



Full wwPDB EM Validation Report ⓘ

Sep 10, 2026 – 04:22 PM EDT

PDB ID : 9ZND / pdb_00009znd
EMDB ID : EMD-74445
Title : Structure of rabbit RyR1 complexed with FKBP12.6 and calmodulin in the presence of dantrolene, ATP, 4-chloro-m-cresol, caffeine, and Mg²⁺
Authors : Kim, K.; Clarke, O.B.
Deposited on : 2025-12-12
Resolution : 3.09 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

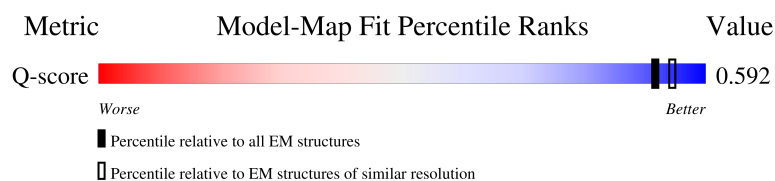
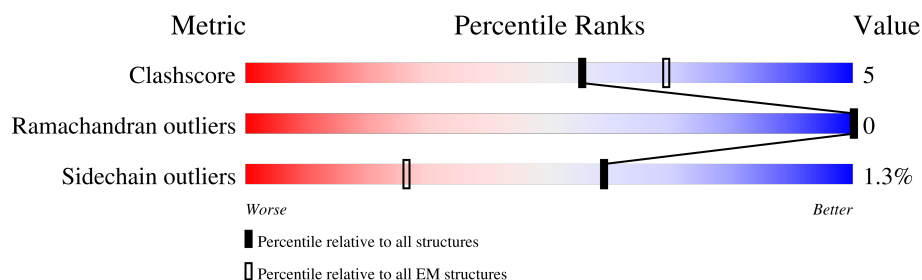
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 3.09 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14003 (2.59 - 3.59)

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

Mol	Chain	Length	Quality of chain
1	E	107	
1	F	107	
1	G	107	
1	H	107	

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Mol	Chain	Length	Quality of chain
2	I	148	
2	J	148	
2	K	148	
2	L	148	
3	A	5037	
3	B	5037	
3	C	5037	
3	D	5037	

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 143134 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 Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
1	F	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
1	G	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
1	H	107	Total	C	N	O	S	0	0
			819	516	144	155	4		

- Molecule 2 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	148	Total	C	N	O	S	0	0
			1005	615	170	214	6		
2	J	148	Total	C	N	O	S	0	0
			1005	615	170	214	6		
2	K	148	Total	C	N	O	S	0	0
			1005	615	170	214	6		
2	L	148	Total	C	N	O	S	0	0
			1005	615	170	214	6		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-1	HIS	-	expression tag	UNP P0DP23
J	-1	HIS	-	expression tag	UNP P0DP23
K	-1	HIS	-	expression tag	UNP P0DP23
L	-1	HIS	-	expression tag	UNP P0DP23

- Molecule 3 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	4262	Total	C	N	O	S	1	0
			33366	21223	5777	6136	230		
3	B	4262	Total	C	N	O	S	1	0
			33366	21223	5777	6136	230		
3	A	4262	Total	C	N	O	S	1	0
			33366	21223	5777	6136	230		
3	C	4262	Total	C	N	O	S	1	0
			33366	21223	5777	6136	230		

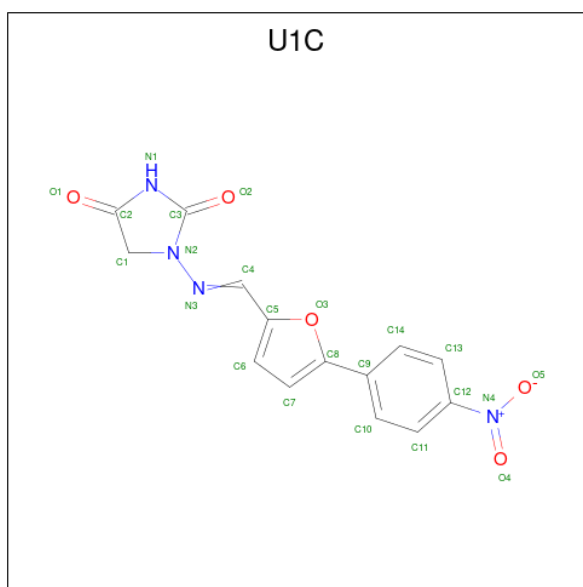
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
4	D	1	Total	Ca	0
			1	1	
4	B	1	Total	Ca	0
			1	1	
4	A	1	Total	Ca	0
			1	1	
4	C	1	Total	Ca	0
			1	1	

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

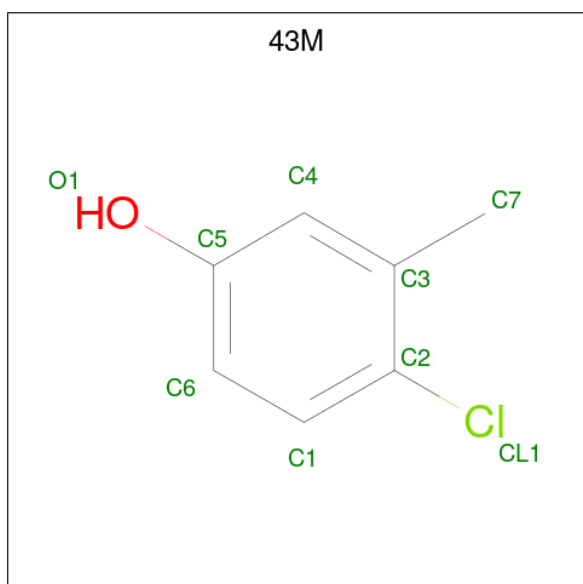
Mol	Chain	Residues	Atoms		AltConf
5	D	1	Total	Zn	0
			1	1	
5	B	1	Total	Zn	0
			1	1	
5	A	1	Total	Zn	0
			1	1	
5	C	1	Total	Zn	0
			1	1	

- Molecule 6 is Dantrolene (CCD ID: U1C) (formula: C₁₄H₁₀N₄O₅) (labeled as "Ligand of Interest" by depositor).



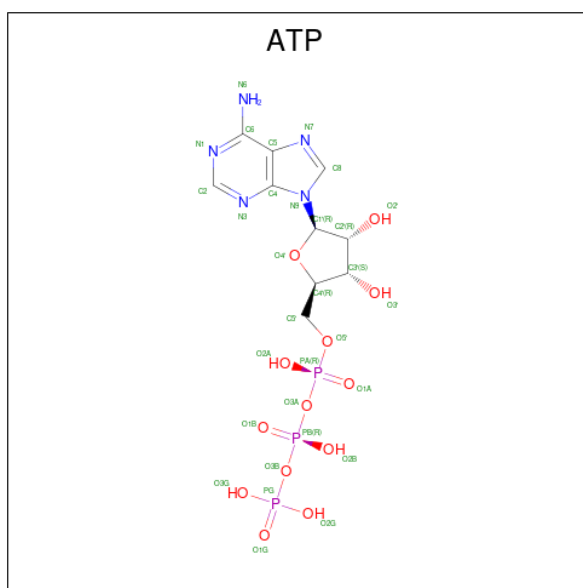
Mol	Chain	Residues	Atoms				AltConf
6	D	1	Total	C	N	O	0
			23	14	4	5	
6	B	1	Total	C	N	O	0
			23	14	4	5	
6	A	1	Total	C	N	O	0
			23	14	4	5	
6	C	1	Total	C	N	O	0
			23	14	4	5	

- Molecule 7 is 4-CHLORO-3-METHYLPHENOL (CCD ID: 43M) (formula: C_7H_7ClO) (labeled as "Ligand of Interest" by depositor).



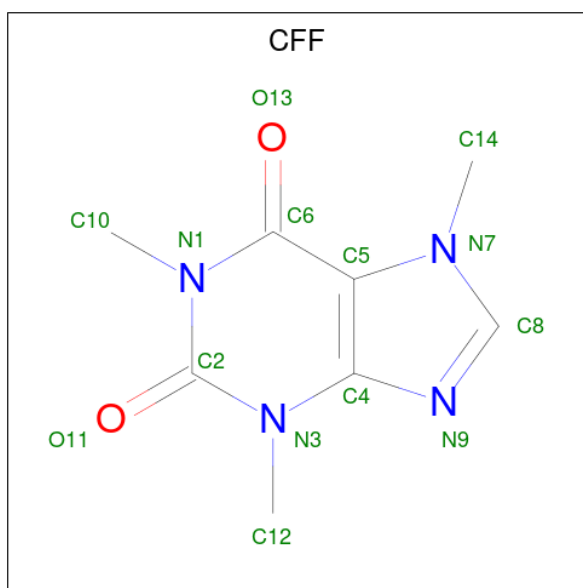
Mol	Chain	Residues	Atoms				AltConf
7	D	1	Total	C	Cl	O	0
			9	7	1	1	
7	D	1	Total	C	Cl	O	0
			9	7	1	1	
7	D	1	Total	C	Cl	O	0
			9	7	1	1	
7	B	1	Total	C	Cl	O	0
			9	7	1	1	
7	B	1	Total	C	Cl	O	0
			9	7	1	1	
7	B	1	Total	C	Cl	O	0
			9	7	1	1	
7	A	1	Total	C	Cl	O	0
			9	7	1	1	
7	A	1	Total	C	Cl	O	0
			9	7	1	1	
7	A	1	Total	C	Cl	O	0
			9	7	1	1	
7	C	1	Total	C	Cl	O	0
			9	7	1	1	
7	C	1	Total	C	Cl	O	0
			9	7	1	1	
7	C	1	Total	C	Cl	O	0
			9	7	1	1	

- Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



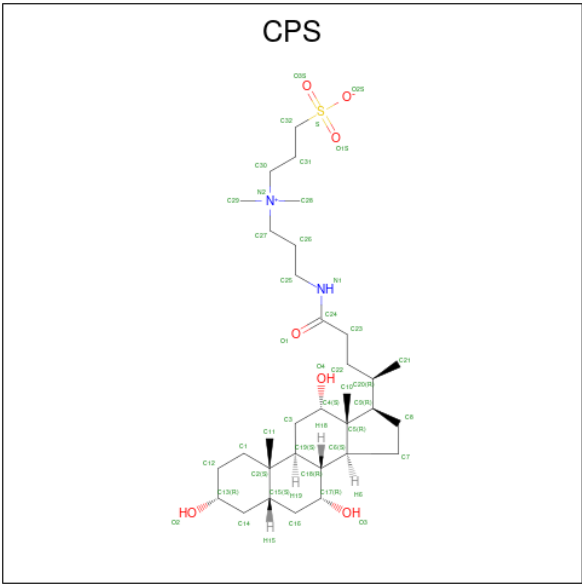
Mol	Chain	Residues	Atoms					AltConf
8	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
8	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
8	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
8	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
8	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
8	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
8	C	1	Total	C	N	O	P	0
			31	10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

- Molecule 9 is CAFFEINE (CCD ID: CFF) (formula: $C_8H_{10}N_4O_2$).



Mol	Chain	Residues	Atoms				AltConf
9	D	1	Total	C	N	O	0
			14	8	4	2	
9	B	1	Total	C	N	O	0
			14	8	4	2	
9	A	1	Total	C	N	O	0
			14	8	4	2	
9	C	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 10 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFONATE (CCD ID: CPS) (formula: C₃₂H₅₈N₂O₇S).



Mol	Chain	Residues	Atoms					AltConf
10	D	1	Total	C	N	O	S	0
			42	32	2	7	1	
10	B	1	Total	C	N	O	S	0
			42	32	2	7	1	
10	A	1	Total	C	N	O	S	0
			42	32	2	7	1	
10	C	1	Total	C	N	O	S	0
			42	32	2	7	1	

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		AltConf
11	E	8	Total	O	0
			8	8	
11	F	7	Total	O	0
			7	7	
11	G	9	Total	O	0
			9	9	
11	H	9	Total	O	0
			9	9	
11	I	29	Total	O	0
			29	29	
11	J	28	Total	O	0
			28	28	

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Mol	Chain	Residues	Atoms		AltConf
11	K	23	Total 23	O 23	0
11	L	31	Total 31	O 31	0
11	D	386	Total 386	O 386	0
11	B	389	Total 389	O 389	0
11	A	387	Total 387	O 387	0
11	C	388	Total 388	O 388	0

3 Residue-property plots [i](#)

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

- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E: 



- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F: 



- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G: 



- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

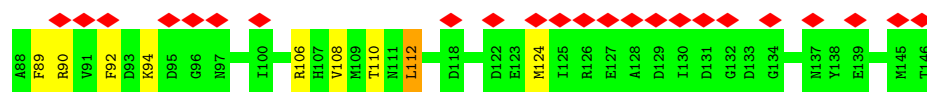
Chain H: 



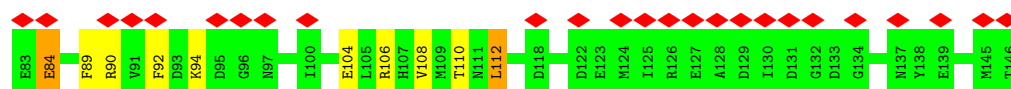
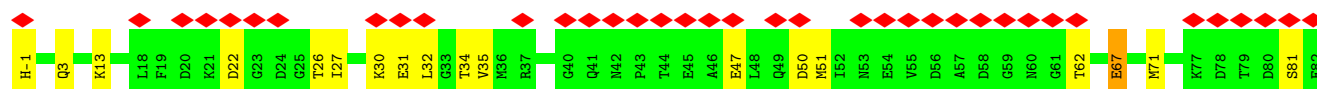
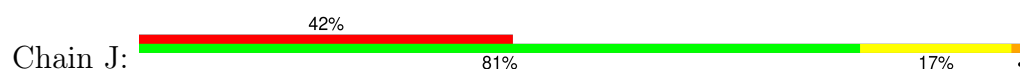
- Molecule 2: Calmodulin-1

Chain I: 

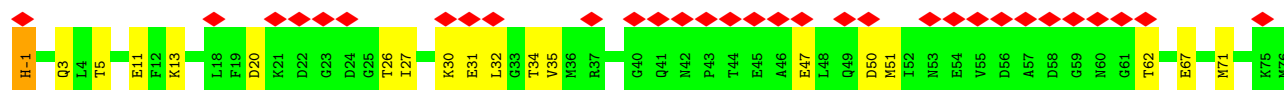
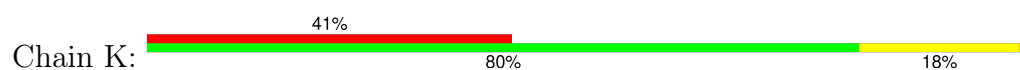




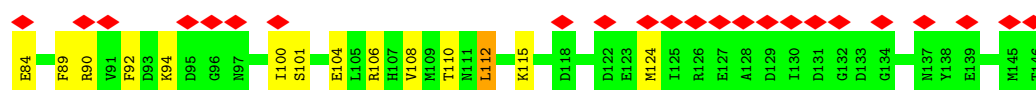
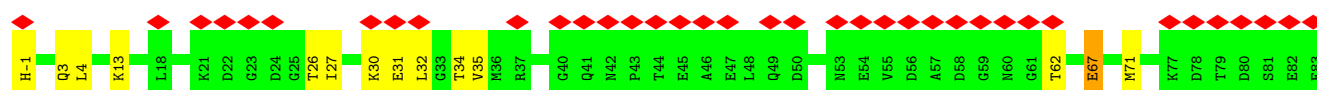
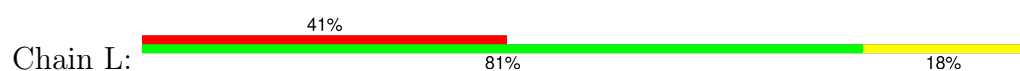
• Molecule 2: Calmodulin-1



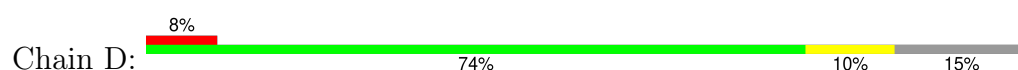
• Molecule 2: Calmodulin-1



• Molecule 2: Calmodulin-1



• Molecule 3: Ryanodine receptor 1





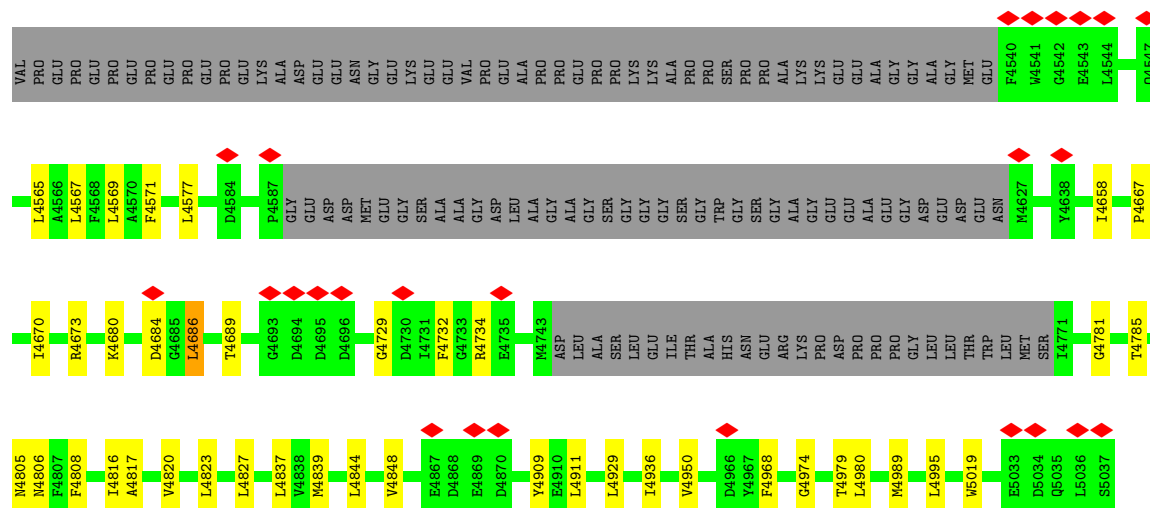
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K3959	K3959	S3979	S3983	A3988	G3991	V3995	F3996	M3999	M4000	M4001	K4002	L4003	Q4009	K4021	D4022	M4023	S4029	E4032	A4041	V4045	V4049	K4060	F4061	M4064	K4067	L4068	K4069	D4070	I4071	V4072	Q4073	S4074	E4075	A4076	D4079	T4082	P4083	P4084	R4085	G4086	L4087																								
I3802	S3803	L3804	D3822	A3834	L3835	M3836	Q3837	T3838	L3842	D3843	Q3850	M3858	V3859	N3860	E3861	D3862	I3866	ASN	ARG	GLN	ASN	GLY	E3872	K3873	D3877	F3880	D3883	L3884	L3903	Q3906	T3907	T3912	L3913	N3914	L3915	L3916	L3917	V3920	L3924	S3929	K3940	D3941	V3942																						
GLU	GLU	VAL	GLU	K3693	K3694	P3695	L3698	H3699	V3702	K3715	L3716	D3717	E3718	D3719	Y3720	M3723	A3724	Y3725	K3731	L3735	GLU	GLU	GLY	GLY	GLU	ASN	GLY	ALA	GLU	GLU	VAL	V3751	E3754	E3755	E3759	Q3767	S3768	R3769	L3770	H3771	T3772	R3773	M3793																						
ASP	ALA	D3587	D3588	P3589	E3590	K3591	L3592	V3593	V3596	Y3604	E3607	T3608	E3610	H3611	P3612	TYR	LYS	SER	LYS	ALA	VAL	THR	LYS	GLY	L3624	K3626	R3629	V3633	A3634	C3635	F3636	R3637	M3638	N3651	E3655	L3663	E3670	M3673	E3682	GLN	GLU	GLU	GLU																						
GLN	GLU	ARG	THR	LYS	LYS	ARG	ASP	ARG	Y3503	S3504	V3505	Q3506	L3509	L3510	L3514	D3531	L3532	M3534	L3535	A3536	Y3540	A3541	L3542	K3543	E3548	V3549	E3551	F3552	L3553	G3561	K3562	V3563	E3564	G3565	S3566	L3569	R3570	V3571	R3577	G3578	L3579	P3580	G3581	R3582	GLU																				
E3388	E3389	G3390	E3391	L3392	L3393	V3394	R3395	D3396	E3397	L3405	Y3409	V3416	D3417	N3418	N3419	R3420	W3423	N3428	W3445	R3453	N3457	Q3461	N3462	E3463	L3464	N3466	M3467	S3468	T3471	ALA	ASP	SER	LYS	SER	LYS	MET	LYS	ALA	GLY	ASP	GLN	SER	GLY	SER	ASP																				
I3229	L3230	E3237	D3242	E3258	K3266	W3284	P3292	PRO	PRO	ALA	LEU	PRO	ALA	GLY	ALA	P3301	T3305	D3310	N3313	L3320	R3321	L3322	V3324	L3327	G3328	L3329	A3332	T3333	S3347	R3348	A3349	L3365	E3377	Q3378	K3380	L3381	E3382	A3383	K3384	A3385	E3386	A3387																							
P3062	D3076	V3080	E3086	I3087	V3107	R3111	L3112	G3113	LYS	VAL	SER	GLN	ALA	ARG	THR	GLN	VAL	K3123	G3124	V3125	G3126	T3130	Y3131	T3132	L3136	D3159	D3160	V3163	L3175	G3176	T3177	T3178	K3179	N3180	T3181	K3185	P3208	S3217	T3221	K3222	S3223	P3224	R3225	A3228																					
ASP	T2948	S2949	S2950	T2951	R2954	F2957	R2965	S2970	E2972	F2973	T2974	A2975	H2976	L2977	E2978	A2979	V2980	V2981	S2982	S2983	G2984	R2985	V2986	E2987	K2988	S2989	P2990	H2991	E2992	Q2993	E2994	T2995	L3003	T3020	P3021	A3022	S3027	H3030	K3034	E3035	K3036	T3039	L3056	T3059																					
W2886	Q2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	D2909	T2910	L2911	T2912	A2913	E2914	K2915	A2916	E2917	R2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	P2929	L2930	Q2931	M2932	N2933	G2934	Y2935	A2936	V2937	T2938	R2939	GLY	LEU	LYS	ASP	MET	GLU	LEU							
ALA	ARG	GLY	GLY	GLU	GLU	THR	THR	LYS	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	ARG	ARG	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	K2795	T2796	F2797	S2798	E2799	K2800	D2801	K2802	E2803	L2804	Y2805	K2806	W2807	P2808	T2809	K2810	E2811	S2812	L2813	A2814	H2815	H2816	T2817	A2818	W2819	E2820	THR	THR	ILE	GLU	LYS



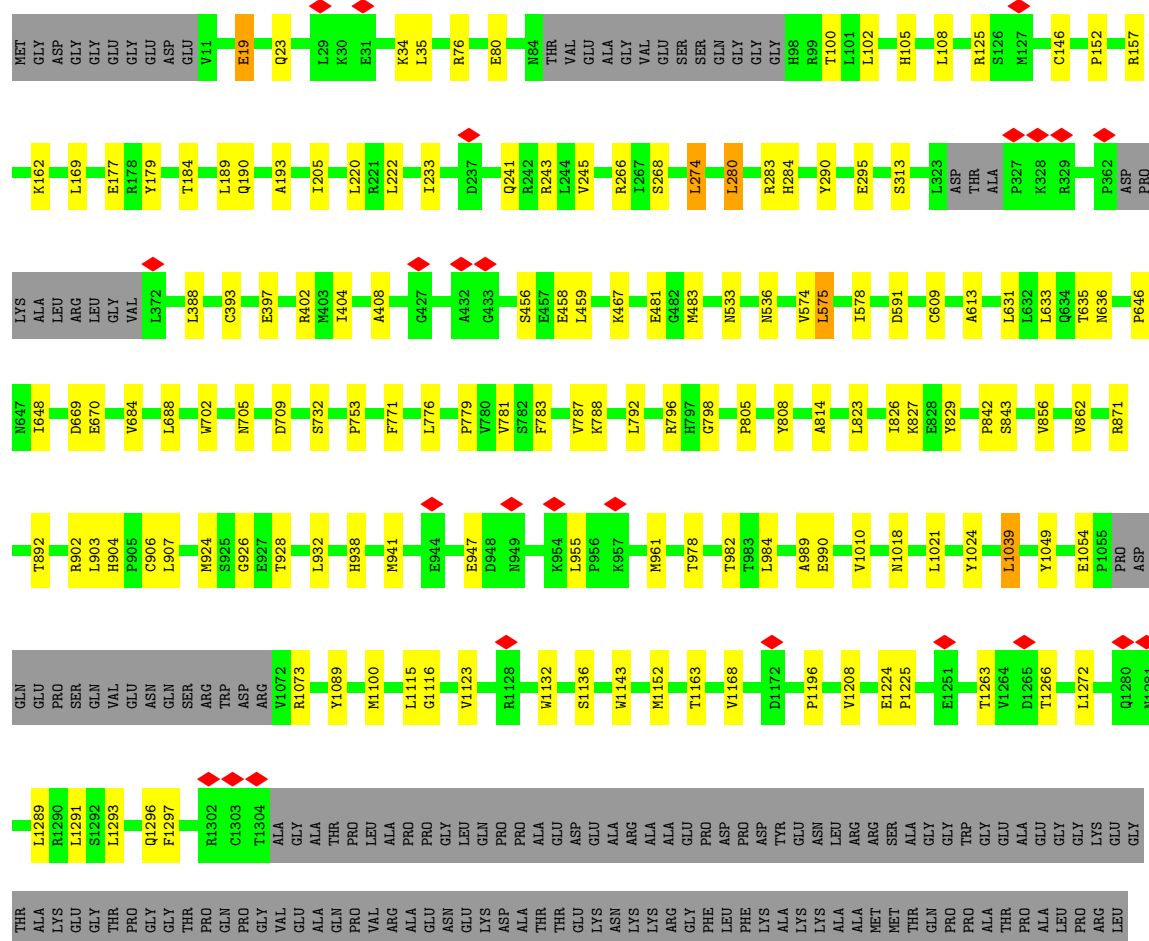
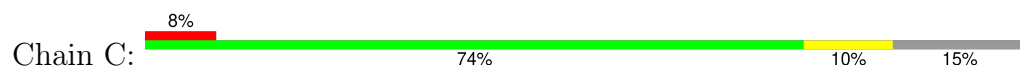






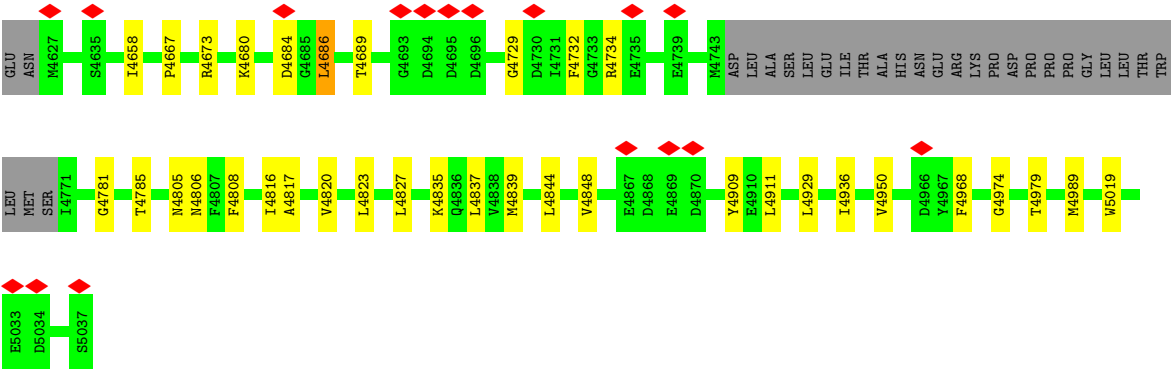


• Molecule 3: Ryanodine receptor 1









4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	71984	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	8.317	Depositor
Minimum map value	0.000	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.119	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	542.72, 542.72, 542.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: ATP, CPS, 43M, U1C, CFF, ZN, 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	E	0.17	0/835	0.31	0/1123
1	F	0.17	0/835	0.32	0/1123
1	G	0.16	0/835	0.33	0/1123
1	H	0.16	0/835	0.32	0/1123
2	I	0.13	0/1014	0.34	0/1373
2	J	0.14	0/1014	0.29	0/1373
2	K	0.16	0/1014	0.31	0/1373
2	L	0.12	0/1014	0.27	0/1373
3	A	0.16	0/34085	0.31	0/46189
3	B	0.16	0/34085	0.31	0/46189
3	C	0.16	0/34085	0.31	0/46189
3	D	0.16	0/34085	0.31	0/46189
All	All	0.16	0/143736	0.31	0/194740

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	E	819	0	824	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	819	0	824	17	0
1	G	819	0	824	16	0
1	H	819	0	824	16	0
2	I	1005	0	810	16	0
2	J	1005	0	810	24	0
2	K	1005	0	810	26	0
2	L	1005	0	810	22	0
3	A	33366	0	32561	322	0
3	B	33366	0	32561	322	0
3	C	33366	0	32561	327	0
3	D	33366	0	32561	318	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	23	0	0	0	0
6	B	23	0	0	0	0
6	C	23	0	0	0	0
6	D	23	0	0	0	0
7	A	27	0	18	0	0
7	B	27	0	18	0	0
7	C	27	0	18	0	0
7	D	27	0	18	0	0
8	A	62	0	24	1	0
8	B	62	0	24	1	0
8	C	62	0	24	1	0
8	D	62	0	24	1	0
9	A	14	0	10	0	0
9	B	14	0	10	0	0
9	C	14	0	10	0	0
9	D	14	0	10	0	0
10	A	42	0	58	1	0
10	B	42	0	58	0	0
10	C	42	0	58	1	0
10	D	42	0	58	1	0
11	A	387	0	0	2	0
11	B	389	0	0	1	0
11	C	388	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	D	386	0	0	1	0
11	E	8	0	0	0	0
11	F	7	0	0	0	0
11	G	9	0	0	0	0
11	H	9	0	0	0	0
11	I	29	0	0	0	0
11	J	28	0	0	0	0
11	K	23	0	0	0	0
11	L	31	0	0	0	0
All	All	143134	0	137220	1392	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 (1392) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:47:GLU:HA	2:K:50:ASP:OD2	1.66	0.96
2:J:47:GLU:HA	2:J:50:ASP:OD2	1.67	0.95
3:C:3996:PHE:HE2	3:C:4023:MET:CE	1.90	0.85
3:B:3996:PHE:HE2	3:B:4023:MET:CE	1.90	0.84
3:A:3996:PHE:HE2	3:A:4023:MET:CE	1.90	0.84
3:D:3996:PHE:HE2	3:D:4023:MET:CE	1.90	0.83
3:D:2204:HIS:HB2	3:D:2250:MET:HE3	1.63	0.81
3:C:2204:HIS:HB2	3:C:2250:MET:HE3	1.63	0.81
3:B:2204:HIS:HB2	3:B:2250:MET:HE3	1.63	0.80
3:D:4068:LEU:HD12	3:D:4111:LEU:HD22	1.65	0.79
3:A:2204:HIS:HB2	3:A:2250:MET:HE3	1.63	0.79
3:B:989:ALA:HA	3:B:1039:LEU:HD13	1.65	0.79
3:A:989:ALA:HA	3:A:1039:LEU:HD13	1.65	0.79
3:D:989:ALA:HA	3:D:1039:LEU:HD13	1.65	0.79
3:A:4068:LEU:HD12	3:A:4111:LEU:HD22	1.65	0.79
3:D:4029:SER:HA	3:D:4032:GLU:HG3	1.65	0.79
3:C:989:ALA:HA	3:C:1039:LEU:HD13	1.65	0.79
3:C:4068:LEU:HD12	3:C:4111:LEU:HD22	1.64	0.79
3:C:3850:GLN:HE21	3:C:3873:LYS:H	1.31	0.78
3:A:4029:SER:HA	3:A:4032:GLU:HG3	1.65	0.78
3:B:3850:GLN:HE21	3:B:3873:LYS:H	1.31	0.78
3:B:4068:LEU:HD12	3:B:4111:LEU:HD22	1.65	0.78
3:B:4029:SER:HA	3:B:4032:GLU:HG3	1.65	0.77
3:A:3850:GLN:HE21	3:A:3873:LYS:H	1.31	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3850:GLN:HE21	3:D:3873:LYS:H	1.31	0.77
3:C:4029:SER:HA	3:C:4032:GLU:HG3	1.65	0.76
3:C:3996:PHE:HE2	3:C:4023:MET:HE3	1.51	0.75
3:D:3996:PHE:HE2	3:D:4023:MET:HE3	1.51	0.74
3:B:3996:PHE:HE2	3:B:4023:MET:HE3	1.51	0.74
3:A:3996:PHE:HE2	3:A:4023:MET:HE3	1.51	0.74
3:B:3533:ILE:HG13	3:B:3596:VAL:HG23	1.71	0.72
2:K:47:GLU:O	2:K:50:ASP:OD1	2.06	0.72
3:C:2175:GLU:HG3	3:C:2228:MET:HB2	1.71	0.72
3:B:3020:THR:HG22	3:B:3022:ALA:H	1.55	0.72
3:C:3533:ILE:HG13	3:C:3596:VAL:HG23	1.71	0.72
3:D:2175:GLU:HG3	3:D:2228:MET:HB2	1.71	0.72
3:A:3020:THR:HG22	3:A:3022:ALA:H	1.55	0.71
3:B:2977:LEU:HD13	3:B:3056:LEU:HD21	1.73	0.71
3:A:3533:ILE:HG13	3:A:3596:VAL:HG23	1.71	0.71
3:D:3533:ILE:HG13	3:D:3596:VAL:HG23	1.71	0.71
3:C:3020:THR:HG22	3:C:3022:ALA:H	1.55	0.71
3:D:4229:GLU:OE2	3:D:4229:GLU:N	2.24	0.71
3:A:2977:LEU:HD13	3:A:3056:LEU:HD21	1.73	0.71
3:A:4229:GLU:OE2	3:A:4229:GLU:N	2.24	0.70
3:C:2977:LEU:HD13	3:C:3056:LEU:HD21	1.73	0.70
3:B:2175:GLU:HG3	3:B:2228:MET:HB2	1.71	0.70
2:J:47:GLU:O	2:J:50:ASP:OD1	2.09	0.70
2:K:84:GLU:HG3	3:C:3637:ARG:HE	1.55	0.70
3:D:2977:LEU:HD13	3:D:3056:LEU:HD21	1.73	0.70
3:D:3020:THR:HG22	3:D:3022:ALA:H	1.55	0.70
3:A:2175:GLU:HG3	3:A:2228:MET:HB2	1.71	0.70
3:C:4229:GLU:N	3:C:4229:GLU:OE2	2.24	0.70
3:B:4092:ASP:HA	3:B:4095:LYS:HE2	1.73	0.70
3:B:4229:GLU:N	3:B:4229:GLU:OE2	2.24	0.70
3:D:4092:ASP:HA	3:D:4095:LYS:HE2	1.73	0.69
3:A:4092:ASP:HA	3:A:4095:LYS:HE2	1.73	0.69
3:C:4092:ASP:HA	3:C:4095:LYS:HE2	1.73	0.69
3:B:3996:PHE:CE2	3:B:4023:MET:CE	2.76	0.69
3:C:3996:PHE:CE2	3:C:4023:MET:CE	2.76	0.68
3:D:3996:PHE:CE2	3:D:4023:MET:CE	2.76	0.68
3:B:3588:ASP:O	3:B:3592:ILE:HD12	1.94	0.67
3:C:3588:ASP:O	3:C:3592:ILE:HD12	1.94	0.67
3:D:3588:ASP:O	3:D:3592:ILE:HD12	1.95	0.67
3:D:3365:LEU:HD13	3:D:3405:LEU:HD23	1.76	0.67
3:A:3588:ASP:O	3:A:3592:ILE:HD12	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3996:PHE:CE2	3:A:4023:MET:CE	2.76	0.67
3:A:796:ARG:NH1	11:A:5601:HOH:O	2.28	0.67
3:B:3365:LEU:HD13	3:B:3405:LEU:HD23	1.76	0.67
3:D:3540:TYR:HB3	3:D:3604:TYR:CD1	2.30	0.67
2:K:27:ILE:HG23	2:K:31:GLU:HB2	1.76	0.67
3:A:3365:LEU:HD13	3:A:3405:LEU:HD23	1.76	0.67
3:D:796:ARG:NH1	11:D:5601:HOH:O	2.28	0.67
3:B:3540:TYR:HB3	3:B:3604:TYR:CD1	2.30	0.67
3:C:796:ARG:NH1	11:C:5601:HOH:O	2.28	0.67
3:C:295:GLU:CD	3:C:295:GLU:H	2.04	0.66
3:C:3540:TYR:HB3	3:C:3604:TYR:CD1	2.30	0.66
3:D:1983:ALA:CB	3:D:1986:MET:HE3	2.26	0.66
3:B:1983:ALA:CB	3:B:1986:MET:HE3	2.26	0.66
3:B:295:GLU:H	3:B:295:GLU:CD	2.04	0.66
3:A:941:MET:HE2	3:A:941:MET:HA	1.78	0.66
3:A:1983:ALA:CB	3:A:1986:MET:HE3	2.26	0.66
3:C:1983:ALA:CB	3:C:1986:MET:HE3	2.26	0.66
3:C:3365:LEU:HD13	3:C:3405:LEU:HD23	1.76	0.66
3:D:295:GLU:H	3:D:295:GLU:CD	2.04	0.66
3:C:1699:GLU:HG3	3:C:1810:LYS:HZ3	1.61	0.66
3:A:3540:TYR:HB3	3:A:3604:TYR:CD1	2.30	0.66
3:D:184:THR:HG22	3:D:189:LEU:HD22	1.78	0.66
3:A:295:GLU:CD	3:A:295:GLU:H	2.04	0.66
3:B:796:ARG:NH1	11:B:5601:HOH:O	2.28	0.65
3:B:102:LEU:HB2	3:B:105:HIS:CD2	2.32	0.65
3:A:184:THR:HG22	3:A:189:LEU:HD22	1.78	0.65
2:J:84:GLU:HG3	3:B:3637:ARG:HE	1.61	0.65
3:D:1520:VAL:HG12	3:D:1527:MET:HG2	1.79	0.65
3:B:1520:VAL:HG12	3:B:1527:MET:HG2	1.79	0.65
3:A:1520:VAL:HG12	3:A:1527:MET:HG2	1.79	0.65
3:A:102:LEU:HB2	3:A:105:HIS:CD2	2.32	0.65
2:K:84:GLU:HG3	3:C:3637:ARG:NE	2.11	0.65
3:D:941:MET:HE2	3:D:941:MET:HA	1.78	0.65
1:G:25:HIS:HD2	1:G:104:LEU:HD11	1.62	0.65
3:B:184:THR:HG22	3:B:189:LEU:HD22	1.78	0.65
3:A:4200:THR:HG22	3:A:4204:GLN:NE2	2.12	0.65
3:C:184:THR:HG22	3:C:189:LEU:HD22	1.78	0.65
3:B:941:MET:HE2	3:B:941:MET:HA	1.78	0.65
2:I:31:GLU:O	2:I:35:VAL:HG13	1.97	0.65
3:B:4200:THR:HG22	3:B:4204:GLN:NE2	2.12	0.65
3:A:1699:GLU:HG3	3:A:1810:LYS:HZ3	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1520:VAL:HG12	3:C:1527:MET:HG2	1.79	0.65
3:D:4200:THR:HG22	3:D:4204:GLN:NE2	2.12	0.64
3:D:102:LEU:HB2	3:D:105:HIS:CD2	2.32	0.64
3:D:1699:GLU:HG3	3:D:1810:LYS:HZ3	1.61	0.64
3:C:102:LEU:HB2	3:C:105:HIS:CD2	2.32	0.64
3:C:4200:THR:HG22	3:C:4204:GLN:NE2	2.12	0.64
3:C:941:MET:HE2	3:C:941:MET:HA	1.78	0.64
2:J:27:ILE:HG23	2:J:31:GLU:HB2	1.77	0.64
2:I:32:LEU:HA	2:I:35:VAL:HG22	1.79	0.64
2:K:84:GLU:OE2	3:C:3637:ARG:NH2	2.29	0.64
3:B:2627:VAL:HG22	3:B:2678:LEU:HB2	1.80	0.63
3:A:2627:VAL:HG22	3:A:2678:LEU:HB2	1.80	0.63
3:B:4160:LEU:O	3:B:4164:LEU:HD22	1.99	0.63
3:C:4151:SER:HB3	3:C:4164:LEU:HD21	1.81	0.63
3:D:2520:HIS:O	3:D:2524:VAL:HG22	1.99	0.63
3:D:4151:SER:HB3	3:D:4164:LEU:HD21	1.81	0.63
3:D:2419:GLY:O	3:D:2423:MET:HG3	1.99	0.63
3:A:4160:LEU:O	3:A:4164:LEU:HD22	1.99	0.62
2:K:84:GLU:CG	3:C:3637:ARG:HE	2.12	0.62
3:B:1870:VAL:HG21	3:B:2097:LEU:HD13	1.81	0.62
3:A:2419:GLY:O	3:A:2423:MET:HG3	1.99	0.62
3:D:4160:LEU:O	3:D:4164:LEU:HD22	1.99	0.62
3:B:1699:GLU:HG3	3:B:1810:LYS:HZ3	1.64	0.62
3:C:2419:GLY:O	3:C:2423:MET:HG3	1.99	0.62
3:C:2520:HIS:O	3:C:2524:VAL:HG22	1.99	0.62
2:J:112:LEU:HD12	3:B:1999:ARG:HD2	1.81	0.62
3:A:4151:SER:HB3	3:A:4164:LEU:HD21	1.81	0.62
3:D:1870:VAL:HG21	3:D:2097:LEU:HD13	1.81	0.62
3:B:2419:GLY:O	3:B:2423:MET:HG3	1.99	0.62
3:A:2520:HIS:O	3:A:2524:VAL:HG22	1.99	0.62
3:C:2627:VAL:HG22	3:C:2678:LEU:HB2	1.80	0.62
3:C:4160:LEU:O	3:C:4164:LEU:HD22	1.99	0.62
3:B:4151:SER:HB3	3:B:4164:LEU:HD21	1.81	0.62
3:D:2627:VAL:HG22	3:D:2678:LEU:HB2	1.80	0.61
3:B:2520:HIS:O	3:B:2524:VAL:HG22	1.99	0.61
3:B:3589:PRO:O	3:B:3593:VAL:HG12	2.00	0.61
3:A:3589:PRO:O	3:A:3593:VAL:HG12	2.00	0.61
3:A:1870:VAL:HG21	3:A:2097:LEU:HD13	1.81	0.61
3:C:1870:VAL:HG21	3:C:2097:LEU:HD13	1.81	0.61
3:D:3589:PRO:O	3:D:3593:VAL:HG12	2.00	0.61
3:A:3996:PHE:CE2	3:A:4023:MET:HE1	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2519:LEU:HD13	3:D:2575:ARG:HG3	1.83	0.61
3:D:3996:PHE:CE2	3:D:4023:MET:HE1	2.35	0.61
3:C:947:GLU:HG3	3:C:1049:TYR:HD1	1.65	0.61
3:A:2519:LEU:HD13	3:A:2575:ARG:HG3	1.83	0.61
3:C:2519:LEU:HD13	3:C:2575:ARG:HG3	1.83	0.61
3:B:947:GLU:HG3	3:B:1049:TYR:HD1	1.65	0.61
3:A:4837:LEU:HD21	3:A:4936:ILE:HD11	1.83	0.61
3:C:3589:PRO:O	3:C:3593:VAL:HG12	2.00	0.61
3:D:408:ALA:HB2	3:D:483:MET:HE1	1.82	0.60
3:D:947:GLU:HG3	3:D:1049:TYR:HD1	1.65	0.60
3:A:947:GLU:HG3	3:A:1049:TYR:HD1	1.65	0.60
3:C:408:ALA:HB2	3:C:483:MET:HE1	1.82	0.60
3:C:4837:LEU:HD21	3:C:4936:ILE:HD11	1.83	0.60
1:E:23:VAL:HG13	1:E:47:LYS:HG2	1.84	0.60
3:D:222:LEU:HB3	3:D:388:LEU:HD13	1.83	0.60
3:C:222:LEU:HB3	3:C:388:LEU:HD13	1.83	0.60
3:B:4837:LEU:HD21	3:B:4936:ILE:HD11	1.83	0.60
3:D:3382:GLU:HB2	3:D:3387:ALA:HB2	1.82	0.60
3:D:4837:LEU:HD21	3:D:4936:ILE:HD11	1.83	0.60
3:B:2519:LEU:HD13	3:B:2575:ARG:HG3	1.83	0.60
3:A:408:ALA:HB2	3:A:483:MET:HE1	1.82	0.60
3:A:3382:GLU:HB2	3:A:3387:ALA:HB2	1.82	0.60
3:B:408:ALA:HB2	3:B:483:MET:HE1	1.82	0.60
3:B:3132:THR:HG23	3:B:3136:LEU:HD23	1.84	0.60
3:B:3382:GLU:HB2	3:B:3387:ALA:HB2	1.83	0.60
3:B:4067:LYS:O	3:B:4071:ILE:HG13	2.02	0.60
3:C:3996:PHE:CE2	3:C:4023:MET:HE1	2.35	0.60
3:D:3834:ALA:O	3:D:3838:THR:HG23	2.02	0.60
3:A:3834:ALA:O	3:A:3838:THR:HG23	2.02	0.60
3:A:4067:LYS:O	3:A:4071:ILE:HG13	2.02	0.60
3:B:3996:PHE:CE2	3:B:4023:MET:HE1	2.35	0.59
1:H:16:PRO:HG3	1:H:106:LEU:HD21	1.84	0.59
3:D:2951:ILE:HA	3:D:2954:ARG:HD2	1.84	0.59
3:C:3056:LEU:HD23	3:C:3056:LEU:O	2.02	0.59
3:B:2951:ILE:HA	3:B:2954:ARG:HD2	1.84	0.59
3:A:3056:LEU:HD23	3:A:3056:LEU:O	2.02	0.59
3:C:3834:ALA:O	3:C:3838:THR:HG23	2.02	0.59
2:I:112:LEU:HD12	3:A:1999:ARG:HD2	1.84	0.59
3:B:3834:ALA:O	3:B:3838:THR:HG23	2.02	0.59
3:C:3382:GLU:HB2	3:C:3387:ALA:HB2	1.83	0.59
1:G:14:THR:HG22	1:G:106:LEU:HD12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:82:TYR:HE1	3:D:1786:LEU:HD13	1.67	0.59
3:D:4067:LYS:O	3:D:4071:ILE:HG13	2.02	0.59
3:B:4909:TYR:OH	3:A:4318:ARG:HD2	2.02	0.59
3:D:3132:THR:HG23	3:D:3136:LEU:HD23	1.84	0.59
3:B:222:LEU:HB3	3:B:388:LEU:HD13	1.83	0.59
3:A:3132:THR:HG23	3:A:3136:LEU:HD23	1.84	0.59
3:C:3132:THR:HG23	3:C:3136:LEU:HD23	1.84	0.59
3:A:222:LEU:HB3	3:A:388:LEU:HD13	1.83	0.59
3:A:2951:ILE:HA	3:A:2954:ARG:HD2	1.84	0.59
3:C:4067:LYS:O	3:C:4071:ILE:HG13	2.02	0.59
3:B:3056:LEU:O	3:B:3056:LEU:HD23	2.02	0.58
3:C:2951:ILE:HA	3:C:2954:ARG:HD2	1.84	0.58
3:B:4318:ARG:HD2	3:C:4909:TYR:OH	2.03	0.58
2:K:112:LEU:HD12	3:C:1999:ARG:HD2	1.84	0.58
3:D:3056:LEU:HD23	3:D:3056:LEU:O	2.02	0.58
3:D:4909:TYR:OH	3:C:4318:ARG:HD2	2.04	0.58
3:B:2519:LEU:HD22	3:B:2578:MET:HE1	1.86	0.58
3:D:871:ARG:HH21	3:D:926:GLY:HA3	1.69	0.58
3:B:871:ARG:HH21	3:B:926:GLY:HA3	1.69	0.58
2:I:34:THR:HA	2:I:37:ARG:HB2	1.85	0.58
3:D:3329:ILE:HD11	3:D:3332:ALA:HB2	1.86	0.58
2:L:112:LEU:HD12	3:D:1999:ARG:HD2	1.86	0.57
3:D:4318:ARG:HD2	3:A:4909:TYR:OH	2.03	0.57
3:B:1986:MET:HG3	3:B:1991:THR:OG1	2.04	0.57
3:C:2588:ARG:HB3	3:C:2588:ARG:CZ	2.34	0.57
2:I:92:PHE:HE1	3:A:1991:THR:HG22	1.68	0.57
3:D:4979:THR:HG21	8:D:5508:ATP:H2'	1.85	0.57
3:B:3536:ALA:HB2	3:B:3553:LEU:HD11	1.86	0.57
3:A:4979:THR:HG21	8:A:5508:ATP:H2'	1.85	0.57
3:C:456:SER:HB2	3:C:458:GLU:OE1	2.04	0.57
3:C:1835:GLU:HG3	3:C:1932:PRO:HG2	1.87	0.57
3:C:1986:MET:HG3	3:C:1991:THR:OG1	2.04	0.57
3:A:456:SER:HB2	3:A:458:GLU:OE1	2.04	0.57
3:A:3457:ASN:O	3:A:3461:GLN:HG2	2.05	0.57
3:C:4979:THR:HG21	8:C:5508:ATP:H2'	1.85	0.57
3:D:3536:ALA:HB2	3:D:3553:LEU:HD11	1.86	0.57
3:A:1986:MET:HG3	3:A:1991:THR:OG1	2.04	0.57
3:A:2588:ARG:HB3	3:A:2588:ARG:CZ	2.34	0.57
1:F:23:VAL:HG13	1:F:47:LYS:HG2	1.87	0.57
3:D:456:SER:HB2	3:D:458:GLU:OE1	2.04	0.57
3:B:456:SER:HB2	3:B:458:GLU:OE1	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2588:ARG:HB3	3:B:2588:ARG:CZ	2.34	0.57
3:A:2519:LEU:HD22	3:A:2578:MET:HE1	1.86	0.57
3:C:3536:ALA:HB2	3:C:3553:LEU:HD11	1.86	0.57
3:D:2004:GLU:O	3:D:2008:MET:HG2	2.04	0.57
3:A:3906:GLN:H	3:A:3912:THR:HG23	1.70	0.57
3:C:3457:ASN:O	3:C:3461:GLN:HG2	2.05	0.57
3:D:2519:LEU:HD22	3:D:2578:MET:HE1	1.86	0.56
3:A:2004:GLU:O	3:A:2008:MET:HG2	2.04	0.56
3:D:1835:GLU:HG3	3:D:1932:PRO:HG2	1.87	0.56
3:B:4979:THR:HG21	8:B:5508:ATP:H2'	1.85	0.56
1:G:4:ILE:HD12	1:G:65:GLN:HG3	1.86	0.56
3:D:1986:MET:HG3	3:D:1991:THR:OG1	2.04	0.56
3:D:3906:GLN:H	3:D:3912:THR:HG23	1.70	0.56
3:B:2004:GLU:O	3:B:2008:MET:HG2	2.04	0.56
3:B:3906:GLN:H	3:B:3912:THR:HG23	1.70	0.56
3:A:3329:ILE:HD11	3:A:3332:ALA:HB2	1.86	0.56
3:A:3536:ALA:HB2	3:A:3553:LEU:HD11	1.86	0.56
3:C:871:ARG:HH21	3:C:926:GLY:HA3	1.69	0.56
3:C:2519:LEU:HD22	3:C:2578:MET:HE1	1.86	0.56
3:C:3329:ILE:HD11	3:C:3332:ALA:HB2	1.86	0.56
1:G:25:HIS:CD2	1:G:104:LEU:HD11	2.41	0.56
2:K:84:GLU:CD	3:C:3637:ARG:HE	2.13	0.56
3:B:1835:GLU:HG3	3:B:1932:PRO:HG2	1.87	0.56
2:K:-1:HIS:O	2:K:3:GLN:HG2	2.05	0.56
3:B:3457:ASN:O	3:B:3461:GLN:HG2	2.05	0.56
3:C:2004:GLU:O	3:C:2008:MET:HG2	2.04	0.56
3:D:3457:ASN:O	3:D:3461:GLN:HG2	2.05	0.56
3:A:871:ARG:HH21	3:A:926:GLY:HA3	1.69	0.56
3:D:2588:ARG:HB3	3:D:2588:ARG:CZ	2.34	0.56
3:D:3324:VAL:HA	3:D:3327:LEU:HG	1.88	0.56
3:A:3324:VAL:HA	3:A:3327:LEU:HG	1.88	0.56
3:A:591:ASP:HA	3:A:631:LEU:HD21	1.89	0.55
3:A:4049:VAL:HG11	3:A:4159:ARG:HD2	1.88	0.55
3:D:591:ASP:HA	3:D:631:LEU:HD21	1.89	0.55
3:A:1835:GLU:HG3	3:A:1932:PRO:HG2	1.87	0.55
3:C:3324:VAL:HA	3:C:3327:LEU:HG	1.88	0.55
3:C:3906:GLN:H	3:C:3912:THR:HG23	1.70	0.55
3:B:3329:ILE:HD11	3:B:3332:ALA:HB2	1.86	0.55
3:D:76:ARG:O	3:D:80:GLU:HG2	2.07	0.55
3:A:100:THR:HG21	3:A:162:LYS:HZ2	1.71	0.55
3:D:4049:VAL:HG11	3:D:4159:ARG:HD2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:591:ASP:HA	3:B:631:LEU:HD21	1.89	0.55
3:B:4049:VAL:HG11	3:B:4159:ARG:HD2	1.88	0.55
3:C:613:ALA:HB2	3:C:1676:LEU:HD12	1.89	0.55
3:B:76:ARG:O	3:B:80:GLU:HG2	2.07	0.55
2:K:13:LYS:HG2	3:C:2189:LYS:HB3	1.89	0.55
3:D:3651:ASN:O	3:D:3655:GLU:HG2	2.07	0.55
3:B:1935:VAL:O	3:B:1939:MET:HG2	2.07	0.55
3:C:591:ASP:HA	3:C:631:LEU:HD21	1.89	0.55
3:C:1935:VAL:O	3:C:1939:MET:HG2	2.07	0.55
3:D:1115:LEU:HD13	3:D:1123:VAL:HG11	1.89	0.54
3:D:2166:LEU:HD11	3:D:2206:THR:HG23	1.89	0.54
3:D:3571:TRP:HZ2	3:A:1224:GLU:HG2	1.73	0.54
3:B:3324:VAL:HA	3:B:3327:LEU:HG	1.88	0.54
3:B:3571:TRP:HZ2	3:C:1224:GLU:HG2	1.72	0.54
3:B:4577:LEU:HD21	3:B:4806:ASN:HB3	1.90	0.54
3:C:2018:GLU:HG2	3:C:2028:ARG:NH1	2.22	0.54
2:L:84:GLU:HG3	3:D:3637:ARG:HE	1.72	0.54
3:D:100:THR:HG21	3:D:162:LYS:HZ2	1.71	0.54
3:D:1935:VAL:O	3:D:1939:MET:HG2	2.07	0.54
3:D:3625:SER:O	3:D:3629:ARG:HG3	2.08	0.54
3:B:613:ALA:HB2	3:B:1676:LEU:HD12	1.89	0.54
3:B:2018:GLU:HG2	3:B:2028:ARG:NH1	2.22	0.54
3:A:1115:LEU:HD13	3:A:1123:VAL:HG11	1.89	0.54
3:A:2166:LEU:HD11	3:A:2206:THR:HG23	1.89	0.54
3:C:76:ARG:O	3:C:80:GLU:HG2	2.07	0.54
3:A:3651:ASN:O	3:A:3655:GLU:HG2	2.07	0.54
3:B:1224:GLU:HG2	3:A:3571:TRP:HZ2	1.72	0.54
3:A:3266:MET:HG3	3:A:3266:MET:O	2.08	0.54
3:C:3266:MET:O	3:C:3266:MET:HG3	2.07	0.54
2:L:-1:HIS:O	2:L:3:GLN:HG2	2.07	0.54
3:D:823:LEU:HD11	3:D:1626:TRP:HB3	1.90	0.54
3:D:4577:LEU:HD21	3:D:4806:ASN:HB3	1.90	0.54
3:B:823:LEU:HD11	3:B:1626:TRP:HB3	1.90	0.54
3:A:4577:LEU:HD21	3:A:4806:ASN:HB3	1.90	0.54
3:B:2166:LEU:HD11	3:B:2206:THR:HG23	1.89	0.54
3:A:1653:LEU:HD13	3:A:1660:GLN:HA	1.90	0.54
3:C:100:THR:HG21	3:C:162:LYS:HZ2	1.73	0.54
3:C:783:PHE:HB2	3:C:787:VAL:HG21	1.89	0.54
2:J:84:GLU:HG3	3:B:3637:ARG:NE	2.22	0.54
3:A:2018:GLU:HG2	3:A:2028:ARG:NH1	2.22	0.54
3:C:1983:ALA:HB1	3:C:1986:MET:HE3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1653:LEU:HD13	3:B:1660:GLN:HA	1.90	0.54
3:A:76:ARG:O	3:A:80:GLU:HG2	2.07	0.54
3:A:783:PHE:HB2	3:A:787:VAL:HG21	1.89	0.54
3:C:1580:PHE:CE2	3:C:1592:PRO:HG2	2.43	0.54
3:C:2166:LEU:HD11	3:C:2206:THR:HG23	1.89	0.54
3:C:3718:GLU:HG3	3:C:3723:MET:HE1	1.90	0.54
3:C:4049:VAL:HG11	3:C:4159:ARG:HD2	1.88	0.54
1:E:16:PRO:HG3	1:E:106:LEU:HD21	1.90	0.54
1:F:25:HIS:HD2	1:F:104:LEU:HD11	1.73	0.54
3:A:1935:VAL:O	3:A:1939:MET:HG2	2.07	0.54
3:A:3625:SER:O	3:A:3629:ARG:HG3	2.08	0.54
2:L:108:VAL:O	2:L:112:LEU:HB2	2.08	0.54
3:D:1653:LEU:HD13	3:D:1660:GLN:HA	1.90	0.54
3:B:902:ARG:HG3	3:B:902:ARG:HH11	1.73	0.54
3:C:823:LEU:HD11	3:C:1626:TRP:HB3	1.90	0.54
3:C:3126:GLY:O	3:C:3130:THR:HG22	2.08	0.54
3:D:613:ALA:HB2	3:D:1676:LEU:HD12	1.89	0.53
3:D:1224:GLU:HG2	3:C:3571:TRP:HZ2	1.73	0.53
3:D:2018:GLU:HG2	3:D:2028:ARG:NH1	2.22	0.53
3:D:3266:MET:HG3	3:D:3266:MET:O	2.08	0.53
3:A:823:LEU:HD11	3:A:1626:TRP:HB3	1.90	0.53
3:A:3718:GLU:HG3	3:A:3723:MET:HE1	1.90	0.53
3:C:3625:SER:O	3:C:3629:ARG:HG3	2.08	0.53
3:C:4247:ILE:HD11	3:C:4667:PRO:HB2	1.90	0.53
3:D:783:PHE:HB2	3:D:787:VAL:HG21	1.89	0.53
3:D:1808:ARG:HG3	3:D:1854:PHE:CE1	2.43	0.53
3:B:1983:ALA:HB1	3:B:1986:MET:HE3	1.90	0.53
3:C:902:ARG:HG3	3:C:902:ARG:HH11	1.73	0.53
3:C:4567:LEU:HD11	3:C:4816:ILE:HG22	1.91	0.53
2:L:-1:HIS:CD2	3:D:2244:ARG:HH11	2.27	0.53
3:D:902:ARG:HH11	3:D:902:ARG:HG3	1.73	0.53
3:D:3391:GLU:HA	3:D:3394:VAL:HG22	1.91	0.53
3:B:1580:PHE:CE2	3:B:1592:PRO:HG2	2.43	0.53
3:A:2596:THR:HB	3:A:2599:GLN:HG3	1.89	0.53
3:C:792:LEU:HA	3:C:798:GLY:HA3	1.91	0.53
1:H:14:THR:HG22	1:H:106:LEU:HD12	1.91	0.53
3:B:792:LEU:HA	3:B:798:GLY:HA3	1.91	0.53
3:B:4567:LEU:HD11	3:B:4816:ILE:HG22	1.91	0.53
3:A:613:ALA:HB2	3:A:1676:LEU:HD12	1.89	0.53
3:C:3651:ASN:O	3:C:3655:GLU:HG2	2.07	0.53
3:C:4577:LEU:HD21	3:C:4806:ASN:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1983:ALA:HB1	3:D:1986:MET:HE3	1.90	0.53
3:D:3126:GLY:O	3:D:3130:THR:HG22	2.08	0.53
3:D:4567:LEU:HD11	3:D:4816:ILE:HG22	1.91	0.53
3:B:783:PHE:HB2	3:B:787:VAL:HG21	1.89	0.53
3:B:3651:ASN:O	3:B:3655:GLU:HG2	2.07	0.53
3:A:902:ARG:HG3	3:A:902:ARG:HH11	1.73	0.53
3:A:1808:ARG:HG3	3:A:1854:PHE:CE1	2.43	0.53
3:A:3126:GLY:O	3:A:3130:THR:HG22	2.08	0.53
3:A:4247:ILE:HD11	3:A:4667:PRO:HB2	1.90	0.53
3:C:1808:ARG:HG3	3:C:1854:PHE:CE1	2.43	0.53
3:C:3416:VAL:O	3:C:3420:ARG:HB2	2.09	0.53
3:D:792:LEU:HA	3:D:798:GLY:HA3	1.91	0.53
3:D:2596:THR:HB	3:D:2599:GLN:HG3	1.89	0.53
3:B:1115:LEU:HD13	3:B:1123:VAL:HG11	1.89	0.53
3:B:2596:THR:HB	3:B:2599:GLN:HG3	1.89	0.53
3:B:3718:GLU:HG3	3:B:3723:MET:HE1	1.90	0.53
3:D:3181:THR:O	3:D:3185:LYS:HG2	2.09	0.53
3:B:3181:THR:O	3:B:3185:LYS:HG2	2.09	0.53
3:B:3924:LEU:HD12	3:B:3988:ALA:HB2	1.91	0.53
3:A:3391:GLU:HA	3:A:3394:VAL:HG22	1.91	0.53
3:A:3416:VAL:O	3:A:3420:ARG:HB2	2.09	0.53
3:A:4567:LEU:HD11	3:A:4816:ILE:HG22	1.91	0.53
3:C:1115:LEU:HD13	3:C:1123:VAL:HG11	1.89	0.53
3:C:3391:GLU:HA	3:C:3394:VAL:HG22	1.91	0.53
2:K:108:VAL:O	2:K:112:LEU:HB2	2.08	0.53
2:L:90:ARG:HA	2:L:94:LYS:HB2	1.89	0.53
3:D:3718:GLU:HG3	3:D:3723:MET:HE1	1.90	0.53
3:B:1808:ARG:HG3	3:B:1854:PHE:CE1	2.43	0.53
3:B:3423:TRP:CD1	3:B:3428:ASN:HD22	2.27	0.53
3:C:3423:TRP:CD1	3:C:3428:ASN:HD22	2.27	0.53
3:B:2358:ILE:HD11	3:C:177:GLU:HG2	1.91	0.52
3:A:1580:PHE:CE2	3:A:1592:PRO:HG2	2.43	0.52
2:I:1:1:HIS:O	2:I:3:GLN:HG2	2.09	0.52
3:D:1580:PHE:CE2	3:D:1592:PRO:HG2	2.43	0.52
3:B:3266:MET:O	3:B:3266:MET:HG3	2.08	0.52
3:B:3625:SER:O	3:B:3629:ARG:HG3	2.08	0.52
3:C:1805:GLU:H	3:C:1805:GLU:CD	2.18	0.52
3:D:670:GLU:HG3	3:D:788:LYS:HB2	1.91	0.52
3:D:4247:ILE:HD11	3:D:4667:PRO:HB2	1.90	0.52
3:A:533:ASN:HB3	3:A:536:ASN:HB2	1.91	0.52
3:A:1983:ALA:HB1	3:A:1986:MET:HE3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3924:LEU:HD12	3:A:3988:ALA:HB2	1.91	0.52
3:C:1653:LEU:HD13	3:C:1660:GLN:HA	1.90	0.52
3:C:2596:THR:HB	3:C:2599:GLN:HG3	1.89	0.52
1:F:16:PRO:HG3	1:F:106:LEU:HD21	1.92	0.52
1:H:25:HIS:HD2	1:H:104:LEU:HD11	1.75	0.52
2:J:92:PHE:HE1	3:B:1991:THR:HG22	1.75	0.52
3:D:633:LEU:HD13	3:D:1639:LEU:HD21	1.91	0.52
3:D:3416:VAL:O	3:D:3420:ARG:HB2	2.09	0.52
3:A:792:LEU:HA	3:A:798:GLY:HA3	1.91	0.52
3:D:3423:TRP:CD1	3:D:3428:ASN:HD22	2.27	0.52
3:B:533:ASN:HB3	3:B:536:ASN:HB2	1.91	0.52
3:B:1805:GLU:CD	3:B:1805:GLU:H	2.18	0.52
3:A:3423:TRP:CD1	3:A:3428:ASN:HD22	2.27	0.52
3:A:4689:THR:HG22	3:A:4732:PHE:CZ	2.45	0.52
3:C:3181:THR:O	3:C:3185:LYS:HG2	2.09	0.52
2:I:90:ARG:HA	2:I:94:LYS:HB2	1.92	0.52
3:D:3056:LEU:HD23	3:D:3056:LEU:C	2.35	0.52
3:D:3320:LEU:O	3:D:3324:VAL:HG23	2.10	0.52
3:B:3391:GLU:HA	3:B:3394:VAL:HG22	1.91	0.52
3:A:3320:LEU:O	3:A:3324:VAL:HG23	2.10	0.52
3:D:2644:LEU:HD13	3:D:2678:LEU:HD21	1.92	0.52
3:B:177:GLU:HG2	3:A:2358:ILE:HD11	1.92	0.52
3:B:3126:GLY:O	3:B:3130:THR:HG22	2.08	0.52
3:A:1811:ALA:HA	3:A:1814:MET:HE2	1.92	0.52
3:A:3181:THR:O	3:A:3185:LYS:HG2	2.09	0.52
3:C:670:GLU:HG3	3:C:788:LYS:HB2	1.91	0.52
1:F:49:ARG:HG2	1:F:49:ARG:HH11	1.75	0.52
3:B:633:LEU:HD13	3:B:1639:LEU:HD21	1.92	0.52
3:B:3635:CYS:HA	3:B:3638:MET:HE2	1.92	0.52
3:A:670:GLU:HG3	3:A:788:LYS:HB2	1.91	0.52
3:A:1805:GLU:CD	3:A:1805:GLU:H	2.18	0.52
3:C:1811:ALA:HA	3:C:1814:MET:HE2	1.92	0.52
3:D:177:GLU:HG2	3:C:2358:ILE:HD11	1.92	0.52
3:D:2470:ILE:HG22	3:D:2525:GLY:HA3	1.92	0.52
3:B:3416:VAL:O	3:B:3420:ARG:HB2	2.09	0.52
3:C:3056:LEU:HD23	3:C:3056:LEU:C	2.35	0.52
1:E:14:THR:HG22	1:E:106:LEU:HD12	1.92	0.52
1:H:4:ILE:HD12	1:H:65:GLN:HG3	1.92	0.52
2:L:92:PHE:HE1	3:D:1991:THR:HG22	1.75	0.52
3:B:684:VAL:HG22	3:B:781:VAL:HG12	1.92	0.52
3:B:1527:MET:HE2	3:B:1540:PHE:HB2	1.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:4689:THR:HG22	3:B:4732:PHE:CZ	2.45	0.52
3:A:2248:ARG:HD2	3:A:2286:LEU:HD21	1.92	0.52
3:C:684:VAL:HG22	3:C:781:VAL:HG12	1.92	0.52
1:H:49:ARG:HH21	1:H:52:LYS:HE2	1.74	0.51
2:J:108:VAL:O	2:J:112:LEU:HB2	2.10	0.51
3:D:1811:ALA:HA	3:D:1814:MET:HE2	1.92	0.51
3:D:2358:ILE:HD11	3:A:177:GLU:HG2	1.92	0.51
3:D:3635:CYS:HA	3:D:3638:MET:HE2	1.92	0.51
3:B:2598:ALA:O	3:B:2602:VAL:HG23	2.10	0.51
3:B:4805:ASN:HB3	3:B:4808:PHE:HD2	1.76	0.51
3:C:533:ASN:HB3	3:C:536:ASN:HB2	1.91	0.51
3:C:2598:ALA:O	3:C:2602:VAL:HG23	2.10	0.51
3:A:684:VAL:HG22	3:A:781:VAL:HG12	1.92	0.51
3:A:2644:LEU:HD13	3:A:2678:LEU:HD21	1.92	0.51
3:D:533:ASN:HB3	3:D:536:ASN:HB2	1.91	0.51
3:D:4689:THR:HG22	3:D:4732:PHE:CZ	2.45	0.51
3:B:3320:LEU:O	3:B:3324:VAL:HG23	2.10	0.51
3:A:2598:ALA:O	3:A:2602:VAL:HG23	2.10	0.51
3:C:1527:MET:HE2	3:C:1540:PHE:HB2	1.93	0.51
3:C:2470:ILE:HG22	3:C:2525:GLY:HA3	1.92	0.51
3:D:177:GLU:O	3:D:177:GLU:HG3	2.11	0.51
3:D:684:VAL:HG22	3:D:781:VAL:HG12	1.92	0.51
3:B:4247:ILE:HD11	3:B:4667:PRO:HB2	1.90	0.51
3:C:2644:LEU:HD13	3:C:2678:LEU:HD21	1.92	0.51
2:J:-1:HIS:O	2:J:3:GLN:HG2	2.10	0.51
2:K:92:PHE:HE1	3:C:1991:THR:HG22	1.76	0.51
3:D:1527:MET:HE2	3:D:1540:PHE:HB2	1.93	0.51
3:D:3924:LEU:HD12	3:D:3988:ALA:HB2	1.91	0.51
3:B:1811:ALA:HA	3:B:1814:MET:HE2	1.92	0.51
3:B:2248:ARG:HD2	3:B:2286:LEU:HD21	1.92	0.51
3:C:633:LEU:HD13	3:C:1639:LEU:HD21	1.91	0.51
3:A:1527:MET:HE2	3:A:1540:PHE:HB2	1.93	0.51
3:C:3320:LEU:O	3:C:3324:VAL:HG23	2.10	0.51
3:C:4805:ASN:HB3	3:C:4808:PHE:HD2	1.76	0.51
1:G:49:ARG:HG2	1:G:49:ARG:HH11	1.75	0.51
2:I:39:LEU:HD13	2:I:72:MET:HE2	1.92	0.51
3:D:1805:GLU:CD	3:D:1805:GLU:H	2.18	0.51
3:D:3604:TYR:HE2	3:D:3608:GLN:NE2	2.08	0.51
3:B:3056:LEU:HD23	3:B:3056:LEU:C	2.35	0.51
3:A:3056:LEU:HD23	3:A:3056:LEU:C	2.35	0.51
3:C:1132:TRP:CE2	3:C:1136:SER:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2248:ARG:HD2	3:C:2286:LEU:HD21	1.92	0.51
3:C:3635:CYS:HA	3:C:3638:MET:HE2	1.92	0.51
1:H:49:ARG:HG2	1:H:49:ARG:HH11	1.75	0.51
3:D:1132:TRP:CE2	3:D:1136:SER:HB2	2.46	0.51
3:D:2598:ALA:O	3:D:2602:VAL:HG23	2.10	0.51
3:B:670:GLU:HG3	3:B:788:LYS:HB2	1.91	0.51
3:A:2470:ILE:HG22	3:A:2525:GLY:HA3	1.92	0.51
3:A:3635:CYS:HA	3:A:3638:MET:HE2	1.92	0.51
3:A:4805:ASN:HB3	3:A:4808:PHE:HD2	1.76	0.51
3:C:1116:GLY:HA3	3:C:1132:TRP:HB3	1.92	0.51
3:C:3604:TYR:HE2	3:C:3608:GLN:NE2	2.08	0.51
3:C:4689:THR:HG22	3:C:4732:PHE:CZ	2.45	0.51
2:J:50:ASP:OD1	2:J:51:MET:N	2.44	0.51
3:B:177:GLU:O	3:B:177:GLU:HG3	2.11	0.51
3:B:1116:GLY:HA3	3:B:1132:TRP:HB3	1.92	0.51
3:A:19:GLU:HB3	3:A:205:ILE:HB	1.93	0.51
3:C:3991:GLY:O	3:C:3995:VAL:HG23	2.11	0.51
1:E:25:HIS:HD2	1:E:104:LEU:HD11	1.77	0.50
1:E:49:ARG:HG2	1:E:49:ARG:HH11	1.75	0.50
3:B:2970:SER:HA	3:B:2973:PHE:CD2	2.46	0.50
3:A:177:GLU:O	3:A:177:GLU:HG3	2.11	0.50
3:A:3604:TYR:HE2	3:A:3608:GLN:NE2	2.08	0.50
3:C:648:ILE:HG23	3:C:814:ALA:HB3	1.93	0.50
3:C:2970:SER:HA	3:C:2973:PHE:CD2	2.46	0.50
1:F:49:ARG:HH21	1:F:52:LYS:HE2	1.77	0.50
1:F:82:TYR:HE1	3:B:1786:LEU:HD13	1.75	0.50
3:D:648:ILE:HG23	3:D:814:ALA:HB3	1.93	0.50
3:D:3991:GLY:O	3:D:3995:VAL:HG23	2.11	0.50
3:B:2470:ILE:HG22	3:B:2525:GLY:HA3	1.92	0.50
3:B:3991:GLY:O	3:B:3995:VAL:HG23	2.11	0.50
3:A:633:LEU:HD13	3:A:1639:LEU:HD21	1.91	0.50
3:A:2970:SER:HA	3:A:2973:PHE:CD2	2.46	0.50
1:G:16:PRO:HG3	1:G:106:LEU:HD21	1.94	0.50
2:J:81:SER:HA	3:B:3637:ARG:NH2	2.27	0.50
3:D:4805:ASN:HB3	3:D:4808:PHE:HD2	1.76	0.50
3:B:2644:LEU:HD13	3:B:2678:LEU:HD21	1.92	0.50
3:B:3914:ASN:HB3	3:B:3917:ILE:HB	1.94	0.50
3:A:1116:GLY:HA3	3:A:1132:TRP:HB3	1.92	0.50
3:B:3107:VAL:HG13	3:B:3175:LEU:HG	1.94	0.50
3:B:3604:TYR:HE2	3:B:3608:GLN:NE2	2.08	0.50
3:A:3755:GLU:O	3:A:3759:GLU:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3914:ASN:HB3	3:A:3917:ILE:HB	1.94	0.50
3:C:904:HIS:CE1	3:C:906:CYS:HB2	2.47	0.50
3:C:3107:VAL:HG13	3:C:3175:LEU:HG	1.94	0.50
1:E:87:HIS:HB3	1:E:90:VAL:HB	1.94	0.50
3:B:1132:TRP:CE2	3:B:1136:SER:HB2	2.46	0.50
3:A:4060:LYS:HD3	3:A:4064:MET:HG3	1.94	0.50
1:H:25:HIS:CD2	1:H:104:LEU:HD11	2.47	0.50
3:D:3755:GLU:O	3:D:3759:GLU:HG2	2.12	0.50
3:B:19:GLU:HB3	3:B:205:ILE:HB	1.93	0.50
3:A:3991:GLY:O	3:A:3995:VAL:HG23	2.11	0.50
3:C:177:GLU:HG3	3:C:177:GLU:O	2.11	0.50
3:C:3836:MET:HG3	3:C:3884:LEU:HD21	1.94	0.50
3:C:3914:ASN:HB3	3:C:3917:ILE:HB	1.94	0.50
3:A:2970:SER:HA	3:A:2973:PHE:CE2	2.47	0.50
3:C:1983:ALA:HB2	3:C:1986:MET:HE3	1.94	0.50
3:C:3755:GLU:O	3:C:3759:GLU:HG2	2.12	0.50
3:D:19:GLU:HB3	3:D:205:ILE:HB	1.93	0.50
3:D:904:HIS:CE1	3:D:906:CYS:HB2	2.47	0.50
3:D:1116:GLY:HA3	3:D:1132:TRP:HB3	1.92	0.50
3:D:2970:SER:HA	3:D:2973:PHE:CE2	2.47	0.50
3:D:3914:ASN:HB3	3:D:3917:ILE:HB	1.94	0.50
3:B:3836:MET:HG3	3:B:3884:LEU:HD21	1.94	0.50
3:A:1132:TRP:CE2	3:A:1136:SER:HB2	2.46	0.50
3:A:4245:MET:HE1	3:A:4989:MET:HE1	1.94	0.50
3:C:266:ARG:HD2	3:C:268:SER:O	2.12	0.50
3:C:3924:LEU:HD12	3:C:3988:ALA:HB2	1.91	0.50
1:G:82:TYR:HE1	3:C:1786:LEU:HD13	1.77	0.50
3:D:2248:ARG:HD2	3:D:2286:LEU:HD21	1.92	0.50
3:D:3107:VAL:HG13	3:D:3175:LEU:HG	1.94	0.50
3:D:3768:SER:HA	3:D:3771:HIS:CD2	2.47	0.50
3:A:2584:HIS:O	3:A:2588:ARG:HG3	2.12	0.50
3:C:2970:SER:HA	3:C:2973:PHE:CE2	2.47	0.50
3:C:3768:SER:HA	3:C:3771:HIS:CD2	2.47	0.50
3:C:4060:LYS:HD3	3:C:4064:MET:HG3	1.94	0.50
1:E:4:ILE:HD12	1:E:65:GLN:HG3	1.94	0.49
3:D:4060:LYS:HD3	3:D:4064:MET:HG3	1.94	0.49
3:B:826:ILE:HG22	3:B:827:LYS:HG2	1.94	0.49
3:B:978:THR:O	3:B:982:THR:HG23	2.12	0.49
3:B:2584:HIS:O	3:B:2588:ARG:HG3	2.12	0.49
3:C:978:THR:O	3:C:982:THR:HG23	2.12	0.49
3:C:2584:HIS:O	3:C:2588:ARG:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:81:SER:HA	3:C:3637:ARG:NH2	2.27	0.49
3:D:2970:SER:HA	3:D:2973:PHE:CD2	2.46	0.49
3:B:648:ILE:HG23	3:B:814:ALA:HB3	1.93	0.49
3:A:978:THR:O	3:A:982:THR:HG23	2.12	0.49
3:A:3107:VAL:HG13	3:A:3175:LEU:HG	1.94	0.49
3:A:3768:SER:HA	3:A:3771:HIS:CD2	2.47	0.49
3:A:4219:PHE:HA	3:A:4950:VAL:HG11	1.95	0.49
3:D:266:ARG:HD2	3:D:268:SER:O	2.12	0.49
3:B:152:PRO:HB3	3:B:157:ARG:HB2	1.94	0.49
3:B:904:HIS:CE1	3:B:906:CYS:HB2	2.47	0.49
1:F:25:HIS:CD2	1:F:104:LEU:HD11	2.47	0.49
1:F:87:HIS:HB3	1:F:90:VAL:HB	1.94	0.49
3:D:2312:MET:O	3:D:2316:LYS:HG2	2.13	0.49
3:D:3836:MET:HG3	3:D:3884:LEU:HD21	1.94	0.49
3:B:3755:GLU:O	3:B:3759:GLU:HG2	2.12	0.49
3:B:3768:SER:HA	3:B:3771:HIS:CD2	2.47	0.49
3:A:266:ARG:HD2	3:A:268:SER:O	2.12	0.49
3:A:648:ILE:HG23	3:A:814:ALA:HB3	1.93	0.49
3:D:978:THR:O	3:D:982:THR:HG23	2.12	0.49
3:D:2266:GLY:H	3:D:2330:ARG:NH1	2.11	0.49
1:F:4:ILE:HD12	1:F:65:GLN:HG3	1.93	0.49
3:D:1983:ALA:HB2	3:D:1986:MET:HE3	1.94	0.49
3:B:4219:PHE:HA	3:B:4950:VAL:HG11	1.95	0.49
3:A:904:HIS:CE1	3:A:906:CYS:HB2	2.47	0.49
3:A:2312:MET:O	3:A:2316:LYS:HG2	2.13	0.49
3:C:826:ILE:HG22	3:C:827:LYS:HG2	1.94	0.49
1:E:25:HIS:CD2	1:E:104:LEU:HD11	2.48	0.49
3:D:23:GLN:HE21	3:D:34:LYS:HG2	1.78	0.49
3:B:266:ARG:HD2	3:B:268:SER:O	2.12	0.49
3:A:152:PRO:HB3	3:A:157:ARG:HB2	1.94	0.49
3:C:19:GLU:HB3	3:C:205:ILE:HB	1.93	0.49
3:D:4219:PHE:HA	3:D:4950:VAL:HG11	1.95	0.49
3:B:1977:TYR:O	3:B:1981:MET:HB2	2.13	0.49
3:A:3673:MET:HE2	3:A:3725:TYR:HE1	1.78	0.49
3:C:4245:MET:HE1	3:C:4989:MET:HE1	1.94	0.49
3:D:938:HIS:ND1	3:D:1054:GLU:HG3	2.28	0.49
3:D:1977:TYR:O	3:D:1981:MET:HB2	2.13	0.49
3:B:2312:MET:O	3:B:2316:LYS:HG2	2.13	0.49
3:B:2970:SER:HA	3:B:2973:PHE:CE2	2.47	0.49
3:B:3767:GLN:HG2	3:B:3804:ILE:HA	1.94	0.49
3:C:3767:GLN:HG2	3:C:3804:ILE:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2266:GLY:H	3:B:2330:ARG:NH1	2.11	0.49
3:B:4232:GLU:HG2	3:B:5019:TRP:HE1	1.78	0.49
3:A:23:GLN:HE21	3:A:34:LYS:HG2	1.78	0.49
3:A:3266:MET:HE1	3:A:3322:ILE:HG12	1.95	0.49
3:A:3836:MET:HG3	3:A:3884:LEU:HD21	1.94	0.49
3:C:636:ASN:HB2	3:C:702:TRP:CZ3	2.48	0.49
3:C:938:HIS:ND1	3:C:1054:GLU:HG3	2.28	0.49
3:C:1208:VAL:HG23	3:C:1225:PRO:HG2	1.95	0.49
3:C:2312:MET:O	3:C:2316:LYS:HG2	2.13	0.49
3:C:4686:LEU:HD23	3:C:4686:LEU:HA	1.72	0.49
3:D:3842:LEU:HB2	3:D:3929:SER:OG	2.13	0.48
3:D:2584:HIS:O	3:D:2588:ARG:HG3	2.12	0.48
3:D:3553:LEU:HD13	3:D:3596:VAL:HG13	1.95	0.48
3:D:3767:GLN:HG2	3:D:3804:ILE:HA	1.94	0.48
3:B:636:ASN:HB2	3:B:702:TRP:CZ3	2.48	0.48
3:B:938:HIS:ND1	3:B:1054:GLU:HG3	2.28	0.48
3:A:3842:LEU:HB2	3:A:3929:SER:OG	2.13	0.48
3:C:3940:LYS:H	3:C:3940:LYS:HD2	1.78	0.48
3:C:4219:PHE:HA	3:C:4950:VAL:HG11	1.95	0.48
2:K:115:LYS:HG2	3:C:3858:MET:HE1	1.95	0.48
3:D:152:PRO:HB3	3:D:157:ARG:HB2	1.94	0.48
3:D:4232:GLU:HG2	3:D:5019:TRP:HE1	1.78	0.48
3:B:4060:LYS:HD3	3:B:4064:MET:HG3	1.94	0.48
3:A:1796:ALA:HB2	3:A:2177:LEU:HD21	1.96	0.48
3:A:3540:TYR:HB3	3:A:3604:TYR:HD1	1.77	0.48
3:C:152:PRO:HB3	3:C:157:ARG:HB2	1.94	0.48
1:G:49:ARG:HH21	1:G:52:LYS:NZ	2.11	0.48
3:D:3940:LYS:H	3:D:3940:LYS:HD2	1.78	0.48
3:B:283:ARG:HB2	3:B:290:TYR:CE2	2.49	0.48
3:B:3553:LEU:HD13	3:B:3596:VAL:HG13	1.95	0.48
3:B:4229:GLU:H	3:B:4229:GLU:CD	2.21	0.48
3:A:283:ARG:HB2	3:A:290:TYR:CE2	2.49	0.48
3:C:2266:GLY:H	3:C:2330:ARG:NH1	2.11	0.48
3:C:3842:LEU:HB2	3:C:3929:SER:OG	2.13	0.48
3:D:636:ASN:HB2	3:D:702:TRP:CZ3	2.48	0.48
3:A:1983:ALA:HB2	3:A:1986:MET:HE3	1.94	0.48
3:A:2266:GLY:H	3:A:2330:ARG:NH1	2.11	0.48
3:A:3940:LYS:H	3:A:3940:LYS:HD2	1.78	0.48
3:C:3673:MET:HE2	3:C:3725:TYR:HE1	1.78	0.48
3:D:3266:MET:HE1	3:D:3322:ILE:HG12	1.95	0.48
3:D:3673:MET:HE2	3:D:3725:TYR:HE1	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4245:MET:HE1	3:D:4989:MET:HE1	1.94	0.48
3:B:1983:ALA:HB2	3:B:1986:MET:HE3	1.94	0.48
3:A:826:ILE:HG22	3:A:827:LYS:HG2	1.94	0.48
3:A:3553:LEU:HD13	3:A:3596:VAL:HG13	1.95	0.48
3:C:1977:TYR:O	3:C:1981:MET:HB2	2.13	0.48
3:D:826:ILE:HG22	3:D:827:LYS:HG2	1.94	0.48
3:B:1796:ALA:HB2	3:B:2177:LEU:HD21	1.96	0.48
3:B:3842:LEU:HB2	3:B:3929:SER:OG	2.13	0.48
3:A:938:HIS:ND1	3:A:1054:GLU:HG3	2.28	0.48
2:K:50:ASP:OD1	2:K:51:MET:N	2.46	0.48
3:D:1293:LEU:O	3:D:1579:MET:HE2	2.14	0.48
3:D:3540:TYR:HB3	3:D:3604:TYR:HD1	1.77	0.48
3:A:1208:VAL:HG23	3:A:1225:PRO:HG2	1.95	0.48
3:C:23:GLN:HE21	3:C:34:LYS:HG2	1.78	0.48
3:D:1796:ALA:HB2	3:D:2177:LEU:HD21	1.96	0.48
3:B:1293:LEU:O	3:B:1579:MET:HE2	2.14	0.48
3:B:4245:MET:HE1	3:B:4989:MET:HE1	1.94	0.48
3:A:1293:LEU:O	3:A:1579:MET:HE2	2.14	0.48
1:E:49:ARG:HH21	1:E:52:LYS:HE2	1.79	0.48
2:L:31:GLU:O	2:L:35:VAL:HG13	2.14	0.48
3:D:283:ARG:HB2	3:D:290:TYR:CE2	2.49	0.48
3:D:3132:THR:HA	3:D:3136:LEU:HB3	1.96	0.48
3:B:3673:MET:HE2	3:B:3725:TYR:HE1	1.78	0.48
3:B:3940:LYS:H	3:B:3940:LYS:HD2	1.78	0.48
3:A:636:ASN:HB2	3:A:702:TRP:CZ3	2.48	0.48
3:A:4229:GLU:H	3:A:4229:GLU:CD	2.21	0.48
3:C:2420:HIS:HA	3:C:2423:MET:HE3	1.96	0.48
2:I:19:PHE:CG	2:I:35:VAL:HG12	2.48	0.47
3:B:3132:THR:HA	3:B:3136:LEU:HB3	1.96	0.47
3:A:924:MET:O	3:A:928:THR:HG23	2.15	0.47
3:A:1977:TYR:O	3:A:1981:MET:HB2	2.13	0.47
3:A:4098:ASP:O	3:A:4101:LYS:HG2	2.14	0.47
3:C:283:ARG:HB2	3:C:290:TYR:CE2	2.49	0.47
3:B:23:GLN:HE21	3:B:34:LYS:HG2	1.78	0.47
3:C:2599:GLN:O	3:C:2603:ILE:HG13	2.15	0.47
3:C:3266:MET:HE1	3:C:3322:ILE:HG12	1.95	0.47
3:C:3553:LEU:HD13	3:C:3596:VAL:HG13	1.95	0.47
1:H:6:THR:HG23	1:H:70:GLN:HE21	1.79	0.47
3:D:2420:HIS:HA	3:D:2423:MET:HE3	1.96	0.47
3:A:3217:SER:O	3:A:3221:THR:HG23	2.14	0.47
3:A:3767:GLN:HG2	3:A:3804:ILE:HA	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3132:THR:HA	3:C:3136:LEU:HB3	1.96	0.47
3:C:3217:SER:O	3:C:3221:THR:HG23	2.14	0.47
3:C:4232:GLU:HG2	3:C:5019:TRP:HE1	1.78	0.47
1:F:31:GLN:HA	1:F:98:ILE:HD12	1.95	0.47
3:D:1208:VAL:HG23	3:D:1225:PRO:HG2	1.95	0.47
3:A:3132:THR:HA	3:A:3136:LEU:HB3	1.96	0.47
3:C:4098:ASP:O	3:C:4101:LYS:HG2	2.14	0.47
2:K:47:GLU:HA	2:K:50:ASP:CG	2.37	0.47
3:D:3384:LYS:H	3:D:3387:ALA:HB3	1.80	0.47
3:B:4098:ASP:O	3:B:4101:LYS:HG2	2.14	0.47
3:B:4686:LEU:HD23	3:B:4686:LEU:HA	1.72	0.47
3:A:3999:MET:HE3	3:A:4003:LEU:HD11	1.96	0.47
1:E:4:ILE:HG12	1:E:74:LEU:CD2	2.45	0.47
3:D:924:MET:O	3:D:928:THR:HG23	2.15	0.47
3:D:3036:LYS:O	3:D:3039:ILE:HG22	2.15	0.47
3:D:3999:MET:HE3	3:D:4003:LEU:HD11	1.96	0.47
3:D:4098:ASP:O	3:D:4101:LYS:HG2	2.14	0.47
3:B:100:THR:HG21	3:B:162:LYS:HZ2	1.80	0.47
3:B:1208:VAL:HG23	3:B:1225:PRO:HG2	1.95	0.47
3:B:3266:MET:HE1	3:B:3322:ILE:HG12	1.95	0.47
3:B:3999:MET:HE3	3:B:4003:LEU:HD11	1.96	0.47
3:A:2973:PHE:CD1	3:A:2973:PHE:C	2.93	0.47
3:A:3036:LYS:O	3:A:3039:ILE:HG22	2.15	0.47
3:A:3384:LYS:H	3:A:3387:ALA:HB3	1.80	0.47
3:A:4232:GLU:HG2	3:A:5019:TRP:HE1	1.78	0.47
3:C:1293:LEU:O	3:C:1579:MET:HE2	2.14	0.47
3:C:1796:ALA:HB2	3:C:2177:LEU:HD21	1.96	0.47
1:E:52:LYS:HA	1:E:52:LYS:HD3	1.62	0.47
3:A:2599:GLN:O	3:A:2603:ILE:HG13	2.15	0.47
3:B:924:MET:O	3:B:928:THR:HG23	2.15	0.47
3:B:3217:SER:O	3:B:3221:THR:HG23	2.14	0.47
3:A:2420:HIS:HA	3:A:2423:MET:HE3	1.96	0.47
3:A:2526:PHE:O	3:A:2530:MET:HG3	2.15	0.47
3:A:3076:ASP:O	3:A:3080:VAL:HG23	2.15	0.47
3:A:4686:LEU:HD23	3:A:4686:LEU:HA	1.72	0.47
3:C:2526:PHE:O	3:C:2530:MET:HG3	2.15	0.47
3:C:3999:MET:HE3	3:C:4003:LEU:HD11	1.96	0.47
1:G:49:ARG:HH21	1:G:52:LYS:HZ2	1.62	0.47
2:K:31:GLU:O	2:K:35:VAL:HG13	2.14	0.47
3:A:990:GLU:HG3	3:A:1024:TYR:CD2	2.50	0.47
3:C:3540:TYR:HB3	3:C:3604:TYR:HD1	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:31:GLN:HA	1:E:98:ILE:HD12	1.97	0.46
3:B:2420:HIS:HA	3:B:2423:MET:HE3	1.96	0.46
3:A:574:VAL:O	3:A:578:ILE:HG12	2.15	0.46
3:A:2680:TRP:O	3:A:2684:ASP:OD2	2.33	0.46
3:A:3021:PRO:HG3	3:A:3030:HIS:CE1	2.50	0.46
2:K:26:THR:HB	2:K:62:THR:HG23	1.96	0.46
3:D:3217:SER:O	3:D:3221:THR:HG23	2.14	0.46
3:B:990:GLU:HG3	3:B:1024:TYR:CD2	2.50	0.46
3:B:2212:VAL:HG11	3:B:2256:TYR:CZ	2.51	0.46
3:B:2599:GLN:O	3:B:2603:ILE:HG13	2.15	0.46
3:B:2957:PHE:CE2	3:B:3034:LYS:HG2	2.51	0.46
3:A:3769:ARG:O	3:A:3773:ARG:HD2	2.16	0.46
3:C:924:MET:O	3:C:928:THR:HG23	2.15	0.46
3:B:829:TYR:CE1	3:B:1608:MET:HG2	2.51	0.46
3:B:3021:PRO:HG3	3:B:3030:HIS:CE1	2.50	0.46
3:B:3076:ASP:O	3:B:3080:VAL:HG23	2.15	0.46
3:A:829:TYR:CE1	3:A:1608:MET:HG2	2.51	0.46
3:A:2957:PHE:CE2	3:A:3034:LYS:HG2	2.51	0.46
3:C:2957:PHE:CE2	3:C:3034:LYS:HG2	2.51	0.46
3:C:2973:PHE:CD1	3:C:2973:PHE:C	2.93	0.46
3:D:574:VAL:O	3:D:578:ILE:HG12	2.15	0.46
3:D:990:GLU:HG3	3:D:1024:TYR:CD2	2.50	0.46
3:D:2599:GLN:O	3:D:2603:ILE:HG13	2.15	0.46
3:D:2680:TRP:O	3:D:2684:ASP:OD2	2.33	0.46
3:D:4229:GLU:H	3:D:4229:GLU:CD	2.21	0.46
3:C:990:GLU:HG3	3:C:1024:TYR:CD2	2.50	0.46
3:C:3384:LYS:H	3:C:3387:ALA:HB3	1.80	0.46
2:J:106:ARG:O	2:J:110:THR:HG23	2.16	0.46
2:L:30:LYS:O	2:L:34:THR:HG22	2.16	0.46
3:D:829:TYR:CE1	3:D:1608:MET:HG2	2.51	0.46
3:D:932:LEU:HD21	3:D:984:LEU:HD21	1.97	0.46
3:D:2973:PHE:CD1	3:D:2973:PHE:C	2.93	0.46
3:D:3021:PRO:HG3	3:D:3030:HIS:CE1	2.50	0.46
3:B:574:VAL:O	3:B:578:ILE:HG12	2.15	0.46
3:B:575:LEU:HD12	3:B:609:CYS:HB2	1.98	0.46
3:B:3384:LYS:H	3:B:3387:ALA:HB3	1.80	0.46
3:B:3769:ARG:O	3:B:3773:ARG:HD2	2.16	0.46
3:B:4181:ILE:HG23	3:B:4195:PHE:HE1	1.81	0.46
3:C:4181:ILE:HG23	3:C:4195:PHE:HE1	1.81	0.46
3:D:3076:ASP:O	3:D:3080:VAL:HG23	2.15	0.46
3:D:3698:LEU:O	3:D:3702:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3769:ARG:O	3:D:3773:ARG:HD2	2.16	0.46
3:D:4844:LEU:O	3:D:4848:VAL:HG23	2.16	0.46
3:B:3540:TYR:HB3	3:B:3604:TYR:HD1	1.77	0.46
3:C:2212:VAL:HG11	3:C:2256:TYR:CZ	2.51	0.46
3:C:3021:PRO:HG3	3:C:3030:HIS:CE1	2.50	0.46
3:C:3036:LYS:O	3:C:3039:ILE:HG22	2.15	0.46
2:L:115:LYS:HG2	3:D:3858:MET:HE1	1.98	0.46
3:D:2212:VAL:HG11	3:D:2256:TYR:CZ	2.51	0.46
3:D:2238:TYR:O	3:D:2242:ILE:HG12	2.16	0.46
3:B:3036:LYS:O	3:B:3039:ILE:HG22	2.15	0.46
3:A:575:LEU:HD12	3:A:609:CYS:HB2	1.98	0.46
3:C:2639:MET:HE3	3:C:2639:MET:HB3	1.89	0.46
3:C:3698:LEU:O	3:C:3702:VAL:HG23	2.16	0.46
2:K:30:LYS:O	2:K:34:THR:HG22	2.16	0.46
3:B:2238:TYR:O	3:B:2242:ILE:HG12	2.16	0.46
3:B:4844:LEU:O	3:B:4848:VAL:HG23	2.16	0.46
3:A:2212:VAL:HG11	3:A:2256:TYR:CZ	2.51	0.46
3:A:2238:TYR:O	3:A:2242:ILE:HG12	2.16	0.46
3:C:574:VAL:O	3:C:578:ILE:HG12	2.15	0.46
3:C:3592:ILE:HD12	3:C:3592:ILE:H	1.81	0.46
1:G:87:HIS:HB3	1:G:90:VAL:HB	1.98	0.46
2:K:104:GLU:O	2:K:108:VAL:HG22	2.16	0.46
2:L:13:LYS:HG2	3:D:2189:LYS:HB3	1.97	0.46
3:B:2526:PHE:O	3:B:2530:MET:HG3	2.15	0.46
3:B:3592:ILE:HD12	3:B:3592:ILE:H	1.81	0.46
3:C:829:TYR:CE1	3:C:1608:MET:HG2	2.51	0.46
3:D:1089:TYR:HD2	3:D:1152:MET:HG3	1.81	0.46
3:D:1619:ARG:HD2	3:D:1626:TRP:CZ2	2.51	0.46
3:D:3592:ILE:HD12	3:D:3592:ILE:H	1.81	0.46
3:D:4181:ILE:HG23	3:D:4195:PHE:HE1	1.81	0.46
3:C:3076:ASP:O	3:C:3080:VAL:HG23	2.15	0.46
3:C:3225:ARG:HE	3:C:3229:ILE:HD11	1.81	0.46
3:C:3769:ARG:O	3:C:3773:ARG:HD2	2.16	0.46
1:F:14:THR:HG22	1:F:106:LEU:HD12	1.98	0.45
3:D:2526:PHE:O	3:D:2530:MET:HG3	2.15	0.45
3:D:2957:PHE:CE2	3:D:3034:LYS:HG2	2.51	0.45
3:D:3550:ARG:HG3	3:D:3593:VAL:CG2	2.46	0.45
3:B:3159:ASP:O	3:B:3163:VAL:HG13	2.17	0.45
3:B:3225:ARG:HE	3:B:3229:ILE:HD11	1.81	0.45
3:A:1089:TYR:HD2	3:A:1152:MET:HG3	1.81	0.45
3:A:3698:LEU:O	3:A:3702:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:4844:LEU:O	3:A:4848:VAL:HG23	2.16	0.45
3:C:3550:ARG:HG3	3:C:3593:VAL:CG2	2.46	0.45
1:E:13:ARG:HB2	1:E:13:ARG:NH1	2.31	0.45
1:G:13:ARG:NH1	1:G:13:ARG:HB2	2.31	0.45
3:D:2582:MET:HE2	3:D:2582:MET:HB3	1.86	0.45
3:B:932:LEU:HD21	3:B:984:LEU:HD21	1.97	0.45
3:B:3445:TRP:CD1	3:B:3510:ILE:HD12	2.51	0.45
3:A:3550:ARG:HG3	3:A:3593:VAL:HG22	1.99	0.45
3:A:4181:ILE:HG23	3:A:4195:PHE:HE1	1.81	0.45
3:C:3159:ASP:O	3:C:3163:VAL:HG13	2.17	0.45
3:C:4844:LEU:O	3:C:4848:VAL:HG23	2.16	0.45
2:J:104:GLU:O	2:J:108:VAL:HG22	2.17	0.45
3:D:575:LEU:HD12	3:D:609:CYS:HB2	1.98	0.45
3:D:1867:GLU:HG3	3:D:2097:LEU:HD11	1.99	0.45
3:D:3159:ASP:O	3:D:3163:VAL:HG13	2.17	0.45
3:B:1867:GLU:HG3	3:B:2097:LEU:HD11	1.99	0.45
3:A:932:LEU:HD21	3:A:984:LEU:HD21	1.97	0.45
3:A:1619:ARG:HD2	3:A:1626:TRP:CZ2	2.51	0.45
3:C:575:LEU:HD12	3:C:609:CYS:HB2	1.98	0.45
1:F:13:ARG:NH1	1:F:13:ARG:HB2	2.31	0.45
3:B:2973:PHE:CD1	3:B:2973:PHE:C	2.93	0.45
3:B:3550:ARG:HG3	3:B:3593:VAL:HG22	1.99	0.45
3:B:3698:LEU:O	3:B:3702:VAL:HG23	2.16	0.45
3:C:1867:GLU:HG3	3:C:2097:LEU:HD11	1.99	0.45
3:C:2680:TRP:O	3:C:2684:ASP:OD2	2.33	0.45
3:D:2991:HIS:O	3:D:2995:ILE:HD13	2.17	0.45
3:B:404:ILE:HG21	3:B:481:GLU:HG3	1.99	0.45
3:B:3405:LEU:O	3:B:3409:TYR:HB2	2.17	0.45
3:A:3550:ARG:HG3	3:A:3593:VAL:CG2	2.46	0.45
3:C:932:LEU:HD21	3:C:984:LEU:HD21	1.97	0.45
3:C:947:GLU:HG3	3:C:1049:TYR:CD1	2.50	0.45
1:G:82:TYR:CE1	3:C:1786:LEU:HD13	2.51	0.45
1:H:87:HIS:H	1:H:91:ILE:HB	1.82	0.45
2:J:67:GLU:O	2:J:71:MET:HG3	2.16	0.45
2:L:101:SER:HB3	2:L:104:GLU:HG3	1.98	0.45
3:D:1018:ASN:HB3	3:D:1021:LEU:HB2	1.99	0.45
3:B:393:CYS:SG	3:B:397:GLU:HB3	2.57	0.45
3:B:2680:TRP:O	3:B:2684:ASP:OD2	2.33	0.45
3:B:3629:ARG:O	3:B:3633:VAL:HG23	2.17	0.45
3:B:4732:PHE:CD1	3:B:4732:PHE:N	2.85	0.45
3:C:1297:PHE:CE2	3:C:1525:GLY:HA2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:108:VAL:O	2:I:112:LEU:HB2	2.17	0.45
3:D:393:CYS:SG	3:D:397:GLU:HB3	2.57	0.45
3:B:902:ARG:HG3	3:B:902:ARG:NH1	2.32	0.45
3:B:1619:ARG:HD2	3:B:1626:TRP:CZ2	2.51	0.45
3:B:1982:ARG:HB2	3:B:1982:ARG:NH1	2.32	0.45
3:A:669:ASP:HB2	3:A:788:LYS:HB3	1.99	0.45
3:A:1297:PHE:CE2	3:A:1525:GLY:HA2	2.52	0.45
3:A:3445:TRP:CD1	3:A:3510:ILE:HD12	2.51	0.45
3:C:1018:ASN:HB3	3:C:1021:LEU:HB2	1.99	0.45
3:C:3445:TRP:CD1	3:C:3510:ILE:HD12	2.51	0.45
2:J:22:ASP:OD1	2:J:22:ASP:C	2.60	0.45
2:L:67:GLU:O	2:L:71:MET:HG3	2.17	0.45
3:D:669:ASP:HB2	3:D:788:LYS:HB3	1.99	0.45
3:B:3550:ARG:HG3	3:B:3593:VAL:CG2	2.46	0.45
3:A:404:ILE:HG21	3:A:481:GLU:HG3	1.99	0.45
3:A:1867:GLU:HG3	3:A:2097:LEU:HD11	1.99	0.45
3:A:2965:ARG:NH1	3:A:2965:ARG:HG2	2.32	0.45
3:C:393:CYS:SG	3:C:397:GLU:HB3	2.57	0.45
3:C:2238:TYR:O	3:C:2242:ILE:HG12	2.16	0.45
2:I:106:ARG:O	2:I:110:THR:HG23	2.16	0.45
3:D:947:GLU:HG3	3:D:1049:TYR:CD1	2.50	0.45
3:D:2965:ARG:NH1	3:D:2965:ARG:HG2	2.32	0.45
3:D:3445:TRP:CD1	3:D:3510:ILE:HD12	2.51	0.45
3:B:1018:ASN:HB3	3:B:1021:LEU:HB2	1.99	0.45
3:B:1297:PHE:CE2	3:B:1525:GLY:HA2	2.52	0.45
3:B:2485:LEU:HD23	3:B:2485:LEU:HA	1.84	0.45
3:A:902:ARG:HG3	3:A:902:ARG:NH1	2.32	0.45
3:A:3225:ARG:HE	3:A:3229:ILE:HD11	1.81	0.45
3:C:404:ILE:HG21	3:C:481:GLU:HG3	1.99	0.45
3:C:1619:ARG:HD2	3:C:1626:TRP:CZ2	2.51	0.45
3:C:3550:ARG:HG3	3:C:3593:VAL:HG22	1.99	0.45
3:D:1297:PHE:CE2	3:D:1525:GLY:HA2	2.52	0.45
3:D:4732:PHE:CD1	3:D:4732:PHE:N	2.85	0.45
3:B:3347:SER:HA	3:B:3418:ASN:ND2	2.32	0.45
3:B:4839:MET:HB3	3:A:4823:LEU:HD21	1.98	0.45
3:A:233:ILE:HG12	3:A:284:HIS:NE2	2.32	0.45
3:A:2204:HIS:HB2	3:A:2250:MET:CE	2.42	0.45
3:C:2965:ARG:NH1	3:C:2965:ARG:HG2	2.32	0.45
3:C:2991:HIS:O	3:C:2995:ILE:HD13	2.17	0.45
1:H:14:THR:HB	1:H:68:LEU:HB2	1.99	0.44
3:D:902:ARG:HG3	3:D:902:ARG:NH1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3225:ARG:HE	3:D:3229:ILE:HD11	1.81	0.44
3:D:3347:SER:HA	3:D:3418:ASN:ND2	2.32	0.44
3:D:3405:LEU:O	3:D:3409:TYR:HB2	2.17	0.44
3:B:1089:TYR:HD2	3:B:1152:MET:HG3	1.81	0.44
3:A:1982:ARG:NH1	3:A:1982:ARG:HB2	2.32	0.44
3:A:3159:ASP:O	3:A:3163:VAL:HG13	2.17	0.44
3:A:3347:SER:HA	3:A:3418:ASN:ND2	2.32	0.44
3:A:3629:ARG:O	3:A:3633:VAL:HG23	2.17	0.44
3:A:4732:PHE:N	3:A:4732:PHE:CD1	2.85	0.44
3:C:4732:PHE:CD1	3:C:4732:PHE:N	2.85	0.44
1:F:82:TYR:CE1	3:B:1786:LEU:HD13	2.52	0.44
2:J:89:PHE:HB3	2:J:94:LYS:HZ1	1.81	0.44
2:K:67:GLU:O	2:K:71:MET:HG3	2.17	0.44
2:L:27:ILE:HG23	2:L:31:GLU:HB3	1.99	0.44
3:D:3550:ARG:HG3	3:D:3593:VAL:HG22	1.99	0.44
3:D:3723:MET:HE2	3:D:3793:MET:HG2	1.99	0.44
3:D:4565:LEU:O	3:D:4569:LEU:HG	2.18	0.44
3:B:233:ILE:HG12	3:B:284:HIS:NE2	2.32	0.44
3:B:3723:MET:HE2	3:B:3793:MET:HG2	1.99	0.44
3:B:4839:MET:HG3	3:A:4820:VAL:HG11	1.99	0.44
3:A:3405:LEU:O	3:A:3409:TYR:HB2	2.17	0.44
3:A:3637:ARG:HA	3:A:3637:ARG:HD2	1.78	0.44
3:C:1982:ARG:HB2	3:C:1982:ARG:NH1	2.32	0.44
3:D:402:ARG:HA	3:D:402:ARG:HD2	1.84	0.44
3:D:2972:GLU:C	3:D:2972:GLU:OE1	2.60	0.44
3:B:2689:LYS:HE2	3:B:2689:LYS:HB3	1.79	0.44
3:B:4823:LEU:HD21	3:C:4839:MET:HB3	1.99	0.44
3:A:393:CYS:SG	3:A:397:GLU:HB3	2.57	0.44
3:A:1018:ASN:HB3	3:A:1021:LEU:HB2	1.99	0.44
3:A:2208:MET:HE3	3:A:2208:MET:HB3	1.83	0.44
3:A:2991:HIS:O	3:A:2995:ILE:HD13	2.17	0.44
3:A:3313:ASN:OD1	3:A:3349:ALA:HA	2.18	0.44
3:C:1089:TYR:HD2	3:C:1152:MET:HG3	1.81	0.44
3:C:3347:SER:HA	3:C:3418:ASN:ND2	2.32	0.44
3:C:4229:GLU:H	3:C:4229:GLU:CD	2.21	0.44
1:H:13:ARG:HB2	1:H:13:ARG:NH1	2.32	0.44
1:H:82:TYR:CE1	3:D:1786:LEU:HD13	2.49	0.44
2:K:84:GLU:OE2	3:C:3637:ARG:NE	2.49	0.44
3:D:1982:ARG:NH1	3:D:1982:ARG:HB2	2.32	0.44
3:D:4820:VAL:HG11	3:A:4839:MET:HG3	1.99	0.44
3:B:669:ASP:HB2	3:B:788:LYS:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:947:GLU:HG3	3:B:1049:TYR:CD1	2.50	0.44
3:B:4729:GLY:O	3:B:4734:ARG:HG2	2.18	0.44
3:A:947:GLU:HG3	3:A:1049:TYR:CD1	2.50	0.44
3:A:2972:GLU:C	3:A:2972:GLU:OE1	2.60	0.44
3:A:4565:LEU:O	3:A:4569:LEU:HG	2.18	0.44
3:C:902:ARG:HG3	3:C:902:ARG:NH1	2.32	0.44
2:I:124:MET:HB3	2:I:124:MET:HE3	1.86	0.44
3:D:233:ILE:HG12	3:D:284:HIS:NE2	2.32	0.44
3:B:2991:HIS:O	3:B:2995:ILE:HD13	2.17	0.44
3:A:3509:LEU:HD12	3:A:3509:LEU:HA	1.84	0.44
3:A:3592:ILE:HD12	3:A:3592:ILE:H	1.81	0.44
3:C:233:ILE:HG12	3:C:284:HIS:NE2	2.32	0.44
3:C:2972:GLU:C	3:C:2972:GLU:OE1	2.60	0.44
10:C:5510:CPS:H28A	10:C:5510:CPS:H261	1.82	0.44
1:E:82:TYR:HE1	3:A:1786:LEU:HD13	1.82	0.44
3:D:3003:LEU:HB2	3:D:3004:PRO:HD3	2.00	0.44
3:D:3313:ASN:OD1	3:D:3349:ALA:HA	2.18	0.44
3:D:3629:ARG:O	3:D:3633:VAL:HG23	2.17	0.44
3:D:4817:ALA:HB1	3:D:4827:LEU:HD11	2.00	0.44
3:B:796:ARG:HG3	3:B:796:ARG:HH11	1.83	0.44
3:B:2972:GLU:OE1	3:B:2972:GLU:C	2.60	0.44
3:A:241:GLN:HB2	3:A:243:ARG:HG2	2.00	0.44
3:A:3003:LEU:HB2	3:A:3004:PRO:HD3	2.00	0.44
1:E:82:TYR:CE1	3:A:1786:LEU:HD13	2.52	0.44
2:I:67:GLU:O	2:I:71:MET:HG3	2.17	0.44
2:J:90:ARG:O	2:J:94:LYS:HB2	2.17	0.44
3:D:404:ILE:HG21	3:D:481:GLU:HG3	1.99	0.44
3:D:2689:LYS:HE2	3:D:2689:LYS:HB3	1.79	0.44
3:A:1802:ILE:HG13	3:A:1803:PRO:HD2	2.00	0.44
3:C:3405:LEU:O	3:C:3409:TYR:HB2	2.17	0.44
3:C:4729:GLY:O	3:C:4734:ARG:HG2	2.18	0.44
3:D:241:GLN:HB2	3:D:243:ARG:HG2	2.00	0.44
3:D:1802:ILE:HG13	3:D:1803:PRO:HD2	2.00	0.44
3:D:3391:GLU:OE1	3:D:3395:ARG:HD2	2.18	0.44
3:B:4565:LEU:O	3:B:4569:LEU:HG	2.18	0.44
3:A:796:ARG:HG3	3:A:796:ARG:HH11	1.83	0.44
3:A:2527:LEU:HD12	3:A:2527:LEU:HA	1.82	0.44
3:A:3723:MET:HE2	3:A:3793:MET:HG2	1.99	0.44
3:C:796:ARG:HG3	3:C:796:ARG:HH11	1.83	0.44
2:L:124:MET:HE3	2:L:124:MET:HB3	1.76	0.44
3:B:2639:MET:HE3	3:B:2639:MET:HB3	1.89	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3059:THR:O	3:A:3062:PRO:HD2	2.18	0.44
3:A:4673:ARG:HA	3:A:4673:ARG:HD3	1.88	0.44
3:C:669:ASP:HB2	3:C:788:LYS:HB3	1.99	0.44
3:C:3310:ASP:OD2	3:C:3310:ASP:C	2.61	0.44
3:C:4565:LEU:O	3:C:4569:LEU:HG	2.18	0.44
2:I:89:PHE:HE2	2:I:108:VAL:HG21	1.83	0.43
3:B:2950:SER:O	3:B:2954:ARG:HG3	2.18	0.43
3:B:3003:LEU:HB2	3:B:3004:PRO:HD3	2.00	0.43
3:B:4820:VAL:HG11	3:C:4839:MET:HG3	1.99	0.43
3:A:4729:GLY:O	3:A:4734:ARG:HG2	2.18	0.43
3:C:3003:LEU:HB2	3:C:3004:PRO:HD3	2.00	0.43
3:C:3723:MET:HE2	3:C:3793:MET:HG2	1.99	0.43
3:D:3579:LEU:HD23	3:D:3580:PRO:HD2	2.00	0.43
3:D:3695:PRO:HB3	3:D:3699:HIS:HB3	2.00	0.43
3:D:4839:MET:HB3	3:C:4823:LEU:HD21	1.98	0.43
3:A:3604:TYR:C	3:A:3604:TYR:CD2	2.96	0.43
3:D:4729:GLY:O	3:D:4734:ARG:HG2	2.18	0.43
3:D:4823:LEU:HD21	3:A:4839:MET:HB3	1.98	0.43
10:D:5510:CPS:H28A	10:D:5510:CPS:H261	1.82	0.43
3:B:3313:ASN:OD1	3:B:3349:ALA:HA	2.18	0.43
3:A:4001:MET:HE2	3:A:4061:PHE:HB2	2.00	0.43
3:C:3629:ARG:O	3:C:3633:VAL:HG23	2.17	0.43
3:C:3695:PRO:HB3	3:C:3699:HIS:HB3	2.01	0.43
2:J:84:GLU:CG	3:B:3637:ARG:HE	2.31	0.43
3:D:1738:LEU:HD22	3:D:1963:GLU:HG3	2.00	0.43
3:D:2135:LEU:HD21	3:D:3663:LEU:HD13	2.01	0.43
3:D:3393:LEU:O	3:D:3397:GLU:HG3	2.19	0.43
3:D:4801:LEU:HD23	3:D:4801:LEU:HA	1.89	0.43
3:D:4839:MET:HG3	3:C:4820:VAL:HG11	1.99	0.43
3:D:4995:LEU:HD23	3:D:4995:LEU:HA	1.89	0.43
3:B:1100:MET:HB2	3:B:1143:TRP:CZ2	2.54	0.43
3:A:4097:MET:HE3	3:A:4097:MET:HB3	1.90	0.43
3:A:4837:LEU:HD12	3:A:4837:LEU:HA	1.84	0.43
3:C:179:TYR:O	3:C:193:ALA:HA	2.18	0.43
3:C:3059:THR:O	3:C:3062:PRO:HD2	2.18	0.43
3:C:4021:LYS:HD2	3:C:4138:ASP:CG	2.44	0.43
3:C:4680:LYS:HA	3:C:4684:ASP:HB2	2.01	0.43
3:C:4817:ALA:HB1	3:C:4827:LEU:HD11	2.00	0.43
1:F:52:LYS:HD3	1:F:52:LYS:HA	1.77	0.43
2:L:90:ARG:O	2:L:94:LYS:HB2	2.19	0.43
3:D:2639:MET:HE3	3:D:2639:MET:HB3	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3715:LYS:HB2	3:D:3715:LYS:HE2	1.87	0.43
3:B:179:TYR:O	3:B:193:ALA:HA	2.18	0.43
3:B:241:GLN:HB2	3:B:243:ARG:HG2	2.00	0.43
3:B:892:THR:O	3:B:903:LEU:HA	2.18	0.43
3:B:2672:LEU:HD23	3:B:2672:LEU:HA	1.88	0.43
3:B:4817:ALA:HB1	3:B:4827:LEU:HD11	2.00	0.43
3:A:2689:LYS:HE2	3:A:2689:LYS:HB3	1.79	0.43
3:A:3310:ASP:C	3:A:3310:ASP:OD2	2.61	0.43
3:A:3579:LEU:HD23	3:A:3580:PRO:HD2	2.00	0.43
3:A:4087:LEU:HD23	3:A:4122:MET:HB3	2.00	0.43
3:C:3391:GLU:OE1	3:C:3395:ARG:HD2	2.18	0.43
3:C:3604:TYR:C	3:C:3604:TYR:CD2	2.96	0.43
3:C:4097:MET:HE3	3:C:4097:MET:HB3	1.90	0.43
3:D:2552:ARG:O	3:D:2556:LEU:HB2	2.19	0.43
3:D:2950:SER:O	3:D:2954:ARG:HG3	2.18	0.43
3:D:3059:THR:O	3:D:3062:PRO:HD2	2.18	0.43
3:B:1738:LEU:HD22	3:B:1963:GLU:HG3	2.00	0.43
3:B:1802:ILE:HG13	3:B:1803:PRO:HD2	2.00	0.43
3:B:3059:THR:O	3:B:3062:PRO:HD2	2.18	0.43
3:B:4087:LEU:HD23	3:B:4122:MET:HB3	2.00	0.43
3:B:4680:LYS:HA	3:B:4684:ASP:HB2	2.01	0.43
3:A:907:LEU:HD13	3:A:961:MET:HE1	2.01	0.43
3:A:3695:PRO:HB3	3:A:3699:HIS:HB3	2.00	0.43
3:C:2443:ILE:HD13	3:C:2443:ILE:HA	1.88	0.43
3:B:907:LEU:HD13	3:B:961:MET:HE1	2.01	0.43
3:C:2135:LEU:HD21	3:C:3663:LEU:HD13	2.01	0.43
2:J:30:LYS:O	2:J:34:THR:HG22	2.19	0.43
3:D:1100:MET:HB2	3:D:1143:TRP:CZ2	2.54	0.43
3:B:1926:LEU:HA	3:B:1929:MET:HE2	2.01	0.43
3:B:3284:TRP:HB3	3:B:3305:THR:HG21	2.01	0.43
3:B:4021:LYS:HD2	3:B:4138:ASP:CG	2.44	0.43
3:B:4134:GLU:HB2	3:B:4135:PRO:HD3	2.01	0.43
3:A:1100:MET:HB2	3:A:1143:TRP:CZ2	2.54	0.43
3:A:1455:PRO:HG3	3:A:1549:PHE:HE1	1.84	0.43
3:A:3208:PRO:HB2	3:A:3237:GLU:HG3	2.01	0.43
3:A:4680:LYS:HA	3:A:4684:ASP:HB2	2.01	0.43
10:A:5510:CPS:H28A	10:A:5510:CPS:H261	1.82	0.43
3:C:1455:PRO:HG3	3:C:1549:PHE:HE1	1.84	0.43
3:C:3393:LEU:O	3:C:3397:GLU:HG3	2.19	0.43
3:C:3637:ARG:HA	3:C:3637:ARG:HD2	1.78	0.43
1:G:31:GLN:HA	1:G:98:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3391:GLU:OE1	3:B:3395:ARG:HD2	2.18	0.43
3:B:3393:LEU:O	3:B:3397:GLU:HG3	2.19	0.43
3:B:3579:LEU:HD23	3:B:3580:PRO:HD2	2.01	0.43
3:A:1263:THR:HG22	3:A:1266:THR:HB	2.00	0.43
3:A:2950:SER:O	3:A:2954:ARG:HG3	2.18	0.43
3:A:3670:GLU:HG2	3:A:3731:LYS:HB2	2.01	0.43
3:C:241:GLN:HB2	3:C:243:ARG:HG2	2.00	0.43
3:C:4001:MET:HE2	3:C:4061:PHE:HB2	2.00	0.43
2:J:13:LYS:HG2	3:B:2189:LYS:HB3	2.01	0.43
3:D:705:ASN:HA	3:D:709:ASP:OD2	2.19	0.43
3:D:1455:PRO:HG3	3:D:1549:PHE:HE1	1.84	0.43
3:B:2135:LEU:HD21	3:B:3663:LEU:HD13	2.01	0.43
3:B:2552:ARG:O	3:B:2556:LEU:HB2	2.19	0.43
3:A:179:TYR:O	3:A:193:ALA:HA	2.18	0.43
3:A:1926:LEU:HA	3:A:1929:MET:HE2	2.01	0.43
3:A:2135:LEU:HD21	3:A:3663:LEU:HD13	2.01	0.43
3:A:3393:LEU:O	3:A:3397:GLU:HG3	2.19	0.43
3:A:4134:GLU:HB2	3:A:4135:PRO:HD3	2.01	0.43
3:C:1263:THR:HG22	3:C:1266:THR:HB	2.00	0.43
3:C:1926:LEU:HA	3:C:1929:MET:HE2	2.01	0.43
3:C:3313:ASN:OD1	3:C:3349:ALA:HA	2.18	0.43
3:C:4087:LEU:HD23	3:C:4122:MET:HB3	2.00	0.43
1:G:57:LYS:HG3	1:G:61:GLU:OE1	2.18	0.42
2:J:47:GLU:HA	2:J:50:ASP:CG	2.42	0.42
3:D:3310:ASP:OD2	3:D:3310:ASP:C	2.61	0.42
3:D:4680:LYS:HA	3:D:4684:ASP:HB2	2.01	0.42
3:B:1163:THR:HG22	3:B:1168:VAL:HA	2.01	0.42
3:B:1263:THR:HG22	3:B:1266:THR:HB	2.00	0.42
3:B:1455:PRO:HG3	3:B:1549:PHE:HE1	1.84	0.42
3:B:2481:LYS:HB2	3:B:2481:LYS:HE2	1.89	0.42
3:B:2965:ARG:NH1	3:B:2965:ARG:HG2	2.32	0.42
3:B:3695:PRO:HB3	3:B:3699:HIS:HB3	2.00	0.42
3:B:4001:MET:HE2	3:B:4061:PHE:HB2	2.00	0.42
3:A:1738:LEU:HD22	3:A:1963:GLU:HG3	2.00	0.42
3:C:402:ARG:HD2	3:C:402:ARG:HA	1.84	0.42
2:I:67:GLU:H	2:I:67:GLU:HG2	1.59	0.42
3:D:796:ARG:HG3	3:D:796:ARG:HH11	1.83	0.42
3:B:705:ASN:HA	3:B:709:ASP:OD2	2.19	0.42
3:A:4817:ALA:HB1	3:A:4827:LEU:HD11	2.00	0.42
3:C:1802:ILE:HG13	3:C:1803:PRO:HD2	2.00	0.42
3:C:2552:ARG:O	3:C:2556:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1263:THR:HG22	3:D:1266:THR:HB	2.00	0.42
3:D:3208:PRO:HB2	3:D:3237:GLU:HG3	2.01	0.42
3:D:4021:LYS:HD2	3:D:4138:ASP:CG	2.44	0.42
3:A:1624:LEU:HD13	3:A:1624:LEU:HA	1.90	0.42
3:A:3284:TRP:HB3	3:A:3305:THR:HG21	2.01	0.42
3:A:3391:GLU:OE1	3:A:3395:ARG:HD2	2.18	0.42
3:C:892:THR:O	3:C:903:LEU:HA	2.18	0.42
3:D:635:THR:HA	3:D:1638:ALA:O	2.20	0.42
3:D:3509:LEU:HD12	3:D:3509:LEU:HA	1.84	0.42
3:D:3604:TYR:C	3:D:3604:TYR:CD2	2.96	0.42
3:A:1643:GLU:HG2	3:A:1644:GLU:N	2.34	0.42
3:A:4781:GLY:O	3:A:4785:THR:HG23	2.19	0.42
3:C:1100:MET:HB2	3:C:1143:TRP:CZ2	2.54	0.42
3:C:2138:LEU:HA	3:C:2138:LEU:HD23	1.75	0.42
3:C:2672:LEU:HD23	3:C:2672:LEU:HA	1.88	0.42
3:C:2950:SER:O	3:C:2954:ARG:HG3	2.18	0.42
3:C:4781:GLY:O	3:C:4785:THR:HG23	2.19	0.42
2:K:106:ARG:O	2:K:110:THR:HG23	2.20	0.42
3:D:3663:LEU:HD12	3:D:3663:LEU:HA	1.87	0.42
3:B:1291:LEU:HD12	3:B:1550:PRO:HG2	2.02	0.42
3:B:4837:LEU:HD12	3:B:4837:LEU:HA	1.84	0.42
3:A:805:PRO:HG2	3:A:808:TYR:CD1	2.54	0.42
3:A:892:THR:O	3:A:903:LEU:HA	2.18	0.42
3:A:4147:LEU:HD23	3:A:4147:LEU:HA	1.95	0.42
3:C:635:THR:HA	3:C:1638:ALA:O	2.20	0.42
3:C:4057:MET:HE3	3:C:4057:MET:HB2	1.90	0.42
1:G:52:LYS:HA	1:G:52:LYS:HD3	1.86	0.42
1:H:2:VAL:HA	1:H:75:THR:O	2.20	0.42
2:L:13:LYS:HD2	2:L:13:LYS:HA	1.84	0.42
2:L:100:ILE:HD13	2:L:100:ILE:HA	1.81	0.42
3:D:3604:TYR:O	3:D:3608:GLN:HG2	2.20	0.42
3:B:2604:GLU:HG2	3:B:2639:MET:HG3	2.02	0.42
3:B:3277:LEU:HD23	3:B:3277:LEU:HA	1.89	0.42
3:A:635:THR:HA	3:A:1638:ALA:O	2.20	0.42
3:A:955:LEU:HD12	3:A:955:LEU:HA	1.90	0.42
3:A:1163:THR:HG22	3:A:1168:VAL:HA	2.01	0.42
3:A:4021:LYS:HD2	3:A:4138:ASP:CG	2.44	0.42
3:A:4670:ILE:HD13	3:A:4670:ILE:HA	1.88	0.42
3:C:108:LEU:HD12	3:C:146:CYS:O	2.20	0.42
3:C:1738:LEU:HD22	3:C:1963:GLU:HG3	2.00	0.42
2:L:106:ARG:O	2:L:110:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:108:LEU:HD12	3:D:146:CYS:O	2.20	0.42
3:D:892:THR:O	3:D:903:LEU:HA	2.18	0.42
3:D:3284:TRP:HB3	3:D:3305:THR:HG21	2.01	0.42
3:B:688:LEU:HA	3:B:776:LEU:O	2.20	0.42
3:B:3208:PRO:HB2	3:B:3237:GLU:HG3	2.01	0.42
3:B:3604:TYR:C	3:B:3604:TYR:CD2	2.96	0.42
3:B:3670:GLU:HG2	3:B:3731:LYS:HB2	2.01	0.42
3:A:688:LEU:HA	3:A:776:LEU:O	2.20	0.42
3:A:2604:GLU:HG2	3:A:2639:MET:HG3	2.02	0.42
3:A:3802:ILE:HD11	3:A:3883:ASP:O	2.20	0.42
3:A:4159:ARG:H	3:A:4159:ARG:HG3	1.65	0.42
3:C:688:LEU:HA	3:C:776:LEU:O	2.20	0.42
3:C:3579:LEU:HD23	3:C:3580:PRO:HD2	2.00	0.42
3:C:3604:TYR:O	3:C:3608:GLN:HG2	2.20	0.42
3:D:955:LEU:HD12	3:D:955:LEU:HA	1.90	0.42
3:D:957:LYS:HD3	3:D:957:LYS:HA	1.85	0.42
3:D:3802:ILE:HD11	3:D:3883:ASP:O	2.20	0.42
3:D:4235:VAL:O	3:D:4239:GLU:HG3	2.20	0.42
3:B:805:PRO:HG2	3:B:808:TYR:CD1	2.55	0.42
3:B:1566:LEU:O	3:B:1589:PRO:HB3	2.20	0.42
3:B:2639:MET:HB3	3:B:2640:PRO:HD3	2.02	0.42
3:A:108:LEU:HD12	3:A:146:CYS:O	2.20	0.42
3:A:2639:MET:HB3	3:A:2640:PRO:HD3	2.02	0.42
3:A:3588:ASP:HB3	3:A:3590:GLU:OE1	2.20	0.42
3:C:1163:THR:HG22	3:C:1168:VAL:HA	2.01	0.42
3:C:1643:GLU:HG2	3:C:1644:GLU:N	2.34	0.42
3:C:2991:HIS:HB3	3:C:2994:GLU:HG3	2.02	0.42
3:C:3284:TRP:HB3	3:C:3305:THR:HG21	2.01	0.42
3:C:3670:GLU:HG2	3:C:3731:LYS:HB2	2.01	0.42
3:C:3802:ILE:HD11	3:C:3883:ASP:O	2.20	0.42
3:C:4235:VAL:O	3:C:4239:GLU:HG3	2.20	0.42
3:D:805:PRO:HG2	3:D:808:TYR:CD1	2.54	0.42
3:D:907:LEU:HD13	3:D:961:MET:HE1	2.01	0.42
3:D:1291:LEU:HD12	3:D:1550:PRO:HG2	2.02	0.42
3:D:1566:LEU:O	3:D:1589:PRO:HB3	2.20	0.42
3:D:1926:LEU:HA	3:D:1929:MET:HE2	2.01	0.42
3:B:635:THR:HA	3:B:1638:ALA:O	2.20	0.42
3:B:2204:HIS:HB2	3:B:2250:MET:CE	2.42	0.42
3:B:2522:LEU:O	3:B:2527:LEU:HB2	2.20	0.42
3:B:3802:ILE:HD11	3:B:3883:ASP:O	2.20	0.42
3:B:4235:VAL:O	3:B:4239:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:842:PRO:O	3:A:1196:PRO:HA	2.20	0.42
3:A:1566:LEU:O	3:A:1589:PRO:HB3	2.20	0.42
3:C:2639:MET:HB3	3:C:2640:PRO:HD3	2.02	0.42
3:D:179:TYR:O	3:D:193:ALA:HA	2.18	0.42
3:D:3588:ASP:HB3	3:D:3590:GLU:OE1	2.20	0.42
3:D:3637:ARG:HD2	3:D:3637:ARG:HA	1.78	0.42
3:D:4001:MET:HE2	3:D:4061:PHE:HB2	2.00	0.42
3:B:459:LEU:HD12	3:B:459:LEU:HA	1.88	0.42
3:B:4781:GLY:O	3:B:4785:THR:HG23	2.19	0.42
3:A:646:PRO:HB2	3:A:648:ILE:HD12	2.02	0.42
3:A:705:ASN:HA	3:A:709:ASP:OD2	2.19	0.42
3:A:2552:ARG:O	3:A:2556:LEU:HB2	2.19	0.42
3:C:805:PRO:HG2	3:C:808:TYR:CD1	2.54	0.42
3:C:1291:LEU:HD12	3:C:1550:PRO:HG2	2.02	0.42
3:C:2212:VAL:HG21	3:C:2256:TYR:OH	2.20	0.42
2:J:26:THR:HB	2:J:62:THR:HG23	2.01	0.41
3:D:2212:VAL:HG21	3:D:2256:TYR:OH	2.20	0.41
3:D:4087:LEU:HD23	3:D:4122:MET:HB3	2.00	0.41
3:D:4781:GLY:O	3:D:4785:THR:HG23	2.19	0.41
3:B:1643:GLU:HG2	3:B:1644:GLU:N	2.34	0.41
3:B:2700:MET:HB3	3:B:2701:PRO:HD3	2.02	0.41
3:B:3979:SER:O	3:B:3983:SER:HB3	2.20	0.41
3:A:3607:GLU:HA	3:A:3607:GLU:OE1	2.20	0.41
3:A:3917:ILE:HD13	3:A:3917:ILE:HA	1.87	0.41
3:A:4235:VAL:O	3:A:4239:GLU:HG3	2.20	0.41
3:A:4929:LEU:HD23	3:A:4929:LEU:HA	1.92	0.41
3:C:705:ASN:HA	3:C:709:ASP:OD2	2.19	0.41
3:C:907:LEU:HD13	3:C:961:MET:HE1	2.01	0.41
3:C:2604:GLU:HG2	3:C:2639:MET:HG3	2.02	0.41
3:C:2965:ARG:HG2	3:C:2965:ARG:HH11	1.85	0.41
3:C:3607:GLU:OE1	3:C:3607:GLU:HA	2.20	0.41
3:C:4134:GLU:HB2	3:C:4135:PRO:HD3	2.01	0.41
2:J:32:LEU:HA	2:J:35:VAL:HG22	2.01	0.41
3:D:22:LEU:HD23	3:D:22:LEU:HA	1.95	0.41
3:D:842:PRO:O	3:D:1196:PRO:HA	2.20	0.41
3:D:1797:ARG:HA	3:D:1797:ARG:HD2	1.90	0.41
3:D:2204:HIS:HB2	3:D:2250:MET:CE	2.42	0.41
3:D:2639:MET:HB3	3:D:2640:PRO:HD3	2.02	0.41
3:D:3379:LEU:HD13	3:D:3390:GLY:HA3	2.02	0.41
3:B:108:LEU:HD12	3:B:146:CYS:O	2.20	0.41
3:B:753:PRO:HB2	3:B:771:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3607:GLU:OE1	3:B:3607:GLU:HA	2.20	0.41
3:A:1249:PRO:HA	3:A:1250:PRO:HD3	1.95	0.41
3:C:1566:LEU:O	3:C:1589:PRO:HB3	2.20	0.41
3:C:3208:PRO:HB2	3:C:3237:GLU:HG3	2.01	0.41
1:G:106:LEU:HA	1:G:106:LEU:HD23	1.69	0.41
2:K:124:MET:HB3	2:K:124:MET:HE3	1.87	0.41
3:B:3194:LEU:HD12	3:B:3194:LEU:HA	1.93	0.41
3:B:3310:ASP:OD2	3:B:3310:ASP:C	2.61	0.41
3:C:1849:LEU:HD23	3:C:1849:LEU:HA	1.94	0.41
3:C:2522:LEU:O	3:C:2527:LEU:HB2	2.20	0.41
3:C:2700:MET:HB3	3:C:2701:PRO:HD3	2.02	0.41
1:H:52:LYS:HA	1:H:52:LYS:HD3	1.68	0.41
2:I:47:GLU:HA	2:I:50:ASP:OD1	2.20	0.41
3:D:2604:GLU:HG2	3:D:2639:MET:HG3	2.02	0.41
3:D:3607:GLU:OE1	3:D:3607:GLU:HA	2.20	0.41
3:D:3670:GLU:HG2	3:D:3731:LYS:HB2	2.01	0.41
3:D:4134:GLU:HB2	3:D:4135:PRO:HD3	2.01	0.41
3:B:1937:LEU:HD12	3:B:1937:LEU:HA	1.92	0.41
3:C:3379:LEU:HD13	3:C:3390:GLY:HA3	2.03	0.41
2:L:89:PHE:HB3	2:L:94:LYS:NZ	2.35	0.41
3:D:1163:THR:HG22	3:D:1168:VAL:HA	2.01	0.41
3:D:2965:ARG:HG2	3:D:2965:ARG:HH11	1.85	0.41
3:D:2991:HIS:HB3	3:D:2994:GLU:HG3	2.02	0.41
3:B:842:PRO:O	3:B:1196:PRO:HA	2.20	0.41
3:B:1448:VAL:HG22	3:B:1554:VAL:HG23	2.03	0.41
3:B:3379:LEU:HD13	3:B:3390:GLY:HA3	2.02	0.41
3:B:4159:ARG:H	3:B:4159:ARG:HG3	1.65	0.41
3:A:4689:THR:HG22	3:A:4732:PHE:CE1	2.56	0.41
3:C:2426:TYR:O	3:C:2430:ILE:HG12	2.21	0.41
3:C:3588:ASP:HB3	3:C:3590:GLU:OE1	2.20	0.41
2:L:26:THR:HB	2:L:62:THR:HG23	2.02	0.41
3:B:402:ARG:HD2	3:B:402:ARG:HA	1.84	0.41
3:B:3274:LEU:HD23	3:B:3274:LEU:HA	1.93	0.41
3:B:3735:LEU:HD12	3:B:3735:LEU:HA	1.91	0.41
3:A:753:PRO:HB2	3:A:771:PHE:CZ	2.55	0.41
3:A:1291:LEU:HD12	3:A:1550:PRO:HG2	2.02	0.41
3:A:2212:VAL:HG21	3:A:2256:TYR:OH	2.20	0.41
3:A:2639:MET:HB3	3:A:2639:MET:HE3	1.89	0.41
3:C:753:PRO:HB2	3:C:771:PHE:CZ	2.55	0.41
3:C:3979:SER:O	3:C:3983:SER:HB3	2.20	0.41
3:C:4673:ARG:HA	3:C:4673:ARG:HD3	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:688:LEU:HA	3:D:776:LEU:O	2.20	0.41
3:D:1643:GLU:HG2	3:D:1644:GLU:N	2.34	0.41
3:B:2527:LEU:HA	3:B:2527:LEU:HD12	1.82	0.41
3:B:2636:PHE:HD1	3:B:2636:PHE:HA	1.78	0.41
3:A:3087:ILE:H	3:A:3087:ILE:HG13	1.72	0.41
3:A:3835:LEU:HD22	3:A:3880:PHE:HZ	1.86	0.41
3:C:2689:LYS:HE2	3:C:2689:LYS:HB3	1.79	0.41
3:C:3194:LEU:HD12	3:C:3194:LEU:HA	1.93	0.41
3:C:3327:LEU:HD23	3:C:3327:LEU:HA	1.89	0.41
1:H:84:ALA:O	1:H:93:PRO:HB3	2.20	0.41
3:D:2426:TYR:O	3:D:2430:ILE:HG12	2.21	0.41
3:D:2679:PHE:HB2	3:D:2706:ILE:HG21	2.03	0.41
3:D:3673:MET:HE2	3:D:3725:TYR:CE1	2.56	0.41
3:D:3835:LEU:HD22	3:D:3880:PHE:HZ	1.86	0.41
3:D:3860:ASN:C	3:D:3861:GLU:HG3	2.46	0.41
3:B:3509:LEU:HD12	3:B:3509:LEU:HA	1.84	0.41
3:B:3588:ASP:HB3	3:B:3590:GLU:OE1	2.20	0.41
3:B:4689:THR:HG22	3:B:4732:PHE:CE1	2.56	0.41
3:A:2700:MET:HB3	3:A:2701:PRO:HD3	2.02	0.41
3:A:2991:HIS:HB3	3:A:2994:GLU:HG3	2.02	0.41
3:A:4980:LEU:HD23	3:A:4980:LEU:HA	1.86	0.41
3:C:842:PRO:O	3:C:1196:PRO:HA	2.20	0.41
3:C:3959:LYS:HG3	3:C:4022:ASP:OD2	2.20	0.41
3:C:4837:LEU:HD12	3:C:4837:LEU:HA	1.84	0.41
1:E:4:ILE:HG12	1:E:74:LEU:HD22	2.02	0.41
1:E:57:LYS:HE3	1:E:57:LYS:HB3	1.75	0.41
1:F:62:GLY:HA3	1:F:74:LEU:HD13	2.03	0.41
1:F:79:ASP:OD1	1:F:80:VAL:HG23	2.21	0.41
3:D:646:PRO:HB2	3:D:648:ILE:HD12	2.02	0.41
3:D:2522:LEU:O	3:D:2527:LEU:HB2	2.20	0.41
3:D:2700:MET:HB3	3:D:2701:PRO:HD3	2.02	0.41
3:D:4168:GLU:HA	3:D:4171:LEU:HD12	2.03	0.41
3:D:4689:THR:HG22	3:D:4732:PHE:CE1	2.56	0.41
3:B:125:ARG:NH2	3:B:190:GLN:HE21	2.19	0.41
3:B:871:ARG:NH2	3:B:926:GLY:HA3	2.36	0.41
3:B:955:LEU:HD12	3:B:955:LEU:HA	1.90	0.41
3:B:1797:ARG:HA	3:B:1797:ARG:HD2	1.90	0.41
3:B:2178:MET:HE3	3:B:2182:ILE:HD11	2.03	0.41
3:B:2212:VAL:HG21	3:B:2256:TYR:OH	2.20	0.41
3:B:2582:MET:HE2	3:B:2582:MET:HB3	1.86	0.41
3:B:2633:LEU:HD13	3:B:2695:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2965:ARG:HG2	3:B:2965:ARG:HH11	1.85	0.41
3:B:3604:TYR:O	3:B:3608:GLN:HG2	2.20	0.41
3:A:402:ARG:HD2	3:A:402:ARG:HA	1.84	0.41
3:A:459:LEU:HD12	3:A:459:LEU:HA	1.88	0.41
3:A:2138:LEU:HD23	3:A:2138:LEU:HA	1.75	0.41
3:A:2522:LEU:O	3:A:2527:LEU:HB2	2.20	0.41
3:A:3379:LEU:HD13	3:A:3390:GLY:HA3	2.02	0.41
3:A:3979:SER:O	3:A:3983:SER:HB3	2.20	0.41
3:C:2178:MET:HE3	3:C:2182:ILE:HD11	2.03	0.41
2:L:67:GLU:H	2:L:67:GLU:HG2	1.55	0.41
3:D:4968:PHE:O	3:D:4974:GLY:HA3	2.21	0.41
3:B:2991:HIS:HB3	3:B:2994:GLU:HG3	2.02	0.41
3:B:4188:ARG:HD3	3:B:4188:ARG:HA	1.94	0.41
3:B:4968:PHE:O	3:B:4974:GLY:HA3	2.21	0.41
3:A:125:ARG:NH2	3:A:190:GLN:HE21	2.19	0.41
3:A:1629:GLN:HG2	11:A:5728:HOH:O	2.21	0.41
3:A:3049:LEU:HD12	3:A:3049:LEU:HA	1.94	0.41
3:C:955:LEU:HD12	3:C:955:LEU:HA	1.90	0.41
3:C:3916:ILE:O	3:C:3920:VAL:HG23	2.21	0.41
3:C:4010:ILE:HD12	3:C:4010:ILE:HA	1.92	0.41
3:C:4168:GLU:HA	3:C:4171:LEU:HD12	2.03	0.41
3:C:4968:PHE:O	3:C:4974:GLY:HA3	2.21	0.41
3:D:753:PRO:HB2	3:D:771:PHE:CZ	2.55	0.40
3:D:955:LEU:HG	3:D:956:PRO:HD2	2.04	0.40
3:B:467:LYS:HA	3:B:467:LYS:HD3	1.84	0.40
3:B:2426:TYR:O	3:B:2430:ILE:HG12	2.21	0.40
3:B:4929:LEU:HD23	3:B:4929:LEU:HA	1.92	0.40
3:A:646:PRO:HD2	3:A:779:PRO:O	2.22	0.40
3:A:2178:MET:HE3	3:A:2182:ILE:HD11	2.03	0.40
3:A:2679:PHE:HB2	3:A:2706:ILE:HG21	2.03	0.40
3:A:3604:TYR:O	3:A:3608:GLN:HG2	2.20	0.40
3:C:2626:LEU:O	3:C:2630:VAL:HG23	2.21	0.40
3:C:2633:LEU:HD13	3:C:2695:LEU:HD11	2.03	0.40
3:C:2641:LEU:HD23	3:C:2641:LEU:HA	1.96	0.40
3:C:3673:MET:HE2	3:C:3725:TYR:CE1	2.56	0.40
3:C:4689:THR:HG22	3:C:4732:PHE:CE1	2.56	0.40
3:C:4835:LYS:HD2	3:C:4835:LYS:HA	1.92	0.40
3:D:177:GLU:OE1	3:C:2359:ARG:NH1	2.55	0.40
3:D:3916:ILE:O	3:D:3920:VAL:HG23	2.21	0.40
3:B:646:PRO:HD2	3:B:779:PRO:O	2.22	0.40
3:B:2225:PHE:N	3:B:2226:PRO:HD3	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3860:ASN:C	3:B:3861:GLU:HG3	2.46	0.40
3:B:3959:LYS:HG3	3:B:4022:ASP:OD2	2.20	0.40
3:B:4980:LEU:HD23	3:B:4980:LEU:HA	1.86	0.40
3:A:274:LEU:HD21	3:A:280:LEU:HD23	2.04	0.40
3:A:4968:PHE:O	3:A:4974:GLY:HA3	2.21	0.40
3:C:467:LYS:HD3	3:C:467:LYS:HA	1.84	0.40
3:C:646:PRO:HB2	3:C:648:ILE:HD12	2.02	0.40
3:C:1272:LEU:HD22	3:C:1289:LEU:HD11	2.03	0.40
2:J:89:PHE:HB3	2:J:94:LYS:NZ	2.37	0.40
3:D:2485:LEU:HD21	3:D:2541:PHE:HE1	1.87	0.40
3:D:3327:LEU:HD23	3:D:3327:LEU:HA	1.89	0.40
3:D:3959:LYS:HG3	3:D:4022:ASP:OD2	2.20	0.40
3:D:4041:ALA:O	3:D:4045:VAL:HG23	2.22	0.40
3:D:4097:MET:HE3	3:D:4097:MET:HB3	1.90	0.40
3:D:4670:ILE:HD13	3:D:4670:ILE:HA	1.88	0.40
3:B:646:PRO:HB2	3:B:648:ILE:HD12	2.02	0.40
3:B:3835:LEU:HD22	3:B:3880:PHE:HZ	1.86	0.40
3:B:4569:LEU:HD22	3:B:4646:LEU:HD22	2.03	0.40
3:A:1849:LEU:HD22	3:A:1945:TYR:CE2	2.56	0.40
3:A:2479:LEU:HD12	3:A:2479:LEU:HA	1.91	0.40
3:A:3312:LEU:HD23	3:A:3345:ILE:HG22	2.04	0.40
3:A:3860:ASN:C	3:A:3861:GLU:HG3	2.46	0.40
3:A:3959:LYS:HG3	3:A:4022:ASP:OD2	2.20	0.40
3:C:646:PRO:HD2	3:C:779:PRO:O	2.22	0.40
3:C:1448:VAL:HG22	3:C:1554:VAL:HG23	2.03	0.40
3:C:3860:ASN:C	3:C:3861:GLU:HG3	2.46	0.40
1:F:2:VAL:HA	1:F:75:THR:O	2.21	0.40
2:K:13:LYS:HD2	2:K:13:LYS:HA	1.82	0.40
3:D:100:THR:HG21	3:D:162:LYS:HG2	2.03	0.40
3:D:878:ILE:HD13	3:D:878:ILE:HA	1.89	0.40
3:D:2626:LEU:O	3:D:2630:VAL:HG23	2.21	0.40
3:D:4721:LYS:HD3	3:D:4741:LEU:HG	2.04	0.40
3:B:1122:TYR:HB3	3:B:1179:PHE:CE2	2.57	0.40
3:A:878:ILE:HD13	3:A:878:ILE:HA	1.89	0.40
3:A:3266:MET:HG3	3:A:3270:ILE:HG13	2.03	0.40
3:A:3673:MET:HE2	3:A:3725:TYR:CE1	2.56	0.40
3:A:4168:GLU:HA	3:A:4171:LEU:HD12	2.03	0.40
3:C:125:ARG:NH2	3:C:190:GLN:HE21	2.19	0.40
3:C:1595:LEU:HD12	3:C:1595:LEU:HA	1.89	0.40
3:C:3971:GLY:N	3:C:3972:PRO:HA	2.37	0.40
3:C:4929:LEU:HD23	3:C:4929:LEU:HA	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:106:LEU:HD23	1:E:106:LEU:HA	1.75	0.40
3:D:646:PRO:HD2	3:D:779:PRO:O	2.22	0.40
3:D:1448:VAL:HG22	3:D:1554:VAL:HG23	2.03	0.40
3:D:3087:ILE:H	3:D:3087:ILE:HG13	1.72	0.40
3:D:3979:SER:O	3:D:3983:SER:HB3	2.20	0.40
3:B:3637:ARG:HA	3:B:3637:ARG:HD2	1.78	0.40
3:A:100:THR:HG21	3:A:162:LYS:HG2	2.03	0.40
3:A:2426:TYR:O	3:A:2430:ILE:HG12	2.21	0.40
3:A:2965:ARG:HG2	3:A:2965:ARG:HH11	1.85	0.40
3:A:4041:ALA:O	3:A:4045:VAL:HG23	2.22	0.40
3:A:4995:LEU:HD23	3:A:4995:LEU:HA	1.89	0.40
3:C:274:LEU:HD21	3:C:280:LEU:HD23	2.04	0.40
3:C:2472:LEU:HD23	3:C:2472:LEU:HA	1.91	0.40
3:C:3266:MET:HG3	3:C:3270:ILE:HG13	2.03	0.40
3:C:4041:ALA:O	3:C:4045:VAL:HG23	2.22	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	E	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
1	F	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
1	G	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
1	H	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
2	I	146/148 (99%)	142 (97%)	4 (3%)	0	100	100
2	J	146/148 (99%)	141 (97%)	5 (3%)	0	100	100
2	K	146/148 (99%)	141 (97%)	5 (3%)	0	100	100
2	L	146/148 (99%)	140 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	4207/5037 (84%)	4134 (98%)	73 (2%)	0	100	100
3	B	4207/5037 (84%)	4133 (98%)	74 (2%)	0	100	100
3	C	4207/5037 (84%)	4133 (98%)	74 (2%)	0	100	100
3	D	4207/5037 (84%)	4134 (98%)	73 (2%)	0	100	100
All	All	17832/21168 (84%)	17499 (98%)	333 (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	E	88/88 (100%)	84 (96%)	4 (4%)	24	56
1	F	88/88 (100%)	84 (96%)	4 (4%)	24	56
1	G	88/88 (100%)	82 (93%)	6 (7%)	14	42
1	H	88/88 (100%)	86 (98%)	2 (2%)	44	70
2	I	80/127 (63%)	77 (96%)	3 (4%)	29	60
2	J	80/127 (63%)	77 (96%)	3 (4%)	29	60
2	K	80/127 (63%)	74 (92%)	6 (8%)	12	39
2	L	80/127 (63%)	76 (95%)	4 (5%)	22	53
3	A	3541/4276 (83%)	3500 (99%)	41 (1%)	63	78
3	B	3541/4276 (83%)	3500 (99%)	41 (1%)	63	78
3	C	3541/4276 (83%)	3498 (99%)	43 (1%)	63	78
3	D	3541/4276 (83%)	3499 (99%)	42 (1%)	63	78
All	All	14836/17964 (83%)	14637 (99%)	199 (1%)	59	77

All (199) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	4	ILE

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Mol	Chain	Res	Type
1	E	22	CYS
1	E	60	GLU
1	E	77	THR
1	F	2	VAL
1	F	22	CYS
1	F	61	GLU
1	F	77	THR
1	G	2	VAL
1	G	3	GLU
1	G	4	ILE
1	G	25	HIS
1	G	61	GLU
1	G	77	THR
1	H	3	GLU
1	H	44	LYS
2	I	32	LEU
2	I	67	GLU
2	I	112	LEU
2	J	67	GLU
2	J	84	GLU
2	J	112	LEU
2	K	-1	HIS
2	K	5	THR
2	K	11	GLU
2	K	20	ASP
2	K	32	LEU
2	K	112	LEU
2	L	4	LEU
2	L	32	LEU
2	L	67	GLU
2	L	112	LEU
3	D	19	GLU
3	D	35	LEU
3	D	169	LEU
3	D	220	LEU
3	D	245	VAL
3	D	274	LEU
3	D	280	LEU
3	D	313	SER
3	D	459	LEU
3	D	575	LEU
3	D	732	SER

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Mol	Chain	Res	Type
3	D	843	SER
3	D	856	VAL
3	D	862	VAL
3	D	1010	VAL
3	D	1039	LEU
3	D	1073	ARG
3	D	1296	GLN
3	D	1489	CYS
3	D	1698	LEU
3	D	2243	SER
3	D	2290	LEU
3	D	2479	LEU
3	D	2636	PHE
3	D	2974	ILE
3	D	2991	HIS
3	D	3160	ASP
3	D	3333	THR
3	D	3514	LEU
3	D	3569	LEU
3	D	3720	TYR
3	D	3903	LEU
3	D	3907	THR
3	D	4009	GLN
3	D	4098	ASP
3	D	4164	LEU
3	D	4221	VAL
3	D	4317	ARG
3	D	4571	PHE
3	D	4658	ILE
3	D	4686	LEU
3	D	4911	LEU
3	B	19	GLU
3	B	35	LEU
3	B	169	LEU
3	B	220	LEU
3	B	245	VAL
3	B	274	LEU
3	B	280	LEU
3	B	313	SER
3	B	459	LEU
3	B	575	LEU
3	B	732	SER

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Mol	Chain	Res	Type
3	B	843	SER
3	B	856	VAL
3	B	862	VAL
3	B	1010	VAL
3	B	1039	LEU
3	B	1073	ARG
3	B	1296	GLN
3	B	1489	CYS
3	B	1698	LEU
3	B	2243	SER
3	B	2290	LEU
3	B	2479	LEU
3	B	2636	PHE
3	B	2974	ILE
3	B	2991	HIS
3	B	3160	ASP
3	B	3333	THR
3	B	3514	LEU
3	B	3569	LEU
3	B	3720	TYR
3	B	3903	LEU
3	B	3907	THR
3	B	4009	GLN
3	B	4098	ASP
3	B	4164	LEU
3	B	4221	VAL
3	B	4317	ARG
3	B	4571	PHE
3	B	4658	ILE
3	B	4686	LEU
3	A	19	GLU
3	A	169	LEU
3	A	220	LEU
3	A	245	VAL
3	A	274	LEU
3	A	280	LEU
3	A	313	SER
3	A	459	LEU
3	A	575	LEU
3	A	732	SER
3	A	856	VAL
3	A	862	VAL

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Mol	Chain	Res	Type
3	A	1010	VAL
3	A	1039	LEU
3	A	1073	ARG
3	A	1296	GLN
3	A	1489	CYS
3	A	1698	LEU
3	A	2243	SER
3	A	2290	LEU
3	A	2308	GLN
3	A	2479	LEU
3	A	2636	PHE
3	A	2974	ILE
3	A	2991	HIS
3	A	3160	ASP
3	A	3333	THR
3	A	3514	LEU
3	A	3569	LEU
3	A	3720	TYR
3	A	3903	LEU
3	A	3907	THR
3	A	4009	GLN
3	A	4098	ASP
3	A	4164	LEU
3	A	4221	VAL
3	A	4317	ARG
3	A	4571	PHE
3	A	4658	ILE
3	A	4686	LEU
3	A	4911	LEU
3	C	19	GLU
3	C	35	LEU
3	C	169	LEU
3	C	220	LEU
3	C	245	VAL
3	C	274	LEU
3	C	280	LEU
3	C	313	SER
3	C	459	LEU
3	C	575	LEU
3	C	732	SER
3	C	843	SER
3	C	856	VAL

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Mol	Chain	Res	Type
3	C	862	VAL
3	C	1010	VAL
3	C	1039	LEU
3	C	1073	ARG
3	C	1296	GLN
3	C	1489	CYS
3	C	1698	LEU
3	C	2243	SER
3	C	2290	LEU
3	C	2333	ASP
3	C	2479	LEU
3	C	2636	PHE
3	C	2974	ILE
3	C	2991	HIS
3	C	3160	ASP
3	C	3333	THR
3	C	3514	LEU
3	C	3569	LEU
3	C	3720	TYR
3	C	3903	LEU
3	C	3907	THR
3	C	4009	GLN
3	C	4098	ASP
3	C	4164	LEU
3	C	4221	VAL
3	C	4317	ARG
3	C	4571	PHE
3	C	4658	ILE
3	C	4686	LEU
3	C	4911	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (136) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	31	GLN
1	G	31	GLN
2	J	53	ASN
3	D	23	GLN
3	D	105	HIS
3	D	181	HIS
3	D	201	ASN
3	D	533	ASN

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Mol	Chain	Res	Type
3	D	576	ASN
3	D	593	HIS
3	D	812	HIS
3	D	838	HIS
3	D	1003	GLN
3	D	1041	GLN
3	D	1052	ASN
3	D	1165	ASN
3	D	1631	GLN
3	D	1702	HIS
3	D	2092	GLN
3	D	2169	GLN
3	D	2187	ASN
3	D	2253	HIS
3	D	2342	ASN
3	D	2599	GLN
3	D	3012	ASN
3	D	3030	HIS
3	D	3128	ASN
3	D	3523	ASN
3	D	3605	HIS
3	D	3850	GLN
3	D	3914	ASN
3	D	4034	ASN
3	D	4037	ASN
3	D	4120	ASN
3	D	4162	ASN
3	D	4662	ASN
3	D	5006	GLN
3	B	23	GLN
3	B	105	HIS
3	B	181	HIS
3	B	533	ASN
3	B	576	ASN
3	B	593	HIS
3	B	636	ASN
3	B	812	HIS
3	B	838	HIS
3	B	1003	GLN
3	B	1041	GLN
3	B	1052	ASN
3	B	1158	ASN

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Mol	Chain	Res	Type
3	B	1165	ASN
3	B	1590	GLN
3	B	1631	GLN
3	B	1702	HIS
3	B	2092	GLN
3	B	2169	GLN
3	B	2342	ASN
3	B	2599	GLN
3	B	2991	HIS
3	B	3012	ASN
3	B	3030	HIS
3	B	3128	ASN
3	B	3605	HIS
3	B	3850	GLN
3	B	3914	ASN
3	B	4034	ASN
3	B	4037	ASN
3	B	4120	ASN
3	B	4162	ASN
3	B	4662	ASN
3	A	23	GLN
3	A	105	HIS
3	A	181	HIS
3	A	201	ASN
3	A	533	ASN
3	A	576	ASN
3	A	593	HIS
3	A	636	ASN
3	A	812	HIS
3	A	838	HIS
3	A	1003	GLN
3	A	1041	GLN
3	A	1052	ASN
3	A	1165	ASN
3	A	1590	GLN
3	A	1631	GLN
3	A	1702	HIS
3	A	2092	GLN
3	A	2169	GLN
3	A	2342	ASN
3	A	2599	GLN
3	A	3012	ASN

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Mol	Chain	Res	Type
3	A	3030	HIS
3	A	3128	ASN
3	A	3605	HIS
3	A	3761	GLN
3	A	3766	GLN
3	A	3850	GLN
3	A	3914	ASN
3	A	4034	ASN
3	A	4037	ASN
3	A	4120	ASN
3	A	4162	ASN
3	A	4662	ASN
3	A	5006	GLN
3	C	23	GLN
3	C	105	HIS
3	C	181	HIS
3	C	201	ASN
3	C	533	ASN
3	C	576	ASN
3	C	636	ASN
3	C	812	HIS
3	C	838	HIS
3	C	1003	GLN
3	C	1041	GLN
3	C	1052	ASN
3	C	1165	ASN
3	C	1590	GLN
3	C	1631	GLN
3	C	1702	HIS
3	C	2169	GLN
3	C	2187	ASN
3	C	2342	ASN
3	C	2599	GLN
3	C	3012	ASN
3	C	3030	HIS
3	C	3128	ASN
3	C	3605	HIS
3	C	3850	GLN
3	C	3914	ASN
3	C	4034	ASN
3	C	4037	ASN
3	C	4120	ASN

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Mol	Chain	Res	Type
3	C	4162	ASN
3	C	4662	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 40 ligands modelled in this entry, 8 are monoatomic - leaving 32 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	$\# Z > 2$
9	CFF	D	5509	-	15,15,15	0.32	0	23,23,23	0.46	0
7	43M	C	5505	-	9,9,9	0.39	0	12,12,12	0.52	0
7	43M	A	5504	-	9,9,9	0.38	0	12,12,12	0.52	0
10	CPS	A	5510	-	45,45,45	0.58	1 (2%)	70,70,70	0.79	0
7	43M	D	5505	-	9,9,9	0.40	0	12,12,12	0.52	0
8	ATP	C	5508	-	32,33,33	0.53	0	48,52,52	0.59	0
7	43M	D	5506	-	9,9,9	0.39	0	12,12,12	0.50	0
9	CFF	B	5509	-	15,15,15	0.32	0	23,23,23	0.46	0
6	U1C	D	5503	-	25,25,25	0.60	0	33,35,35	0.51	0
10	CPS	D	5510	-	45,45,45	0.58	1 (2%)	70,70,70	0.79	0
7	43M	B	5505	-	9,9,9	0.40	0	12,12,12	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	43M	A	5506	-	9,9,9	0.39	0	12,12,12	0.50	0
7	43M	C	5504	-	9,9,9	0.38	0	12,12,12	0.52	0
7	43M	B	5506	-	9,9,9	0.39	0	12,12,12	0.50	0
10	CPS	C	5510	-	45,45,45	0.58	1 (2%)	70,70,70	0.79	0
9	CFF	A	5509	-	15,15,15	0.33	0	23,23,23	0.46	0
8	ATP	D	5507	-	32,33,33	0.38	0	48,52,52	0.38	0
8	ATP	A	5507	-	32,33,33	0.38	0	48,52,52	0.38	0
8	ATP	A	5508	-	32,33,33	0.52	0	48,52,52	0.58	0
6	U1C	A	5503	-	25,25,25	0.60	0	33,35,35	0.51	0
6	U1C	C	5503	-	25,25,25	0.61	0	33,35,35	0.51	0
6	U1C	B	5503	-	25,25,25	0.60	0	33,35,35	0.51	0
7	43M	C	5506	-	9,9,9	0.39	0	12,12,12	0.50	0
8	ATP	B	5508	-	32,33,33	0.52	0	48,52,52	0.58	0
8	ATP	C	5507	-	32,33,33	0.38	0	48,52,52	0.38	0
9	CFF	C	5509	-	15,15,15	0.32	0	23,23,23	0.46	0
7	43M	A	5505	-	9,9,9	0.40	0	12,12,12	0.52	0
8	ATP	D	5508	-	32,33,33	0.52	0	48,52,52	0.58	0
10	CPS	B	5510	-	45,45,45	0.58	1 (2%)	70,70,70	0.79	0
8	ATP	B	5507	-	32,33,33	0.38	0	48,52,52	0.38	0
7	43M	D	5504	-	9,9,9	0.38	0	12,12,12	0.52	0
7	43M	B	5504	-	9,9,9	0.38	0	12,12,12	0.53	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CFF	D	5509	-	-	-	0/2/2/2
7	43M	C	5505	-	-	-	0/1/1/1
7	43M	A	5504	-	-	-	0/1/1/1
10	CPS	A	5510	-	-	18/25/90/90	0/4/4/4
8	ATP	C	5508	-	-	4/22/38/38	0/3/3/3
7	43M	D	5505	-	-	-	0/1/1/1
7	43M	D	5506	-	-	-	0/1/1/1
9	CFF	B	5509	-	-	-	0/2/2/2
6	U1C	D	5503	-	-	0/11/25/25	0/3/3/3
10	CPS	D	5510	-	-	18/25/90/90	0/4/4/4
7	43M	B	5505	-	-	-	0/1/1/1
7	43M	A	5506	-	-	-	0/1/1/1
7	43M	C	5504	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CPS	C	5510	-	-	18/25/90/90	0/4/4/4
7	43M	B	5506	-	-	-	0/1/1/1
9	CFF	A	5509	-	-	-	0/2/2/2
8	ATP	D	5507	-	-	2/22/38/38	0/3/3/3
8	ATP	A	5507	-	-	2/22/38/38	0/3/3/3
8	ATP	A	5508	-	-	4/22/38/38	0/3/3/3
6	U1C	A	5503	-	-	0/11/25/25	0/3/3/3
6	U1C	C	5503	-	-	0/11/25/25	0/3/3/3
6	U1C	B	5503	-	-	0/11/25/25	0/3/3/3
8	ATP	B	5508	-	-	4/22/38/38	0/3/3/3
8	ATP	C	5507	-	-	2/22/38/38	0/3/3/3
7	43M	C	5506	-	-	-	0/1/1/1
9	CFF	C	5509	-	-	-	0/2/2/2
7	43M	A	5505	-	-	-	0/1/1/1
8	ATP	D	5508	-	-	4/22/38/38	0/3/3/3
10	CPS	B	5510	-	-	18/25/90/90	0/4/4/4
8	ATP	B	5507	-	-	2/22/38/38	0/3/3/3
7	43M	D	5504	-	-	-	0/1/1/1
7	43M	B	5504	-	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	5510	CPS	C32-S	2.31	1.80	1.77
10	B	5510	CPS	C32-S	2.31	1.80	1.77
10	A	5510	CPS	C32-S	2.31	1.80	1.77
10	C	5510	CPS	C32-S	2.31	1.80	1.77

There are no bond angle outliers.

There are no chirality outliers.

All (96) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	5507	ATP	C5'-O5'-PA-O1A
8	D	5508	ATP	PB-O3B-PG-O3G
8	D	5508	ATP	C5'-O5'-PA-O1A
8	B	5507	ATP	C5'-O5'-PA-O1A
8	B	5508	ATP	PB-O3B-PG-O3G
8	B	5508	ATP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
8	A	5507	ATP	C5'-O5'-PA-O1A
8	A	5508	ATP	PB-O3B-PG-O3G
8	A	5508	ATP	C5'-O5'-PA-O1A
8	C	5507	ATP	C5'-O5'-PA-O1A
8	C	5508	ATP	PB-O3B-PG-O3G
8	C	5508	ATP	C5'-O5'-PA-O1A
10	D	5510	CPS	N2-C30-C31-C32
10	D	5510	CPS	C31-C30-N2-C27
10	B	5510	CPS	N2-C30-C31-C32
10	B	5510	CPS	C31-C30-N2-C27
10	A	5510	CPS	N2-C30-C31-C32
10	A	5510	CPS	C31-C30-N2-C27
10	C	5510	CPS	N2-C30-C31-C32
10	C	5510	CPS	C31-C30-N2-C27
10	D	5510	CPS	C23-C24-N1-C25
10	B	5510	CPS	C23-C24-N1-C25
10	A	5510	CPS	C23-C24-N1-C25
10	C	5510	CPS	C23-C24-N1-C25
10	D	5510	CPS	C26-C27-N2-C29
10	D	5510	CPS	C31-C30-N2-C28
10	D	5510	CPS	C31-C30-N2-C29
10	B	5510	CPS	C26-C27-N2-C29
10	B	5510	CPS	C31-C30-N2-C28
10	B	5510	CPS	C31-C30-N2-C29
10	A	5510	CPS	C26-C27-N2-C29
10	A	5510	CPS	C31-C30-N2-C28
10	A	5510	CPS	C31-C30-N2-C29
10	C	5510	CPS	C26-C27-N2-C29
10	C	5510	CPS	C31-C30-N2-C28
10	C	5510	CPS	C31-C30-N2-C29
10	D	5510	CPS	O1-C24-N1-C25
10	B	5510	CPS	O1-C24-N1-C25
10	A	5510	CPS	O1-C24-N1-C25
10	C	5510	CPS	O1-C24-N1-C25
8	D	5508	ATP	O4'-C4'-C5'-O5'
8	B	5508	ATP	O4'-C4'-C5'-O5'
8	A	5508	ATP	O4'-C4'-C5'-O5'
8	C	5508	ATP	O4'-C4'-C5'-O5'
10	D	5510	CPS	C26-C27-N2-C28
10	B	5510	CPS	C26-C27-N2-C28
10	A	5510	CPS	C26-C27-N2-C28
10	C	5510	CPS	C26-C27-N2-C28

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Mol	Chain	Res	Type	Atoms
10	D	5510	CPS	C31-C32-S-O2S
10	B	5510	CPS	C31-C32-S-O2S
10	A	5510	CPS	C31-C32-S-O2S
10	C	5510	CPS	C31-C32-S-O2S
8	D	5508	ATP	C3'-C4'-C5'-O5'
8	B	5508	ATP	C3'-C4'-C5'-O5'
8	A	5508	ATP	C3'-C4'-C5'-O5'
8	C	5508	ATP	C3'-C4'-C5'-O5'
10	D	5510	CPS	C25-C26-C27-N2
10	B	5510	CPS	C25-C26-C27-N2
10	A	5510	CPS	C25-C26-C27-N2
10	C	5510	CPS	C25-C26-C27-N2
10	D	5510	CPS	C26-C27-N2-C30
10	B	5510	CPS	C26-C27-N2-C30
10	A	5510	CPS	C26-C27-N2-C30
10	C	5510	CPS	C26-C27-N2-C30
10	D	5510	CPS	C31-C32-S-O3S
10	D	5510	CPS	C31-C32-S-O1S
10	B	5510	CPS	C31-C32-S-O3S
10	B	5510	CPS	C31-C32-S-O1S
10	A	5510	CPS	C31-C32-S-O3S
10	A	5510	CPS	C31-C32-S-O1S
10	C	5510	CPS	C31-C32-S-O3S
10	C	5510	CPS	C31-C32-S-O1S
10	D	5510	CPS	C22-C20-C9-C5
10	B	5510	CPS	C22-C20-C9-C5
10	C	5510	CPS	C22-C20-C9-C5
10	D	5510	CPS	C21-C20-C9-C5
10	A	5510	CPS	C21-C20-C9-C5
10	C	5510	CPS	C21-C20-C9-C5
10	A	5510	CPS	C22-C20-C9-C5
10	B	5510	CPS	C21-C20-C9-C5
10	D	5510	CPS	C22-C20-C9-C8
10	C	5510	CPS	C22-C20-C9-C8
10	B	5510	CPS	C22-C20-C9-C8
10	A	5510	CPS	C22-C20-C9-C8
8	D	5507	ATP	C4'-C5'-O5'-PA
8	B	5507	ATP	C4'-C5'-O5'-PA
8	A	5507	ATP	C4'-C5'-O5'-PA
8	C	5507	ATP	C4'-C5'-O5'-PA
10	D	5510	CPS	C9-C20-C22-C23
10	B	5510	CPS	C9-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
10	A	5510	CPS	C9-C20-C22-C23
10	C	5510	CPS	C9-C20-C22-C23
10	D	5510	CPS	C20-C22-C23-C24
10	B	5510	CPS	C20-C22-C23-C24
10	A	5510	CPS	C20-C22-C23-C24
10	C	5510	CPS	C20-C22-C23-C24

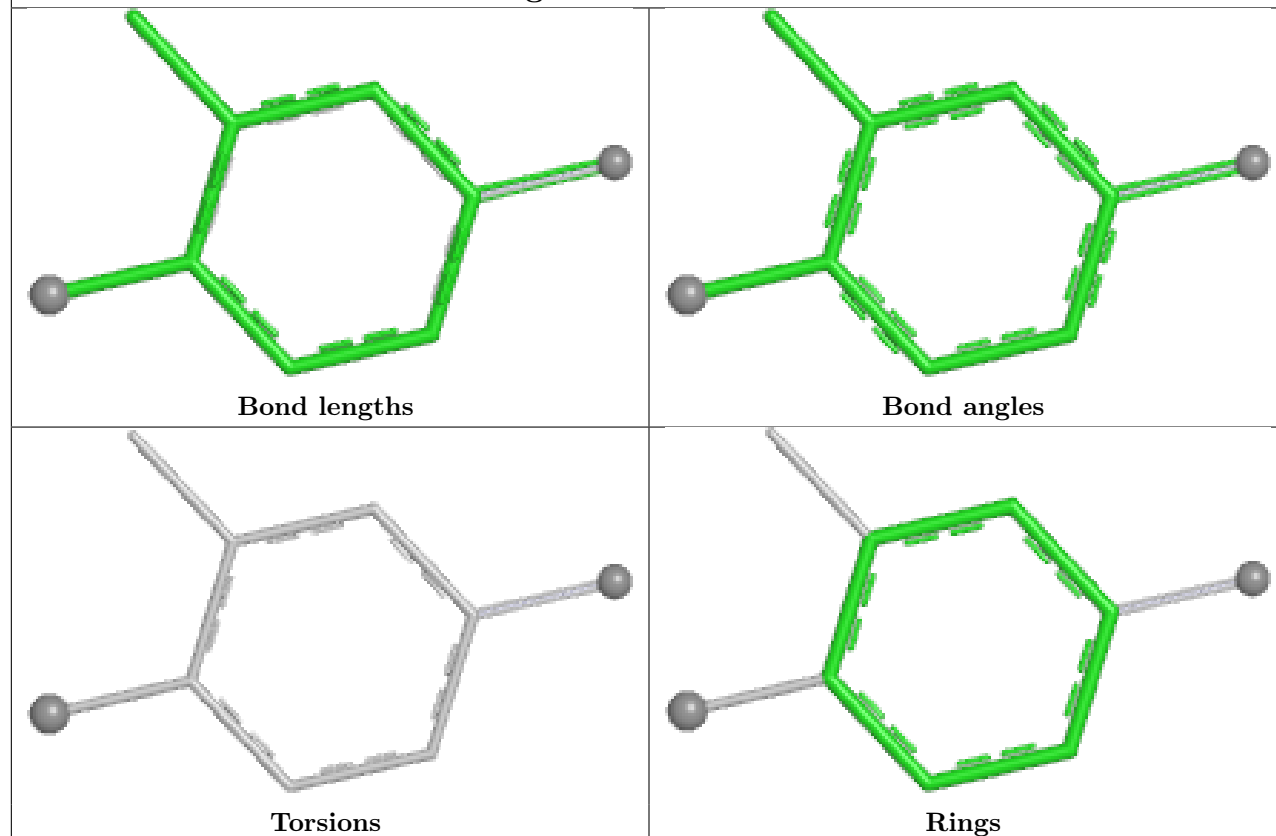
There are no ring outliers.

7 monomers are involved in 7 short contacts:

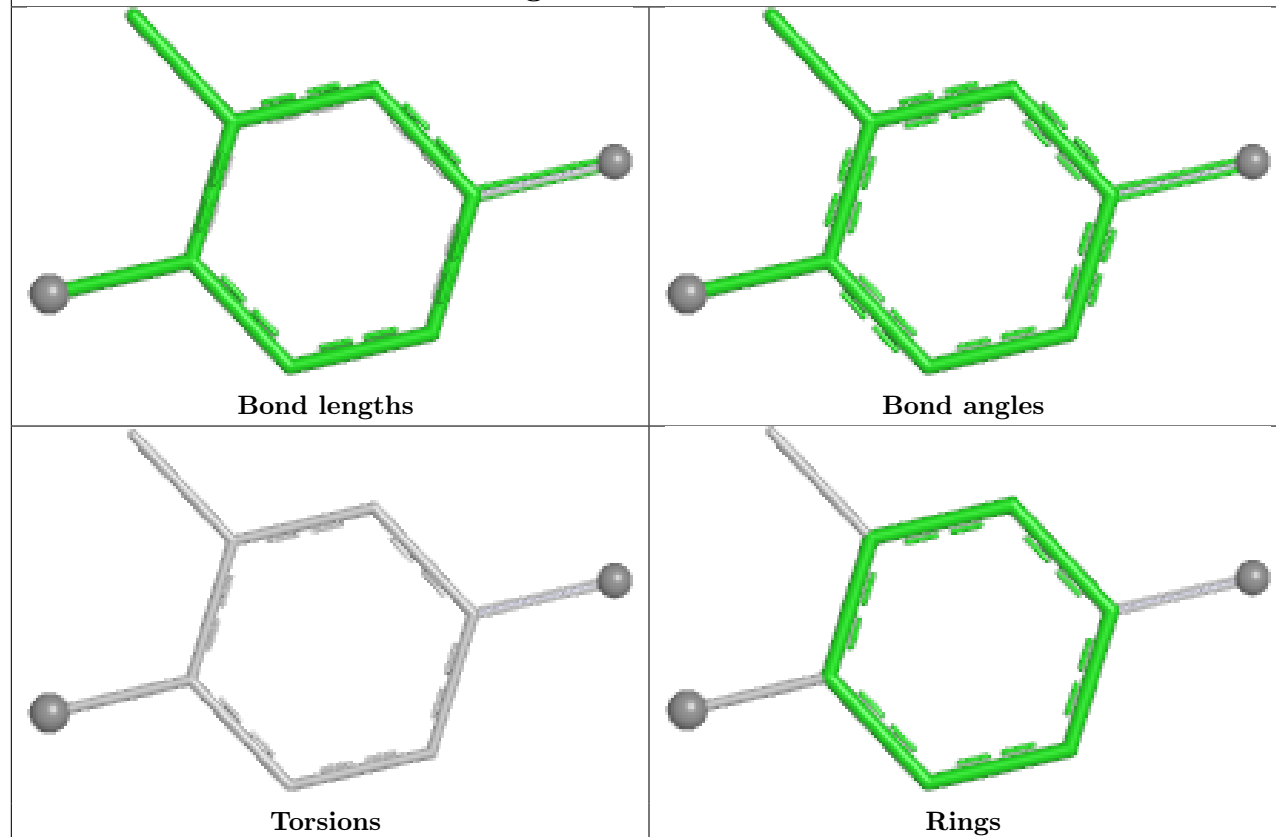
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	5510	CPS	1	0
8	C	5508	ATP	1	0
10	D	5510	CPS	1	0
10	C	5510	CPS	1	0
8	A	5508	ATP	1	0
8	B	5508	ATP	1	0
8	D	5508	ATP	1	0

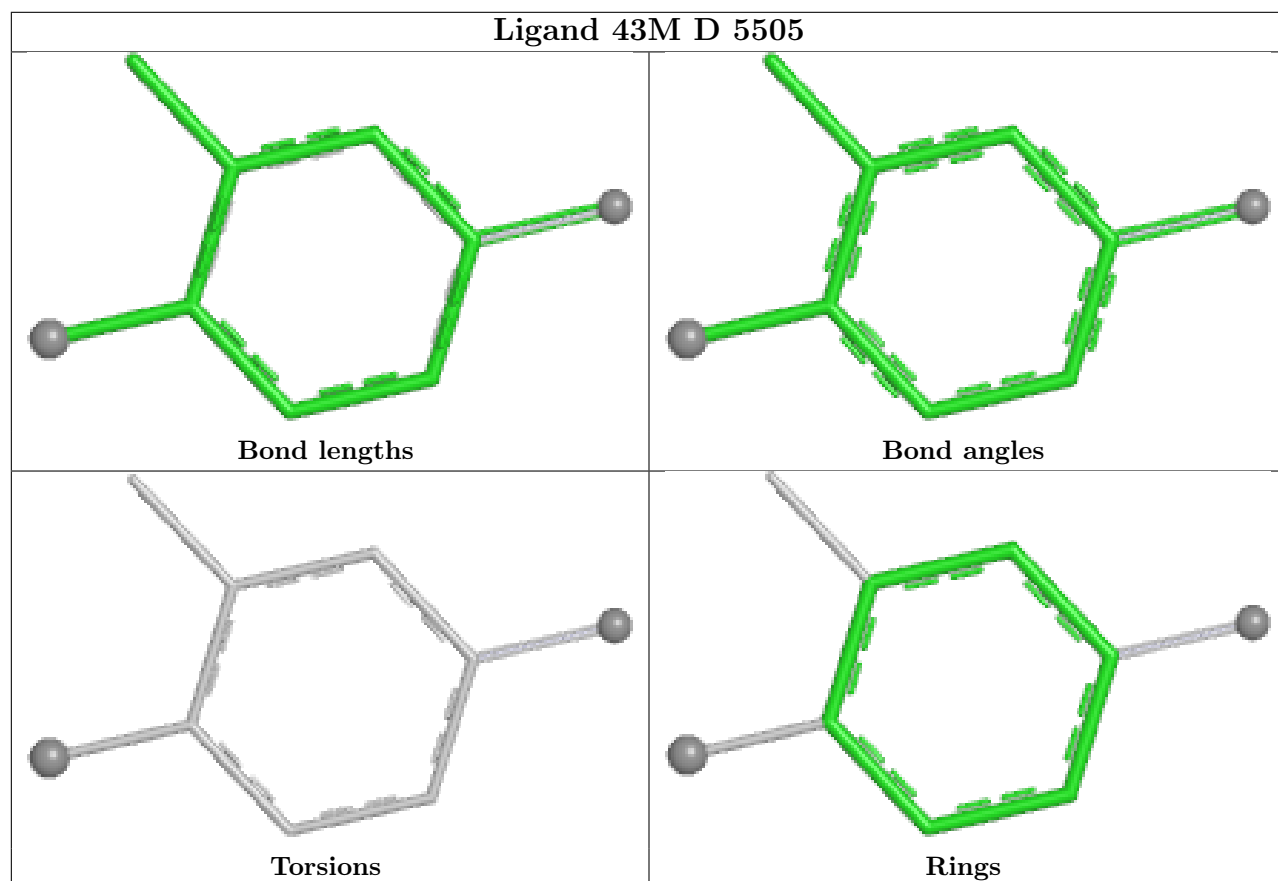
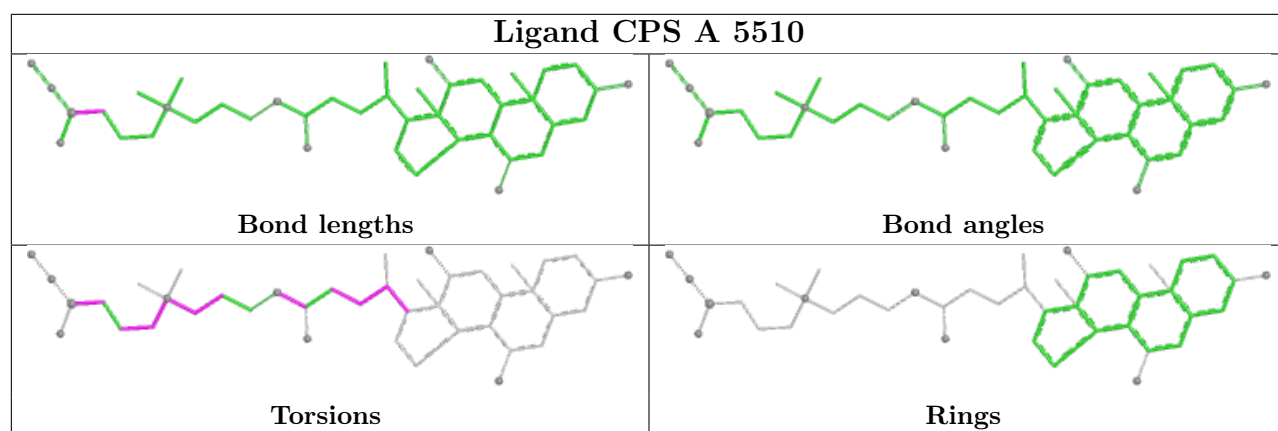
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

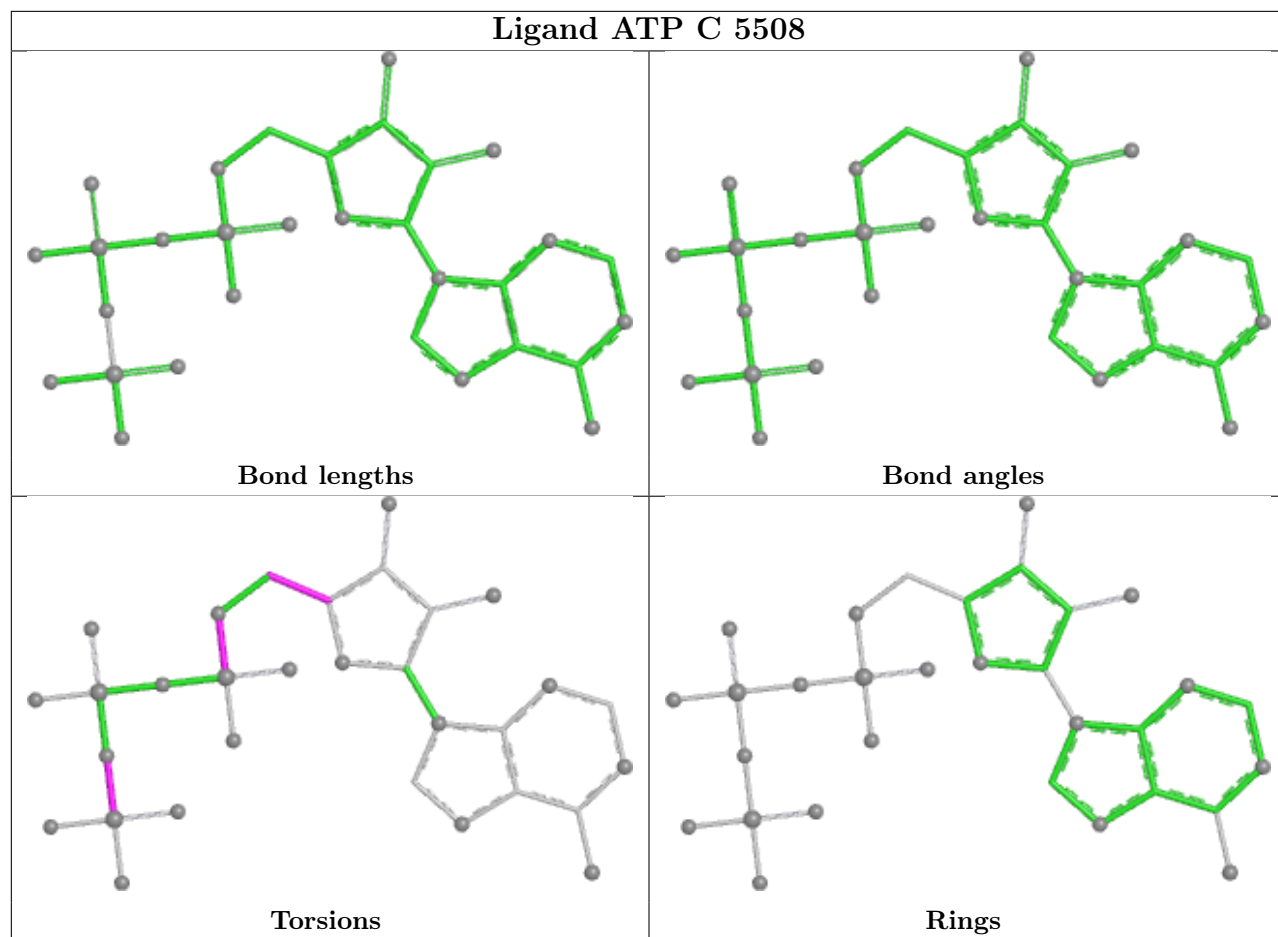
Ligand 43M C 5505

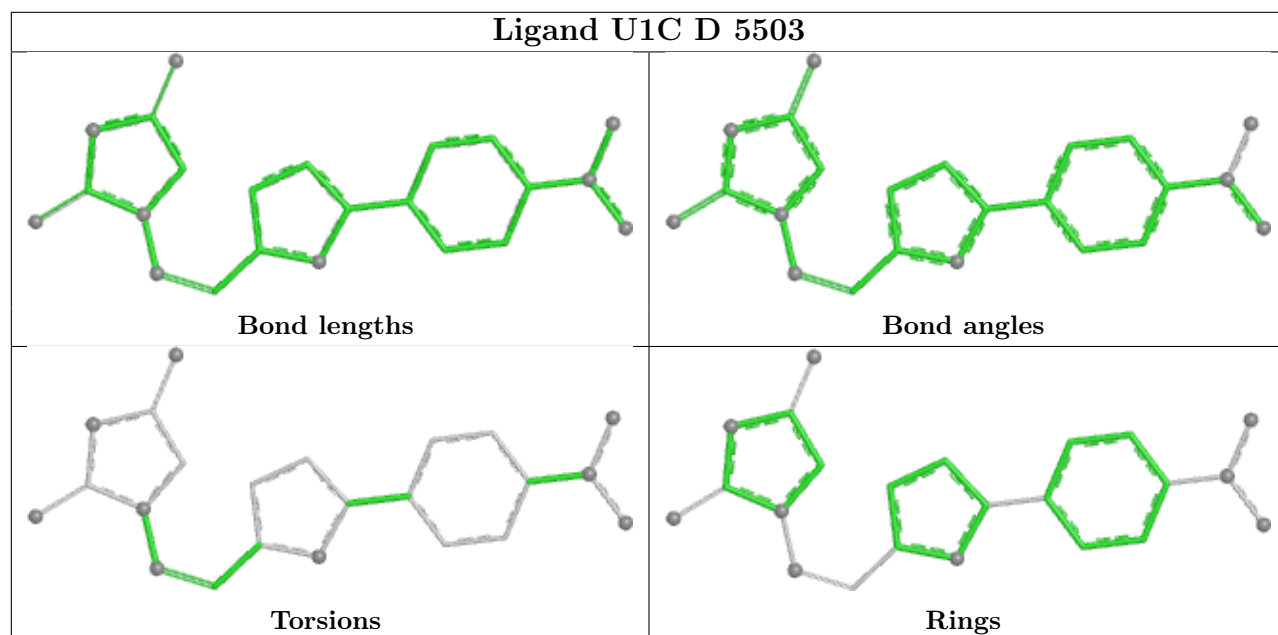
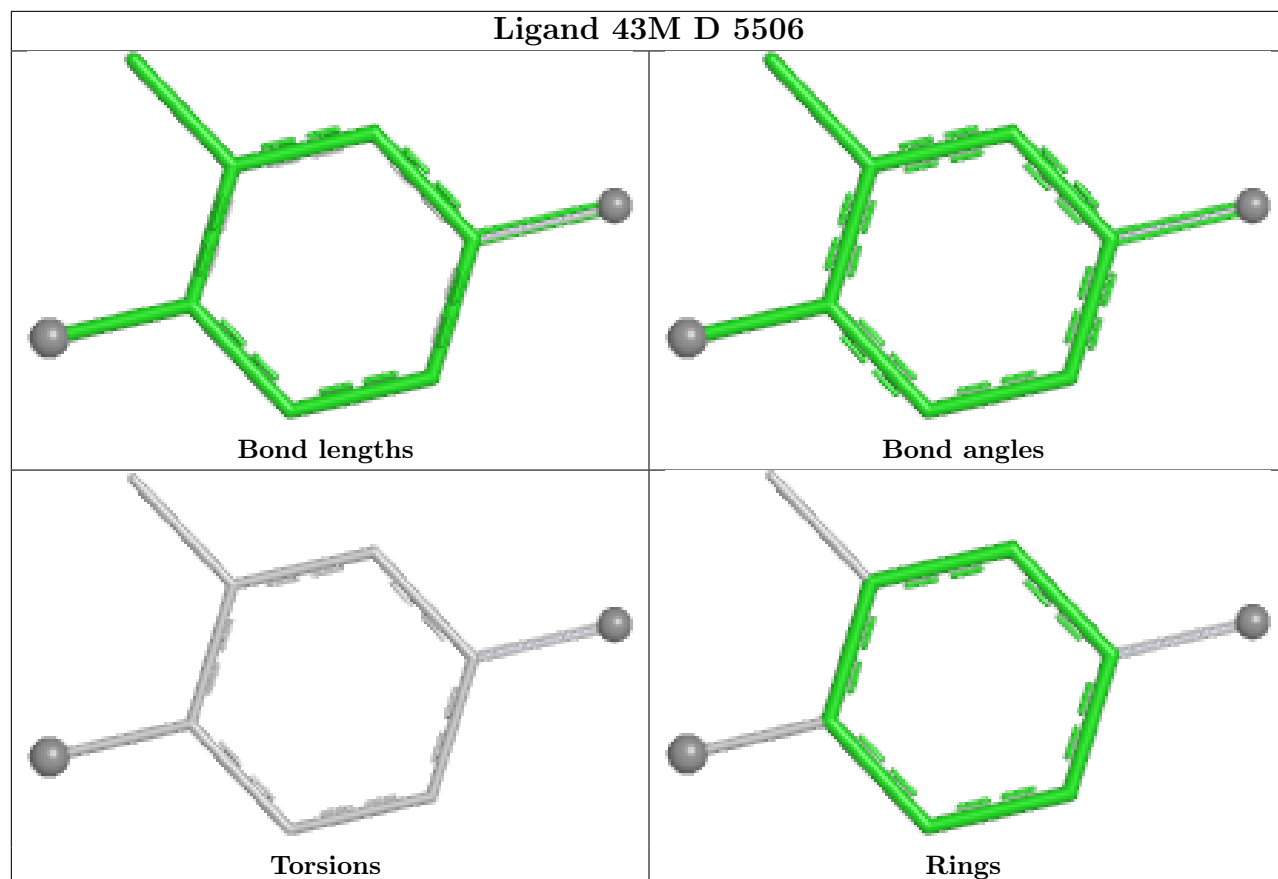


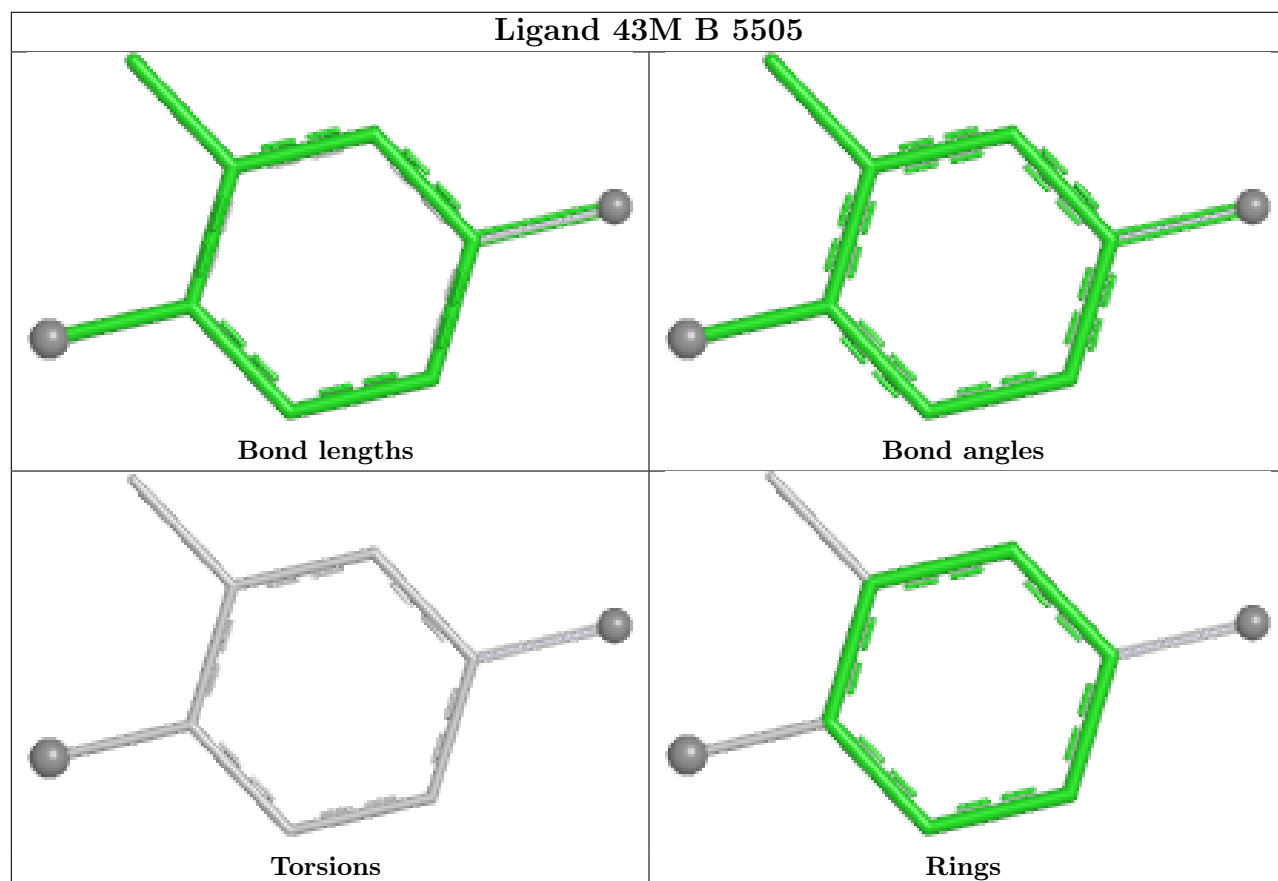
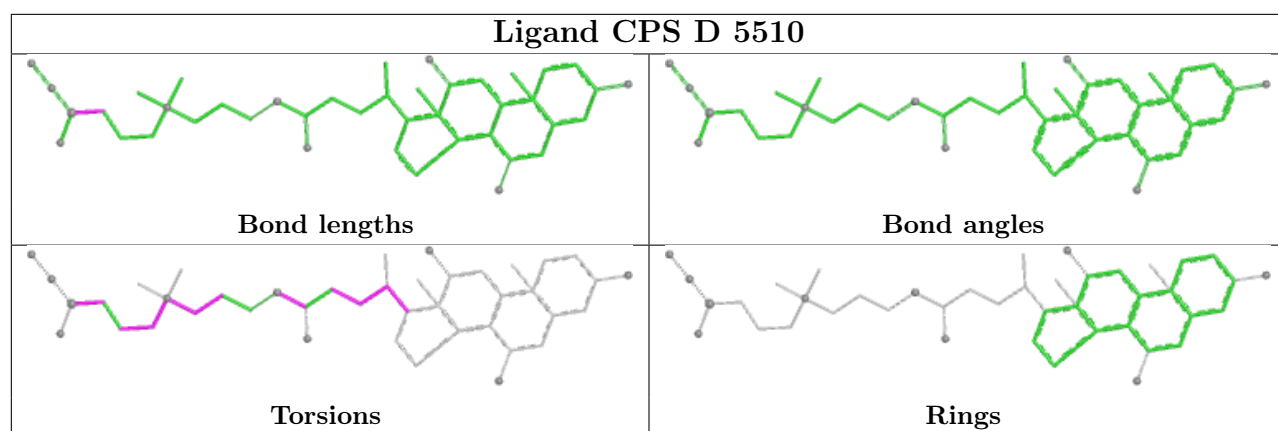
Ligand 43M A 5504



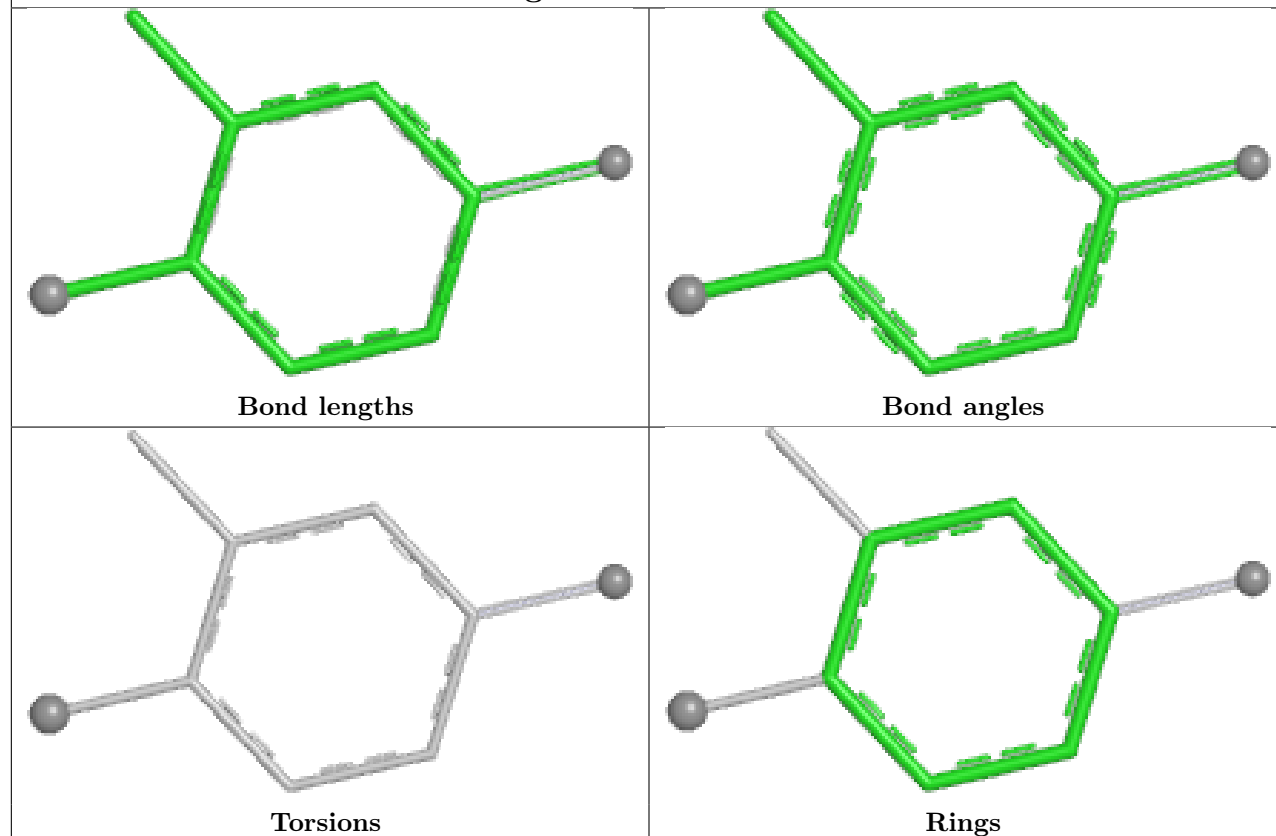




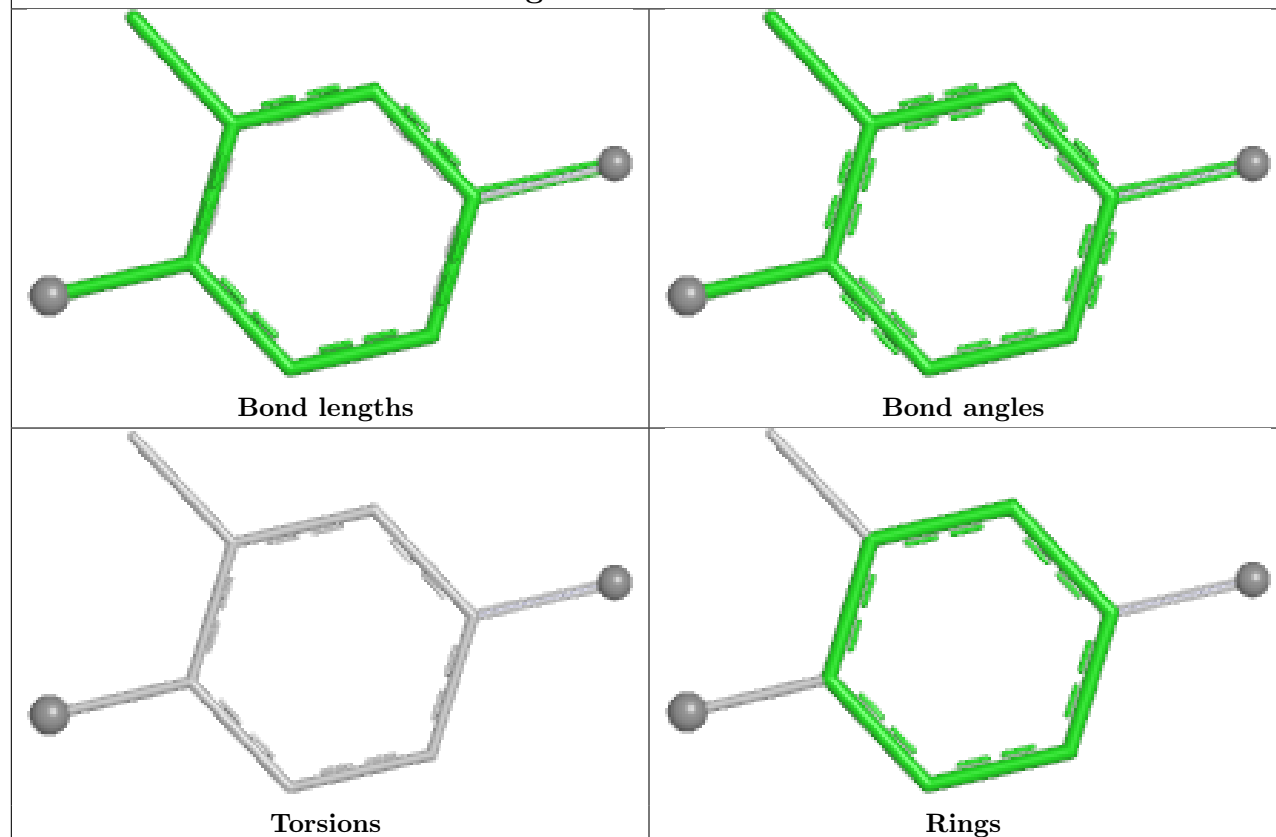


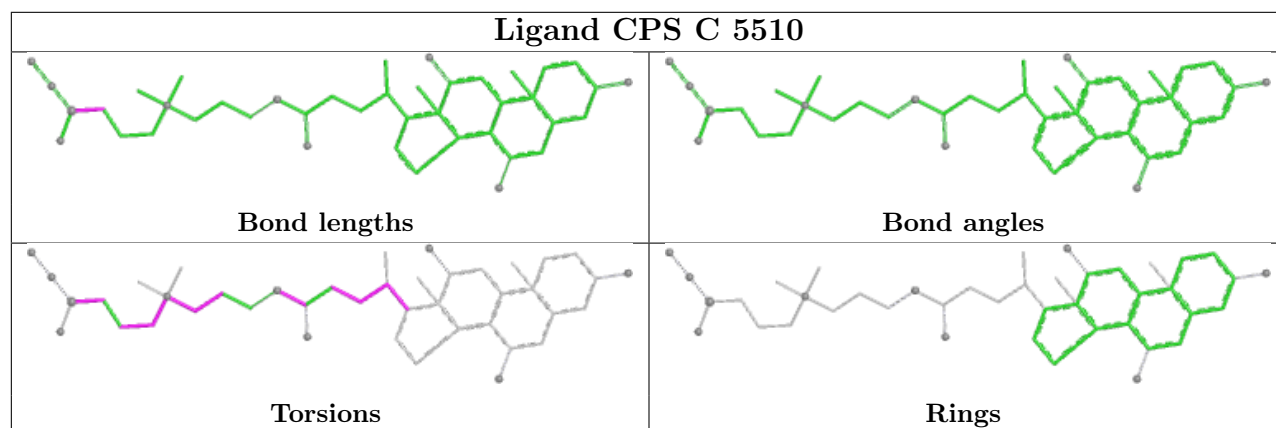
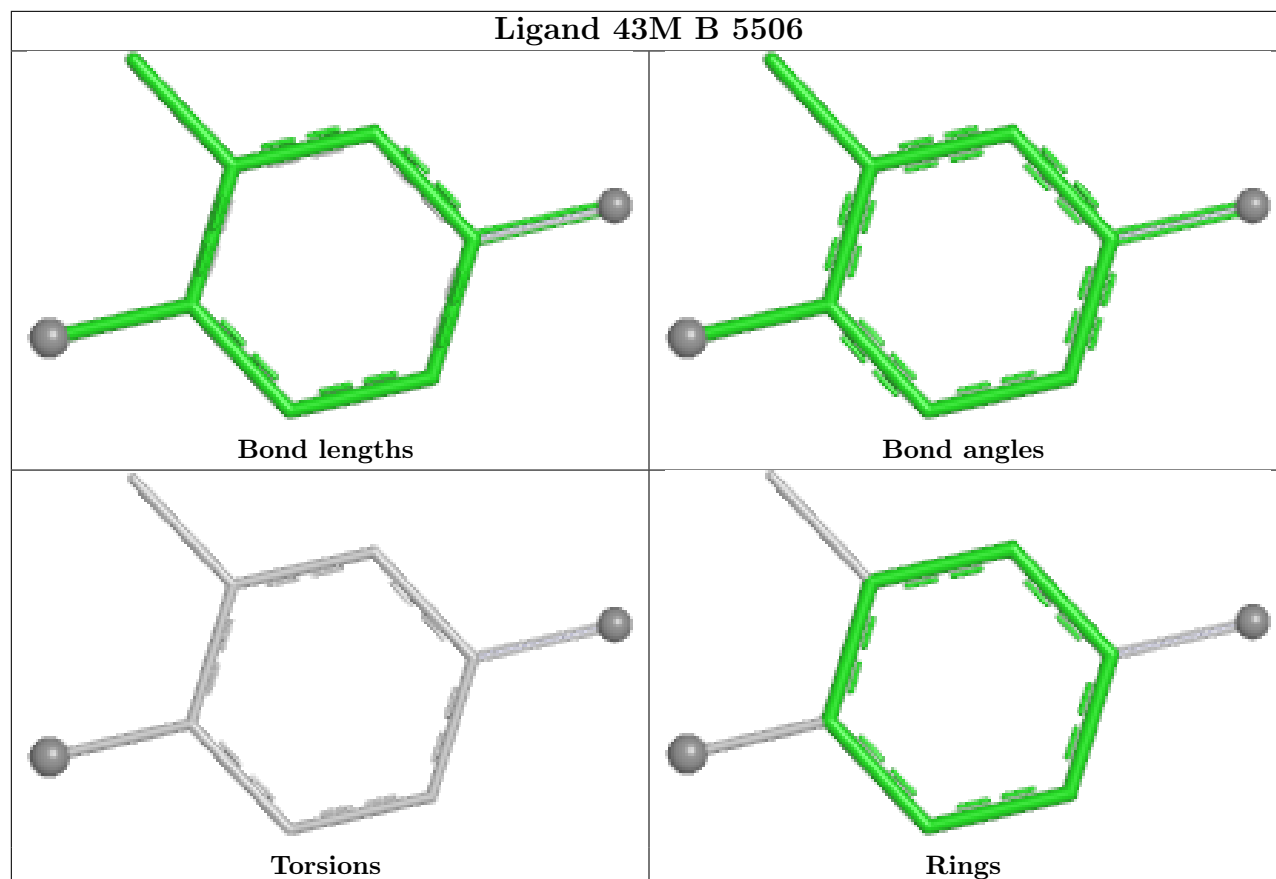


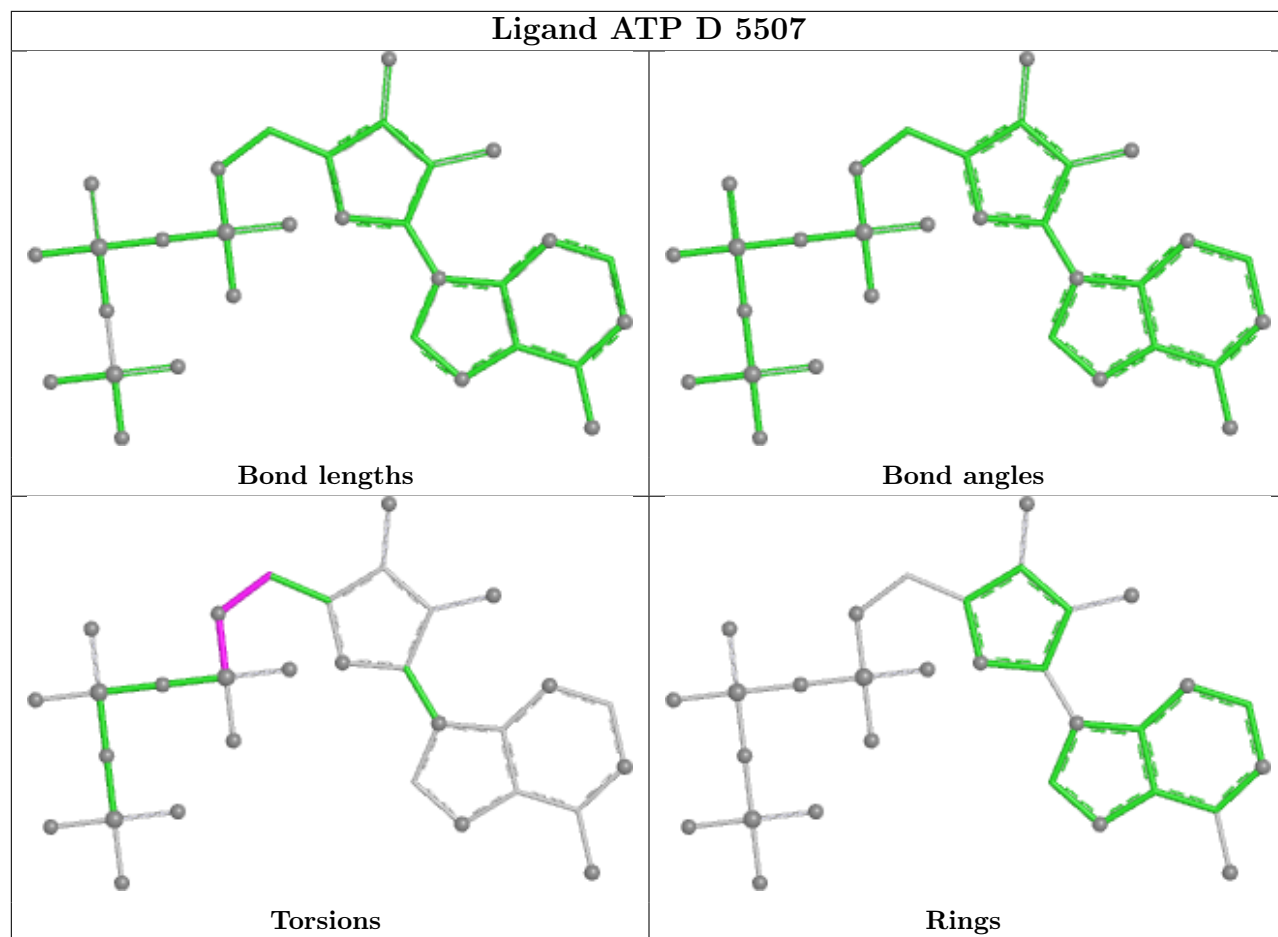
Ligand 43M A 5506

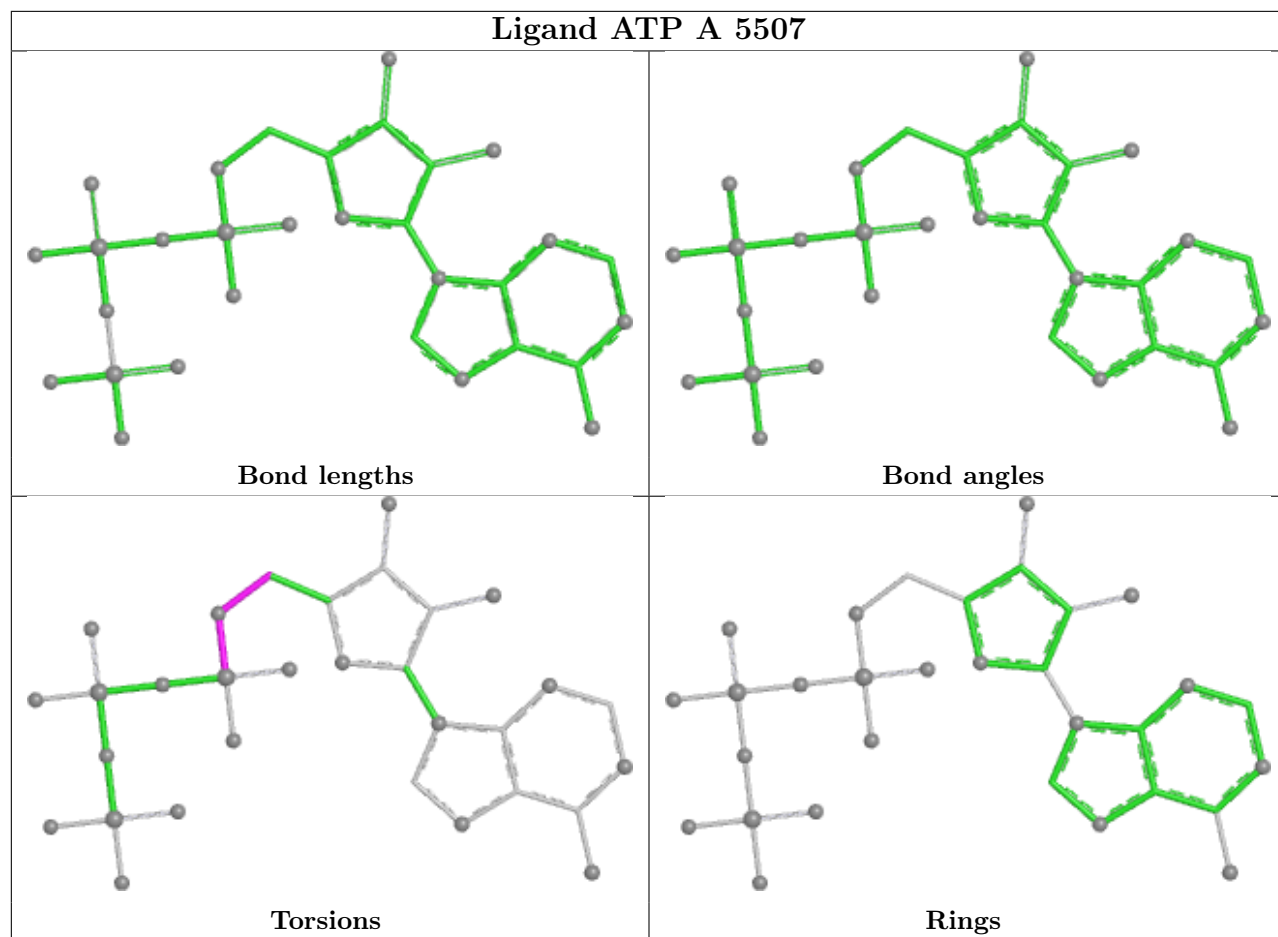


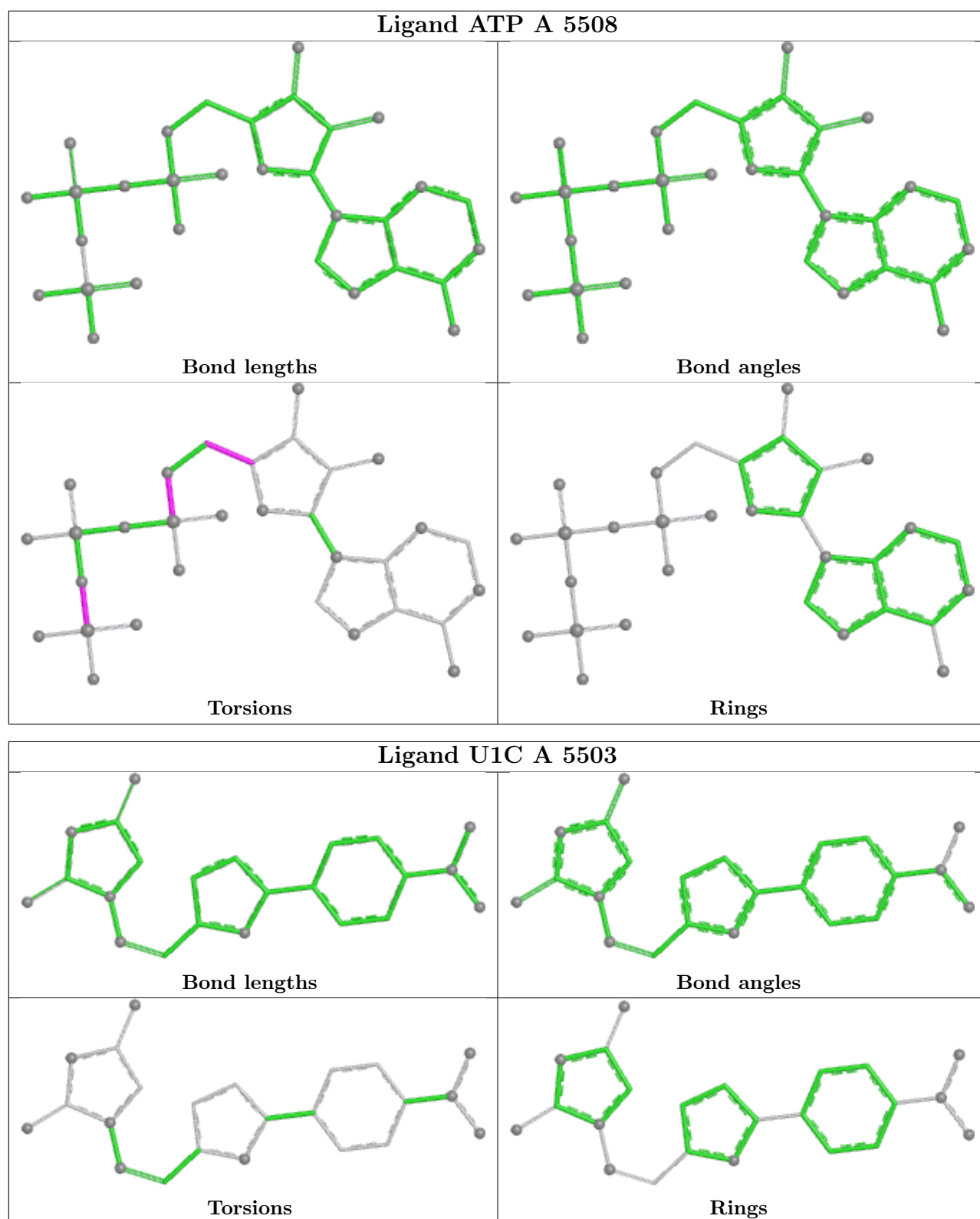
Ligand 43M C 5504

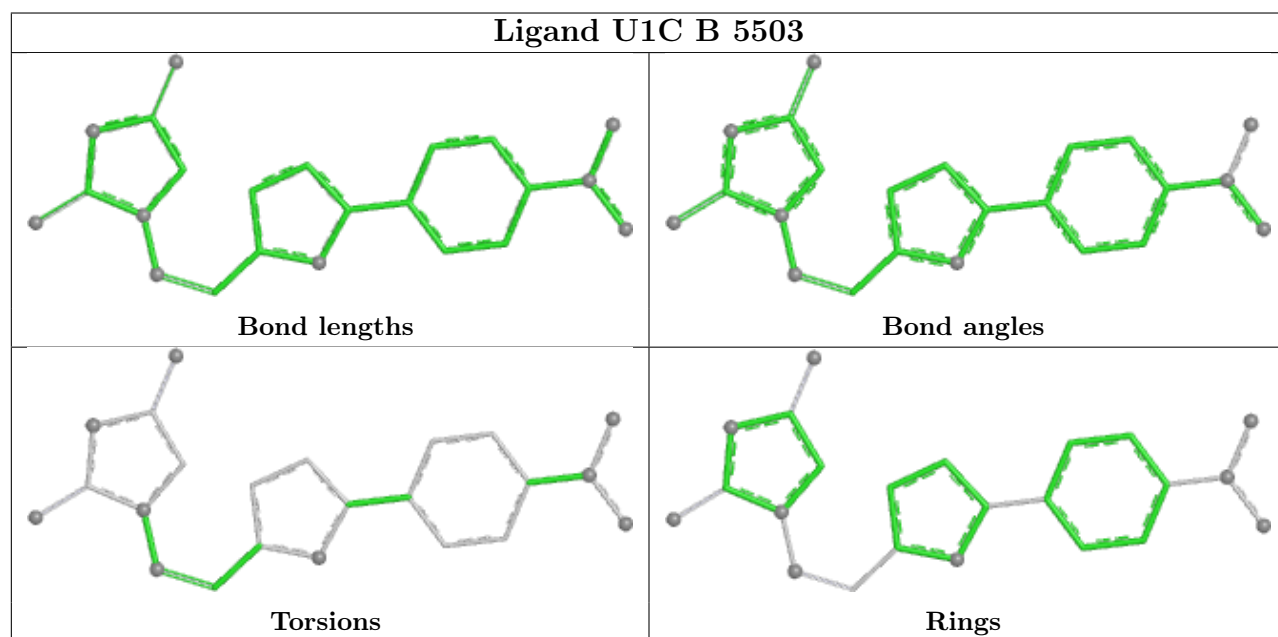
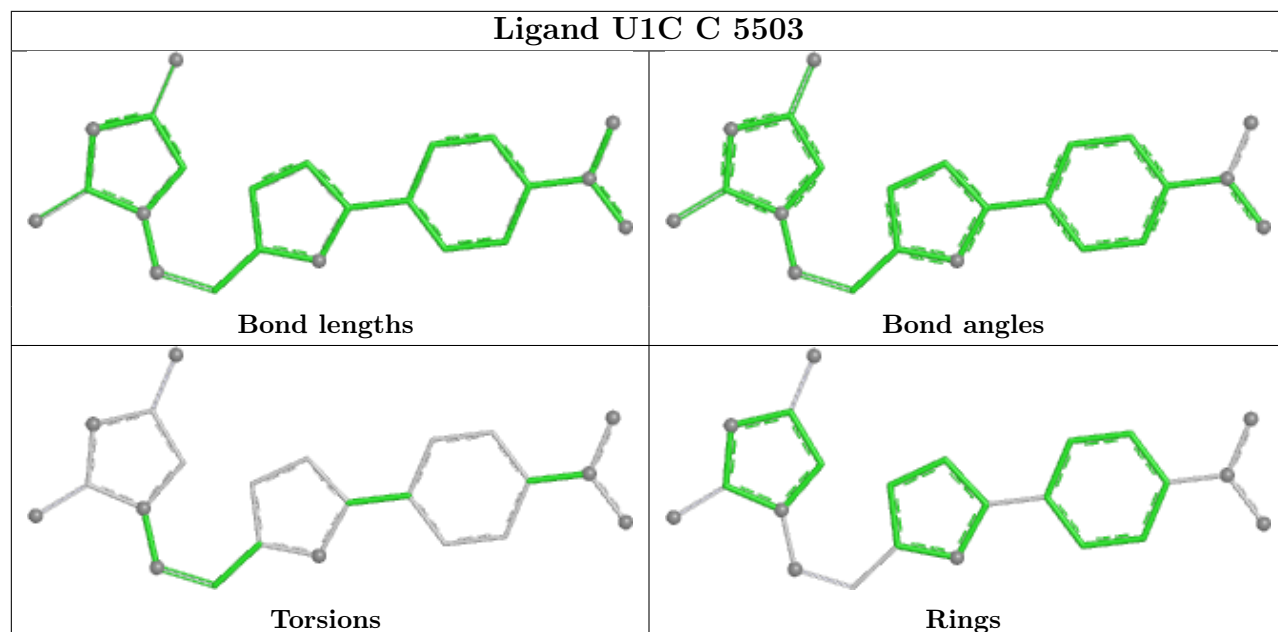


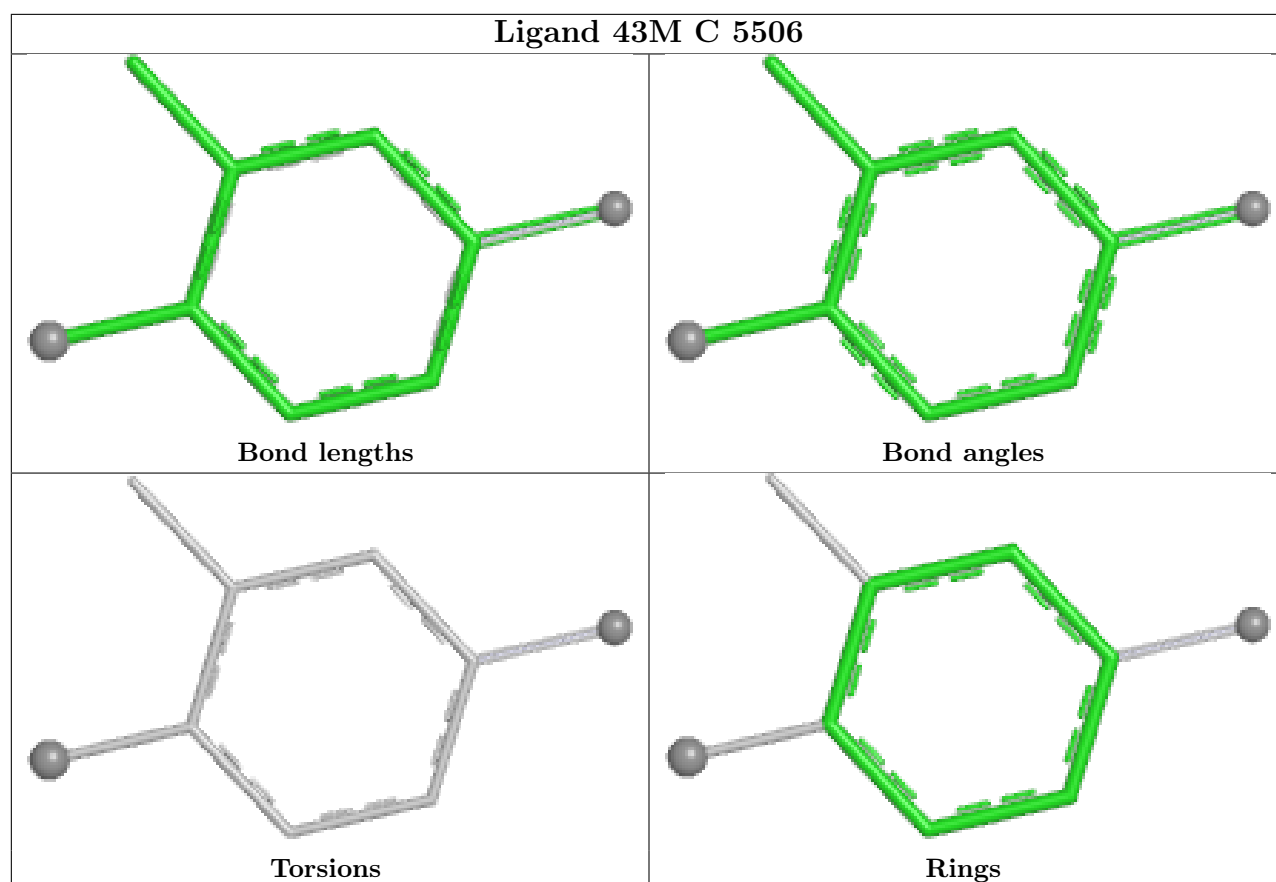


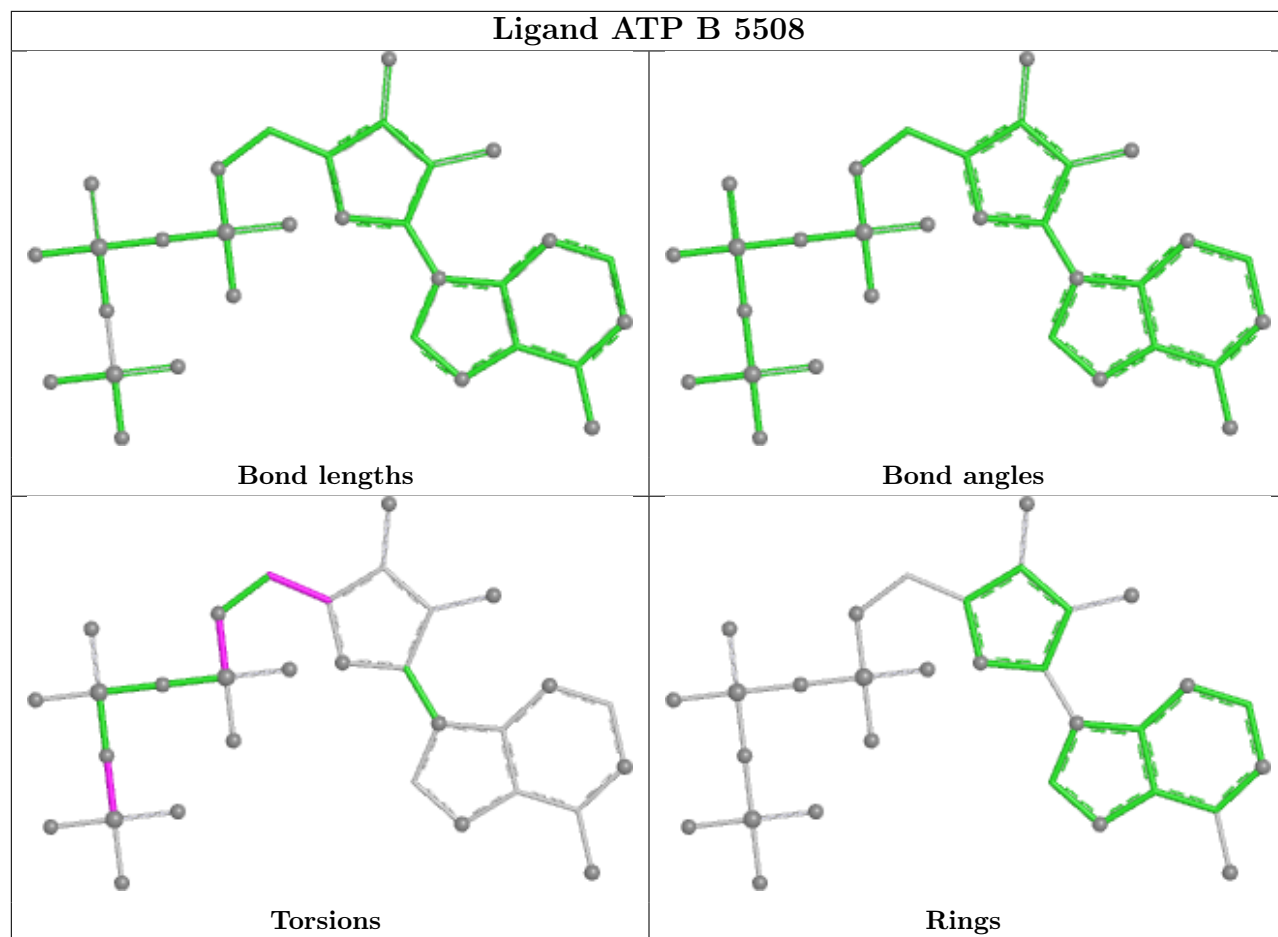


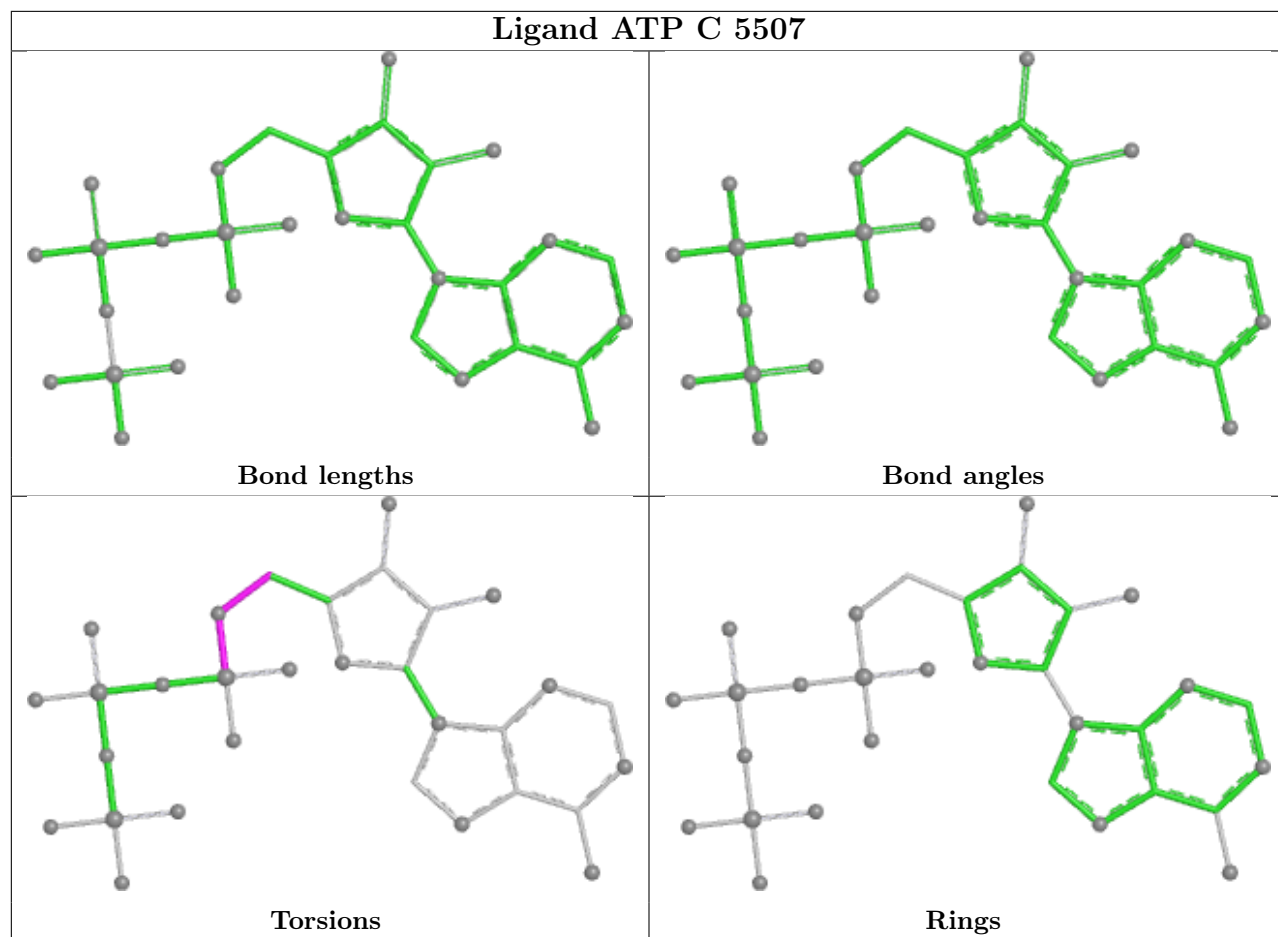


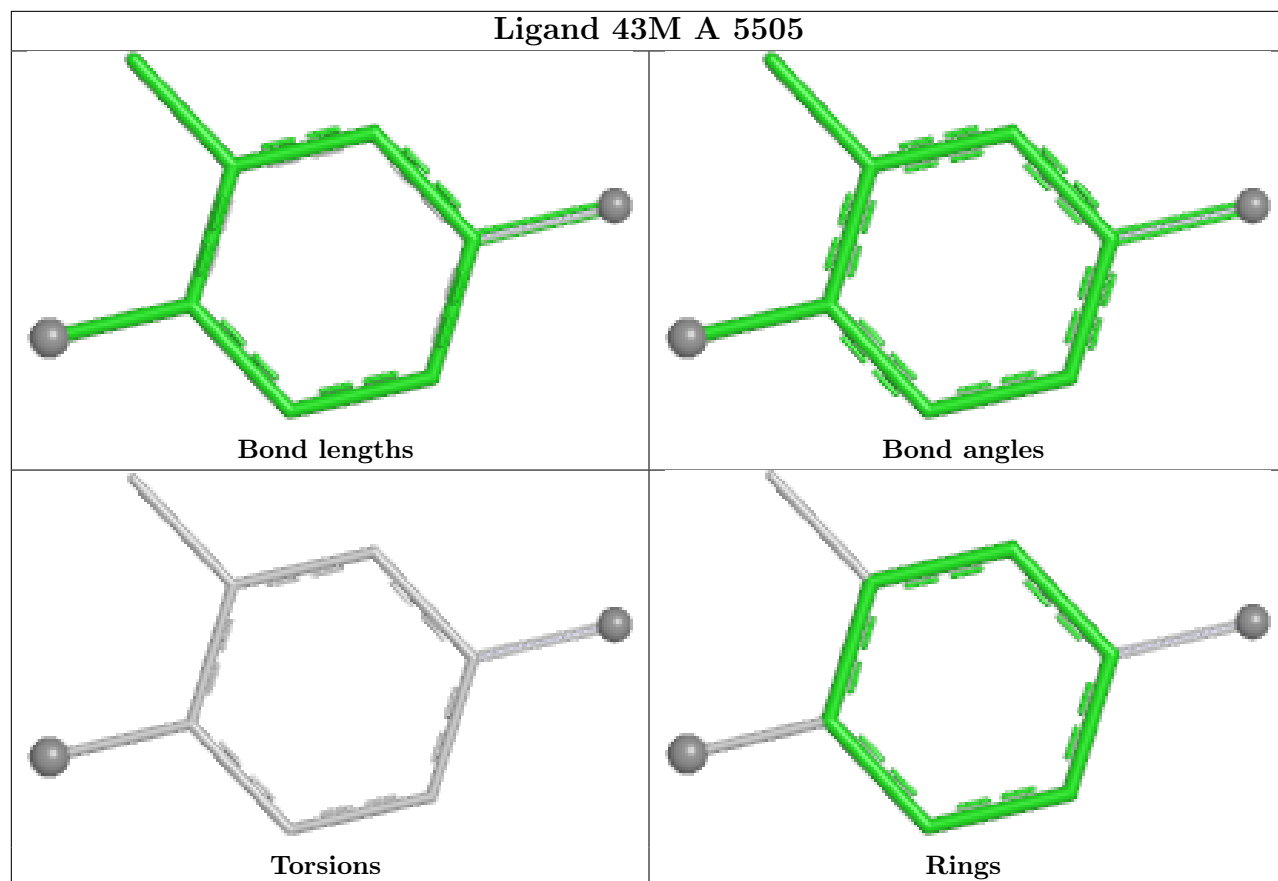


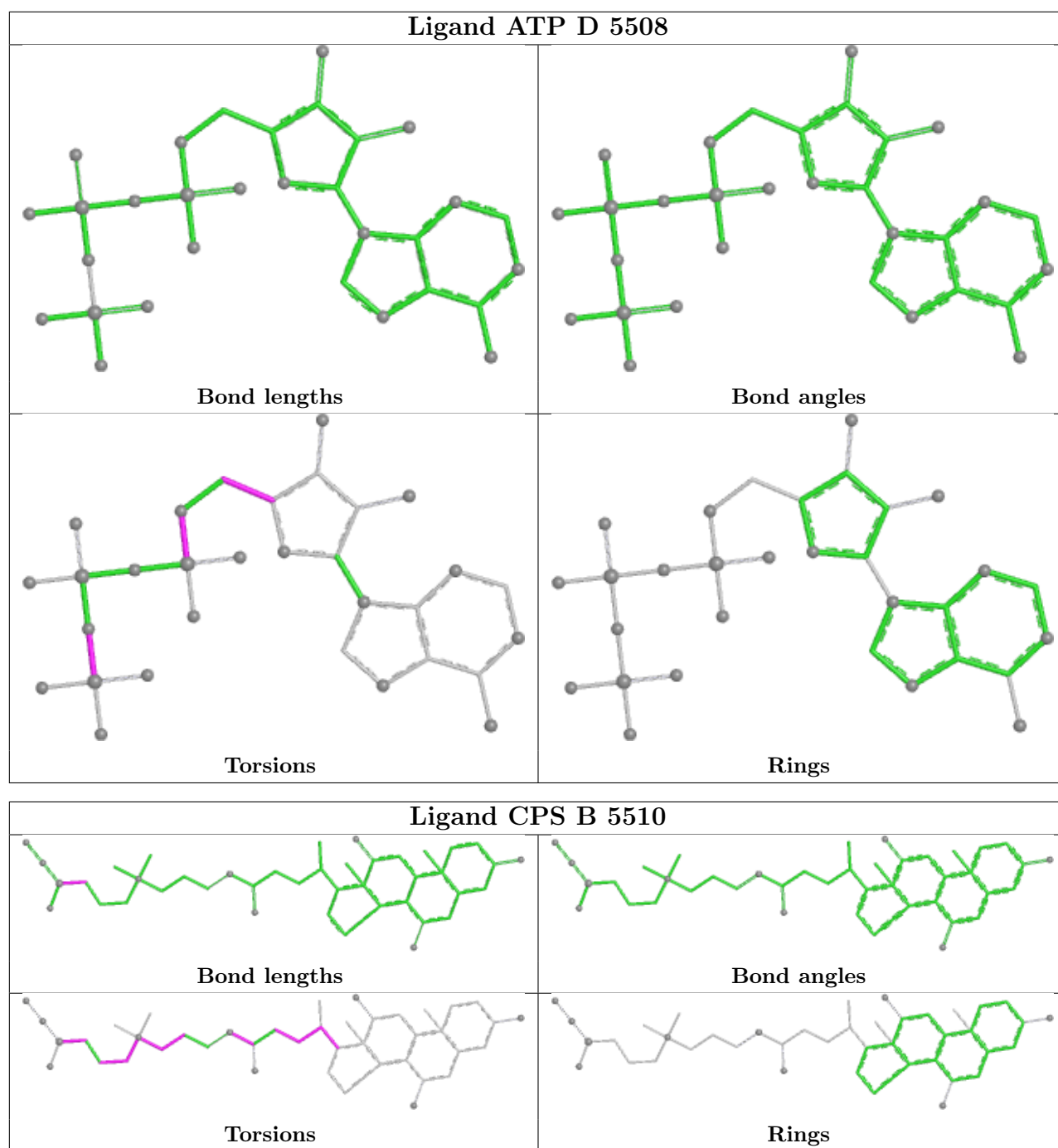


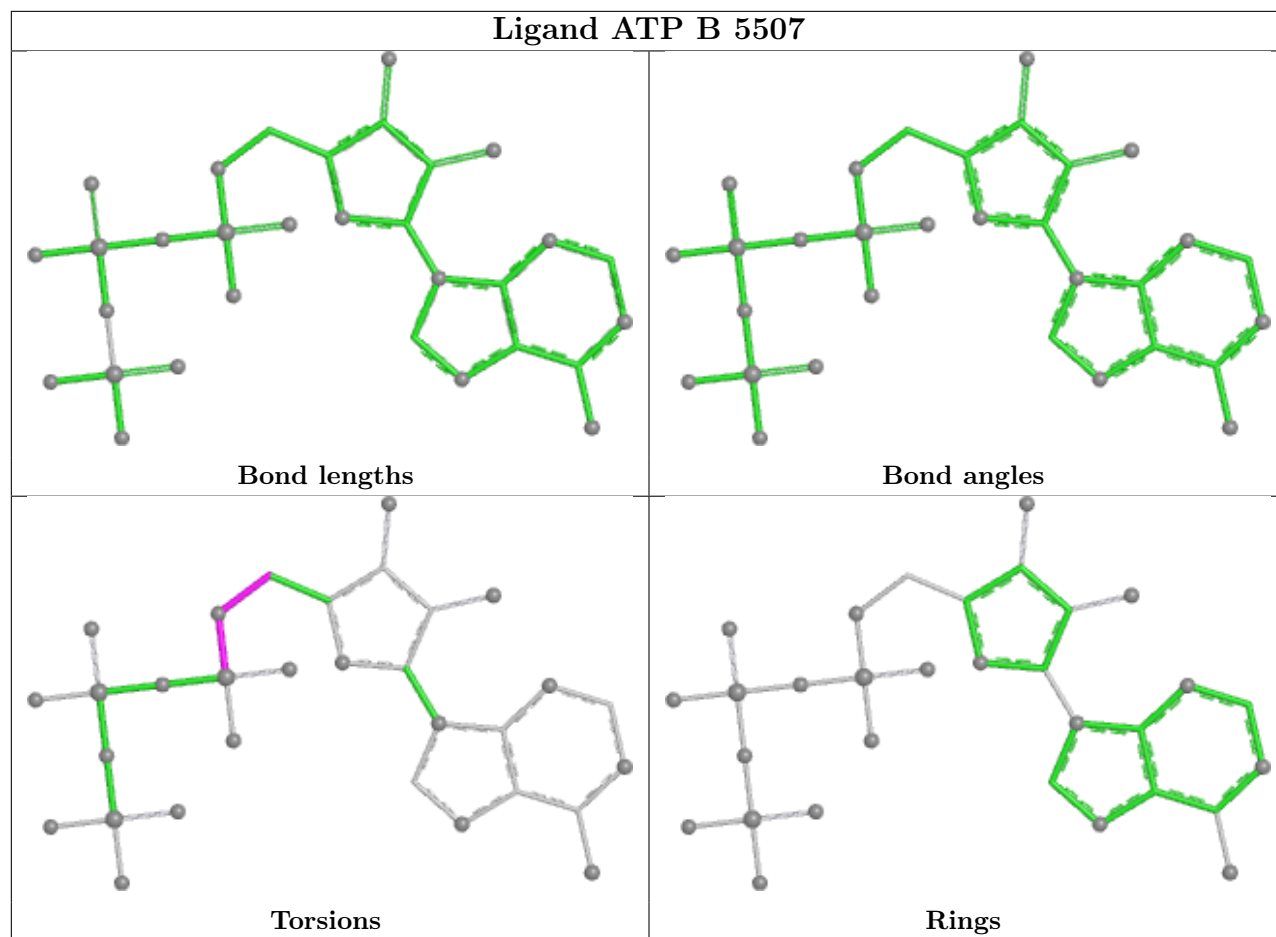




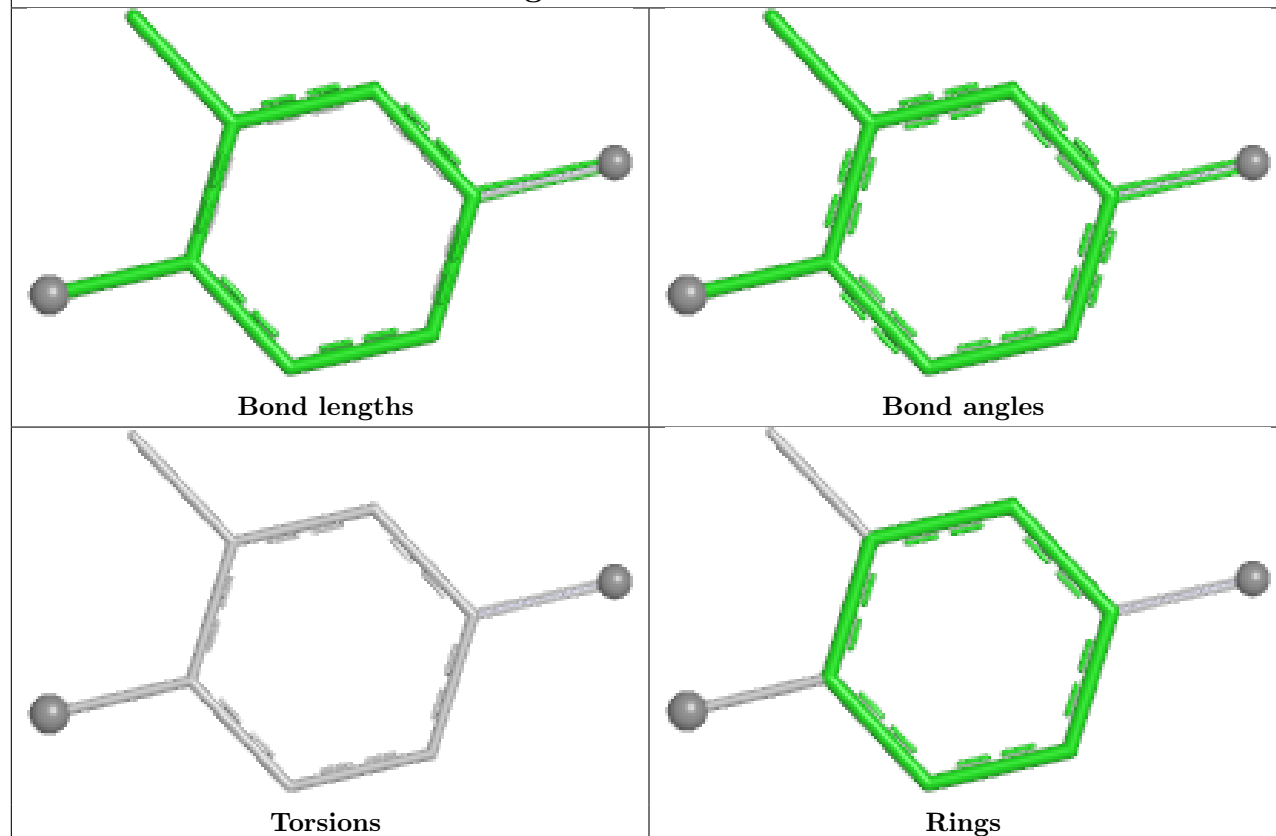




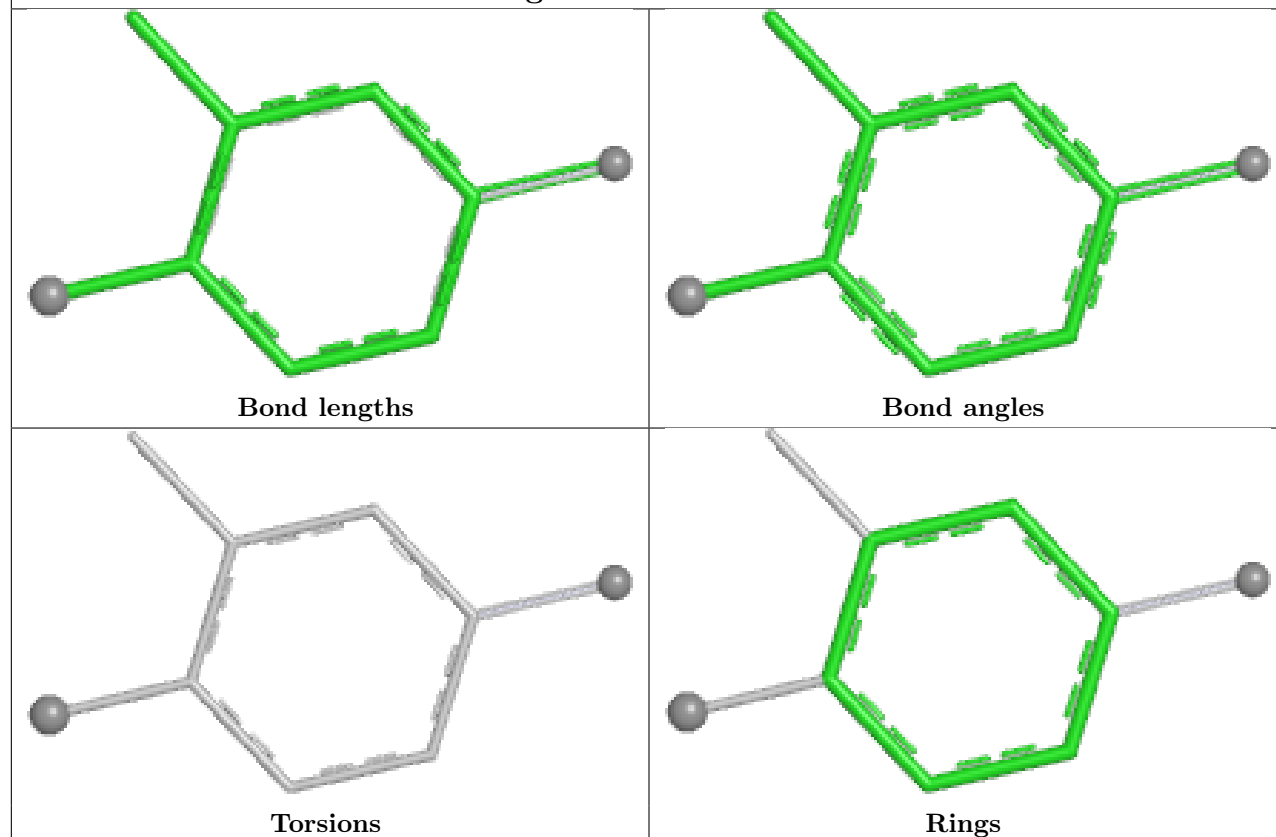




Ligand 43M D 5504



Ligand 43M B 5504



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

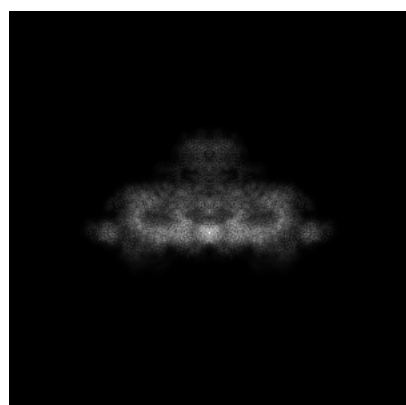
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-74445. These allow visual inspection of the internal detail of the map and identification of artifacts.

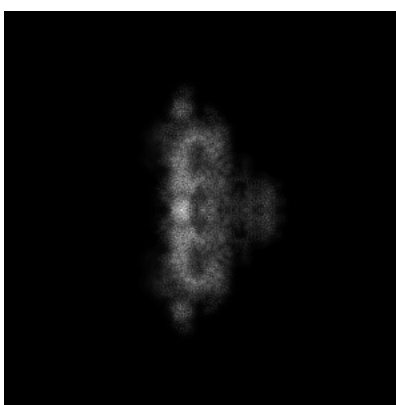
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

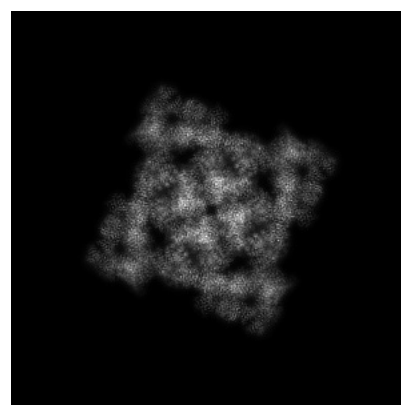
6.1.1 Primary map



X



Y

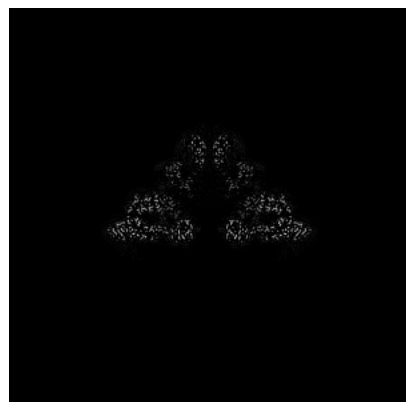


Z

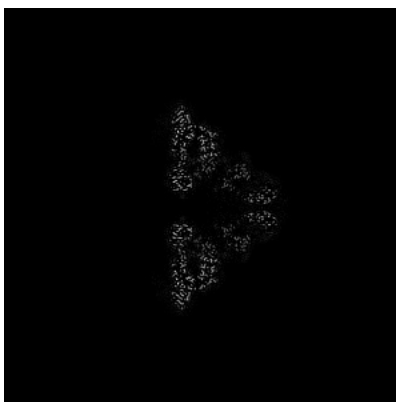
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

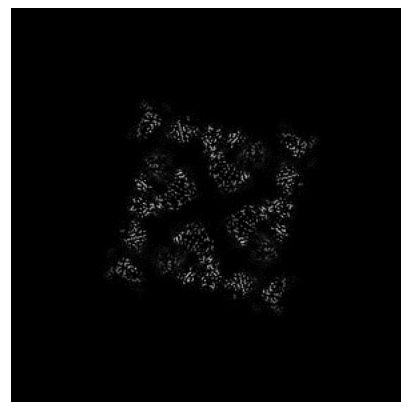
6.2.1 Primary map



X Index: 256



Y Index: 256

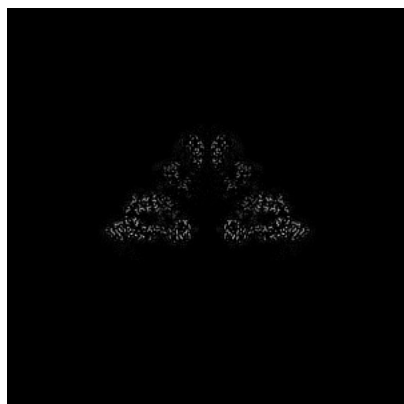


Z Index: 256

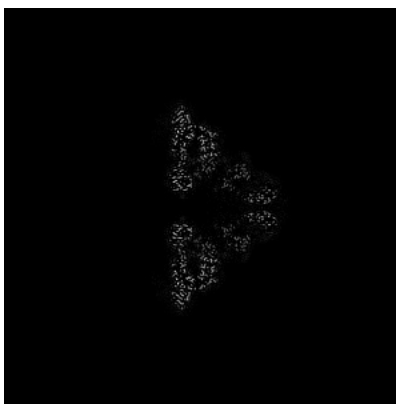
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

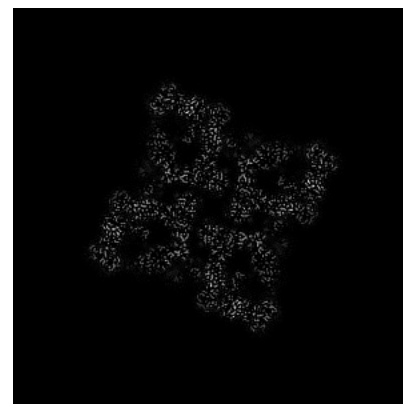
6.3.1 Primary map



X Index: 256



Y Index: 256

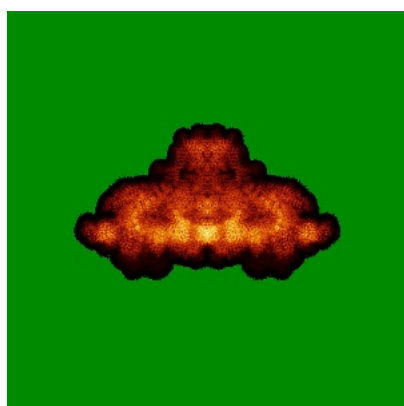


Z Index: 225

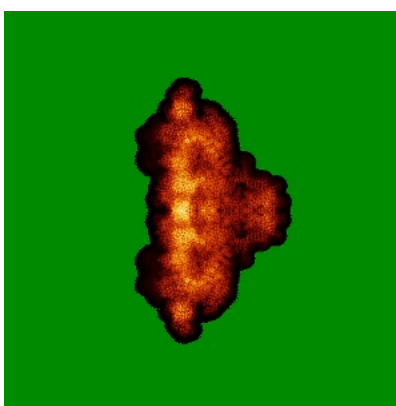
The images above show the largest variance slices of the map in three orthogonal directions.

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

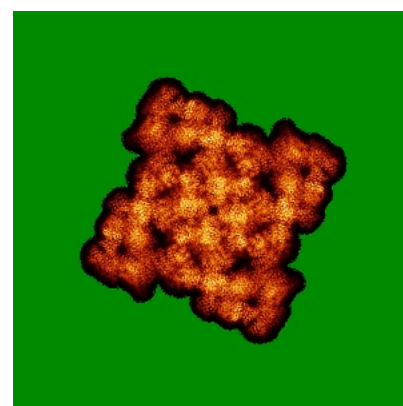
6.4.1 Primary map



X



Y

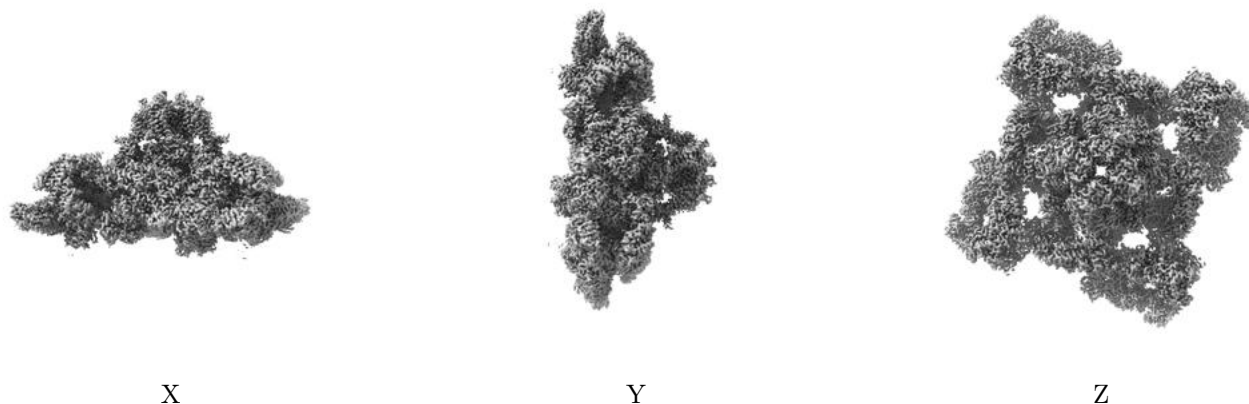


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

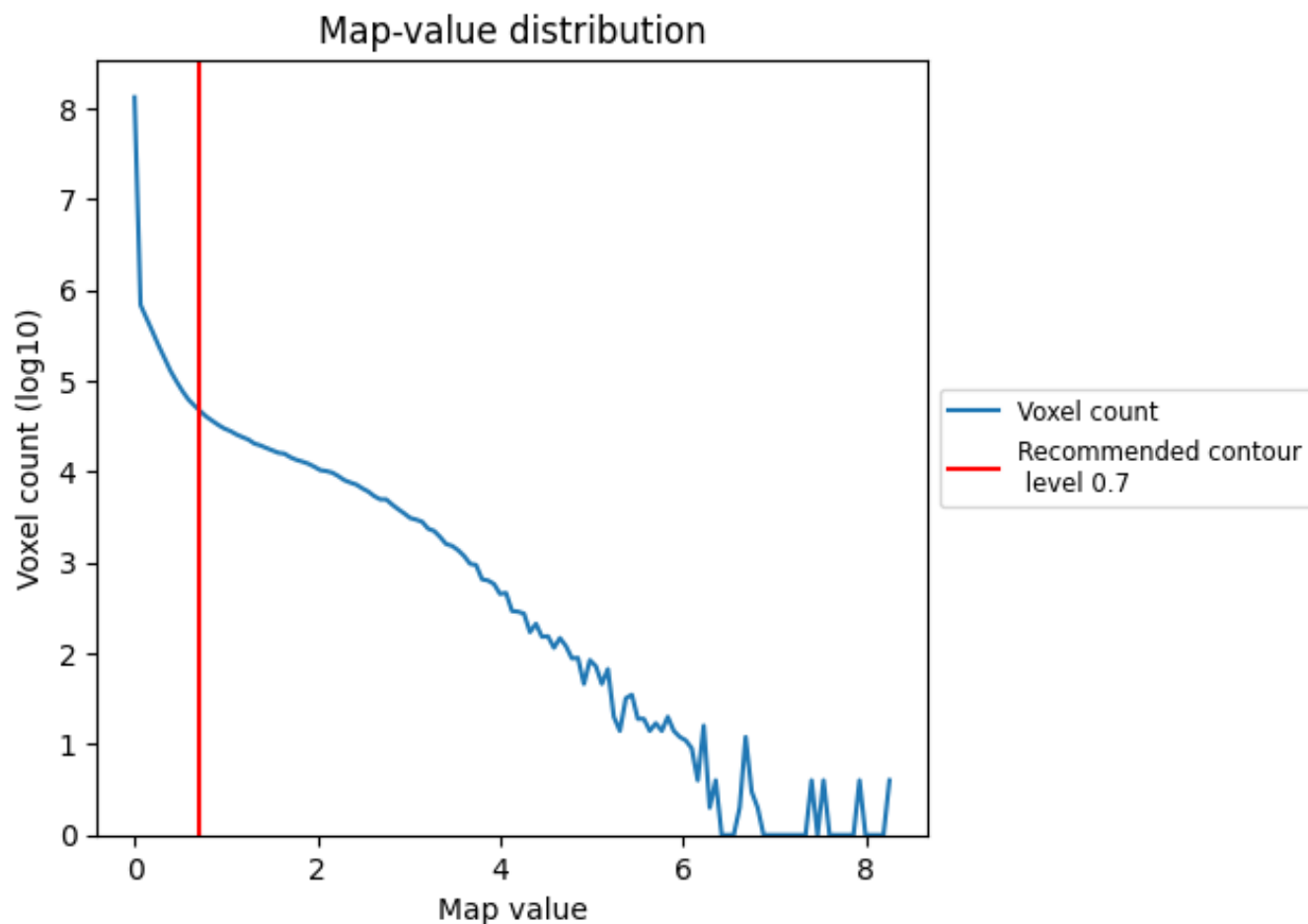
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

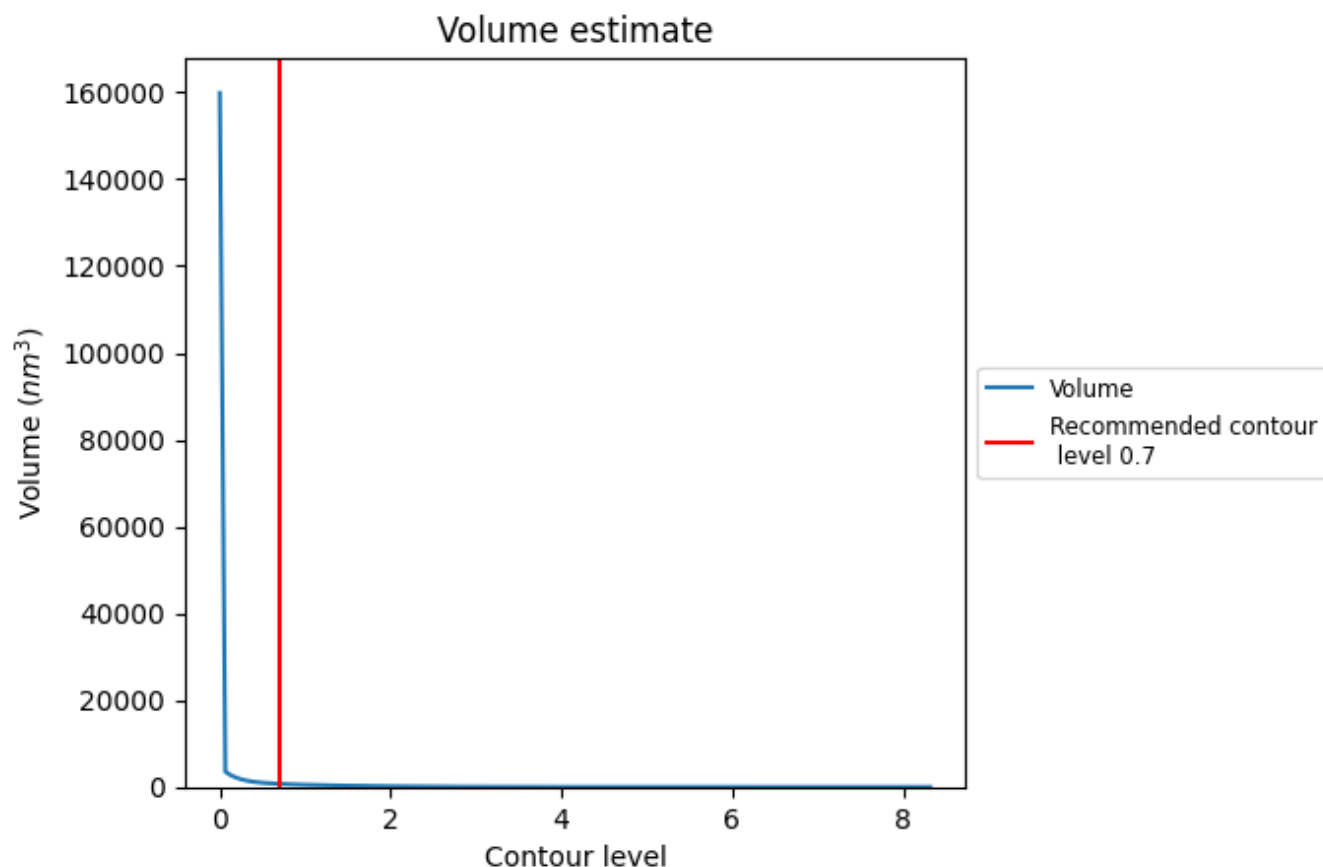
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

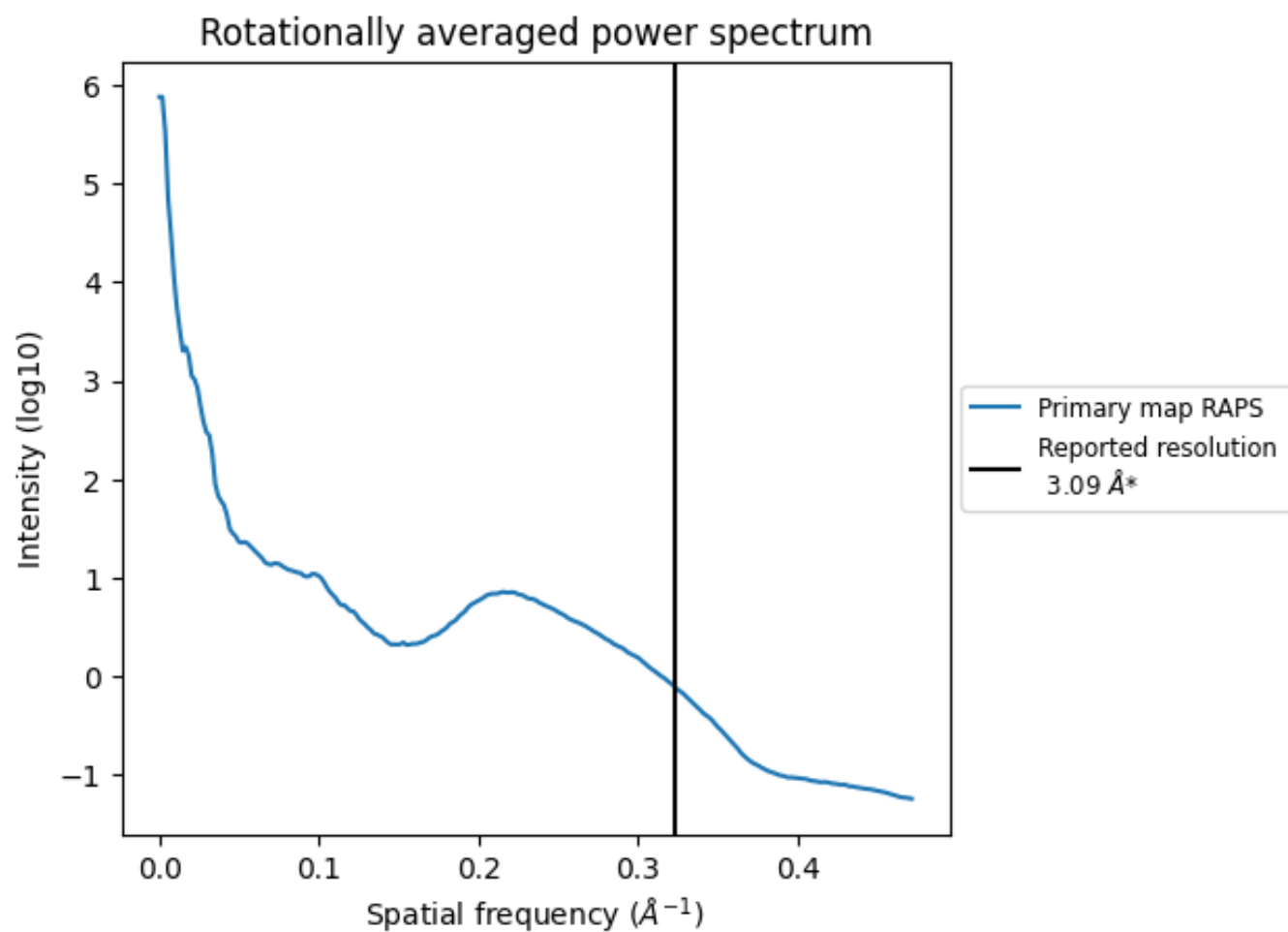
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 716 nm^3 ; this corresponds to an approximate mass of 647 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 0.324 Å⁻¹

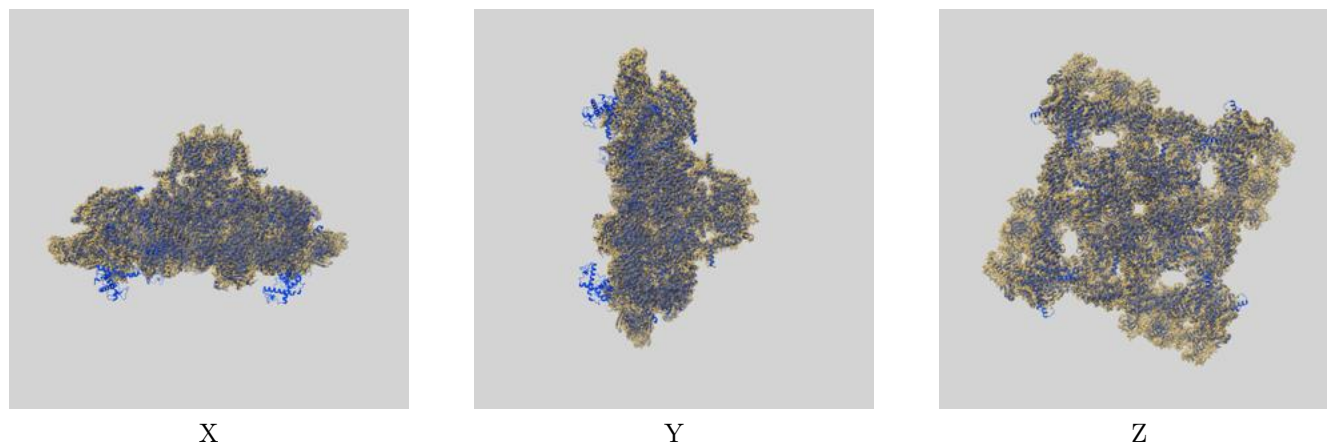
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

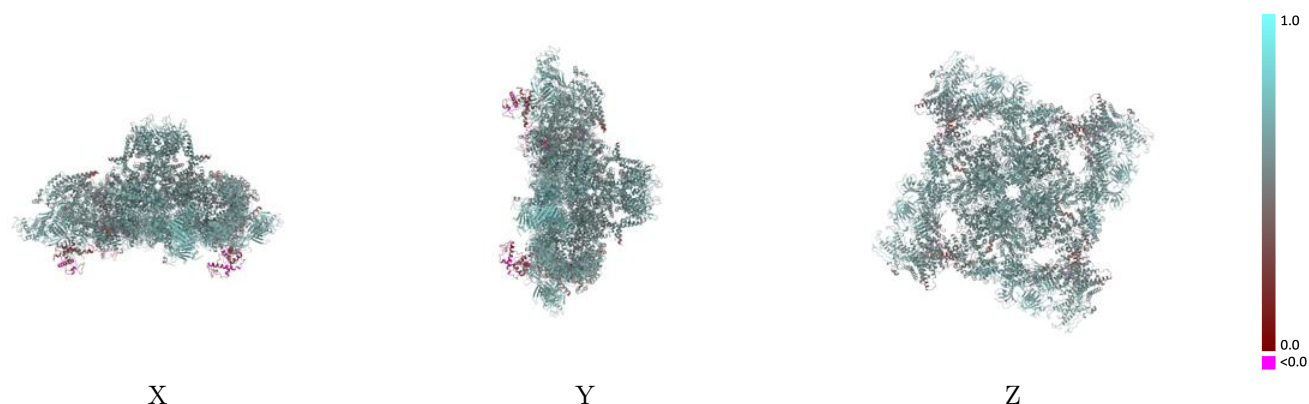
This section contains information regarding the fit between EMDB map EMD-74445 and PDB model 9ZND. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



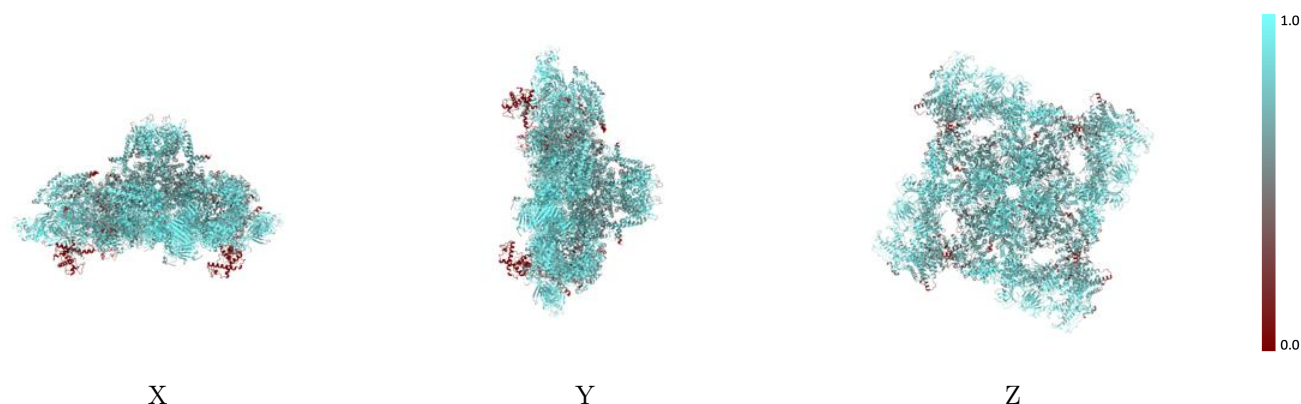
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



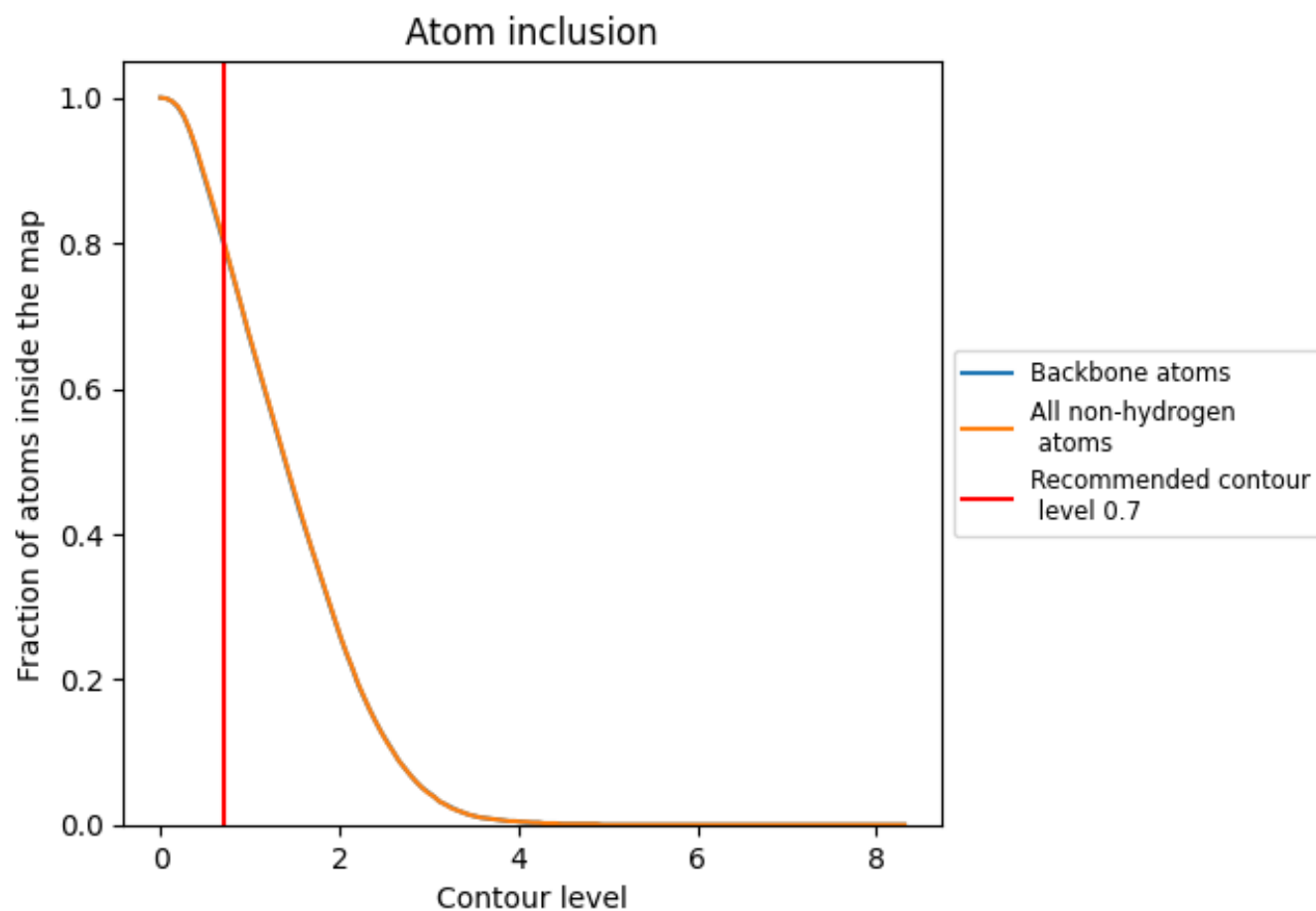
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 81% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8060	0.5920
A	0.8190	0.5950
B	0.8180	0.5960
C	0.8180	0.5960
D	0.8180	0.5960
E	0.8930	0.6250
F	0.8950	0.6290
G	0.8900	0.6280
H	0.8920	0.6260
I	0.4730	0.4540
J	0.4760	0.4410
K	0.4700	0.4460
L	0.4740	0.4490

