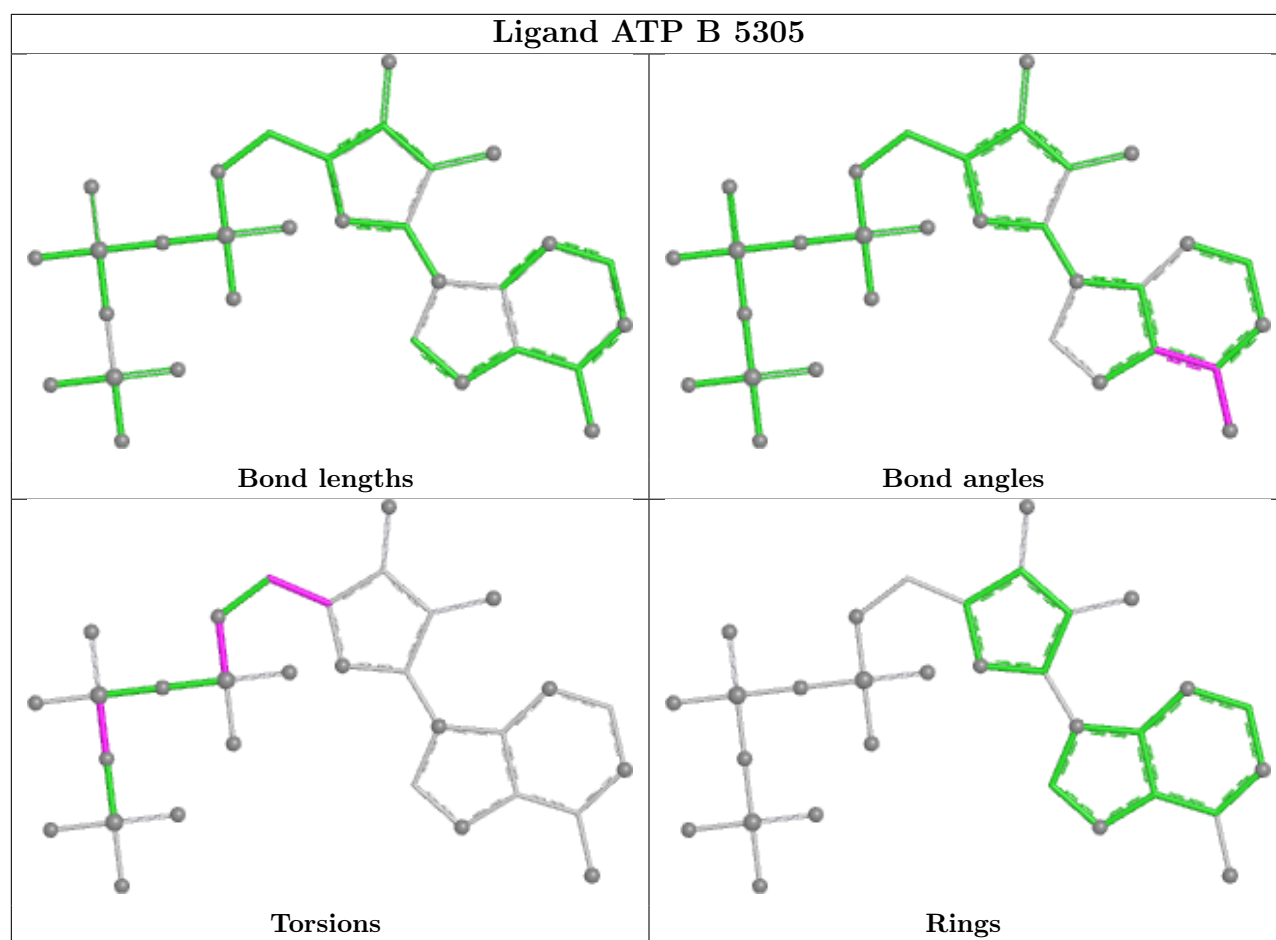


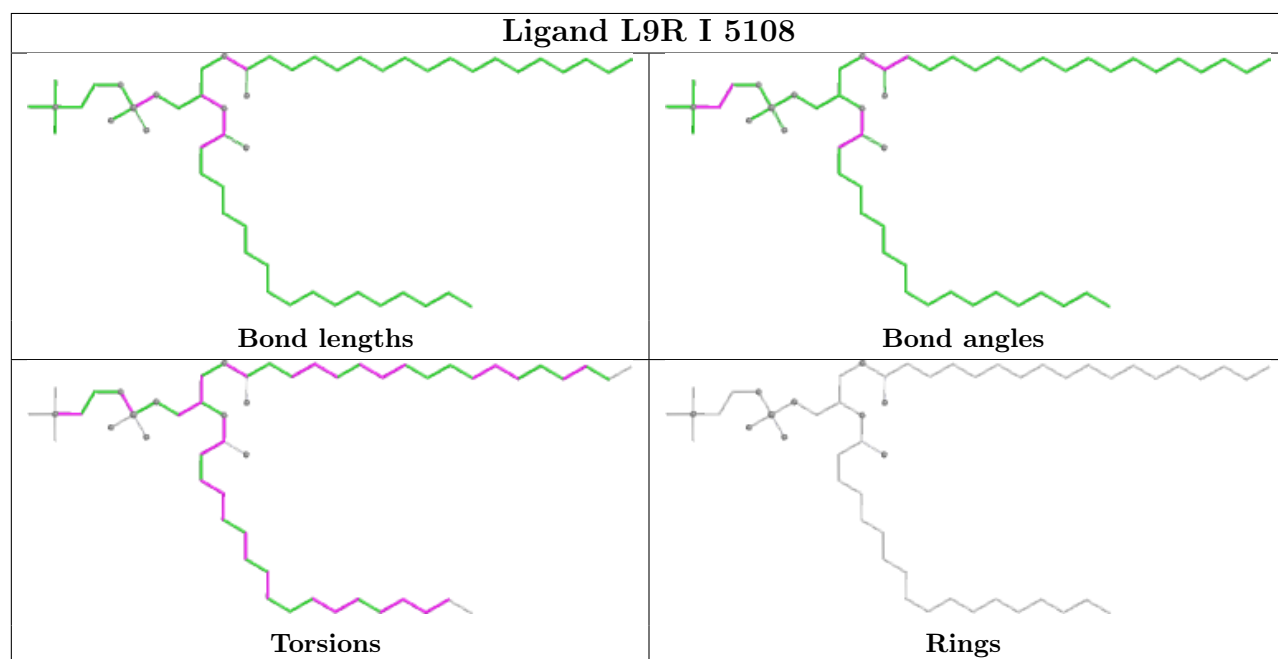
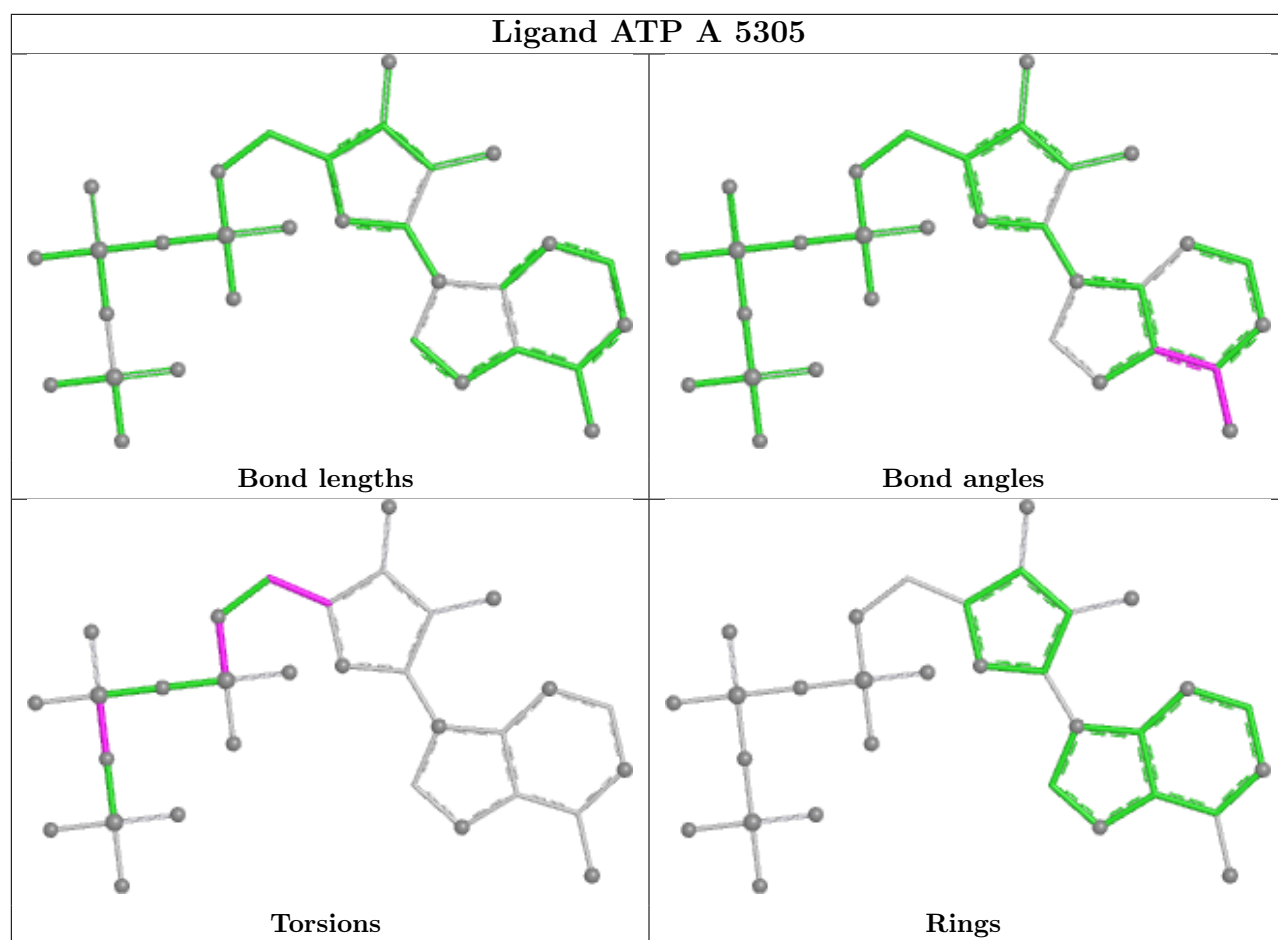


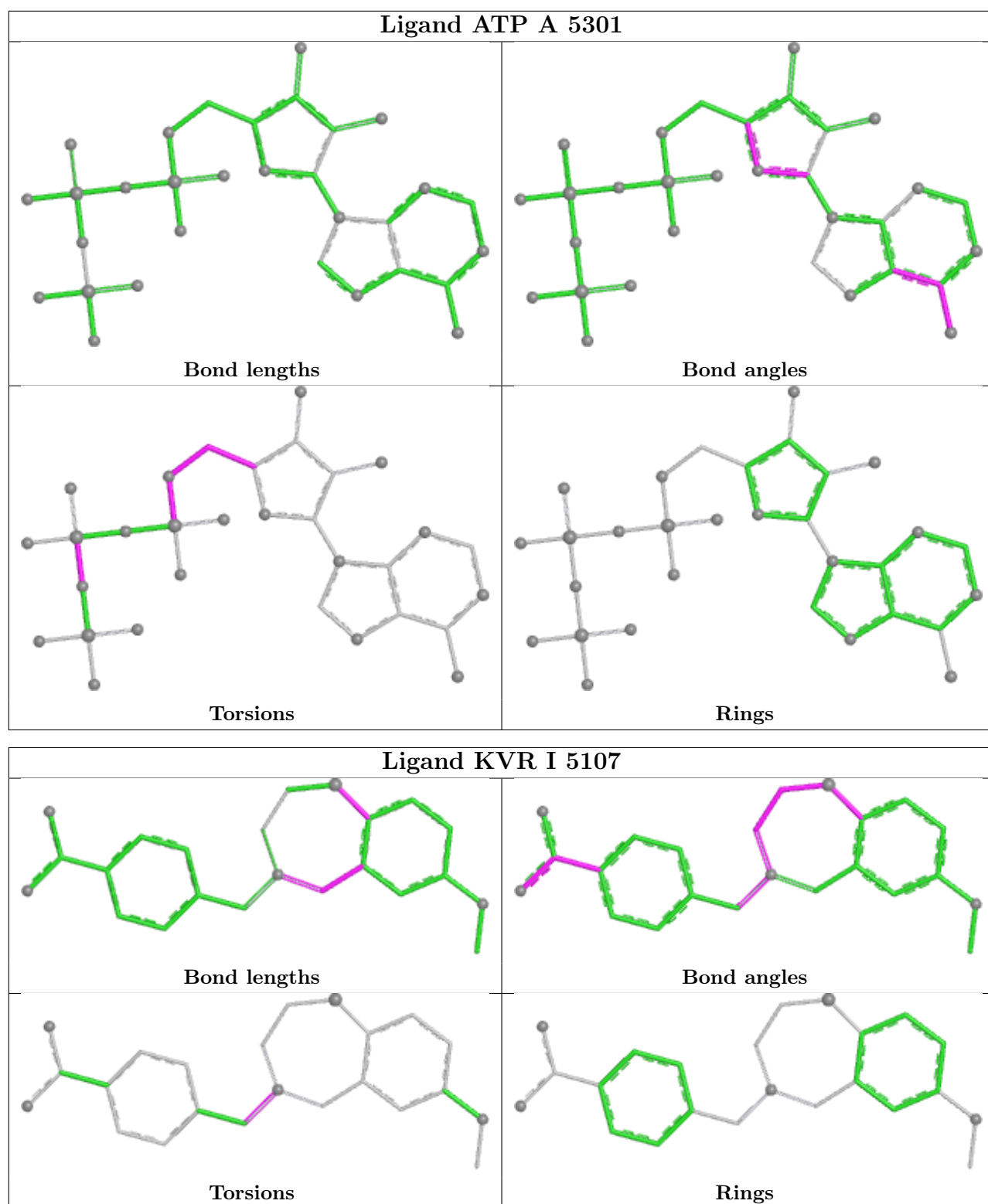


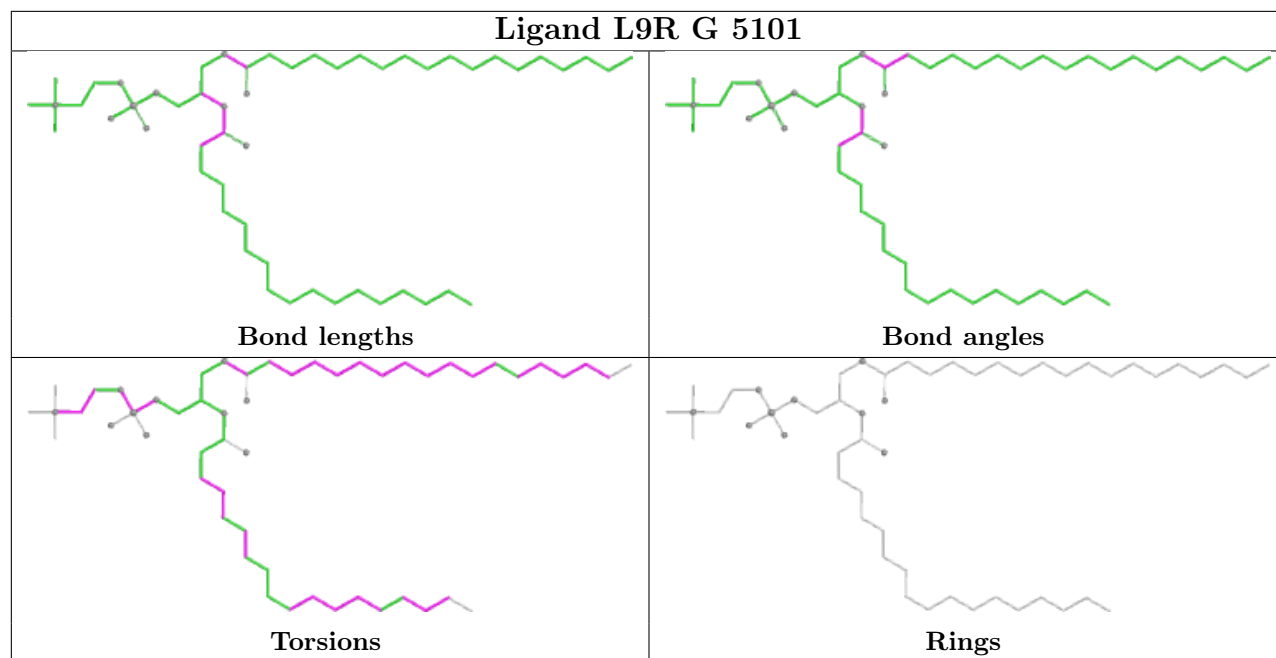












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

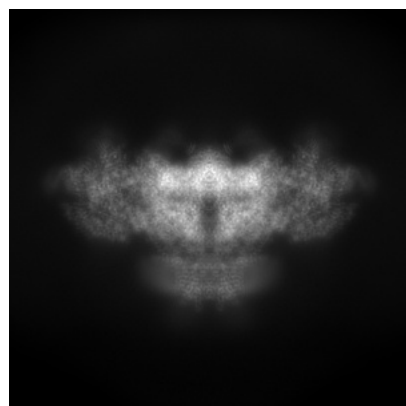
## 6 Map visualisation [i](#)

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.

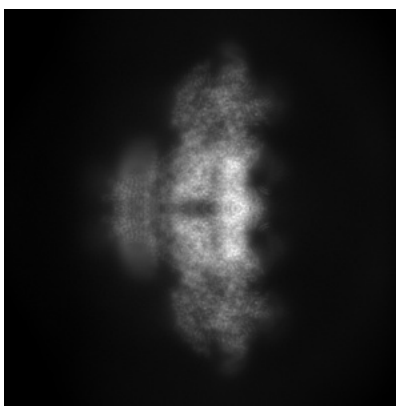
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

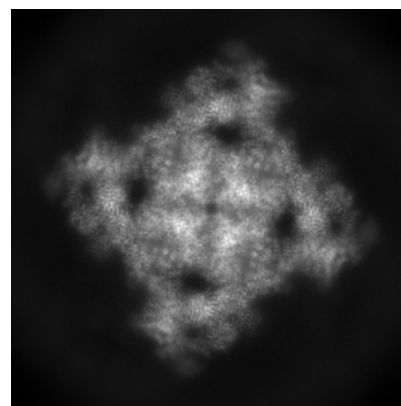
#### 6.1.1 Primary map



X

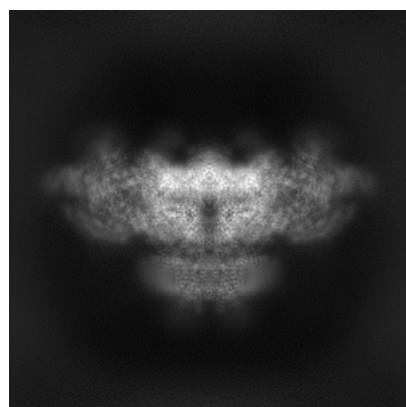


Y

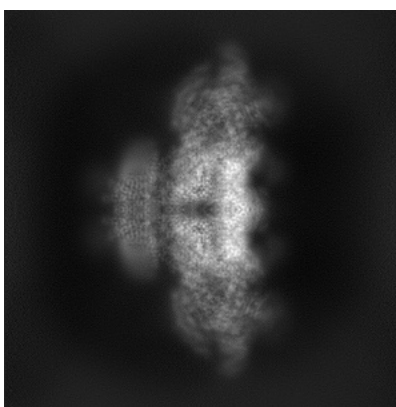


Z

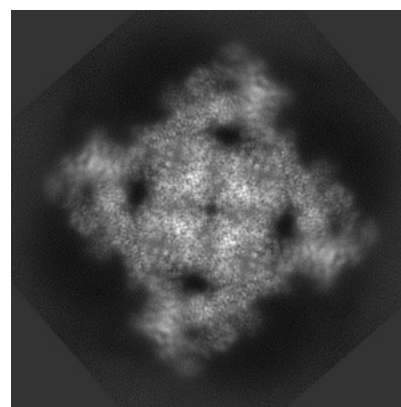
#### 6.1.2 Raw map



X



Y



Z

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

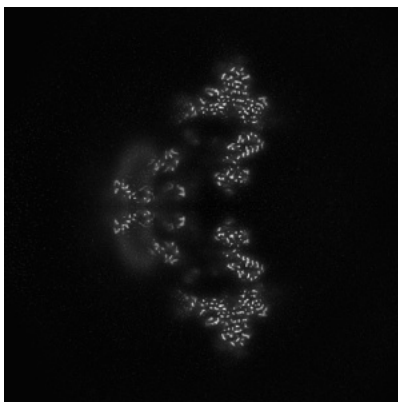


## 6.2 Central slices [i](#)

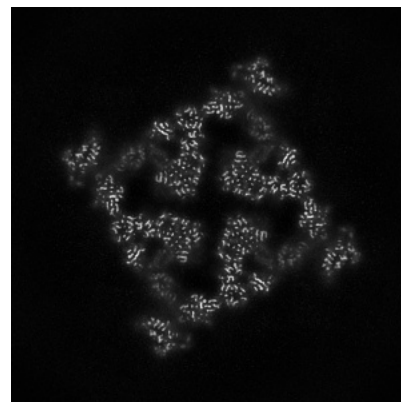
### 6.2.1 Primary map



X Index: 256

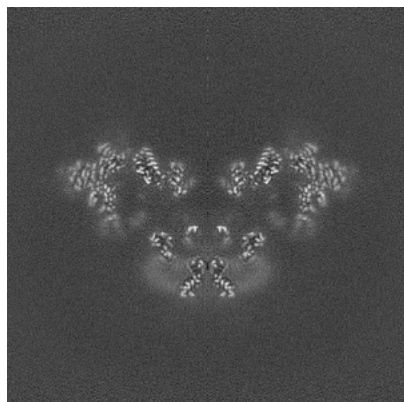


Y Index: 256

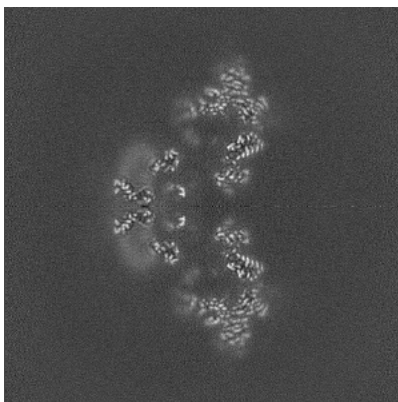


Z Index: 256

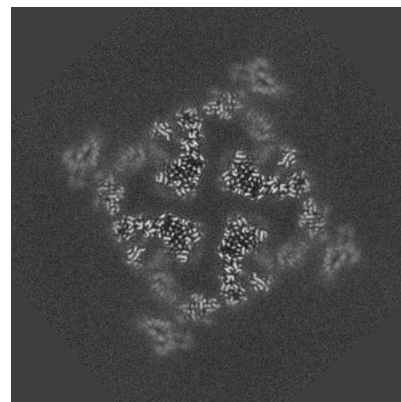
### 6.2.2 Raw map



X Index: 256



Y Index: 256

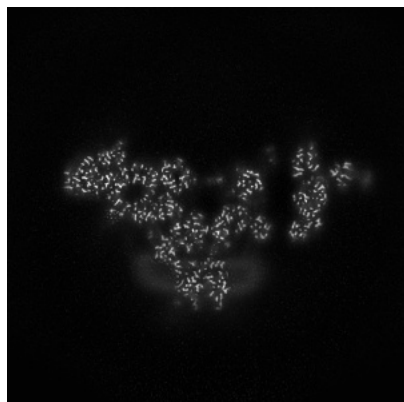


Z Index: 256

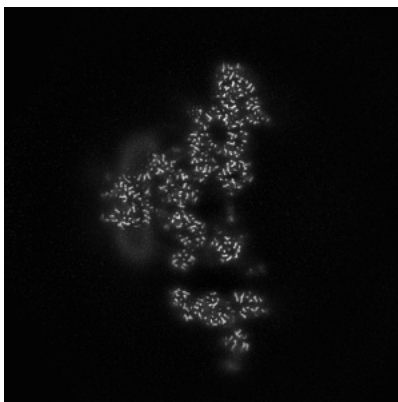
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

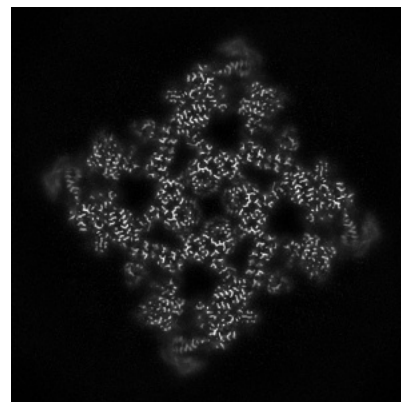
### 6.3.1 Primary map



X Index: 272

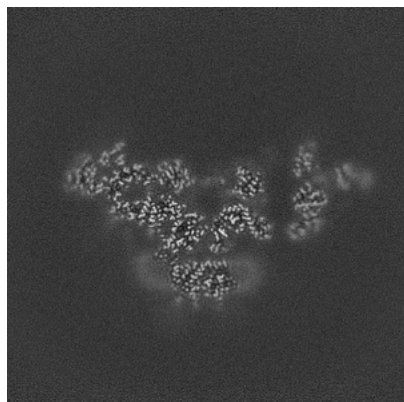


Y Index: 272

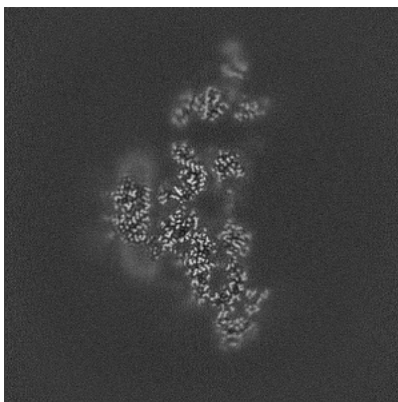


Z Index: 286

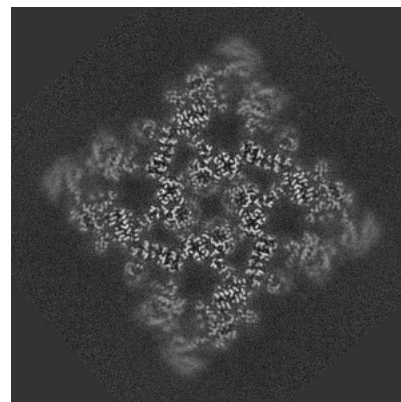
### 6.3.2 Raw map



X Index: 275



Y Index: 237

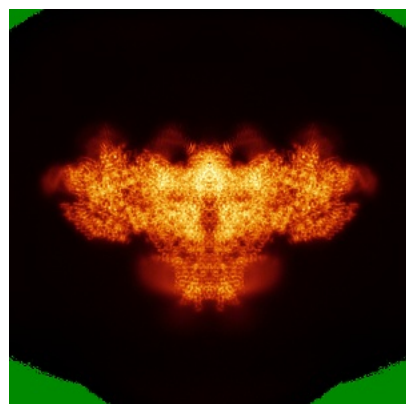


Z Index: 286

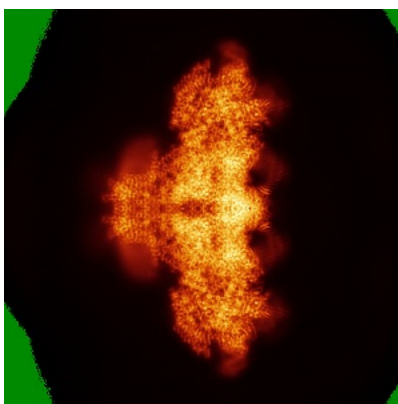
The images above show the largest variance slices of the map in three orthogonal directions.

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

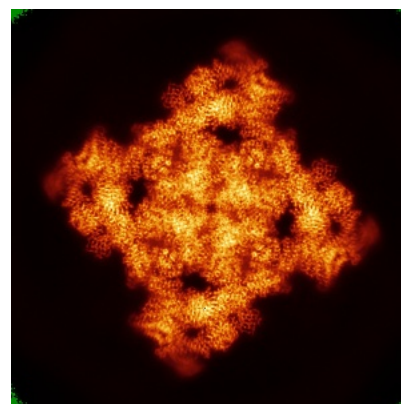
### 6.4.1 Primary map



X



Y

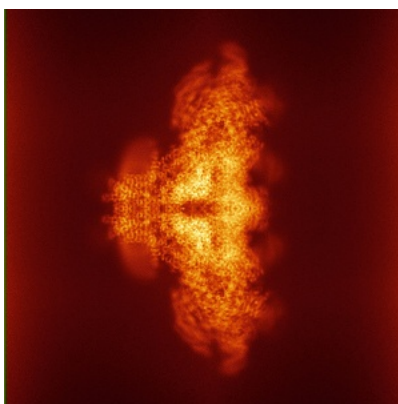


Z

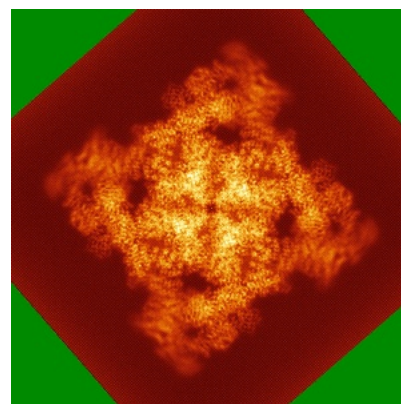
### 6.4.2 Raw map



X



Y

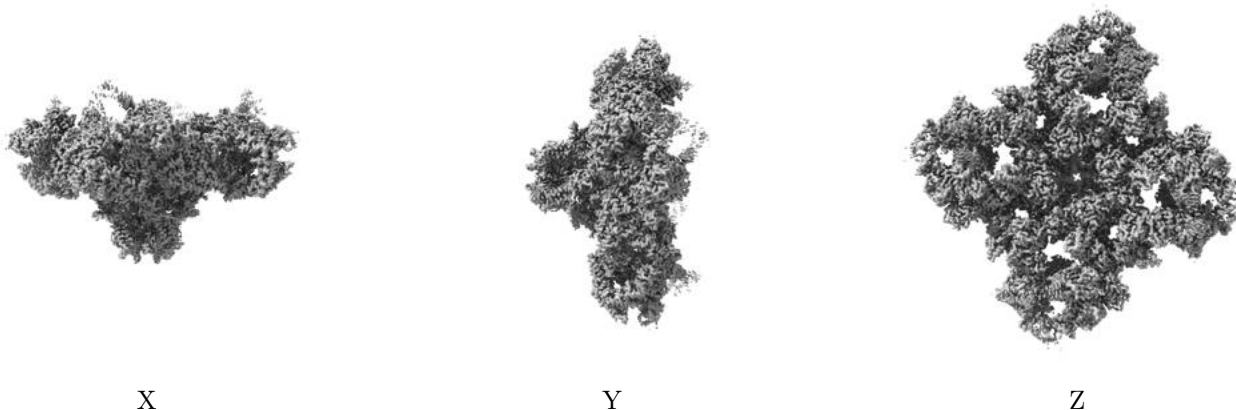


Z

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.

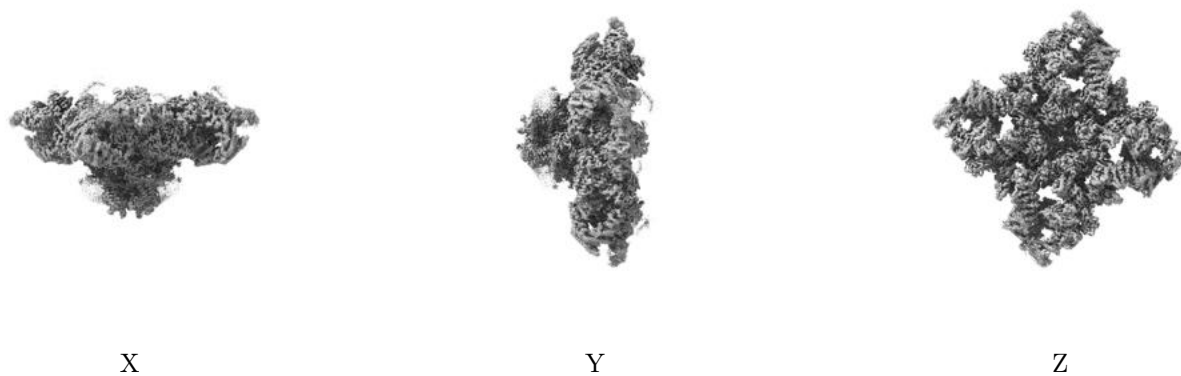
## 6.5 Orthogonal surface views [i](#)

### 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.



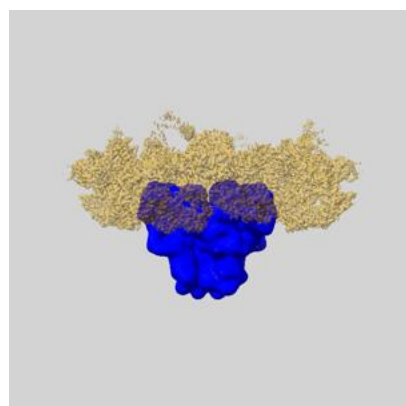
## 6.6 Mask visualisation [i](#)

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

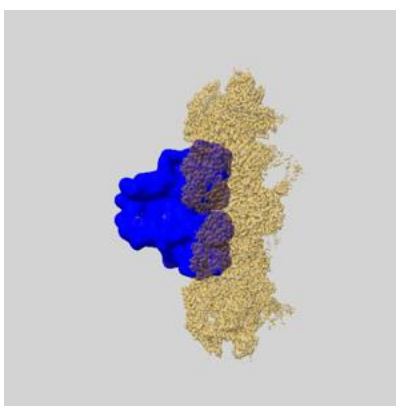
A mask typically either:

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

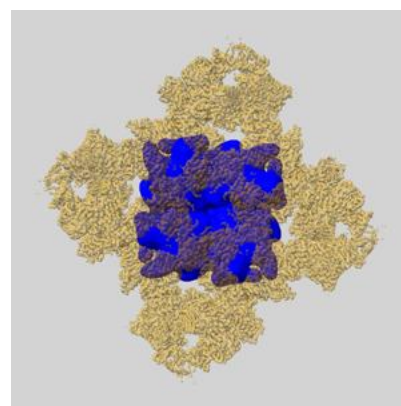
### 6.6.1 emd\_26205\_msk\_1.map [i](#)



X

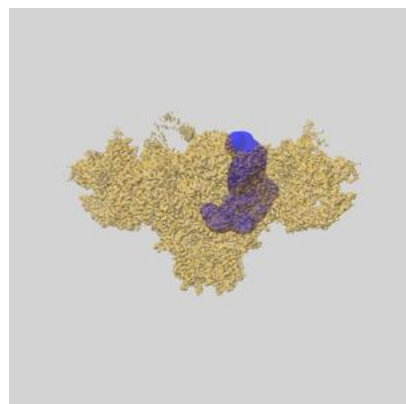


Y

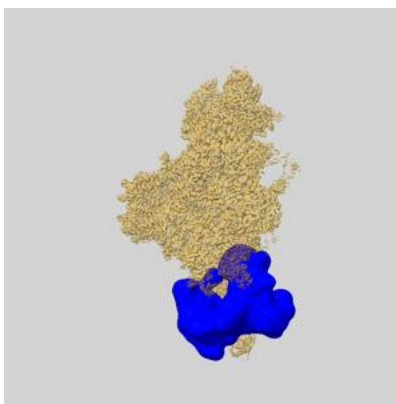


Z

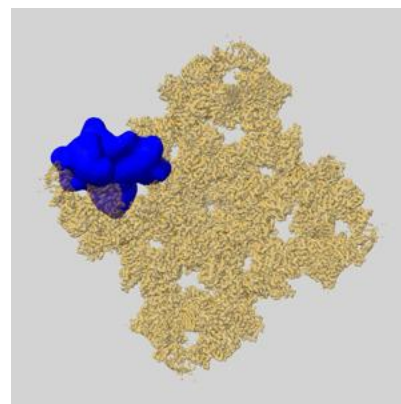
### 6.6.2 emd\_26205\_msk\_2.map [i](#)



X

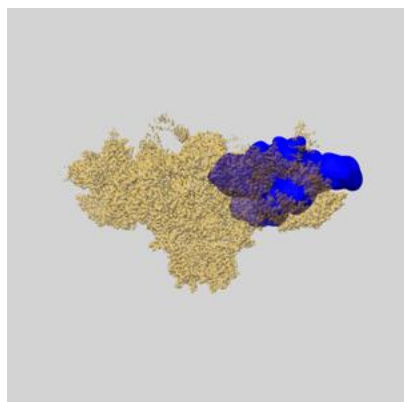


Y

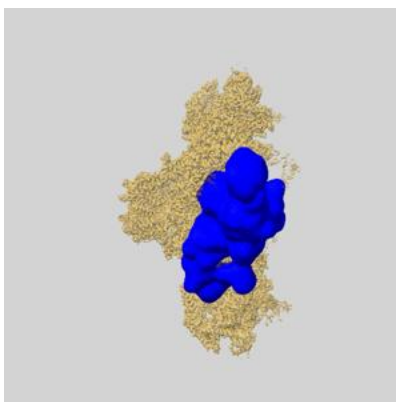


Z

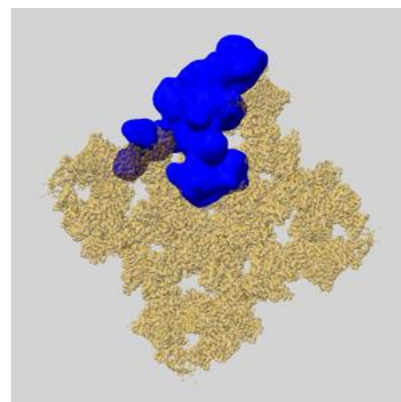
### 6.6.3 emd\_26205\_msk\_3.map [i](#)



X



Y

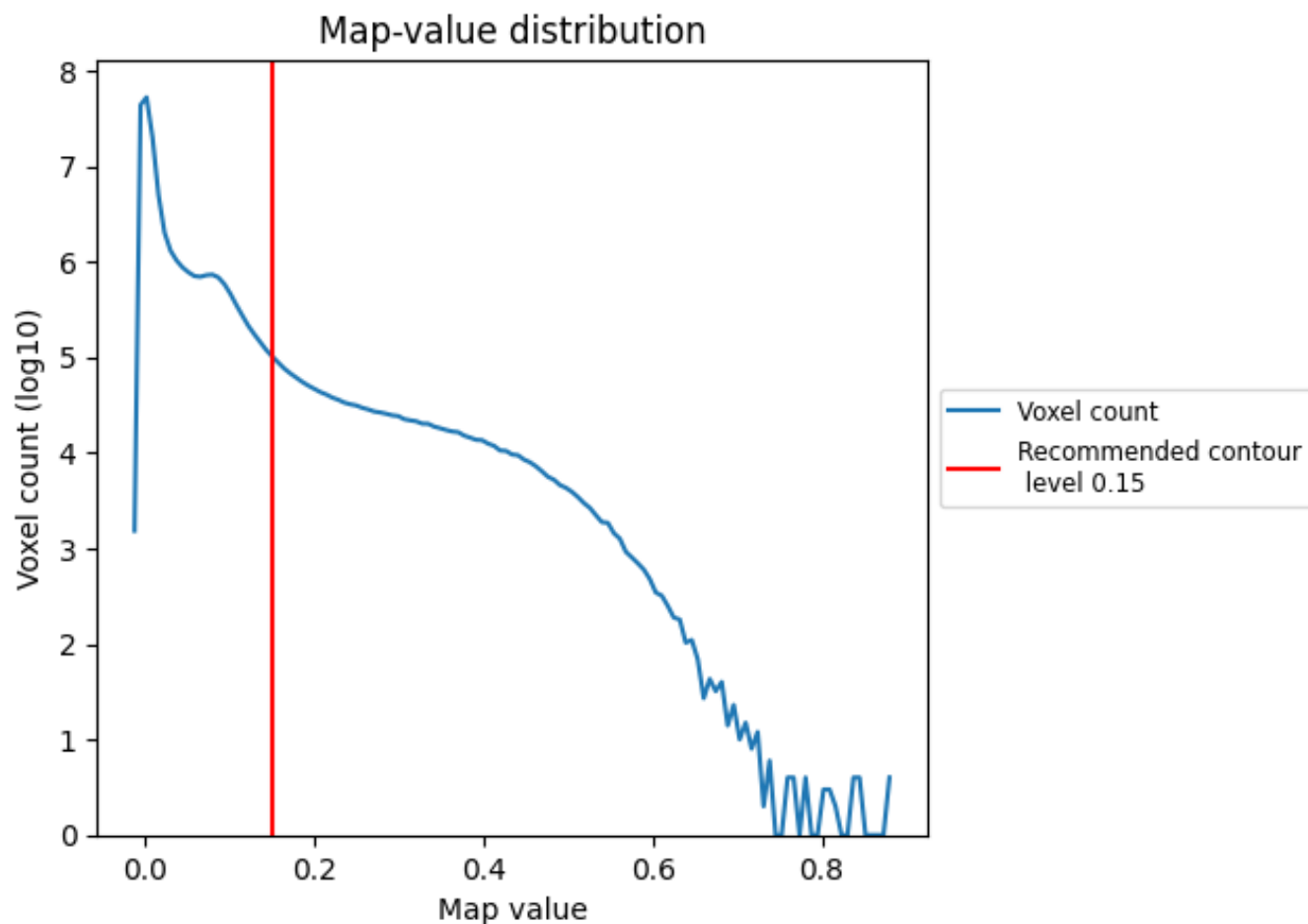


Z

## 7 Map analysis [i](#)

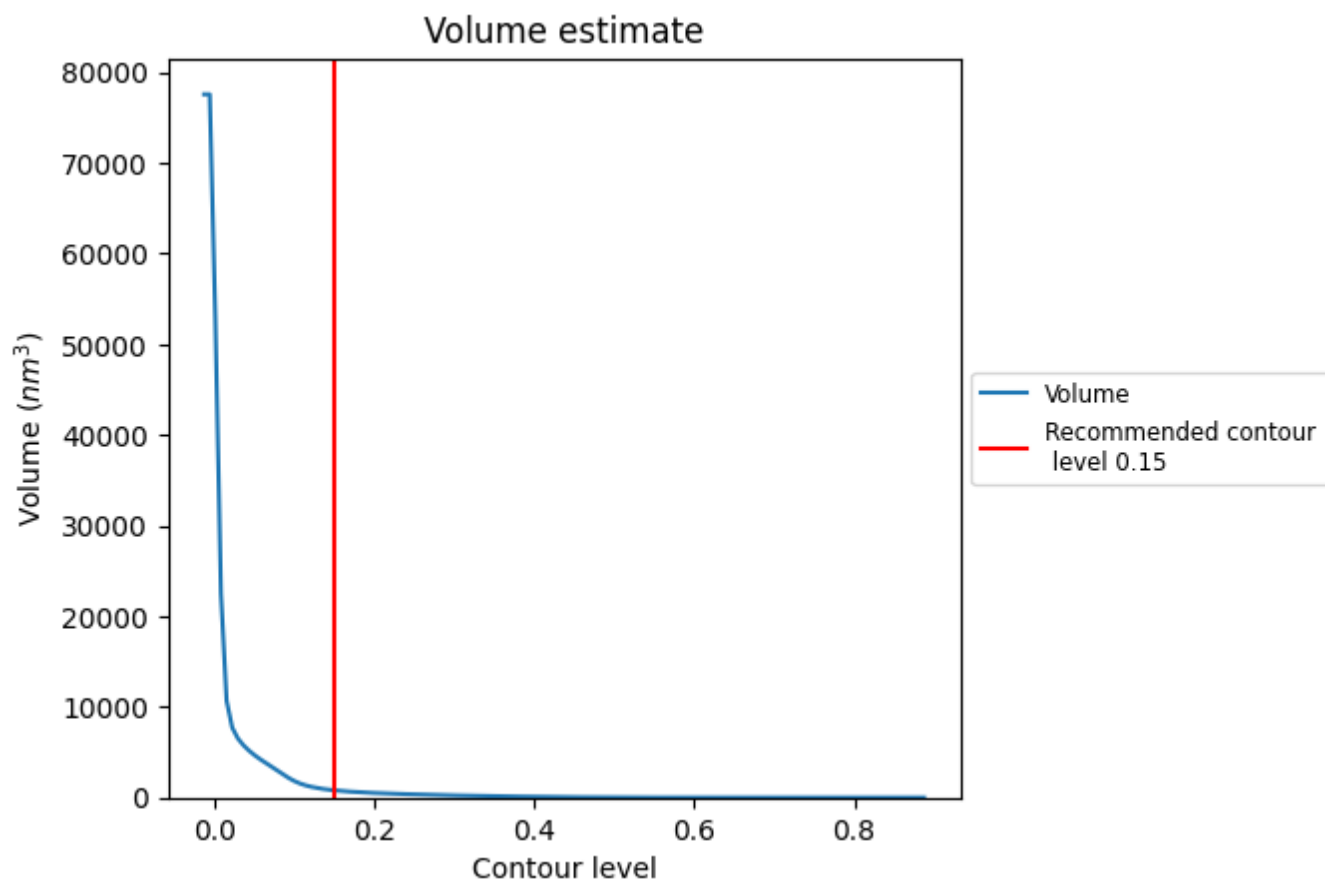
This section contains the results of statistical analysis of the map.

### 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](#)

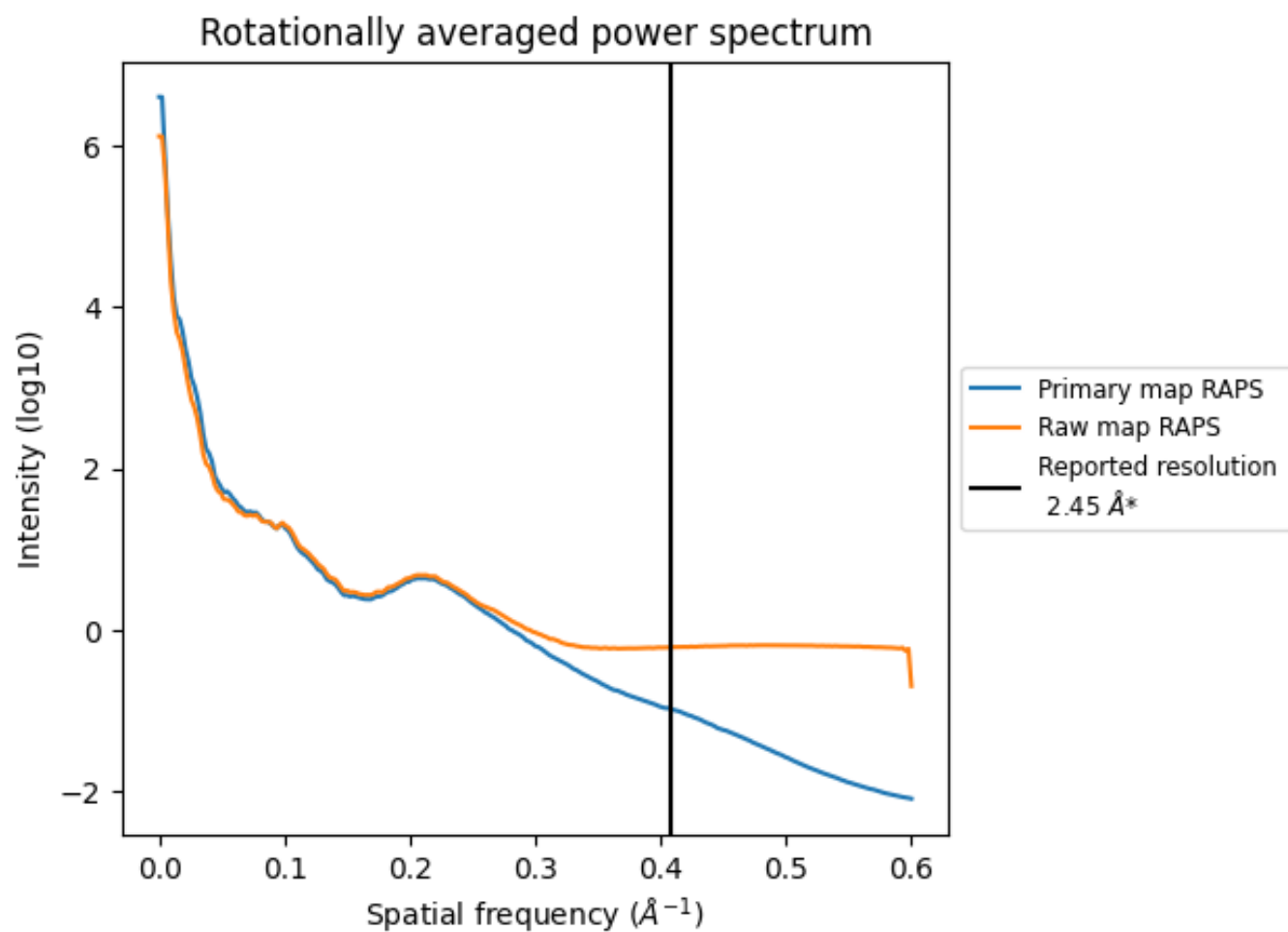


The volume at the recommended contour level is 800 nm<sup>3</sup>; this corresponds to an approximate mass of 723 kDa.

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 ⓘ

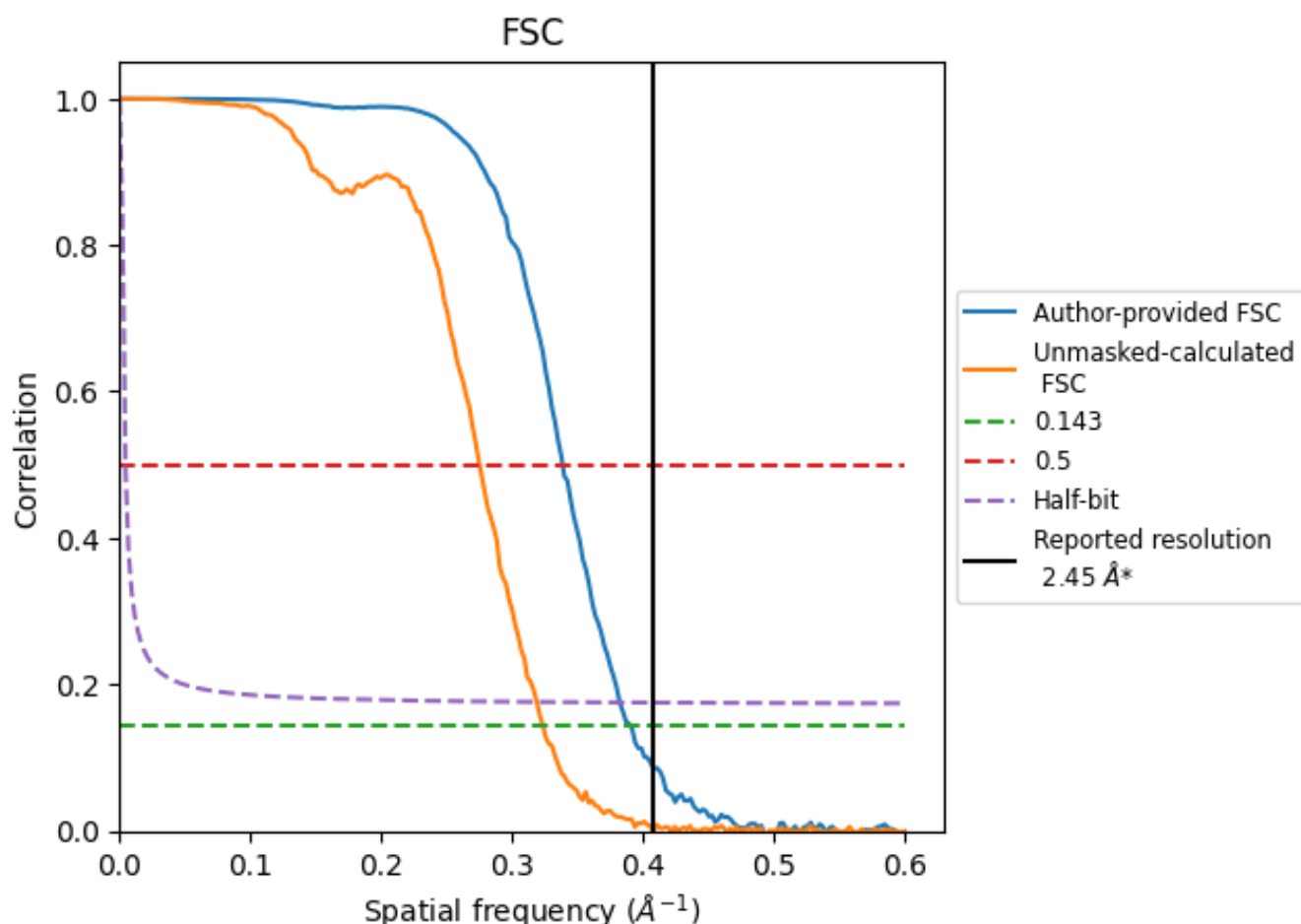


\*Reported resolution corresponds to spatial frequency of 0.408 Å<sup>-1</sup>

## 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](#)

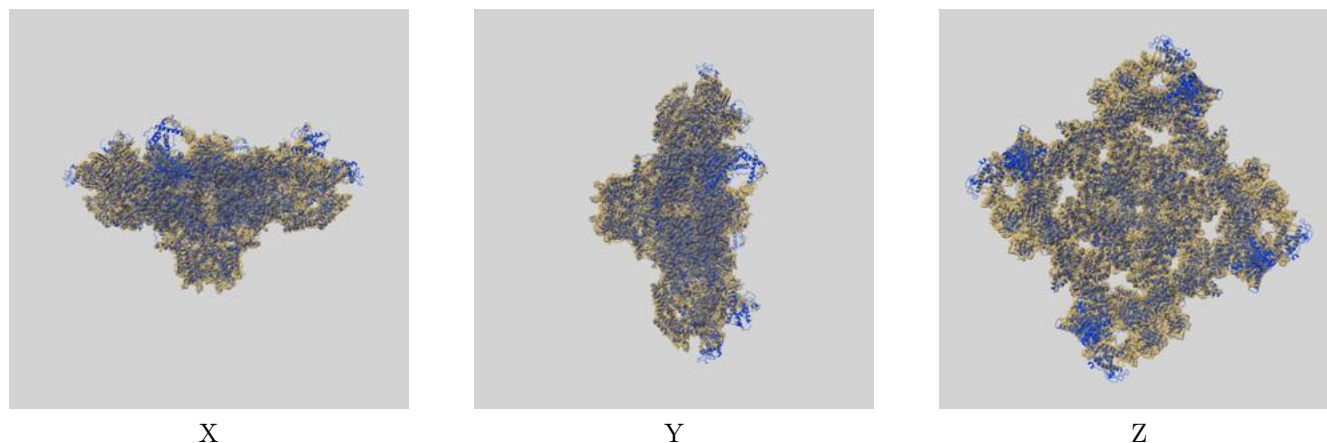
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.45	-	-
Author-provided FSC curve	2.56	2.95	2.62
Unmasked-calculated*	3.09	3.63	3.14

\*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](#)

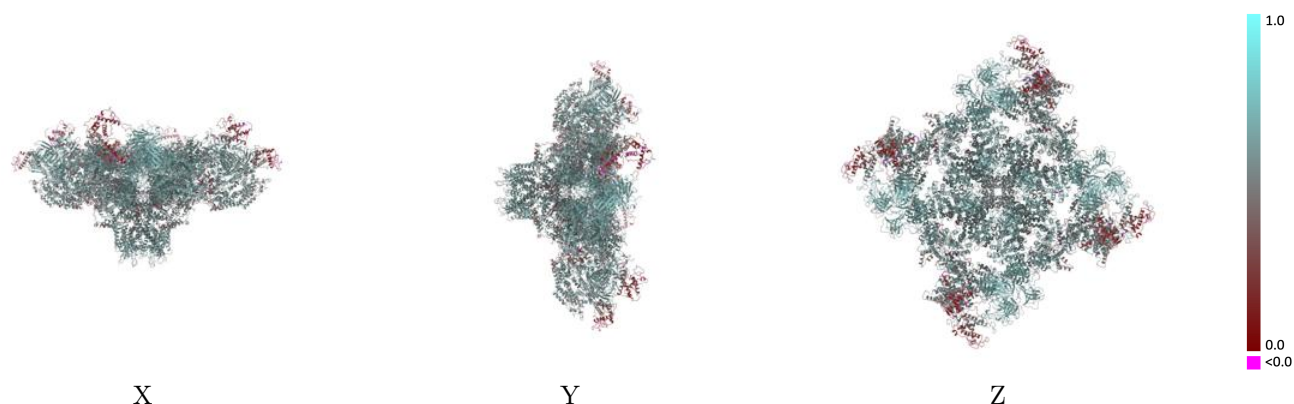
This section contains information regarding the fit between EMDB map EMD-26205 and PDB model 7TZC. Per-residue inclusion information can be found in section 3 on page 10.

### 9.1 Map-model overlay [i](#)



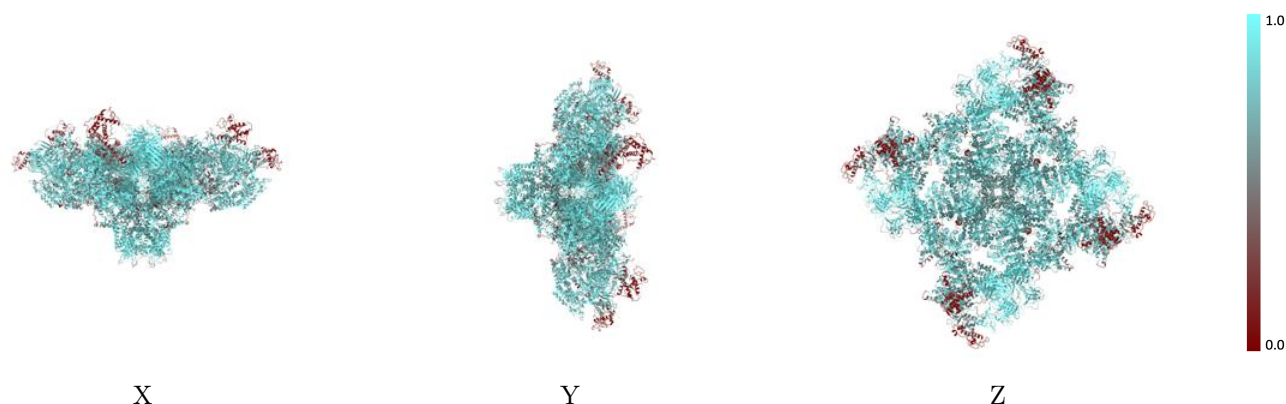
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



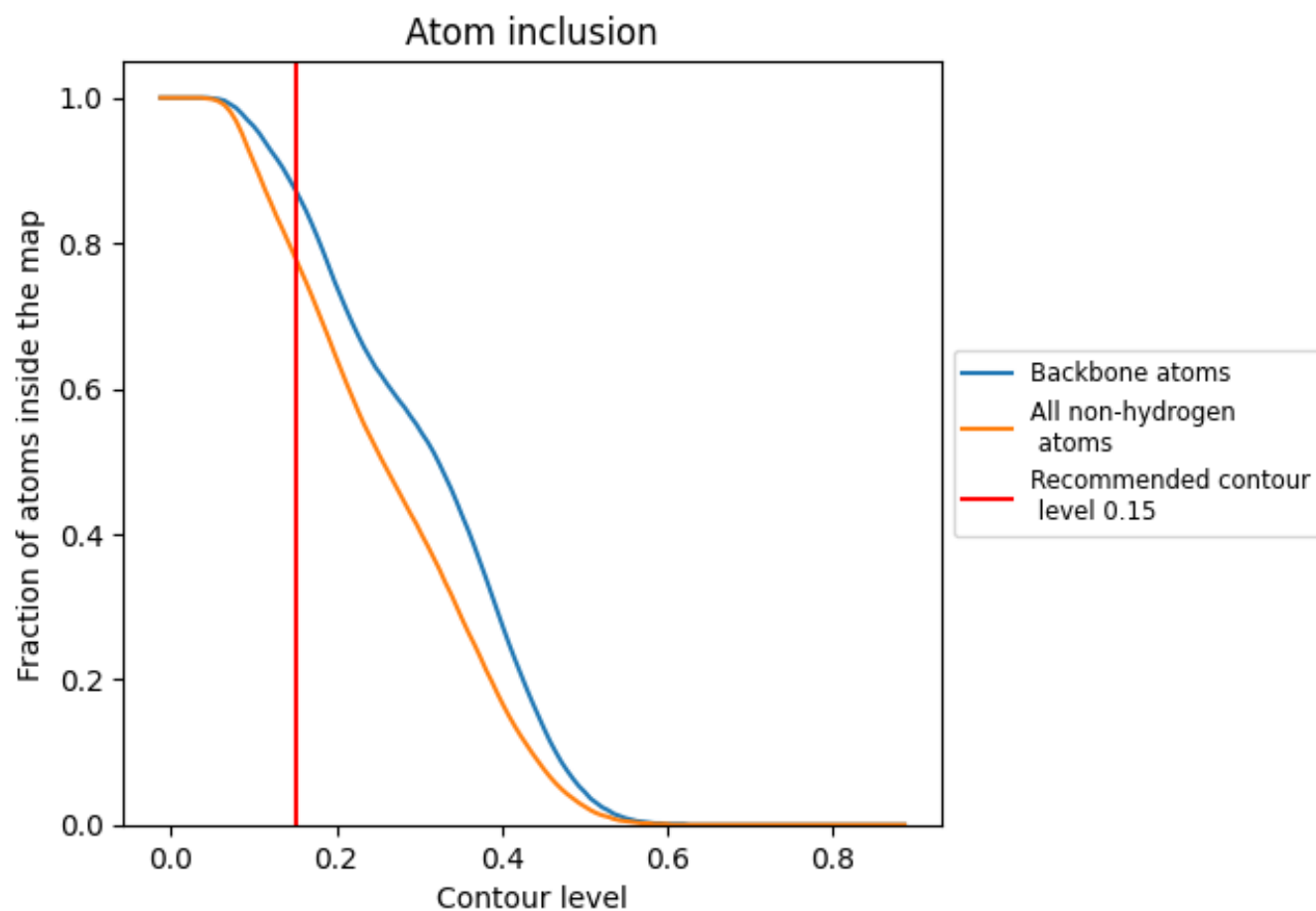
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	<div></div> 0.7810	<div></div> 0.5400
A	<div></div> 0.7900	<div></div> 0.5430
B	<div></div> 0.7890	<div></div> 0.5400
C	<div></div> 0.5240	<div></div> 0.4370
D	<div></div> 0.5310	<div></div> 0.4320
E	<div></div> 0.5310	<div></div> 0.4390
F	<div></div> 0.8040	<div></div> 0.6020
G	<div></div> 0.7890	<div></div> 0.5410
H	<div></div> 0.7930	<div></div> 0.6020
I	<div></div> 0.7890	<div></div> 0.5420
J	<div></div> 0.7890	<div></div> 0.6020
K	<div></div> 0.5280	<div></div> 0.4400
O	<div></div> 0.8020	<div></div> 0.6030

