



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 10:58 PM UTC

PDB ID : 9NMP / pdb_00009nmp
EMDB ID : EMD-49536
Title : Structure of mouse RyR1 with simvastatin (Ca²⁺/CFF/ATP dataset; open pore)
Authors : Weninger, G.; Marks, A.R.
Deposited on : 2025-03-04
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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

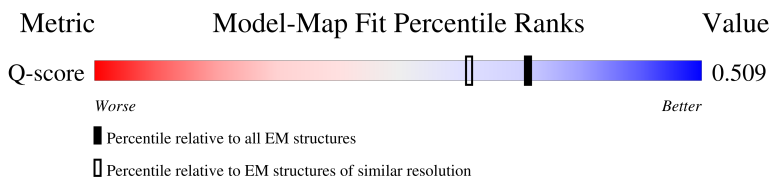
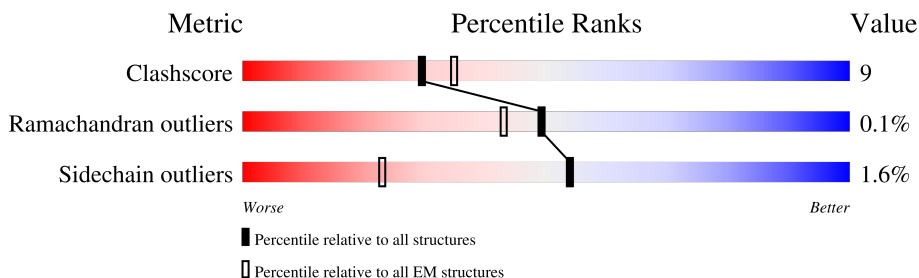
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.09 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	108	 81% 18% .
1	F	108	 81% 19% .
1	G	108	 81% 19% .
1	H	108	 81% 19% .

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Mol	Chain	Length	Quality of chain
2	A	5035	
2	B	5035	
2	C	5035	
2	D	5035	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CFF	A	8002	-	X	-	-
4	CFF	B	8002	-	X	-	-
4	CFF	C	8002	-	X	-	-
4	CFF	D	8002	-	X	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 143492 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 FKBP1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	107	Total	C	N	O	S	0	0
			830	526	146	155	3		
1	F	107	Total	C	N	O	S	0	0
			830	526	146	155	3		
1	G	107	Total	C	N	O	S	0	0
			830	526	146	155	3		
1	H	107	Total	C	N	O	S	0	0
			830	526	146	155	3		

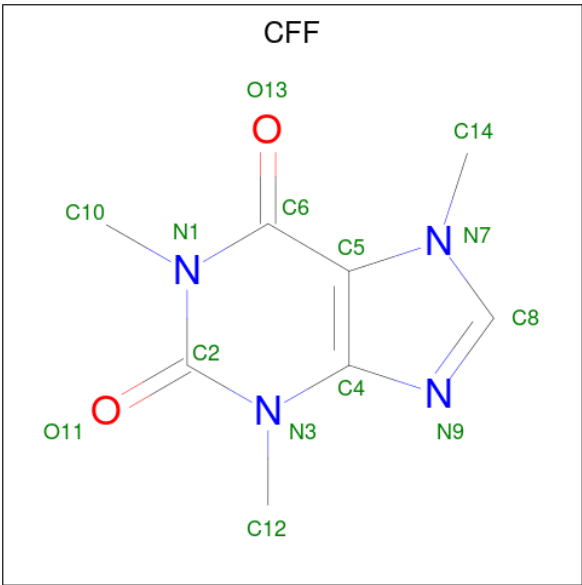
- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	4373	Total	C	N	O	S	0	0
			34797	22132	5983	6445	237		
2	A	4373	Total	C	N	O	S	0	0
			34797	22132	5983	6445	237		
2	B	4373	Total	C	N	O	S	0	0
			34797	22132	5983	6445	237		
2	C	4373	Total	C	N	O	S	0	0
			34797	22132	5983	6445	237		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

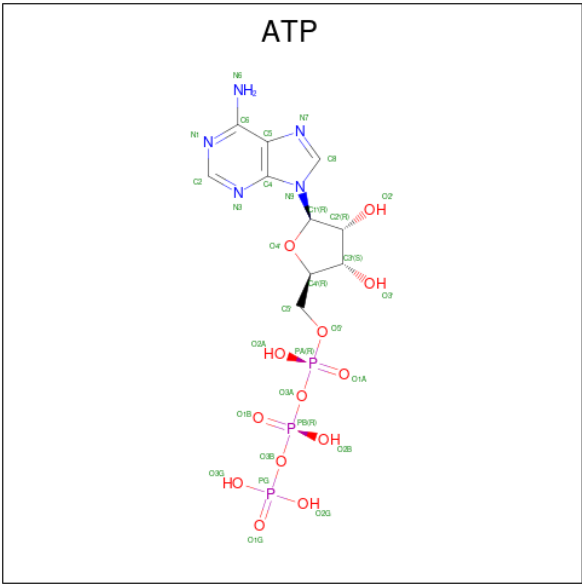
Mol	Chain	Residues	Atoms		AltConf
3	D	1	Total	Zn	0
			1	1	
3	A	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	

- Molecule 4 is CAFFEINE (CCD ID: CFF) (formula: C₈H₁₀N₄O₂).



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

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

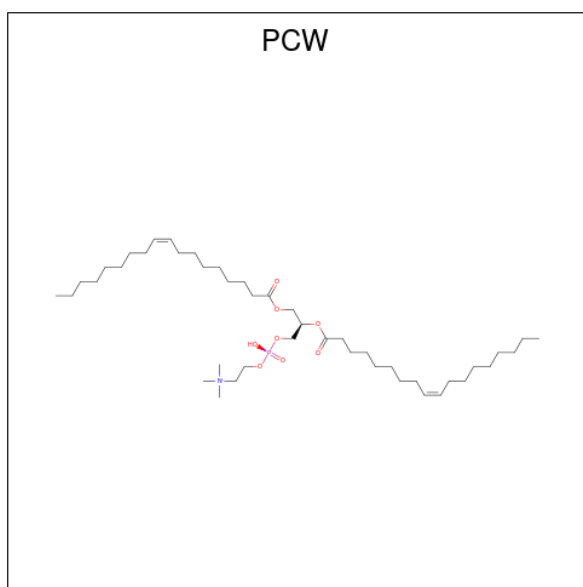


Mol	Chain	Residues	Atoms					AltConf
5	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	C	1	Total	C	N	O	P	0
			31	10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

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

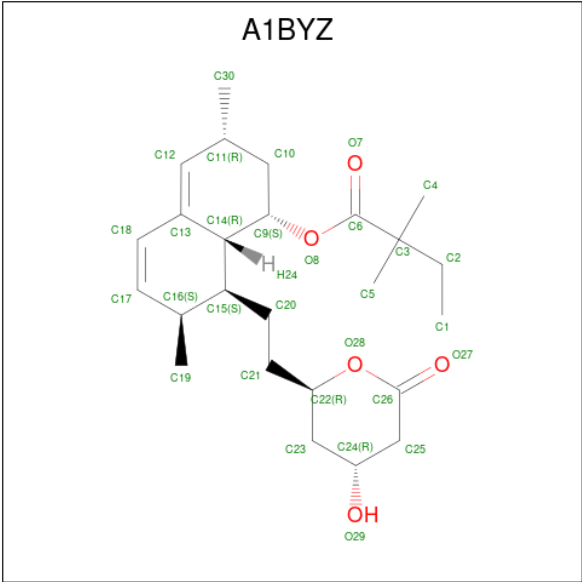
Mol	Chain	Residues	Atoms		AltConf
6	D	1	Total	Ca	0
			1	1	
6	A	1	Total	Ca	0
			1	1	
6	B	1	Total	Ca	0
			1	1	
6	C	1	Total	Ca	0
			1	1	

- Molecule 7 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: C₄₄H₈₅NO₈P).



Mol	Chain	Residues	Atoms					AltConf
7	D	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	D	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	C	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	C	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 8 is Simvastatin (CCD ID: A1BYZ) (formula: $C_{25}H_{38}O_5$) (labeled as "Ligand of Interest" by depositor).



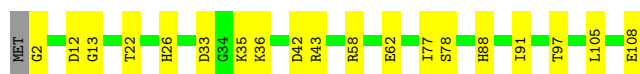
Mol	Chain	Residues	Atoms			AltConf
8	D	1	Total	C	O	0
			30	25	5	
8	D	1	Total	C	O	0
			30	25	5	
8	A	1	Total	C	O	0
			30	25	5	
8	A	1	Total	C	O	0
			30	25	5	
8	B	1	Total	C	O	0
			30	25	5	
8	B	1	Total	C	O	0
			30	25	5	
8	C	1	Total	C	O	0
			30	25	5	
8	C	1	Total	C	O	0
			30	25	5	

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 FKBP1A

Chain E: 



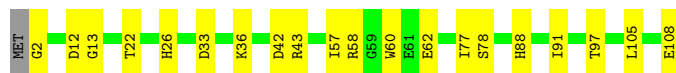
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain F: 



- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain G: 



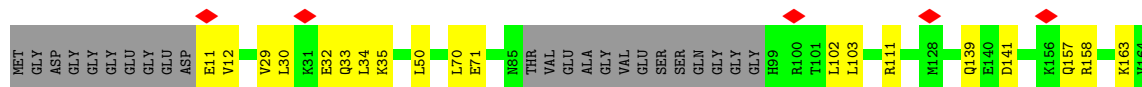
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1A

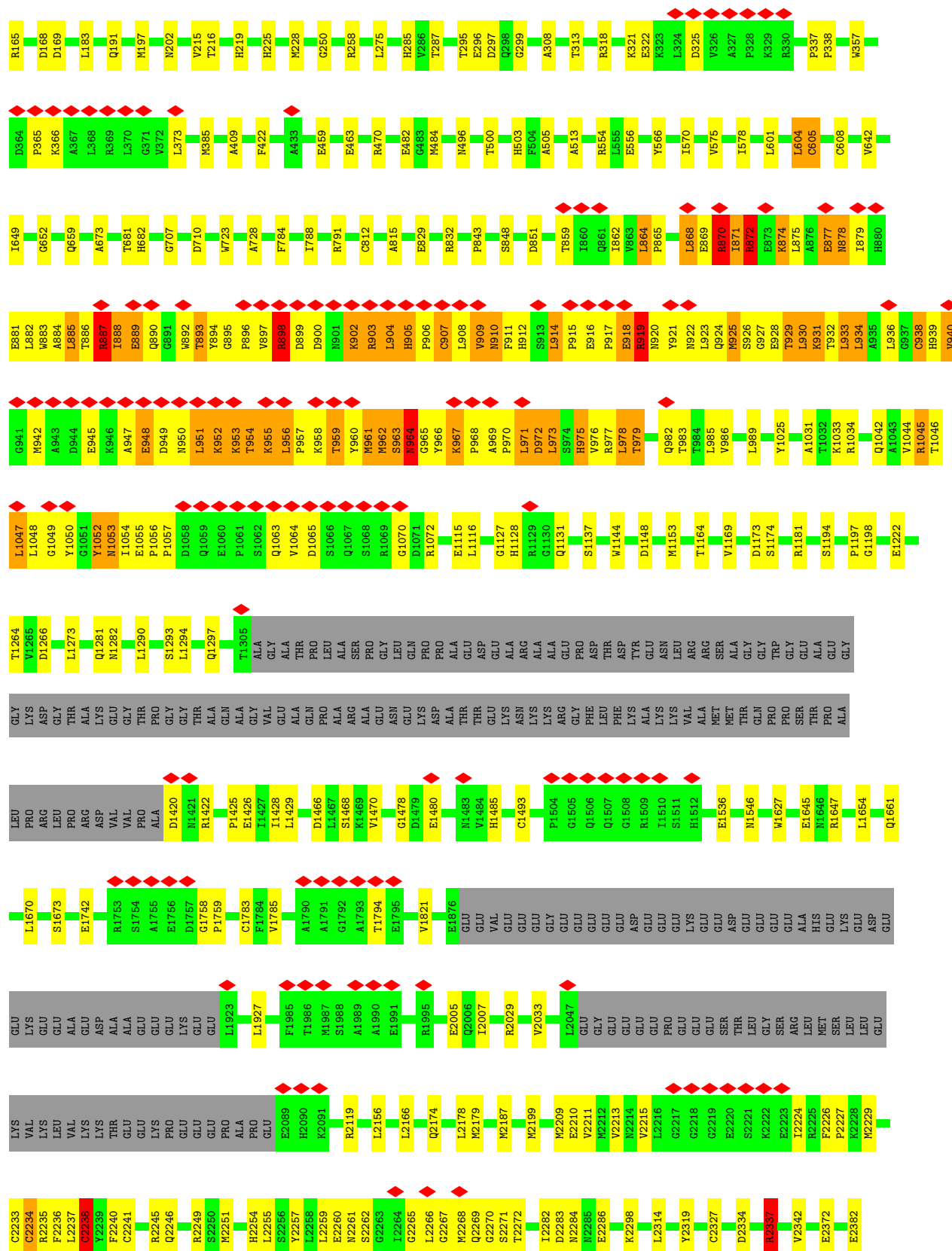
Chain H: 



- Molecule 2: Ryanodine receptor 1

Chain D: 

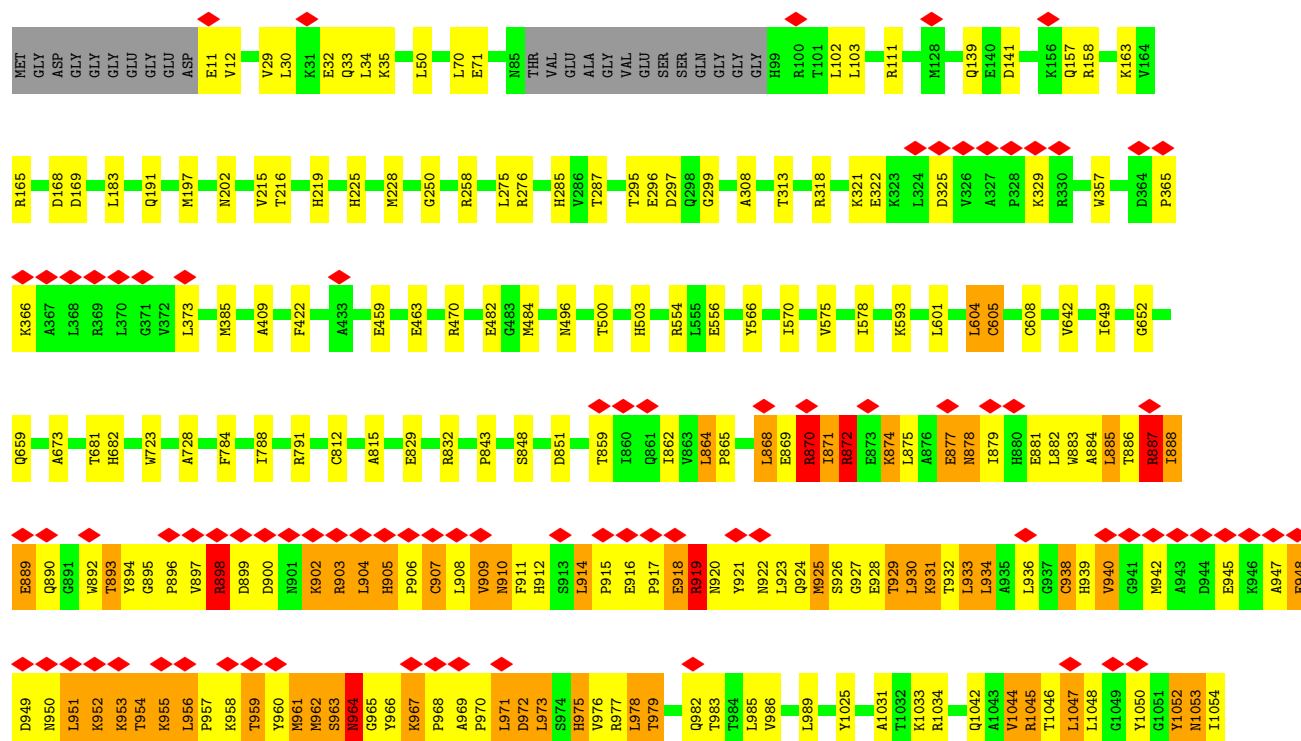




M3653	K3574	D3672	V3580	Q3684	E3685	E3686	E3687	E3688	E3689	V3691	E3692	E3693	L3711	T3712	E3713	D3720	H3735	E3737	GLU	GLY	GLY	GLU	ASN	GLY	GLU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
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S4055	L3859	D3672	V3580	L3406	T3309	C3166	V3025	L2927	T2867	12747
S4056	G3860	E3683	F3581	L3409	S3310	L3170	L3026	L2928	L2868	12748
D4086	M3861	E3684	G3582	Y3410	D3311	G3177	G3027	K2929	W2808	P2749
F4087	N3862	Q3685	R3583	P3411	H3312	G3176	K3035	F2930	E2750	E2750
R4088	N3863	E3686	E3584	L3412	G3317	G3177	T3041	L2931	K2811	K2751
G4089	E3864	E3687	E3585	L3413	G3318	T3178	T3041	L2932	E2812	L2752
L4090	E3865	E3688	E3586	L3414	N3319	T3179	T3041	M2933	S2813	D2753
D4095	D3865	E3689	A3587	R3415	R3322	N3181	V3055	N2934	K2814	S2754
F4096	T3867	E3690	D3588	E3434	I3323	N3182	S3056	G2935	K2815	F2755
M4100	V3868	V3691	D3589	L3435	I3324	V3183	L3057	G2936	A2816	T2756
E4122	I3869	E3692	E3591	M3438	D3331	E3184	D3061	A2937	M2817	M2757
E4129	N3870	E3693	F3592	V3439	K3337	L3195	A3062	V2938	L2818	K2758
M4133	R3871	L3711	I3593	G3440	K3337	L3198	P3063	T2939	A2819	F2759
N4133	Q3872	L3712	R3594	F3443	V3341	L3198	D3077	R2940	W2820	A2760
I4142	N3873	E3713	R3595	L3444	P3203	N3202	R3079	G2941	E2821	E2761
D4160	G3874	E3713	V3597	W3445	Q3344	P3203	T3080	L2942	W2822	Y2762
D4160	D3881	D3720	Q3598	M3518	V3204	V3204	V3081	K2943	T2823	T2763
I4173	E3882	H3735	N3524	M3524	V3347	V3220	M3082	D2944	V2824	H2764
E3736	L3736	E3737	M3525	M3525	V3347	V3220	K3083	M2945	E2825	E2765
E3737	L3607	E3737	T3529	T3529	R3226	R3226	I3088	E2946	K2826	K2766
G3895	T3610	G3895	D3530	L3354	R3226	R3226	E3105	L2947	A2827	E2767
E3896	E3611	E3896	G3531	R3356	T3230	T3230	R3106	D2948	R2828	A2768
F3902	H3612	G3896	D3532	S3357	L3231	L3231	M3107	T2949	E2829	F2769
Y3940	T3613	Y3940	T3534	I3360	V3237	V3237	V3108	K2892	G2830	D2770
K3943	L3613	L3613	V3535	P3361	E3238	E3238	E3109	K2893	E2831	K2771
D4219	L3613	L3613	L3536	L3366	E3239	E3239	N3110	Q2893	GLU	L2772
V3945	L3613	L3613	L3536	L3366	E3240	E3240	L3111	E2894	GLU	Q2773
K3962	L3613	L3613	L3536	V3373	C3241	C3241	L3111	L2895	THR	W2774
E3970	L3613	L3613	L3536	E3377	V3246	V3246	L3113	E2896	GLU	W2775
Y3971	L3613	L3613	L3536	E3377	L3247	L3247	GLY	A2897	LYS	W2776
I3972	L3613	L3613	L3536	E3377	L3247	L3247	LYS	Q2971	LYS	S2777
Q3973	L3613	L3613	L3536	E3377	L3247	L3247	VAL	Q2972	LYS	Y2778
G3974	L3613	L3613	L3536	E3377	L3247	L3247	SER	E2973	THR	Y2778
P3975	L3613	L3613	L3536	E3377	L3247	L3247	GLN	G2974	ARG	G2779
L3983	L3613	L3613	L3536	E3377	L3247	L3247	ALA	L2975	LYS	E2780
F3989	L3613	L3613	L3536	E3377	L3247	L3247	ARG	A2976	ILE	E2781
K4005	L3613	L3613	L3536	E3377	L3247	L3247	THR	H2977	GLN	I2782
D4009	L3613	L3613	L3536	E3377	L3247	L3247	VAL	L2978	THR	D2783
S4010	L3613	L3613	L3536	E3377	L3247	L3247	VAL	E2979	ALA	E2784
L4019	L3613	L3613	L3536	E3377	L3247	L3247	VAL	A2980	GLN	E2785
D4021	L3613	L3613	L3536	E3377	L3247	L3247	VAL	G3125	THR	E2786
ASP	L3613	L3613	L3536	E3377	L3247	L3247	VAL	V2981	TYR	L2786
GLU	L3613	L3613	L3536	E3377	L3247	L3247	VAL	V2982	ASP	K2787
PRO	L3613	L3613	L3536	E3377	L3247	L3247	VAL	S2983	ARG	T2788
GLU	L3613	L3613	L3536	E3377	L3247	L3247	VAL	G2985	GLU	H2789
ASP	L3613	L3613	L3536	E3377	L3247	L3247	VAL	R2986	GLY	P2790
GLU	L3613	L3613	L3536	E3377	L3247	L3247	VAL	V2987	LYS	L2791
ASP	L3613	L3613	L3536	E3377	L3247	L3247	VAL	E2988	THR	L2792
ASP	L3613	L3613	L3536	E3377	L3247	L3247	VAL	K2989	GLY	R2793
GLU	L3613	L3613	L3536	E3377	L3247	L3247	VAL	E2990	GLY	P2794
ALA	L3613	L3613	L3536	E3377	L3247	L3247	VAL	E2993	GLY	Y2795
	L3613	L3613	L3536	E3377	L3247	L3247	VAL	E2993	GLY	K2796
	L3613	L3613	L3536	E3377	L3247	L3247	VAL	E2993	GLY	T2797
	L3613	L3613	L3536	E3377	L3247	L3247	VAL	E2993	GLY	F2798
	L3613	L3613	L3536	E3377	L3247	L3247	VAL	E2993	GLY	S2799
	L3613	L3613	L3536	E3377	L3247	L3247	VAL	E2993	GLY	E2800
	L3613	L3613	L3536	E3377	L3247	L3247	VAL	E2993	GLY	K2801
	L3613	L3613	L3536	E3377	L3247	L3247	VAL	E2993	GLY	D2802
	L3613	L3613	L3536	E3377	L3247	L3247	VAL	E2993	GLY	K2803
	L3613	L3613	L3536	E3377	L3247	L3247	VAL	E2993	GLY	E2804
	L3613	L3613	L3536	E3377	L3247	L3247	VAL	E2993	GLY	Y2805

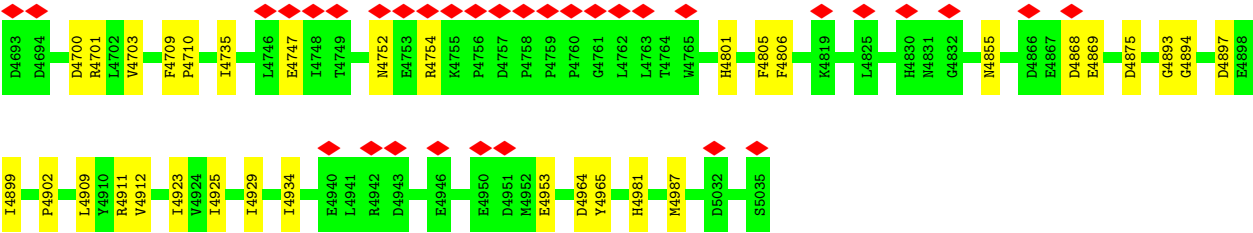












4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25791	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)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.628	Depositor
Minimum map value	0.000	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	424.448, 424.448, 424.448	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.829, 0.829, 0.829	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1BYZ, CFF, PCW, ATP, 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	0.24	0/848	0.40	0/1143
1	F	0.25	0/848	0.40	0/1143
1	G	0.25	0/848	0.41	0/1143
1	H	0.24	0/848	0.40	0/1143
2	A	0.29	0/35586	0.47	13/48203 (0.0%)
2	B	0.29	0/35586	0.47	14/48203 (0.0%)
2	C	0.29	0/35586	0.47	13/48203 (0.0%)
2	D	0.29	0/35586	0.47	13/48203 (0.0%)
All	All	0.29	0/145736	0.47	53/197384 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	10
2	B	0	10
2	C	0	10
2	D	0	10
All	All	0	40

There are no bond length outliers.

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2238	CYS	CA-CB-SG	9.57	136.40	114.40
2	B	2238	CYS	CA-CB-SG	9.57	136.40	114.40
2	C	2238	CYS	CA-CB-SG	9.57	136.40	114.40
2	A	2238	CYS	CA-CB-SG	9.55	136.37	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3241	CYS	CA-CB-SG	7.71	132.13	114.40
2	B	3241	CYS	CA-CB-SG	7.71	132.13	114.40
2	C	3241	CYS	CA-CB-SG	7.71	132.13	114.40
2	A	3241	CYS	CA-CB-SG	7.71	132.12	114.40
2	A	1052	TYR	N-CA-CB	7.00	120.27	109.85
2	B	1052	TYR	N-CA-CB	6.97	120.24	109.85
2	D	1052	TYR	N-CA-CB	6.96	120.22	109.85
2	C	1052	TYR	N-CA-CB	6.96	120.22	109.85
2	A	2233	CYS	CA-C-N	-6.61	108.92	121.54
2	A	2233	CYS	C-N-CA	-6.61	108.92	121.54
2	C	2233	CYS	CA-C-N	-6.60	108.93	121.54
2	C	2233	CYS	C-N-CA	-6.60	108.93	121.54
2	D	2233	CYS	CA-C-N	-6.60	108.93	121.54
2	D	2233	CYS	C-N-CA	-6.60	108.93	121.54
2	B	2233	CYS	CA-C-N	-6.60	108.93	121.54
2	B	2233	CYS	C-N-CA	-6.60	108.93	121.54
2	D	604	LEU	CA-C-N	-6.49	113.13	122.67
2	D	604	LEU	C-N-CA	-6.49	113.13	122.67
2	B	604	LEU	CA-C-N	-6.49	113.13	122.67
2	B	604	LEU	C-N-CA	-6.49	113.13	122.67
2	C	604	LEU	CA-C-N	-6.49	113.13	122.67
2	C	604	LEU	C-N-CA	-6.49	113.13	122.67
2	A	604	LEU	CA-C-N	-6.47	113.16	122.67
2	A	604	LEU	C-N-CA	-6.47	113.16	122.67
2	D	2234	CYS	N-CA-CB	6.40	121.31	110.49
2	C	2234	CYS	N-CA-CB	6.40	121.31	110.49
2	B	2234	CYS	N-CA-CB	6.39	121.28	110.49
2	A	2234	CYS	N-CA-CB	6.38	121.27	110.49
2	D	2238	CYS	CB-CA-C	6.11	119.82	109.55
2	B	2238	CYS	CB-CA-C	6.11	119.82	109.55
2	C	2238	CYS	CB-CA-C	6.11	119.82	109.55
2	A	2238	CYS	CB-CA-C	6.11	119.81	109.55
2	D	2234	CYS	CA-CB-SG	5.84	127.82	114.40
2	C	2234	CYS	CA-CB-SG	5.84	127.82	114.40
2	A	2234	CYS	CA-CB-SG	5.83	127.81	114.40
2	B	2234	CYS	CA-CB-SG	5.83	127.82	114.40
2	C	964	ASN	N-CA-C	-5.82	105.02	111.71
2	D	964	ASN	N-CA-C	-5.79	105.06	111.71
2	B	964	ASN	N-CA-C	-5.79	105.06	111.71
2	A	964	ASN	N-CA-C	-5.78	105.07	111.71
2	A	2238	CYS	N-CA-CB	-5.55	102.49	110.65
2	D	2238	CYS	N-CA-CB	-5.53	102.53	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2238	CYS	N-CA-CB	-5.53	102.53	110.65
2	B	2238	CYS	N-CA-CB	-5.50	102.56	110.65
2	B	2238	CYS	N-CA-C	-5.13	107.05	113.72
2	D	2238	CYS	N-CA-C	-5.12	107.06	113.72
2	A	2238	CYS	N-CA-C	-5.12	107.06	113.72
2	C	2238	CYS	N-CA-C	-5.12	107.06	113.72
2	B	1044	VAL	N-CA-C	-5.01	105.66	110.72

There are no chirality outliers.

All (40) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	1045	ARG	Sidechain
2	A	2238	CYS	Peptide
2	A	2337	ARG	Sidechain
2	A	605	CYS	Peptide
2	A	870	ARG	Sidechain
2	A	872	ARG	Sidechain
2	A	887	ARG	Sidechain
2	A	898	ARG	Sidechain
2	A	903	ARG	Sidechain
2	A	919	ARG	Sidechain
2	B	1045	ARG	Sidechain
2	B	2238	CYS	Peptide
2	B	2337	ARG	Sidechain
2	B	605	CYS	Peptide
2	B	870	ARG	Sidechain
2	B	872	ARG	Sidechain
2	B	887	ARG	Sidechain
2	B	898	ARG	Sidechain
2	B	903	ARG	Sidechain
2	B	919	ARG	Sidechain
2	C	1045	ARG	Sidechain
2	C	2238	CYS	Peptide
2	C	2337	ARG	Sidechain
2	C	605	CYS	Peptide
2	C	870	ARG	Sidechain
2	C	872	ARG	Sidechain
2	C	887	ARG	Sidechain
2	C	898	ARG	Sidechain
2	C	903	ARG	Sidechain
2	C	919	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	D	1045	ARG	Sidechain
2	D	2238	CYS	Peptide
2	D	2337	ARG	Sidechain
2	D	605	CYS	Peptide
2	D	870	ARG	Sidechain
2	D	872	ARG	Sidechain
2	D	887	ARG	Sidechain
2	D	898	ARG	Sidechain
2	D	903	ARG	Sidechain
2	D	919	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	830	0	828	16	0
1	F	830	0	828	15	0
1	G	830	0	828	16	0
1	H	830	0	828	16	0
2	A	34797	0	34382	638	0
2	B	34797	0	34382	643	0
2	C	34797	0	34382	644	0
2	D	34797	0	34382	642	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	14	0	10	0	0
4	B	14	0	10	0	0
4	C	14	0	10	0	0
4	D	14	0	10	0	0
5	A	62	0	24	1	0
5	B	62	0	24	1	0
5	C	62	0	24	1	0
5	D	62	0	24	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	1	0	0	0	0
7	A	108	0	168	5	0
7	B	108	0	168	5	0
7	C	108	0	168	5	0
7	D	108	0	168	5	0
8	A	60	0	0	2	0
8	B	60	0	0	3	0
8	C	60	0	0	3	0
8	D	60	0	0	2	0
All	All	143492	0	141648	2626	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 9.

All (2626) 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:B:899:ASP:HB3	2:B:902:LYS:HB2	1.30	1.10
2:A:899:ASP:HB3	2:A:902:LYS:HB2	1.30	1.09
2:D:899:ASP:HB3	2:D:902:LYS:HB2	1.30	1.08
2:C:899:ASP:HB3	2:C:902:LYS:HB2	1.30	1.08
1:H:2:GLY:N	1:H:78:SER:HG	1.55	1.03
1:F:2:GLY:N	1:F:78:SER:HG	1.53	1.03
2:C:2156:LEU:HD21	2:C:2199:MET:HE1	1.42	1.01
2:A:2156:LEU:HD21	2:A:2199:MET:HE1	1.42	0.99
2:B:879:ILE:HA	2:B:882:LEU:HD12	1.44	0.99
2:B:902:LYS:HB3	2:B:904:LEU:HG	1.45	0.99
2:C:879:ILE:HA	2:C:882:LEU:HD12	1.45	0.99
2:A:902:LYS:HB3	2:A:904:LEU:HG	1.45	0.98
2:B:2156:LEU:HD21	2:B:2199:MET:HE1	1.42	0.97
2:A:879:ILE:HA	2:A:882:LEU:HD12	1.45	0.97
2:C:902:LYS:HB3	2:C:904:LEU:HG	1.45	0.97
2:D:902:LYS:HB3	2:D:904:LEU:HG	1.45	0.97
2:D:2156:LEU:HD21	2:D:2199:MET:HE1	1.42	0.97
2:D:879:ILE:HA	2:D:882:LEU:HD12	1.44	0.97
2:D:3529:THR:HG23	2:D:3574:MET:HE3	1.47	0.97
2:B:2215:VAL:HG11	2:B:2229:MET:HE1	1.48	0.96
2:C:3529:THR:HG23	2:C:3574:MET:HE3	1.47	0.95
2:C:2215:VAL:HG11	2:C:2229:MET:HE1	1.48	0.95
2:A:3529:THR:HG23	2:A:3574:MET:HE3	1.47	0.95
2:A:2215:VAL:HG11	2:A:2229:MET:HE1	1.48	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2:GLY:N	1:G:78:SER:HG	1.64	0.94
2:B:3529:THR:HG23	2:B:3574:MET:HE3	1.47	0.93
2:D:2215:VAL:HG11	2:D:2229:MET:HE1	1.48	0.93
2:B:887:ARG:HG2	2:B:908:LEU:HD11	1.52	0.92
1:E:2:GLY:N	1:E:78:SER:HG	1.68	0.91
2:D:887:ARG:HG2	2:D:908:LEU:HD11	1.52	0.91
2:A:887:ARG:HG2	2:A:908:LEU:HD11	1.52	0.91
2:C:2766:LYS:NZ	2:C:2861:PRO:O	2.04	0.91
2:D:2912:LEU:O	2:D:2917:LYS:NZ	2.04	0.91
2:A:2766:LYS:NZ	2:A:2861:PRO:O	2.04	0.90
2:B:942:MET:HA	2:B:1052:TYR:HA	1.53	0.90
2:B:2766:LYS:NZ	2:B:2861:PRO:O	2.04	0.90
2:C:2912:LEU:O	2:C:2917:LYS:NZ	2.04	0.90
2:C:894:TYR:CG	2:C:964:ASN:HB3	2.07	0.90
2:C:887:ARG:HG2	2:C:908:LEU:HD11	1.52	0.90
2:D:2766:LYS:NZ	2:D:2861:PRO:O	2.04	0.89
2:A:2912:LEU:O	2:A:2917:LYS:NZ	2.04	0.89
2:B:902:LYS:HE3	2:B:904:LEU:HD21	1.55	0.89
2:A:942:MET:HA	2:A:1052:TYR:HA	1.53	0.89
2:B:2912:LEU:O	2:B:2917:LYS:NZ	2.04	0.89
2:D:894:TYR:CG	2:D:964:ASN:HB3	2.07	0.89
2:A:902:LYS:HE3	2:A:904:LEU:HD21	1.55	0.89
2:C:902:LYS:HE3	2:C:904:LEU:HD21	1.55	0.89
2:A:894:TYR:CG	2:A:964:ASN:HB3	2.07	0.88
2:B:894:TYR:CG	2:B:964:ASN:HB3	2.07	0.88
2:C:942:MET:HA	2:C:1052:TYR:HA	1.53	0.88
2:D:902:LYS:HE3	2:D:904:LEU:HD21	1.55	0.88
2:C:1131:GLN:NE2	2:C:1137:SER:OG	2.07	0.88
2:A:894:TYR:HB3	2:A:964:ASN:H	1.38	0.87
2:B:894:TYR:HB3	2:B:964:ASN:H	1.38	0.87
2:A:1131:GLN:NE2	2:A:1137:SER:OG	2.07	0.87
2:B:1131:GLN:NE2	2:B:1137:SER:OG	2.07	0.87
2:D:942:MET:HA	2:D:1052:TYR:HA	1.53	0.87
2:D:1131:GLN:NE2	2:D:1137:SER:OG	2.07	0.87
2:B:3525:MET:O	2:B:3596:ARG:NH2	2.09	0.86
2:C:3525:MET:O	2:C:3596:ARG:NH2	2.08	0.86
2:D:3525:MET:O	2:D:3596:ARG:NH2	2.09	0.85
2:A:956:LEU:HB2	2:A:967:LYS:HE2	1.59	0.85
2:C:894:TYR:HB3	2:C:964:ASN:H	1.38	0.85
2:D:894:TYR:HB3	2:D:964:ASN:H	1.38	0.85
2:B:956:LEU:HB2	2:B:967:LYS:HE2	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3525:MET:O	2:A:3596:ARG:NH2	2.09	0.85
2:D:829:GLU:OE2	2:D:832:ARG:NH1	2.11	0.84
2:B:3962:LYS:NZ	2:B:4021:ASP:OD2	2.11	0.84
2:D:956:LEU:HB2	2:D:967:LYS:HE2	1.59	0.84
2:C:956:LEU:HB2	2:C:967:LYS:HE2	1.59	0.84
2:D:2573:THR:O	2:D:2575:HIS:N	2.11	0.84
2:D:3962:LYS:NZ	2:D:4021:ASP:OD2	2.11	0.83
2:A:3962:LYS:NZ	2:A:4021:ASP:OD2	2.11	0.83
2:C:829:GLU:OE2	2:C:832:ARG:NH1	2.11	0.83
2:D:894:TYR:H	2:D:963:SER:H	1.26	0.83
2:A:2573:THR:O	2:A:2575:HIS:N	2.11	0.83
2:B:829:GLU:OE2	2:B:832:ARG:NH1	2.11	0.83
2:D:605:CYS:SG	2:D:1673:SER:OG	2.37	0.83
2:A:829:GLU:OE2	2:A:832:ARG:NH1	2.11	0.83
2:B:2573:THR:O	2:B:2575:HIS:N	2.11	0.83
2:C:2573:THR:O	2:C:2575:HIS:N	2.11	0.83
2:C:894:TYR:H	2:C:963:SER:H	1.26	0.83
2:C:3962:LYS:NZ	2:C:4021:ASP:OD2	2.11	0.83
2:A:605:CYS:SG	2:A:1673:SER:OG	2.37	0.83
2:C:3178:THR:O	2:C:3180:ARG:NH1	2.12	0.83
2:D:888:ILE:HD13	2:D:960:TYR:HA	1.60	0.83
2:D:1025:TYR:O	2:D:1033:LYS:NZ	2.12	0.83
2:A:888:ILE:HD13	2:A:960:TYR:HA	1.60	0.83
2:D:2209:MET:HE2	2:D:2251:MET:HE1	1.61	0.82
2:A:1025:TYR:O	2:A:1033:LYS:NZ	2.12	0.82
2:C:2209:MET:HE2	2:C:2251:MET:HE1	1.61	0.82
2:B:3178:THR:O	2:B:3180:ARG:NH1	2.12	0.82
2:A:2209:MET:HE2	2:A:2251:MET:HE1	1.61	0.82
2:C:605:CYS:SG	2:C:1673:SER:OG	2.37	0.82
2:A:3178:THR:O	2:A:3180:ARG:NH1	2.12	0.82
2:C:888:ILE:HD13	2:C:960:TYR:HA	1.60	0.82
2:B:605:CYS:SG	2:B:1673:SER:OG	2.37	0.82
2:C:2723:LYS:NZ	2:C:2725:GLU:OE1	2.13	0.82
2:D:3178:THR:O	2:D:3180:ARG:NH1	2.12	0.81
2:B:888:ILE:HD13	2:B:960:TYR:HA	1.60	0.81
2:D:2723:LYS:NZ	2:D:2725:GLU:OE1	2.13	0.81
2:C:1025:TYR:O	2:C:1033:LYS:NZ	2.12	0.81
2:A:2234:CYS:O	2:A:2235:ARG:C	2.23	0.81
2:B:894:TYR:H	2:B:963:SER:H	1.26	0.81
2:A:894:TYR:H	2:A:963:SER:H	1.26	0.81
2:B:1025:TYR:O	2:B:1033:LYS:NZ	2.12	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2209:MET:HE2	2:B:2251:MET:HE1	1.61	0.81
2:D:2234:CYS:O	2:D:2235:ARG:C	2.23	0.81
2:B:2723:LYS:NZ	2:B:2725:GLU:OE1	2.13	0.81
2:A:2723:LYS:NZ	2:A:2725:GLU:OE1	2.13	0.81
2:A:496:ASN:OD1	2:A:554:ARG:NH1	2.15	0.80
2:C:496:ASN:OD1	2:C:554:ARG:NH1	2.15	0.80
2:C:956:LEU:HD13	2:C:960:TYR:HB3	1.64	0.80
2:D:496:ASN:OD1	2:D:554:ARG:NH1	2.15	0.80
2:C:2234:CYS:O	2:C:2235:ARG:C	2.23	0.80
2:D:956:LEU:HD13	2:D:960:TYR:HB3	1.64	0.80
2:A:956:LEU:HD13	2:A:960:TYR:HB3	1.64	0.80
2:B:496:ASN:OD1	2:B:554:ARG:NH1	2.15	0.79
2:D:899:ASP:HB3	2:D:902:LYS:CB	2.12	0.79
2:B:956:LEU:HD13	2:B:960:TYR:HB3	1.64	0.79
2:B:2234:CYS:O	2:B:2235:ARG:C	2.23	0.79
2:C:899:ASP:HB3	2:C:902:LYS:CB	2.12	0.79
2:C:961:MET:HG3	2:C:965:GLY:HA2	1.65	0.79
2:D:961:MET:HG3	2:D:965:GLY:HA2	1.65	0.79
2:A:903:ARG:HH21	2:A:903:ARG:HA	1.47	0.79
2:B:961:MET:HG3	2:B:965:GLY:HA2	1.65	0.79
2:B:903:ARG:HA	2:B:903:ARG:HH21	1.47	0.79
2:B:894:TYR:HB2	2:B:962:MET:HB3	1.65	0.79
2:A:961:MET:HG3	2:A:965:GLY:HA2	1.65	0.78
2:A:899:ASP:HB3	2:A:902:LYS:CB	2.12	0.78
2:C:894:TYR:HB2	2:C:962:MET:HB3	1.65	0.78
2:A:894:TYR:HB2	2:A:962:MET:HB3	1.65	0.78
2:D:903:ARG:HA	2:D:903:ARG:HH21	1.47	0.78
2:A:2372:GLU:HG2	2:B:197:MET:HE1	1.66	0.78
2:A:2234:CYS:O	2:A:2236:PHE:N	2.17	0.78
2:C:903:ARG:HH21	2:C:903:ARG:HA	1.47	0.77
2:D:2234:CYS:O	2:D:2236:PHE:N	2.17	0.77
2:D:2372:GLU:HG2	2:A:197:MET:HE1	1.67	0.77
2:D:894:TYR:HB2	2:D:962:MET:HB3	1.65	0.77
2:B:899:ASP:HB3	2:B:902:LYS:CB	2.12	0.77
2:B:2234:CYS:O	2:B:2236:PHE:N	2.17	0.77
2:D:197:MET:HE1	2:C:2372:GLU:HG2	1.67	0.76
2:B:2372:GLU:HG2	2:C:197:MET:HE1	1.67	0.76
2:B:865:PRO:HD2	2:B:868:LEU:HB2	1.68	0.76
2:A:951:LEU:HD23	2:A:975:HIS:CE1	2.21	0.76
2:B:871:ILE:HG13	2:B:1050:TYR:CD2	2.21	0.76
2:A:865:PRO:HD2	2:A:868:LEU:HB2	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:871:ILE:HG13	2:C:1050:TYR:CD2	2.21	0.76
2:C:2234:CYS:O	2:C:2236:PHE:N	2.17	0.76
2:D:865:PRO:HD2	2:D:868:LEU:HB2	1.68	0.75
2:D:951:LEU:HD23	2:D:975:HIS:CE1	2.21	0.75
2:A:871:ILE:HG13	2:A:1050:TYR:CD2	2.21	0.75
2:B:951:LEU:HD23	2:B:975:HIS:CE1	2.21	0.75
2:B:951:LEU:HD23	2:B:975:HIS:HE1	1.51	0.75
2:C:865:PRO:HD2	2:C:868:LEU:HB2	1.68	0.75
2:D:871:ILE:HG13	2:D:1050:TYR:CD2	2.21	0.75
2:A:951:LEU:HD23	2:A:975:HIS:HE1	1.51	0.74
2:B:859:THR:HA	2:B:862:ILE:HD12	1.69	0.74
2:C:951:LEU:HD23	2:C:975:HIS:CE1	2.21	0.74
2:B:3309:THR:OG1	2:B:3311:ASP:OD1	2.06	0.74
2:D:888:ILE:HG12	2:D:960:TYR:CG	2.23	0.74
2:B:956:LEU:HD12	2:B:968:PRO:HD2	1.70	0.74
2:A:859:THR:HA	2:A:862:ILE:HD12	1.69	0.74
7:D:8006:PCW:H482	7:A:8005:PCW:H271	1.70	0.74
2:C:859:THR:HA	2:C:862:ILE:HD12	1.69	0.74
2:A:888:ILE:HG12	2:A:960:TYR:CG	2.23	0.73
2:A:3309:THR:OG1	2:A:3311:ASP:OD1	2.06	0.73
2:A:3859:LEU:HD11	2:A:3871:ARG:HH22	1.52	0.73
2:D:956:LEU:HD12	2:D:968:PRO:HD2	1.70	0.73
2:C:888:ILE:HG12	2:C:960:TYR:CG	2.23	0.73
2:C:3309:THR:OG1	2:C:3311:ASP:OD1	2.06	0.73
2:B:3859:LEU:HD11	2:B:3871:ARG:HH22	1.53	0.73
2:C:951:LEU:HD23	2:C:975:HIS:HE1	1.51	0.73
2:D:864:LEU:HD11	2:D:930:LEU:HB2	1.70	0.73
2:C:3859:LEU:HD11	2:C:3871:ARG:HH22	1.52	0.73
2:C:956:LEU:HD12	2:C:968:PRO:HD2	1.70	0.73
2:D:898:ARG:HB3	2:D:906:PRO:HD2	1.71	0.73
2:C:898:ARG:HB3	2:C:906:PRO:HD2	1.71	0.73
2:D:951:LEU:HD23	2:D:975:HIS:HE1	1.51	0.72
2:B:864:LEU:HD11	2:B:930:LEU:HB2	1.70	0.72
2:D:859:THR:HA	2:D:862:ILE:HD12	1.69	0.72
2:D:3309:THR:OG1	2:D:3311:ASP:OD1	2.06	0.72
2:D:3859:LEU:HD11	2:D:3871:ARG:HH22	1.52	0.72
2:B:888:ILE:HG12	2:B:960:TYR:CG	2.23	0.72
2:B:3881:ASP:OD2	2:B:3882:GLU:N	2.23	0.72
2:A:3881:ASP:OD2	2:A:3882:GLU:N	2.23	0.72
7:B:8006:PCW:H482	7:C:8005:PCW:H271	1.72	0.72
7:D:8005:PCW:H271	7:C:8006:PCW:H482	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:956:LEU:HD12	2:A:968:PRO:HD2	1.70	0.72
2:C:864:LEU:HD11	2:C:930:LEU:HB2	1.70	0.72
2:C:2824:VAL:HG22	2:C:2938:VAL:HG23	1.72	0.72
2:D:3881:ASP:OD2	2:D:3882:GLU:N	2.23	0.71
2:B:898:ARG:HB3	2:B:906:PRO:HD2	1.71	0.71
2:D:953:LYS:HA	2:D:971:LEU:HA	1.72	0.71
2:A:898:ARG:HB3	2:A:906:PRO:HD2	1.71	0.71
2:C:953:LYS:HA	2:C:971:LEU:HA	1.72	0.71
2:C:3881:ASP:OD2	2:C:3882:GLU:N	2.23	0.71
2:A:864:LEU:HD11	2:A:930:LEU:HB2	1.70	0.71
2:A:914:LEU:HD21	2:A:919:ARG:HA	1.73	0.71
2:C:3107:MET:O	2:C:3111:LEU:HD23	1.91	0.71
2:C:2949:THR:O	2:C:2954:LYS:NZ	2.25	0.70
2:D:2824:VAL:HG22	2:D:2938:VAL:HG23	1.72	0.70
2:A:953:LYS:HA	2:A:971:LEU:HA	1.72	0.70
2:B:2949:THR:O	2:B:2954:LYS:NZ	2.25	0.70
2:D:2949:THR:O	2:D:2954:LYS:NZ	2.25	0.70
2:A:2824:VAL:HG22	2:A:2938:VAL:HG23	1.72	0.70
2:B:953:LYS:HA	2:B:971:LEU:HA	1.72	0.70
2:B:3870:ASN:O	2:B:3872:GLN:NE2	2.25	0.70
2:D:973:LEU:HB2	2:D:976:VAL:HG23	1.74	0.70
2:A:3870:ASN:O	2:A:3872:GLN:NE2	2.25	0.70
2:B:973:LEU:HB2	2:B:976:VAL:HG23	1.74	0.70
2:D:3107:MET:O	2:D:3111:LEU:HD23	1.91	0.69
2:A:973:LEU:HB2	2:A:976:VAL:HG23	1.74	0.69
2:A:3107:MET:O	2:A:3111:LEU:HD23	1.91	0.69
2:C:973:LEU:HB2	2:C:976:VAL:HG23	1.74	0.69
1:H:88:HIS:ND1	1:H:91:ILE:HD13	2.08	0.69
2:B:914:LEU:HD21	2:B:919:ARG:HA	1.73	0.69
2:B:3107:MET:O	2:B:3111:LEU:HD23	1.91	0.69
2:C:914:LEU:HD21	2:C:919:ARG:HA	1.73	0.69
1:E:88:HIS:ND1	1:E:91:ILE:HD13	2.08	0.69
1:G:88:HIS:ND1	1:G:91:ILE:HD13	2.08	0.69
2:A:2949:THR:O	2:A:2954:LYS:NZ	2.25	0.69
2:B:885:LEU:O	2:B:888:ILE:HG23	1.93	0.69
2:B:2824:VAL:HG22	2:B:2938:VAL:HG23	1.72	0.69
1:F:88:HIS:ND1	1:F:91:ILE:HD13	2.08	0.69
2:A:1466:ASP:OD2	2:A:1468:SER:OG	2.11	0.69
2:C:2414:GLU:O	2:C:2418:HIS:NE2	2.26	0.69
2:A:894:TYR:CB	2:A:964:ASN:H	2.06	0.68
2:B:894:TYR:CB	2:B:964:ASN:H	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:885:LEU:O	2:C:888:ILE:HG23	1.93	0.68
2:B:2414:GLU:O	2:B:2418:HIS:NE2	2.26	0.68
2:C:3870:ASN:O	2:C:3872:GLN:NE2	2.25	0.68
2:B:2948:ASP:O	2:B:2949:THR:OG1	2.10	0.68
2:C:250:GLY:H	2:C:373:LEU:HD11	1.58	0.68
2:D:894:TYR:CB	2:D:964:ASN:H	2.07	0.68
2:D:914:LEU:HD21	2:D:919:ARG:HA	1.73	0.68
2:A:2414:GLU:O	2:A:2418:HIS:NE2	2.26	0.68
2:B:911:PHE:CZ	2:B:922:ASN:HB2	2.29	0.68
2:C:894:TYR:CB	2:C:964:ASN:H	2.07	0.68
2:A:885:LEU:O	2:A:888:ILE:HG23	1.93	0.68
2:D:914:LEU:HD12	2:D:915:PRO:HD2	1.75	0.68
2:A:911:PHE:CZ	2:A:922:ASN:HB2	2.29	0.68
2:B:1222:GLU:N	2:B:1222:GLU:OE1	2.27	0.68
2:C:914:LEU:HD12	2:C:915:PRO:HD2	1.75	0.68
1:G:12:ASP:OD1	1:G:13:GLY:N	2.26	0.68
1:H:12:ASP:OD1	1:H:13:GLY:N	2.27	0.68
2:D:250:GLY:H	2:D:373:LEU:HD11	1.58	0.68
2:D:885:LEU:O	2:D:888:ILE:HG23	1.93	0.68
2:D:3870:ASN:O	2:D:3872:GLN:NE2	2.25	0.68
2:D:872:ARG:HG3	2:D:927:GLY:HA2	1.76	0.68
2:A:1222:GLU:OE1	2:A:1222:GLU:N	2.27	0.68
2:B:911:PHE:HA	2:B:914:LEU:HD23	1.76	0.67
2:C:911:PHE:CZ	2:C:922:ASN:HB2	2.29	0.67
2:D:2414:GLU:O	2:D:2418:HIS:NE2	2.26	0.67
2:A:914:LEU:HD12	2:A:915:PRO:HD2	1.75	0.67
2:B:914:LEU:HD12	2:B:915:PRO:HD2	1.74	0.67
2:C:911:PHE:HA	2:C:914:LEU:HD23	1.76	0.67
2:D:898:ARG:CB	2:D:906:PRO:HD2	2.24	0.67
2:D:911:PHE:HZ	2:D:922:ASN:HB2	1.59	0.67
2:A:250:GLY:H	2:A:373:LEU:HD11	1.58	0.67
2:B:872:ARG:HG3	2:B:927:GLY:HA2	1.76	0.67
2:A:898:ARG:CB	2:A:906:PRO:HD2	2.24	0.67
2:C:865:PRO:HD2	2:C:868:LEU:CB	2.25	0.67
2:C:982:GLN:HA	2:C:985:LEU:HD12	1.76	0.67
2:D:911:PHE:CZ	2:D:922:ASN:HB2	2.29	0.67
2:D:1222:GLU:OE1	2:D:1222:GLU:N	2.27	0.67
2:A:911:PHE:HA	2:A:914:LEU:HD23	1.76	0.67
2:B:250:GLY:H	2:B:373:LEU:HD11	1.58	0.67
2:B:871:ILE:HA	2:B:874:LYS:HD3	1.77	0.67
2:C:898:ARG:CB	2:C:906:PRO:HD2	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:12:ASP:OD1	1:E:13:GLY:N	2.28	0.67
2:D:911:PHE:HA	2:D:914:LEU:HD23	1.76	0.67
2:B:1466:ASP:OD2	2:B:1468:SER:OG	2.11	0.67
2:A:2749:PRO:HD2	2:A:2752:LEU:HD12	1.77	0.67
2:C:872:ARG:HG3	2:C:927:GLY:HA2	1.76	0.67
1:F:12:ASP:OD1	1:F:13:GLY:N	2.28	0.67
2:D:865:PRO:HD2	2:D:868:LEU:CB	2.25	0.67
2:C:1466:ASP:OD2	2:C:1468:SER:OG	2.11	0.67
2:C:911:PHE:HZ	2:C:922:ASN:HB2	1.59	0.66
2:D:2948:ASP:O	2:D:2949:THR:OG1	2.10	0.66
2:A:3377:GLU:OE1	2:A:3449:SER:OG	2.12	0.66
2:A:872:ARG:HG3	2:A:927:GLY:HA2	1.76	0.66
2:B:982:GLN:HA	2:B:985:LEU:HD12	1.76	0.66
2:C:1222:GLU:OE1	2:C:1222:GLU:N	2.27	0.66
2:D:3377:GLU:OE1	2:D:3449:SER:OG	2.12	0.66
2:A:911:PHE:HZ	2:A:922:ASN:HB2	1.59	0.66
2:B:898:ARG:CB	2:B:906:PRO:HD2	2.24	0.66
2:D:871:ILE:HA	2:D:874:LYS:HD3	1.77	0.66
2:B:2564:THR:HG22	2:B:2607:CYS:HA	1.78	0.66
2:D:982:GLN:HA	2:D:985:LEU:HD12	1.76	0.66
2:C:2749:PRO:HD2	2:C:2752:LEU:HD12	1.77	0.66
2:A:859:THR:HB	2:A:931:LYS:HB3	1.78	0.66
2:A:865:PRO:HD2	2:A:868:LEU:CB	2.25	0.66
2:B:865:PRO:HD2	2:B:868:LEU:CB	2.25	0.66
2:C:2564:THR:HG22	2:C:2607:CYS:HA	1.78	0.66
2:B:859:THR:HB	2:B:931:LYS:HB3	1.78	0.66
2:D:986:VAL:HG22	2:D:1044:VAL:HG21	1.78	0.66
2:A:871:ILE:HA	2:A:874:LYS:HD3	1.77	0.66
2:B:2749:PRO:HD2	2:B:2752:LEU:HD12	1.77	0.66
2:C:4048:VAL:HG11	2:C:4160:ASP:OD2	1.96	0.66
2:A:887:ARG:HG3	2:A:892:TRP:CD1	2.32	0.65
2:B:911:PHE:HZ	2:B:922:ASN:HB2	1.59	0.65
2:D:887:ARG:HG3	2:D:892:TRP:CD1	2.32	0.65
2:B:4048:VAL:HG11	2:B:4160:ASP:OD2	1.96	0.65
2:C:887:ARG:HG3	2:C:892:TRP:CD1	2.32	0.65
1:F:62:GLU:N	1:F:62:GLU:OE1	2.29	0.65
1:H:62:GLU:OE1	1:H:62:GLU:N	2.30	0.65
2:D:868:LEU:HD13	2:D:930:LEU:HB3	1.79	0.65
2:B:894:TYR:CD2	2:B:964:ASN:HB3	2.31	0.65
2:C:940:VAL:HA	2:C:1053:ASN:O	1.96	0.65
1:E:36:LYS:NZ	1:E:42:ASP:OD2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:982:GLN:HA	2:A:985:LEU:HD12	1.76	0.65
2:B:887:ARG:HG3	2:B:892:TRP:CD1	2.32	0.65
2:B:940:VAL:HA	2:B:1053:ASN:O	1.96	0.65
2:B:1420:ASP:OD1	2:B:1422:ARG:NH1	2.30	0.65
2:A:2564:THR:HG22	2:A:2607:CYS:HA	1.78	0.65
2:D:1420:ASP:OD1	2:D:1422:ARG:NH1	2.30	0.65
2:D:1466:ASP:OD2	2:D:1468:SER:OG	2.11	0.65
2:D:4048:VAL:HG11	2:D:4160:ASP:OD2	1.96	0.65
2:B:2560:LEU:O	2:B:2564:THR:HG23	1.97	0.65
2:C:1420:ASP:OD1	2:C:1422:ARG:NH1	2.30	0.65
2:A:940:VAL:HA	2:A:1053:ASN:O	1.96	0.65
2:C:986:VAL:HG22	2:C:1044:VAL:HG21	1.78	0.65
1:H:36:LYS:NZ	1:H:42:ASP:OD2	2.29	0.65
2:D:914:LEU:HD21	2:D:919:ARG:HB2	1.79	0.65
2:C:894:TYR:CD2	2:C:964:ASN:HB3	2.31	0.65
2:A:894:TYR:CD2	2:A:964:ASN:HB3	2.31	0.65
2:D:2564:THR:HG22	2:D:2607:CYS:HA	1.78	0.65
2:D:2749:PRO:HD2	2:D:2752:LEU:HD12	1.77	0.65
2:A:919:ARG:HA	2:A:922:ASN:ND2	2.12	0.65
2:C:871:ILE:HA	2:C:874:LYS:HD3	1.77	0.65
2:B:4925:ILE:O	2:B:4929:ILE:HD12	1.97	0.64
2:C:914:LEU:HD21	2:C:919:ARG:HB2	1.79	0.64
2:D:859:THR:HB	2:D:931:LYS:HB3	1.78	0.64
2:A:2560:LEU:O	2:A:2564:THR:HG23	1.97	0.64
1:F:36:LYS:NZ	1:F:42:ASP:OD2	2.30	0.64
2:D:894:TYR:CD2	2:D:964:ASN:HB3	2.31	0.64
2:D:919:ARG:HA	2:D:922:ASN:ND2	2.12	0.64
2:D:2866:VAL:HG12	2:D:2933:MET:HE3	1.79	0.64
2:A:986:VAL:HG22	2:A:1044:VAL:HG21	1.78	0.64
2:B:986:VAL:HG22	2:B:1044:VAL:HG21	1.78	0.64
2:C:859:THR:HB	2:C:931:LYS:HB3	1.78	0.64
2:C:868:LEU:HD13	2:C:930:LEU:HB3	1.79	0.64
2:C:2245:ARG:NH2	2:C:2284:ASN:OD1	2.31	0.64
1:G:36:LYS:NZ	1:G:42:ASP:OD1	2.30	0.64
2:D:940:VAL:HA	2:D:1053:ASN:O	1.96	0.64
2:D:4925:ILE:O	2:D:4929:ILE:HD12	1.97	0.64
2:A:868:LEU:HD13	2:A:930:LEU:HB3	1.79	0.64
2:D:2245:ARG:NH2	2:D:2284:ASN:OD1	2.31	0.64
2:A:914:LEU:HD21	2:A:919:ARG:HB2	1.79	0.64
2:A:2245:ARG:NH2	2:A:2284:ASN:OD1	2.31	0.64
7:A:8006:PCW:H482	7:B:8005:PCW:H271	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:GLU:OE1	1:E:62:GLU:N	2.31	0.64
2:D:2560:LEU:O	2:D:2564:THR:HG23	1.97	0.64
2:D:3529:THR:HG23	2:D:3574:MET:CE	2.25	0.64
2:A:1042:GLN:O	2:A:1046:THR:HG23	1.98	0.64
2:B:3972:ILE:HG21	2:B:3983:LEU:HD12	1.80	0.64
2:A:3392:GLU:OE2	2:A:3396:ARG:NE	2.30	0.64
2:A:4925:ILE:O	2:A:4929:ILE:HD12	1.97	0.64
1:G:62:GLU:OE1	1:G:62:GLU:N	2.30	0.64
2:C:919:ARG:HA	2:C:922:ASN:ND2	2.12	0.64
2:C:2866:VAL:HG12	2:C:2933:MET:HE3	1.79	0.64
2:A:4048:VAL:HG11	2:A:4160:ASP:OD2	1.96	0.64
2:B:1042:GLN:O	2:B:1046:THR:HG23	1.98	0.64
2:B:919:ARG:HA	2:B:922:ASN:ND2	2.12	0.64
2:C:3377:GLU:OE1	2:C:3449:SER:OG	2.12	0.64
2:C:3392:GLU:OE2	2:C:3396:ARG:NE	2.30	0.64
2:D:3392:GLU:OE2	2:D:3396:ARG:NE	2.30	0.63
2:A:3506:VAL:O	2:A:3509:SER:OG	2.13	0.63
2:A:4752:ASN:OD1	2:A:4754:ARG:NH2	2.31	0.63
2:B:1070:GLY:N	2:B:1115:GLU:OE1	2.32	0.63
2:C:2560:LEU:O	2:C:2564:THR:HG23	1.97	0.63
2:C:4752:ASN:OD1	2:C:4754:ARG:NH2	2.31	0.63
2:A:1420:ASP:OD1	2:A:1422:ARG:NH1	2.30	0.63
2:B:2245:ARG:NH2	2:B:2284:ASN:OD1	2.31	0.63
2:B:3392:GLU:OE2	2:B:3396:ARG:NE	2.30	0.63
2:D:1042:GLN:O	2:D:1046:THR:HG23	1.98	0.63
2:A:2779:GLY:N	2:A:2789:HIS:O	2.31	0.63
2:A:3972:ILE:HG21	2:A:3983:LEU:HD12	1.80	0.63
2:B:318:ARG:NH2	2:B:322:GLU:O	2.32	0.63
2:B:868:LEU:HD13	2:B:930:LEU:HB3	1.79	0.63
2:A:2866:VAL:HG12	2:A:2933:MET:HE3	1.79	0.63
2:B:914:LEU:HD21	2:B:919:ARG:HB2	1.79	0.63
2:B:4752:ASN:OD1	2:B:4754:ARG:NH2	2.31	0.63
2:C:1042:GLN:O	2:C:1046:THR:HG23	1.98	0.63
2:D:1070:GLY:N	2:D:1115:GLU:OE1	2.32	0.63
2:D:4752:ASN:OD1	2:D:4754:ARG:NH2	2.31	0.63
2:B:2866:VAL:HG12	2:B:2933:MET:HE3	1.79	0.63
2:C:952:LYS:HZ2	2:C:952:LYS:H	1.47	0.63
2:C:4925:ILE:O	2:C:4929:ILE:HD12	1.97	0.63
2:A:3529:THR:HG23	2:A:3574:MET:CE	2.25	0.63
2:C:882:LEU:HG	2:C:970:PRO:HB3	1.81	0.63
2:D:894:TYR:HB3	2:D:964:ASN:N	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3972:ILE:HG21	2:D:3983:LEU:HD12	1.80	0.62
2:C:2259:LEU:O	2:C:2262:SER:OG	2.16	0.62
2:C:3972:ILE:HG21	2:C:3983:LEU:HD12	1.80	0.62
2:A:2259:LEU:O	2:A:2262:SER:OG	2.16	0.62
2:C:1070:GLY:N	2:C:1115:GLU:OE1	2.32	0.62
2:B:952:LYS:HZ2	2:B:952:LYS:H	1.47	0.62
2:B:3529:THR:HG23	2:B:3574:MET:CE	2.25	0.62
2:A:894:TYR:HB3	2:A:964:ASN:N	2.13	0.62
2:B:882:LEU:HG	2:B:970:PRO:HB3	1.81	0.62
2:C:2779:GLY:N	2:C:2789:HIS:O	2.31	0.62
2:A:1070:GLY:N	2:A:1115:GLU:OE1	2.32	0.62
2:D:318:ARG:NH2	2:D:322:GLU:O	2.32	0.62
2:A:882:LEU:HG	2:A:970:PRO:HB3	1.81	0.62
2:A:1794:THR:HG22	2:A:2174:GLN:OE1	2.00	0.62
2:B:1794:THR:HG22	2:B:2174:GLN:OE1	2.00	0.62
2:C:940:VAL:HB	2:C:1054:ILE:HG13	1.81	0.62
2:A:318:ARG:NH2	2:A:322:GLU:O	2.32	0.62
2:A:952:LYS:HZ2	2:A:952:LYS:H	1.47	0.62
2:C:3529:THR:HG23	2:C:3574:MET:CE	2.25	0.62
2:A:2156:LEU:CD2	2:A:2199:MET:HE1	2.24	0.62
2:C:3541:TYR:OH	2:C:3598:GLN:NE2	2.31	0.62
2:D:882:LEU:HG	2:D:970:PRO:HB3	1.81	0.61
2:D:2259:LEU:O	2:D:2262:SER:OG	2.16	0.61
2:D:1794:THR:HG22	2:D:2174:GLN:OE1	2.00	0.61
2:A:940:VAL:HB	2:A:1054:ILE:HG13	1.81	0.61
2:C:2817:MET:HE1	2:C:2931:LEU:HD11	1.82	0.61
2:B:169:ASP:OD1	2:B:202:ASN:ND2	2.32	0.61
2:B:973:LEU:HA	2:B:975:HIS:CE1	2.36	0.61
2:B:2740:PRO:HG3	2:B:2886:THR:HG22	1.83	0.61
2:C:894:TYR:HB3	2:C:964:ASN:N	2.13	0.61
2:C:973:LEU:HB2	2:C:976:VAL:CG2	2.31	0.61
2:C:1794:THR:HG22	2:C:2174:GLN:OE1	2.00	0.61
2:A:2674:HIS:ND1	2:A:2717:ASP:OD2	2.34	0.61
2:A:2817:MET:HE1	2:A:2931:LEU:HD11	1.82	0.61
2:B:940:VAL:HB	2:B:1054:ILE:HG13	1.81	0.61
2:C:3435:LEU:HD23	2:C:3518:MET:HE2	1.82	0.61
2:A:932:THR:O	2:A:936:LEU:HG	2.01	0.61
2:A:3435:LEU:HD23	2:A:3518:MET:HE2	1.82	0.61
2:D:2740:PRO:HG3	2:D:2886:THR:HG22	1.83	0.61
2:B:318:ARG:NH1	2:B:325:ASP:OD2	2.34	0.61
2:B:973:LEU:HB2	2:B:976:VAL:CG2	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2779:GLY:N	2:B:2789:HIS:O	2.31	0.61
2:D:2968:MET:O	2:D:2971:SER:OG	2.17	0.61
2:A:169:ASP:OD1	2:A:202:ASN:ND2	2.32	0.61
2:B:2674:HIS:ND1	2:B:2717:ASP:OD2	2.34	0.61
2:C:318:ARG:NH1	2:C:325:ASP:OD2	2.34	0.61
2:D:318:ARG:NH1	2:D:325:ASP:OD2	2.34	0.61
2:D:928:GLU:O	2:D:932:THR:HG22	2.01	0.61
2:C:870:ARG:HH21	2:C:874:LYS:HD3	1.66	0.61
2:D:2674:HIS:ND1	2:D:2717:ASP:OD2	2.34	0.61
2:D:2817:MET:HE1	2:D:2931:LEU:HD11	1.82	0.61
2:A:2740:PRO:HG3	2:A:2886:THR:HG22	1.83	0.61
2:B:898:ARG:HA	2:B:904:LEU:O	2.01	0.61
2:B:902:LYS:HB3	2:B:904:LEU:CG	2.28	0.61
2:C:318:ARG:NH2	2:C:322:GLU:O	2.32	0.61
2:B:932:THR:O	2:B:936:LEU:HG	2.01	0.60
2:B:3435:LEU:HD23	2:B:3518:MET:HE2	1.82	0.60
2:C:936:LEU:HB2	2:C:938:CYS:SG	2.41	0.60
2:C:2674:HIS:ND1	2:C:2717:ASP:OD2	2.34	0.60
2:D:898:ARG:HA	2:D:904:LEU:O	2.01	0.60
2:D:1264:THR:OG1	2:D:1266:ASP:OD1	2.20	0.60
2:A:973:LEU:HA	2:A:975:HIS:CE1	2.36	0.60
2:C:898:ARG:HA	2:C:904:LEU:O	2.01	0.60
2:D:169:ASP:OD1	2:D:202:ASN:ND2	2.32	0.60
2:D:936:LEU:HB2	2:D:938:CYS:SG	2.41	0.60
2:D:2779:GLY:N	2:D:2789:HIS:O	2.31	0.60
2:A:895:GLY:CA	2:A:904:LEU:HB2	2.31	0.60
2:C:2156:LEU:CD2	2:C:2199:MET:HE1	2.24	0.60
2:D:932:THR:O	2:D:936:LEU:HG	2.01	0.60
2:A:649:ILE:HG23	2:A:815:ALA:HB3	1.84	0.60
2:A:898:ARG:HA	2:A:904:LEU:O	2.01	0.60
2:A:936:LEU:HB2	2:A:938:CYS:SG	2.41	0.60
2:B:2817:MET:HE1	2:B:2931:LEU:HD11	1.82	0.60
2:B:4129:GLU:OE2	2:B:4133:ASN:ND2	2.35	0.60
2:C:169:ASP:OD1	2:C:202:ASN:ND2	2.32	0.60
2:C:884:ALA:HB1	2:C:968:PRO:HG3	1.83	0.60
2:C:1264:THR:OG1	2:C:1266:ASP:OD1	2.20	0.60
2:C:2740:PRO:HG3	2:C:2886:THR:HG22	1.83	0.60
2:D:870:ARG:HH21	2:D:874:LYS:HD3	1.66	0.60
2:D:973:LEU:HA	2:D:975:HIS:CE1	2.36	0.60
2:A:928:GLU:O	2:A:932:THR:HG22	2.01	0.60
2:B:928:GLU:O	2:B:932:THR:HG22	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2156:LEU:CD2	2:B:2199:MET:HE1	2.24	0.60
2:B:2259:LEU:O	2:B:2262:SER:OG	2.16	0.60
2:C:932:THR:O	2:C:936:LEU:HG	2.01	0.60
2:A:884:ALA:HB1	2:A:968:PRO:HG3	1.83	0.60
2:B:2246:GLN:N	2:B:2246:GLN:OE1	2.35	0.60
2:D:2383:GLU:HA	2:D:2386:ARG:NH2	2.17	0.60
2:A:318:ARG:NH1	2:A:325:ASP:OD2	2.34	0.60
2:A:4129:GLU:OE2	2:A:4133:ASN:ND2	2.35	0.60
2:C:928:GLU:O	2:C:932:THR:HG22	2.01	0.60
2:C:2948:ASP:O	2:C:2949:THR:OG1	2.10	0.60
2:D:884:ALA:HB1	2:D:968:PRO:HG3	1.83	0.60
2:D:895:GLY:CA	2:D:904:LEU:HB2	2.31	0.60
2:D:940:VAL:HB	2:D:1054:ILE:HG13	1.81	0.60
2:D:973:LEU:HB2	2:D:976:VAL:CG2	2.31	0.60
2:D:3435:LEU:HD23	2:D:3518:MET:HE2	1.82	0.60
2:A:3541:TYR:OH	2:A:3598:GLN:NE2	2.31	0.60
2:C:973:LEU:HA	2:C:975:HIS:CE1	2.36	0.60
2:B:883:TRP:HH2	2:B:907:CYS:HB3	1.67	0.60
2:B:3506:VAL:O	2:B:3509:SER:OG	2.13	0.60
2:A:973:LEU:HB2	2:A:976:VAL:CG2	2.31	0.59
2:B:2383:GLU:HA	2:B:2386:ARG:NH2	2.17	0.59
2:C:881:GLU:HB3	2:C:969:ALA:H	1.67	0.59
2:C:985:LEU:HD21	2:C:1057:PRO:HD2	1.84	0.59
2:A:3754:VAL:HG13	2:A:3758:GLU:OE2	2.02	0.59
2:B:936:LEU:HB2	2:B:938:CYS:SG	2.41	0.59
2:B:2968:MET:O	2:B:2971:SER:OG	2.17	0.59
2:B:3754:VAL:HG13	2:B:3758:GLU:OE2	2.02	0.59
2:B:3856:ALA:HB1	2:B:3871:ARG:NE	2.17	0.59
2:C:895:GLY:CA	2:C:904:LEU:HB2	2.31	0.59
2:C:3506:VAL:O	2:C:3509:SER:OG	2.13	0.59
2:C:3962:LYS:NZ	2:C:4025:ASP:OD1	2.36	0.59
2:D:2156:LEU:CD2	2:D:2199:MET:HE1	2.24	0.59
2:B:884:ALA:HB1	2:B:968:PRO:HG3	1.83	0.59
2:B:3962:LYS:NZ	2:B:4025:ASP:OD1	2.36	0.59
2:A:881:GLU:HB3	2:A:969:ALA:H	1.67	0.59
2:B:895:GLY:CA	2:B:904:LEU:HB2	2.31	0.59
2:B:919:ARG:HA	2:B:922:ASN:HD22	1.67	0.59
2:B:985:LEU:HD21	2:B:1057:PRO:HD2	1.84	0.59
2:D:3524:ASN:O	2:D:3583:ARG:NH2	2.36	0.59
2:D:3541:TYR:OH	2:D:3598:GLN:NE2	2.31	0.59
2:B:3524:ASN:O	2:B:3583:ARG:NH2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:649:ILE:HG23	2:C:815:ALA:HB3	1.84	0.59
2:C:3828:GLU:OE1	2:C:3828:GLU:N	2.33	0.59
2:D:3440:GLY:O	2:D:3444:ILE:HG13	2.02	0.59
2:B:870:ARG:HH21	2:B:874:LYS:HD3	1.66	0.59
2:B:929:THR:HA	2:B:932:THR:HG22	1.85	0.59
2:C:3856:ALA:HB1	2:C:3871:ARG:NE	2.17	0.59
2:D:3856:ALA:HB1	2:D:3871:ARG:NE	2.17	0.59
2:A:912:HIS:HA	2:A:919:ARG:NH1	2.17	0.59
2:A:2383:GLU:HA	2:A:2386:ARG:NH2	2.17	0.59
2:B:649:ILE:HG23	2:B:815:ALA:HB3	1.84	0.59
2:B:3440:GLY:O	2:B:3444:ILE:HG13	2.02	0.59
2:C:929:THR:HA	2:C:932:THR:HG22	1.85	0.59
2:C:4129:GLU:OE2	2:C:4133:ASN:ND2	2.35	0.59
2:D:3754:VAL:HG13	2:D:3758:GLU:OE2	2.02	0.59
2:A:870:ARG:HH21	2:A:874:LYS:HD3	1.66	0.59
2:A:3524:ASN:O	2:A:3583:ARG:NH2	2.36	0.59
2:C:883:TRP:HH2	2:C:907:CYS:HB3	1.67	0.59
2:C:2246:GLN:OE1	2:C:2246:GLN:N	2.35	0.59
2:C:2383:GLU:HA	2:C:2386:ARG:NH2	2.17	0.59
2:C:3344:GLN:OE1	2:C:3415:ARG:NH2	2.36	0.59
2:D:912:HIS:HA	2:D:919:ARG:NH1	2.18	0.59
2:A:1173:ASP:OD1	2:A:1174:SER:N	2.36	0.59
2:A:3856:ALA:HB1	2:A:3871:ARG:NE	2.17	0.59
2:B:912:HIS:HA	2:B:919:ARG:NH1	2.18	0.59
2:C:1173:ASP:OD1	2:C:1174:SER:N	2.36	0.59
2:C:2249:ARG:NH2	2:C:2286:GLU:OE2	2.36	0.59
2:D:649:ILE:HG23	2:D:815:ALA:HB3	1.84	0.59
2:D:929:THR:HA	2:D:932:THR:HG22	1.85	0.59
2:D:4129:GLU:OE2	2:D:4133:ASN:ND2	2.35	0.59
2:A:902:LYS:HB3	2:A:904:LEU:CG	2.28	0.59
2:A:985:LEU:HD21	2:A:1057:PRO:HD2	1.84	0.59
2:B:1173:ASP:OD1	2:B:1174:SER:N	2.36	0.59
2:C:912:HIS:HA	2:C:919:ARG:NH1	2.18	0.59
2:C:2863:LEU:HD12	2:C:2926:GLU:OE1	2.03	0.59
2:D:895:GLY:HA3	2:D:904:LEU:HB2	1.84	0.58
2:D:898:ARG:HH12	2:D:907:CYS:HB2	1.68	0.58
2:D:985:LEU:HD21	2:D:1057:PRO:HD2	1.84	0.58
2:B:1264:THR:OG1	2:B:1266:ASP:OD1	2.20	0.58
2:C:3754:VAL:HG13	2:C:3758:GLU:OE2	2.02	0.58
2:A:919:ARG:HA	2:A:922:ASN:HD22	1.67	0.58
2:A:3344:GLN:OE1	2:A:3415:ARG:NH2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:163:LYS:O	2:C:165:ARG:NH1	2.36	0.58
2:C:877:GLU:HA	2:C:911:PHE:CD2	2.39	0.58
2:C:3440:GLY:O	2:C:3444:ILE:HG13	2.02	0.58
2:D:883:TRP:HH2	2:D:907:CYS:HB3	1.67	0.58
2:D:2863:LEU:HD12	2:D:2926:GLU:OE1	2.03	0.58
2:A:895:GLY:HA3	2:A:904:LEU:HB2	1.84	0.58
2:A:929:THR:HA	2:A:932:THR:HG22	1.85	0.58
2:A:2863:LEU:HD12	2:A:2926:GLU:OE1	2.03	0.58
2:C:914:LEU:HD21	2:C:919:ARG:CA	2.33	0.58
2:C:3761:MET:HE3	2:C:3761:MET:HA	1.85	0.58
2:D:3962:LYS:NZ	2:D:4025:ASP:OD1	2.36	0.58
2:A:888:ILE:CD1	2:A:960:TYR:HA	2.32	0.58
2:A:3962:LYS:NZ	2:A:4025:ASP:OD1	2.36	0.58
2:A:4868:ASP:OD1	2:A:4869:GLU:N	2.36	0.58
2:B:881:GLU:HB3	2:B:969:ALA:H	1.67	0.58
2:B:2249:ARG:NH2	2:B:2286:GLU:OE2	2.36	0.58
2:C:2695:GLU:OE1	2:C:2698:ARG:NH2	2.37	0.58
2:A:898:ARG:HH12	2:A:907:CYS:HB2	1.69	0.58
2:A:2249:ARG:NH2	2:A:2286:GLU:OE2	2.36	0.58
2:D:287:THR:HG21	2:D:482:GLU:OE2	2.04	0.58
2:D:877:GLU:HA	2:D:911:PHE:CD2	2.39	0.58
2:D:1173:ASP:OD1	2:D:1174:SER:N	2.36	0.58
2:D:2249:ARG:NH2	2:D:2286:GLU:OE2	2.36	0.58
2:D:3761:MET:HA	2:D:3761:MET:HE3	1.85	0.58
2:A:3440:GLY:O	2:A:3444:ILE:HG13	2.02	0.58
2:B:163:LYS:O	2:B:165:ARG:NH1	2.36	0.58
2:B:877:GLU:HA	2:B:911:PHE:CD2	2.39	0.58
2:B:3943:LYS:O	2:B:4005:LYS:NZ	2.36	0.58
2:B:4868:ASP:OD1	2:B:4869:GLU:N	2.37	0.58
2:C:914:LEU:CD2	2:C:919:ARG:HB2	2.34	0.58
2:C:919:ARG:HA	2:C:922:ASN:HD22	1.67	0.58
2:C:919:ARG:HG2	2:C:920:ASN:N	2.18	0.58
2:D:881:GLU:HB3	2:D:969:ALA:H	1.67	0.58
2:B:2863:LEU:HD12	2:B:2926:GLU:OE1	2.03	0.58
2:C:888:ILE:CD1	2:C:960:TYR:HA	2.32	0.58
2:D:4868:ASP:OD1	2:D:4869:GLU:N	2.37	0.58
2:A:877:GLU:HA	2:A:911:PHE:CD2	2.39	0.58
2:A:1264:THR:OG1	2:A:1266:ASP:OD1	2.20	0.58
2:A:2265:GLY:HA2	2:A:2268:MET:HE1	1.86	0.58
2:B:895:GLY:HA3	2:B:904:LEU:HB2	1.84	0.58
2:B:914:LEU:CD2	2:B:919:ARG:HB2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3170:LEU:HD12	2:B:3195:LEU:HD11	1.86	0.58
2:C:225:HIS:O	2:C:228:MET:HE2	2.04	0.58
2:D:2695:GLU:OE1	2:D:2698:ARG:NH2	2.37	0.58
2:D:3344:GLN:OE1	2:D:3415:ARG:NH2	2.36	0.58
2:A:50:LEU:HD11	2:A:183:LEU:HD13	1.86	0.58
2:A:287:THR:HG21	2:A:482:GLU:OE2	2.04	0.58
2:A:914:LEU:CD2	2:A:919:ARG:HB2	2.34	0.58
2:A:2948:ASP:O	2:A:2949:THR:OG1	2.10	0.58
2:B:914:LEU:HD21	2:B:919:ARG:CA	2.33	0.58
2:B:3344:GLN:OE1	2:B:3415:ARG:NH2	2.36	0.58
2:D:888:ILE:HG12	2:D:960:TYR:CD2	2.39	0.58
2:D:914:LEU:HD21	2:D:919:ARG:CA	2.33	0.58
2:A:914:LEU:HD21	2:A:919:ARG:CA	2.33	0.58
2:A:1654:LEU:O	2:A:1661:GLN:NE2	2.36	0.58
2:B:225:HIS:O	2:B:228:MET:HE2	2.04	0.58
2:C:895:GLY:HA3	2:C:904:LEU:HB2	1.84	0.58
2:C:898:ARG:HH12	2:C:907:CYS:HB2	1.68	0.58
2:C:2265:GLY:HA2	2:C:2268:MET:HE1	1.86	0.58
2:D:225:HIS:O	2:D:228:MET:HE2	2.04	0.57
2:D:905:HIS:CE1	2:D:907:CYS:HB2	2.39	0.57
2:A:2246:GLN:OE1	2:A:2246:GLN:N	2.35	0.57
2:A:2695:GLU:OE1	2:A:2698:ARG:NH2	2.36	0.57
2:B:894:TYR:HB3	2:B:964:ASN:N	2.13	0.57
2:D:919:ARG:HA	2:D:922:ASN:HD22	1.67	0.57
2:D:3111:LEU:HD13	2:D:3183:TYR:CE2	2.40	0.57
2:A:883:TRP:HH2	2:A:907:CYS:HB3	1.67	0.57
2:C:3111:LEU:HD13	2:C:3183:TYR:CE2	2.40	0.57
2:C:3524:ASN:O	2:C:3583:ARG:NH2	2.36	0.57
2:C:3524:ASN:O	2:C:3583:ARG:NH1	2.37	0.57
2:D:163:LYS:O	2:D:165:ARG:NH1	2.36	0.57
2:A:29:VAL:HG12	2:A:30:LEU:HG	1.86	0.57
2:C:888:ILE:HG12	2:C:960:TYR:CD2	2.39	0.57
2:C:2968:MET:O	2:C:2971:SER:OG	2.17	0.57
2:C:3170:LEU:HD12	2:C:3195:LEU:HD11	1.86	0.57
2:D:50:LEU:HD11	2:D:183:LEU:HD13	1.86	0.57
2:A:919:ARG:HG2	2:A:920:ASN:N	2.18	0.57
2:B:3366:LEU:HD11	2:B:3409:LEU:HD12	1.87	0.57
2:B:3384:ALA:O	2:B:3388:ALA:N	2.36	0.57
2:C:905:HIS:CE1	2:C:907:CYS:HB2	2.39	0.57
2:C:2209:MET:HE1	2:C:2254:HIS:ND1	2.20	0.57
2:C:3366:LEU:HD11	2:C:3409:LEU:HD12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:4868:ASP:OD1	2:C:4869:GLU:N	2.37	0.57
2:D:3943:LYS:O	2:D:4005:LYS:NZ	2.36	0.57
2:A:163:LYS:O	2:A:165:ARG:NH1	2.36	0.57
2:B:898:ARG:HH12	2:B:907:CYS:HB2	1.68	0.57
2:B:2265:GLY:HA2	2:B:2268:MET:HE1	1.86	0.57
2:B:3828:GLU:OE1	2:B:3828:GLU:N	2.33	0.57
2:C:29:VAL:HG12	2:C:30:LEU:HG	1.86	0.57
2:D:919:ARG:HG2	2:D:920:ASN:N	2.18	0.57
2:D:2246:GLN:OE1	2:D:2246:GLN:N	2.35	0.57
2:D:3170:LEU:HD12	2:D:3195:LEU:HD11	1.86	0.57
2:A:929:THR:HA	2:A:932:THR:CG2	2.35	0.57
2:A:957:PRO:HG2	2:A:960:TYR:CD1	2.40	0.57
2:C:50:LEU:HD11	2:C:183:LEU:HD13	1.86	0.57
2:D:2209:MET:HE1	2:D:2254:HIS:ND1	2.20	0.57
2:A:225:HIS:O	2:A:228:MET:HE2	2.04	0.57
2:A:3111:LEU:HD13	2:A:3183:TYR:CE2	2.40	0.57
2:B:892:TRP:HA	2:B:903:ARG:HE	1.70	0.57
2:C:3943:LYS:O	2:C:4005:LYS:NZ	2.36	0.57
2:D:29:VAL:HG12	2:D:30:LEU:HG	1.86	0.57
2:D:914:LEU:CD2	2:D:919:ARG:HB2	2.34	0.57
2:A:1281:GLN:O	2:A:1282:ASN:OD1	2.23	0.57
2:B:50:LEU:HD11	2:B:183:LEU:HD13	1.86	0.57
2:B:287:THR:HG21	2:B:482:GLU:OE2	2.04	0.57
2:B:2695:GLU:OE1	2:B:2698:ARG:NH2	2.37	0.57
2:C:287:THR:HG21	2:C:482:GLU:OE2	2.04	0.57
2:C:892:TRP:HA	2:C:903:ARG:HE	1.70	0.57
2:A:892:TRP:HA	2:A:903:ARG:HE	1.70	0.57
2:A:2968:MET:O	2:A:2971:SER:OG	2.17	0.57
2:A:3170:LEU:HD12	2:A:3195:LEU:HD11	1.86	0.57
2:A:3761:MET:HA	2:A:3761:MET:HE3	1.85	0.57
1:H:22:THR:N	1:H:108:GLU:O	2.37	0.57
2:D:2768:ALA:HB3	2:D:2858:PRO:HB3	1.87	0.57
2:B:3856:ALA:HB1	2:B:3871:ARG:HE	1.70	0.57
2:C:1281:GLN:O	2:C:1282:ASN:OD1	2.23	0.57
2:C:4675:LEU:HD23	2:C:4709:PHE:HE1	1.70	0.57
1:E:22:THR:N	1:E:108:GLU:O	2.38	0.56
2:D:929:THR:HA	2:D:932:THR:CG2	2.35	0.56
2:D:2166:LEU:HD21	2:D:2178:LEU:HD23	1.87	0.56
8:D:8009:A1BYZ:C5	8:D:8009:A1BYZ:C9	2.83	0.56
2:A:3524:ASN:O	2:A:3583:ARG:NH1	2.37	0.56
2:B:2209:MET:HE1	2:B:2254:HIS:ND1	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4675:LEU:HD23	2:B:4709:PHE:HE1	1.70	0.56
2:C:3856:ALA:HB1	2:C:3871:ARG:HE	1.70	0.56
2:D:902:LYS:HB3	2:D:904:LEU:CG	2.28	0.56
2:D:2265:GLY:HA2	2:D:2268:MET:HE1	1.86	0.56
2:D:2877:GLU:OE2	2:D:2921:ARG:NE	2.38	0.56
2:D:3366:LEU:HD11	2:D:3409:LEU:HD12	1.87	0.56
2:D:3894:LEU:HB3	2:D:3902:PHE:CE2	2.41	0.56
2:A:3943:LYS:O	2:A:4005:LYS:NZ	2.36	0.56
2:B:2166:LEU:HD21	2:B:2178:LEU:HD23	1.87	0.56
2:B:3761:MET:HA	2:B:3761:MET:HE3	1.85	0.56
8:B:8009:A1BYZ:C5	8:B:8009:A1BYZ:C9	2.83	0.56
1:G:22:THR:N	1:G:108:GLU:O	2.38	0.56
2:D:3856:ALA:HB1	2:D:3871:ARG:HE	1.70	0.56
2:A:888:ILE:HG12	2:A:960:TYR:CD2	2.39	0.56
2:A:2166:LEU:HD21	2:A:2178:LEU:HD23	1.87	0.56
2:A:2209:MET:HE1	2:A:2254:HIS:ND1	2.20	0.56
2:A:2746:VAL:HG21	2:A:2818:ILE:HG22	1.87	0.56
2:A:3366:LEU:HD11	2:A:3409:LEU:HD12	1.87	0.56
2:A:3894:LEU:HB3	2:A:3902:PHE:CE2	2.41	0.56
2:B:888:ILE:HG12	2:B:960:TYR:CD2	2.39	0.56
2:B:888:ILE:CD1	2:B:960:TYR:HA	2.32	0.56
2:C:250:GLY:N	2:C:373:LEU:HD11	2.21	0.56
1:G:60:TRP:CZ2	2:C:1785:VAL:HG11	2.41	0.56
2:D:957:PRO:HG2	2:D:960:TYR:CD1	2.40	0.56
2:D:3384:ALA:O	2:D:3388:ALA:N	2.36	0.56
2:A:905:HIS:CE1	2:A:907:CYS:HB2	2.39	0.56
2:A:3384:ALA:O	2:A:3388:ALA:N	2.36	0.56
2:A:3856:ALA:HB1	2:A:3871:ARG:HE	1.70	0.56
2:B:905:HIS:CE1	2:B:907:CYS:HB2	2.39	0.56
2:B:914:LEU:HD11	2:B:919:ARG:N	2.21	0.56
2:B:929:THR:HA	2:B:932:THR:CG2	2.35	0.56
2:B:1281:GLN:O	2:B:1282:ASN:OD1	2.23	0.56
2:B:3111:LEU:HD13	2:B:3183:TYR:CE2	2.40	0.56
2:C:929:THR:HA	2:C:932:THR:CG2	2.35	0.56
2:C:2166:LEU:HD21	2:C:2178:LEU:HD23	1.87	0.56
2:C:2768:ALA:HB3	2:C:2858:PRO:HB3	1.87	0.56
8:C:8009:A1BYZ:C5	8:C:8009:A1BYZ:C9	2.83	0.56
2:D:892:TRP:HA	2:D:903:ARG:HE	1.70	0.56
2:B:2971:SER:HA	2:B:2974:PHE:CE1	2.41	0.56
1:F:22:THR:N	1:F:108:GLU:O	2.38	0.56
2:D:899:ASP:CB	2:D:902:LYS:HB2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3557:ASN:HB3	2:D:3560:LEU:HD12	1.88	0.56
2:A:2971:SER:HA	2:A:2974:PHE:CE1	2.41	0.56
2:B:29:VAL:HG12	2:B:30:LEU:HG	1.86	0.56
2:B:919:ARG:HG2	2:B:920:ASN:N	2.18	0.56
2:B:2746:VAL:HG21	2:B:2818:ILE:HG22	1.87	0.56
2:C:2234:CYS:SG	2:C:2271:SER:HB3	2.46	0.56
2:C:2971:SER:HA	2:C:2974:PHE:CE1	2.41	0.56
2:C:3384:ALA:O	2:C:3388:ALA:N	2.36	0.56
2:D:250:GLY:N	2:D:373:LEU:HD11	2.21	0.56
2:A:554:ARG:NE	2:A:556:GLU:OE2	2.39	0.56
2:A:881:GLU:HB3	2:A:969:ALA:N	2.21	0.56
2:B:957:PRO:HG2	2:B:960:TYR:CD1	2.40	0.56
2:B:3111:LEU:HD13	2:B:3183:TYR:HE2	1.71	0.56
2:B:3347:VAL:HG11	2:B:3415:ARG:HB2	1.88	0.56
2:D:914:LEU:HD11	2:D:919:ARG:N	2.21	0.56
2:A:250:GLY:N	2:A:373:LEU:HD11	2.21	0.56
2:C:914:LEU:HD11	2:C:919:ARG:N	2.21	0.56
2:C:2746:VAL:HG21	2:C:2818:ILE:HG22	1.87	0.56
2:C:3347:VAL:HG11	2:C:3415:ARG:HB2	1.88	0.56
2:D:888:ILE:CD1	2:D:960:TYR:HA	2.32	0.56
2:A:914:LEU:HD11	2:A:919:ARG:N	2.21	0.56
2:A:2877:GLU:OE2	2:A:2921:ARG:NE	2.38	0.56
2:A:4675:LEU:HD23	2:A:4709:PHE:HE1	1.70	0.56
8:A:8009:A1BYZ:C5	8:A:8009:A1BYZ:C9	2.83	0.56
2:B:3894:LEU:HB3	2:B:3902:PHE:CE2	2.41	0.56
2:C:902:LYS:HB3	2:C:904:LEU:CG	2.28	0.56
2:C:3686:GLU:OE1	2:C:3686:GLU:N	2.39	0.56
2:D:881:GLU:HB3	2:D:969:ALA:N	2.21	0.55
2:D:1281:GLN:O	2:D:1282:ASN:OD1	2.23	0.55
2:D:2234:CYS:SG	2:D:2271:SER:HB3	2.46	0.55
2:D:3111:LEU:HD13	2:D:3183:TYR:HE2	1.71	0.55
2:A:916:GLU:HA	2:A:919:ARG:NE	2.21	0.55
2:A:2234:CYS:SG	2:A:2271:SER:HB3	2.46	0.55
2:A:3686:GLU:OE1	2:A:3686:GLU:N	2.39	0.55
2:B:2234:CYS:SG	2:B:2271:SER:HB3	2.46	0.55
2:B:2947:LEU:O	2:B:2954:LYS:NZ	2.39	0.55
2:C:881:GLU:HB3	2:C:969:ALA:N	2.21	0.55
2:C:957:PRO:HG2	2:C:960:TYR:CD1	2.40	0.55
2:B:3377:GLU:OE1	2:B:3449:SER:OG	2.12	0.55
2:C:3894:LEU:HB3	2:C:3902:PHE:CE2	2.41	0.55
2:D:554:ARG:NE	2:D:556:GLU:OE2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3828:GLU:OE1	2:D:3828:GLU:N	2.33	0.55
2:B:554:ARG:NE	2:B:556:GLU:OE2	2.39	0.55
2:B:2768:ALA:HB3	2:B:2858:PRO:HB3	1.87	0.55
2:C:1654:LEU:O	2:C:1661:GLN:NE2	2.36	0.55
2:D:2746:VAL:HG21	2:D:2818:ILE:HG22	1.87	0.55
2:B:881:GLU:O	2:B:968:PRO:HB3	2.07	0.55
2:C:2947:LEU:O	2:C:2954:LYS:NZ	2.39	0.55
2:D:4675:LEU:HD23	2:D:4709:PHE:HE1	1.70	0.55
2:A:881:GLU:O	2:A:968:PRO:HB3	2.07	0.55
2:A:2768:ALA:HB3	2:A:2858:PRO:HB3	1.87	0.55
2:B:916:GLU:HA	2:B:919:ARG:NE	2.21	0.55
2:C:554:ARG:NE	2:C:556:GLU:OE2	2.39	0.55
2:C:2877:GLU:OE2	2:C:2921:ARG:NE	2.38	0.55
2:D:881:GLU:O	2:D:968:PRO:HB3	2.07	0.55
2:D:3531:GLN:HA	2:D:3534:ILE:HD12	1.89	0.55
2:D:3686:GLU:N	2:D:3686:GLU:OE1	2.39	0.55
2:B:409:ALA:HB2	2:B:484:MET:HE1	1.89	0.55
2:B:3166:CYS:HB3	2:B:3202:MET:HE1	1.89	0.55
2:C:864:LEU:HD11	2:C:930:LEU:CB	2.37	0.55
2:D:952:LYS:HZ2	2:D:952:LYS:H	1.55	0.55
2:D:2971:SER:HA	2:D:2974:PHE:CE1	2.41	0.55
2:A:884:ALA:CB	2:A:968:PRO:HG3	2.37	0.55
2:B:881:GLU:HB3	2:B:969:ALA:N	2.21	0.55
2:B:899:ASP:CB	2:B:902:LYS:HB2	2.21	0.55
2:C:884:ALA:CB	2:C:968:PRO:HG3	2.37	0.55
2:C:3111:LEU:HD13	2:C:3183:TYR:HE2	1.71	0.55
2:A:3531:GLN:HA	2:A:3534:ILE:HD12	1.89	0.55
2:A:3557:ASN:HB3	2:A:3560:LEU:HD12	1.88	0.55
2:B:914:LEU:HD21	2:B:919:ARG:CB	2.37	0.55
2:B:3524:ASN:O	2:B:3583:ARG:NH1	2.37	0.55
2:C:1425:PRO:O	2:C:1429:LEU:HD23	2.07	0.55
2:C:2628:VAL:HG21	2:C:2675:LEU:HG	1.89	0.55
2:D:3524:ASN:O	2:D:3583:ARG:NH1	2.37	0.55
2:B:2257:TYR:O	2:B:2261:ASN:ND2	2.40	0.55
2:C:601:LEU:HD23	2:C:604:LEU:HD12	1.89	0.55
2:D:409:ALA:HB2	2:D:484:MET:HE1	1.89	0.55
2:D:916:GLU:HA	2:D:919:ARG:NE	2.21	0.55
2:A:3347:VAL:HG11	2:A:3415:ARG:HB2	1.88	0.55
2:C:916:GLU:HA	2:C:919:ARG:NE	2.21	0.55
2:C:942:MET:HE2	2:C:1052:TYR:CE1	2.42	0.55
2:C:3166:CYS:HB3	2:C:3202:MET:HE1	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:942:MET:HE2	2:D:1052:TYR:CE1	2.42	0.54
2:D:2257:TYR:O	2:D:2261:ASN:ND2	2.40	0.54
2:D:2928:LEU:HA	2:D:2931:LEU:HD12	1.89	0.54
2:D:2947:LEU:O	2:D:2954:LYS:NZ	2.39	0.54
2:A:2928:LEU:HA	2:A:2931:LEU:HD12	1.89	0.54
2:A:3111:LEU:HD13	2:A:3183:TYR:HE2	1.71	0.54
2:A:3166:CYS:HB3	2:A:3202:MET:HE1	1.89	0.54
2:B:864:LEU:HD11	2:B:930:LEU:CB	2.37	0.54
2:D:3166:CYS:HB3	2:D:3202:MET:HE1	1.89	0.54
2:C:409:ALA:HB2	2:C:484:MET:HE1	1.89	0.54
2:C:2260:GLU:OE2	2:C:2298:LYS:NZ	2.41	0.54
2:D:601:LEU:HD23	2:D:604:LEU:HD12	1.89	0.54
2:D:2628:VAL:HG21	2:D:2675:LEU:HG	1.89	0.54
2:D:3506:VAL:O	2:D:3509:SER:OG	2.13	0.54
2:A:956:LEU:HD13	2:A:960:TYR:CB	2.36	0.54
2:B:884:ALA:CB	2:B:968:PRO:HG3	2.37	0.54
2:B:2628:VAL:HG21	2:B:2675:LEU:HG	1.89	0.54
2:B:3531:GLN:HA	2:B:3534:ILE:HD12	1.89	0.54
2:C:881:GLU:O	2:C:968:PRO:HB3	2.07	0.54
2:D:956:LEU:HD13	2:D:960:TYR:CB	2.36	0.54
2:D:3347:VAL:HG11	2:D:3415:ARG:HB2	1.88	0.54
2:A:942:MET:HE2	2:A:1052:TYR:CE1	2.42	0.54
2:A:3828:GLU:N	2:A:3828:GLU:OE1	2.33	0.54
2:B:3557:ASN:HB3	2:B:3560:LEU:HD12	1.88	0.54
2:C:2257:TYR:O	2:C:2261:ASN:ND2	2.40	0.54
1:G:26:HIS:CE1	1:G:105:LEU:HD11	2.43	0.54
2:A:409:ALA:HB2	2:A:484:MET:HE1	1.89	0.54
2:B:2877:GLU:OE2	2:B:2921:ARG:NE	2.38	0.54
2:B:3686:GLU:OE1	2:B:3686:GLU:N	2.39	0.54
2:C:914:LEU:HD21	2:C:919:ARG:CB	2.37	0.54
2:A:3077:ASP:O	2:A:3081:VAL:HG23	2.08	0.54
2:B:1425:PRO:O	2:B:1429:LEU:HD23	2.07	0.54
2:B:2260:GLU:OE2	2:B:2298:LYS:NZ	2.41	0.54
2:D:884:ALA:CB	2:D:968:PRO:HG3	2.37	0.54
2:A:3443:PHE:CG	2:A:3515:LEU:HD22	2.43	0.54
2:C:139:GLN:NE2	2:C:141:ASP:O	2.41	0.54
2:B:884:ALA:HB3	2:B:968:PRO:HB3	1.90	0.54
2:C:3531:GLN:HA	2:C:3534:ILE:HD12	1.89	0.54
1:H:26:HIS:CE1	1:H:105:LEU:HD11	2.43	0.54
2:D:139:GLN:NE2	2:D:141:ASP:O	2.41	0.54
2:D:1425:PRO:O	2:D:1429:LEU:HD23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3443:PHE:CG	2:D:3515:LEU:HD22	2.43	0.54
8:D:8009:A1BYZ:C9	8:D:8009:A1BYZ:C4	2.86	0.54
2:A:874:LYS:HB2	2:A:874:LYS:NZ	2.23	0.54
2:A:914:LEU:HD21	2:A:919:ARG:CB	2.37	0.54
2:A:2260:GLU:OE2	2:A:2298:LYS:NZ	2.41	0.54
2:A:2947:LEU:O	2:A:2954:LYS:NZ	2.39	0.54
2:B:250:GLY:N	2:B:373:LEU:HD11	2.21	0.54
2:B:942:MET:HE2	2:B:1052:TYR:CE1	2.42	0.54
2:B:2928:LEU:HA	2:B:2931:LEU:HD12	1.89	0.54
2:B:3541:TYR:OH	2:B:3598:GLN:NE2	2.31	0.54
2:C:1821:VAL:HG22	2:C:1927:LEU:HD21	1.90	0.54
2:C:3388:ALA:O	2:C:3392:GLU:N	2.39	0.54
2:A:139:GLN:NE2	2:A:141:ASP:O	2.41	0.54
2:B:139:GLN:NE2	2:B:141:ASP:O	2.41	0.54
2:B:2878:GLN:OE1	2:B:2940:ARG:NH1	2.41	0.54
2:B:3443:PHE:CG	2:B:3515:LEU:HD22	2.43	0.54
2:C:2382:GLU:C	2:C:2386:ARG:HH12	2.16	0.54
2:D:215:VAL:HG12	2:D:275:LEU:HD12	1.90	0.53
2:D:905:HIS:ND1	2:D:907:CYS:HB2	2.23	0.53
2:D:1821:VAL:HG22	2:D:1927:LEU:HD21	1.90	0.53
2:A:1425:PRO:O	2:A:1429:LEU:HD23	2.07	0.53
2:A:2878:GLN:OE1	2:A:2940:ARG:NH1	2.41	0.53
8:A:8009:A1BYZ:C9	8:A:8009:A1BYZ:C4	2.86	0.53
2:B:2802:ASP:OD1	2:B:2803:LYS:N	2.41	0.53
2:C:956:LEU:HD13	2:C:960:TYR:CB	2.36	0.53
2:C:2878:GLN:OE1	2:C:2940:ARG:NH1	2.41	0.53
1:E:58:ARG:O	1:E:62:GLU:OE1	2.26	0.53
2:D:2878:GLN:OE1	2:D:2940:ARG:NH1	2.41	0.53
2:D:3672:ASP:OD1	2:D:3735:HIS:NE2	2.36	0.53
2:A:884:ALA:HB3	2:A:968:PRO:HB3	1.90	0.53
2:B:872:ARG:HH12	2:B:923:LEU:HD22	1.72	0.53
2:B:2314:LEU:HD11	2:B:2417:VAL:HG11	1.90	0.53
2:C:942:MET:HB2	2:C:1052:TYR:CE1	2.43	0.53
1:F:26:HIS:CE1	1:F:105:LEU:HD11	2.43	0.53
2:D:872:ARG:HH12	2:D:923:LEU:HD22	1.72	0.53
2:A:864:LEU:HD11	2:A:930:LEU:CB	2.37	0.53
2:A:2628:VAL:HG21	2:A:2675:LEU:HG	1.89	0.53
2:A:3108:VAL:HG12	2:A:3176:LEU:HD12	1.91	0.53
2:B:942:MET:HB2	2:B:1052:TYR:CE1	2.43	0.53
2:C:215:VAL:HG12	2:C:275:LEU:HD12	1.90	0.53
2:C:872:ARG:HH12	2:C:923:LEU:HD22	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3557:ASN:HB3	2:C:3560:LEU:HD12	1.88	0.53
8:C:8009:A1BYZ:C9	8:C:8009:A1BYZ:C4	2.86	0.53
2:D:884:ALA:HB3	2:D:968:PRO:HB3	1.90	0.53
2:D:2260:GLU:OE2	2:D:2298:LYS:NZ	2.41	0.53
2:D:2314:LEU:HD11	2:D:2417:VAL:HG11	1.90	0.53
2:D:2802:ASP:OD1	2:D:2803:LYS:N	2.41	0.53
2:B:903:ARG:HA	2:B:903:ARG:NH2	2.21	0.53
2:B:3108:VAL:HG12	2:B:3176:LEU:HD12	1.91	0.53
2:B:3515:LEU:HD21	2:B:3603:VAL:HG13	1.91	0.53
8:B:8009:A1BYZ:C9	8:B:8009:A1BYZ:C4	2.86	0.53
2:C:905:HIS:ND1	2:C:907:CYS:HB2	2.24	0.53
2:C:2913:THR:HG23	2:C:2916:GLU:OE1	2.08	0.53
2:C:2928:LEU:HA	2:C:2931:LEU:HD12	1.89	0.53
2:A:601:LEU:HD23	2:A:604:LEU:HD12	1.89	0.53
2:A:2802:ASP:OD1	2:A:2803:LYS:N	2.41	0.53
2:B:1654:LEU:O	2:B:1661:GLN:NE2	2.36	0.53
2:B:3672:ASP:OD1	2:B:3735:HIS:NE2	2.36	0.53
2:C:3077:ASP:O	2:C:3081:VAL:HG23	2.08	0.53
2:C:3443:PHE:CG	2:C:3515:LEU:HD22	2.43	0.53
2:D:914:LEU:HD21	2:D:919:ARG:CB	2.37	0.53
2:D:1654:LEU:O	2:D:1661:GLN:NE2	2.36	0.53
2:D:2382:GLU:C	2:D:2386:ARG:HH12	2.16	0.53
2:A:215:VAL:HG12	2:A:275:LEU:HD12	1.90	0.53
2:A:3380:LEU:HD21	2:A:3395:VAL:HG21	1.91	0.53
2:B:905:HIS:ND1	2:B:907:CYS:HB2	2.23	0.53
2:B:958:LYS:HA	2:B:961:MET:HE3	1.91	0.53
2:B:1821:VAL:HG22	2:B:1927:LEU:HD21	1.90	0.53
2:C:958:LYS:HA	2:C:961:MET:HE3	1.91	0.53
2:D:864:LEU:HD11	2:D:930:LEU:CB	2.37	0.53
2:A:899:ASP:CB	2:A:902:LYS:HB2	2.21	0.53
2:A:3344:GLN:O	2:A:3347:VAL:HG12	2.09	0.53
2:B:3077:ASP:O	2:B:3081:VAL:HG23	2.08	0.53
2:C:2802:ASP:OD1	2:C:2803:LYS:N	2.41	0.53
2:C:3311:ASP:OD1	2:C:3312:HIS:N	2.42	0.53
2:C:3515:LEU:HD21	2:C:3603:VAL:HG13	1.91	0.53
2:D:168:ASP:OD1	2:C:385:MET:HE1	2.09	0.53
2:D:898:ARG:HH11	2:D:906:PRO:HD2	1.74	0.53
2:A:1758:GLY:N	2:A:1759:PRO:CD	2.72	0.53
2:A:2913:THR:HG23	2:A:2916:GLU:OE1	2.08	0.53
2:C:2314:LEU:HD11	2:C:2417:VAL:HG11	1.90	0.53
2:C:3380:LEU:HD21	2:C:3395:VAL:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:58:ARG:O	1:H:62:GLU:OE1	2.27	0.53
2:A:385:MET:HE1	2:B:168:ASP:OD1	2.09	0.53
2:B:2382:GLU:C	2:B:2386:ARG:HH12	2.16	0.53
1:E:26:HIS:CE1	1:E:105:LEU:HD11	2.44	0.53
1:G:58:ARG:O	1:G:62:GLU:OE1	2.26	0.53
2:D:32:GLU:OE2	2:D:33:GLN:N	2.42	0.53
2:D:942:MET:HB2	2:D:1052:TYR:CE1	2.43	0.53
2:D:2913:THR:HG23	2:D:2916:GLU:OE1	2.08	0.53
2:D:3344:GLN:O	2:D:3347:VAL:HG12	2.09	0.53
2:D:3380:LEU:HD21	2:D:3395:VAL:HG21	1.91	0.53
2:A:872:ARG:HH12	2:A:923:LEU:HD22	1.72	0.53
2:A:905:HIS:ND1	2:A:907:CYS:HB2	2.24	0.53
2:B:3344:GLN:O	2:B:3347:VAL:HG12	2.09	0.53
2:B:3380:LEU:HD21	2:B:3395:VAL:HG21	1.91	0.53
2:B:4675:LEU:HD23	2:B:4709:PHE:CE1	2.44	0.53
2:C:3108:VAL:HG12	2:C:3176:LEU:HD12	1.91	0.53
2:D:874:LYS:NZ	2:D:874:LYS:HB2	2.23	0.52
2:D:3077:ASP:O	2:D:3081:VAL:HG23	2.08	0.52
2:A:32:GLU:OE2	2:A:33:GLN:N	2.42	0.52
2:A:912:HIS:HA	2:A:919:ARG:CZ	2.39	0.52
2:A:2382:GLU:C	2:A:2386:ARG:HH12	2.16	0.52
2:B:32:GLU:OE2	2:B:33:GLN:N	2.42	0.52
2:B:956:LEU:HD13	2:B:960:TYR:CB	2.36	0.52
2:B:1758:GLY:N	2:B:1759:PRO:CD	2.72	0.52
2:C:874:LYS:HB2	2:C:874:LYS:NZ	2.23	0.52
2:D:912:HIS:HA	2:D:919:ARG:CZ	2.40	0.52
2:A:2382:GLU:O	2:A:2386:ARG:NH1	2.42	0.52
2:A:3515:LEU:HD21	2:A:3603:VAL:HG13	1.91	0.52
2:B:874:LYS:HB2	2:B:874:LYS:NZ	2.23	0.52
2:C:32:GLU:OE2	2:C:33:GLN:N	2.42	0.52
2:D:2382:GLU:O	2:D:2386:ARG:NH1	2.42	0.52
2:A:942:MET:HB2	2:A:1052:TYR:CE1	2.43	0.52
2:A:2257:TYR:O	2:A:2261:ASN:ND2	2.40	0.52
2:B:215:VAL:HG12	2:B:275:LEU:HD12	1.90	0.52
2:B:601:LEU:HD23	2:B:604:LEU:HD12	1.89	0.52
2:B:912:HIS:HA	2:B:919:ARG:CZ	2.40	0.52
2:B:2913:THR:HG23	2:B:2916:GLU:OE1	2.08	0.52
2:C:2382:GLU:O	2:C:2386:ARG:NH1	2.42	0.52
2:C:3672:ASP:OD1	2:C:3735:HIS:NE2	2.36	0.52
2:D:979:THR:O	2:D:983:THR:HG23	2.10	0.52
2:D:2737:ASP:OD1	2:D:2739:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3108:VAL:HG12	2:D:3176:LEU:HD12	1.91	0.52
2:D:3515:LEU:HD21	2:D:3603:VAL:HG13	1.91	0.52
2:B:898:ARG:HH11	2:B:906:PRO:HD2	1.74	0.52
2:C:884:ALA:HB3	2:C:968:PRO:HB3	1.90	0.52
2:D:2005:GLU:N	2:D:2005:GLU:OE1	2.43	0.52
2:A:3584:GLU:OE1	2:A:3584:GLU:N	2.37	0.52
2:B:2005:GLU:OE1	2:B:2005:GLU:N	2.43	0.52
2:C:912:HIS:HA	2:C:919:ARG:CZ	2.40	0.52
2:C:979:THR:O	2:C:983:THR:HG23	2.10	0.52
2:C:1758:GLY:N	2:C:1759:PRO:CD	2.72	0.52
2:C:2737:ASP:OD1	2:C:2739:ARG:NH1	2.43	0.52
2:C:3344:GLN:O	2:C:3347:VAL:HG12	2.09	0.52
2:D:3311:ASP:OD1	2:D:3312:HIS:N	2.42	0.52
2:A:898:ARG:HH11	2:A:906:PRO:HD2	1.74	0.52
2:A:1821:VAL:HG22	2:A:1927:LEU:HD21	1.90	0.52
2:A:2737:ASP:OD1	2:A:2739:ARG:NH1	2.43	0.52
2:A:3311:ASP:OD1	2:A:3312:HIS:N	2.42	0.52
2:B:385:MET:HE1	2:C:168:ASP:OD1	2.09	0.52
2:B:2382:GLU:O	2:B:2386:ARG:NH1	2.42	0.52
2:B:3079:ARG:NH1	2:B:3156:ASP:OD2	2.43	0.52
2:C:3584:GLU:OE1	2:C:3584:GLU:N	2.37	0.52
2:A:2314:LEU:HD11	2:A:2417:VAL:HG11	1.90	0.52
2:C:898:ARG:HH11	2:C:906:PRO:HD2	1.74	0.52
2:C:2213:VAL:HG11	2:C:2257:TYR:OH	2.10	0.52
2:C:3079:ARG:NH1	2:C:3156:ASP:OD2	2.43	0.52
2:C:4981:HIS:O	5:C:8003:ATP:N6	2.43	0.52
2:D:1758:GLY:N	2:D:1759:PRO:CD	2.72	0.52
2:D:2741:VAL:HG11	2:D:2820:TRP:NE1	2.25	0.52
2:A:958:LYS:HA	2:A:961:MET:HE3	1.91	0.52
2:A:1164:THR:HG22	2:A:1169:VAL:HA	1.92	0.52
2:A:2741:VAL:HG11	2:A:2820:TRP:NE1	2.25	0.52
2:B:2226:PHE:N	2:B:2227:PRO:HD3	2.25	0.52
2:C:71:GLU:OE1	2:C:111:ARG:NH2	2.42	0.52
2:C:2226:PHE:N	2:C:2227:PRO:HD3	2.25	0.52
2:D:958:LYS:HA	2:D:961:MET:HE3	1.91	0.52
2:A:2213:VAL:HG11	2:A:2257:TYR:OH	2.10	0.52
2:A:2226:PHE:N	2:A:2227:PRO:HD3	2.25	0.52
2:B:605:CYS:SG	2:B:1670:LEU:HD12	2.50	0.52
2:D:103:LEU:HD23	2:D:163:LYS:HA	1.92	0.52
2:D:868:LEU:HD13	2:D:930:LEU:HG	1.92	0.52
2:A:868:LEU:HD13	2:A:930:LEU:HG	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2005:GLU:N	2:A:2005:GLU:OE1	2.43	0.52
2:A:4675:LEU:HD23	2:A:4709:PHE:CE1	2.44	0.52
2:B:103:LEU:HD23	2:B:163:LYS:HA	1.92	0.52
2:B:2863:LEU:HD22	2:B:2929:LYS:HB3	1.93	0.52
2:B:3311:ASP:OD1	2:B:3312:HIS:N	2.42	0.52
2:C:4675:LEU:HD23	2:C:4709:PHE:CE1	2.44	0.52
2:D:2007:ILE:HD11	2:D:3642:LEU:HD21	1.93	0.51
2:A:605:CYS:SG	2:A:1670:LEU:HD12	2.50	0.51
2:B:979:THR:O	2:B:983:THR:HG23	2.10	0.51
2:B:2737:ASP:OD1	2:B:2739:ARG:NH1	2.43	0.51
2:C:2005:GLU:OE1	2:C:2005:GLU:N	2.43	0.51
2:D:71:GLU:OE1	2:D:111:ARG:NH2	2.42	0.51
2:D:4675:LEU:HD23	2:D:4709:PHE:CE1	2.44	0.51
2:D:4981:HIS:O	5:D:8003:ATP:N6	2.43	0.51
2:A:898:ARG:O	2:A:898:ARG:HG2	2.11	0.51
2:A:2007:ILE:HD11	2:A:3642:LEU:HD21	1.92	0.51
2:B:608:CYS:SG	2:B:1673:SER:OG	2.69	0.51
2:C:1164:THR:HG22	2:C:1169:VAL:HA	1.92	0.51
2:C:2741:VAL:HG11	2:C:2820:TRP:NE1	2.25	0.51
2:D:1164:THR:HG22	2:D:1169:VAL:HA	1.92	0.51
2:D:2226:PHE:N	2:D:2227:PRO:HD3	2.25	0.51
2:D:3337:LYS:O	2:D:3341:VAL:HG23	2.11	0.51
2:A:2542:PHE:O	2:A:2545:THR:OG1	2.28	0.51
2:B:1164:THR:HG22	2:B:1169:VAL:HA	1.92	0.51
2:B:2741:VAL:HG11	2:B:2820:TRP:NE1	2.25	0.51
2:C:2007:ILE:HD11	2:C:3642:LEU:HD21	1.93	0.51
2:C:4953:GLU:N	2:C:4953:GLU:OE2	2.44	0.51
1:F:58:ARG:O	1:F:62:GLU:OE1	2.28	0.51
2:D:2213:VAL:HG11	2:D:2257:TYR:OH	2.10	0.51
2:A:2863:LEU:HD22	2:A:2929:LYS:HB3	1.93	0.51
2:A:4964:ASP:OD1	2:A:4965:TYR:N	2.44	0.51
2:B:942:MET:HB2	2:B:1052:TYR:CD1	2.46	0.51
2:B:2213:VAL:HG11	2:B:2257:TYR:OH	2.10	0.51
2:B:4981:HIS:O	5:B:8003:ATP:N6	2.43	0.51
2:D:1063:GLN:OE1	2:D:1063:GLN:N	2.44	0.51
2:D:4964:ASP:OD1	2:D:4965:TYR:N	2.44	0.51
2:A:1063:GLN:OE1	2:A:1063:GLN:N	2.44	0.51
2:C:605:CYS:SG	2:C:1670:LEU:HD12	2.50	0.51
2:C:4964:ASP:OD1	2:C:4965:TYR:N	2.44	0.51
2:D:605:CYS:SG	2:D:1670:LEU:HD12	2.50	0.51
2:D:1116:LEU:HD12	2:D:1194:SER:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3079:ARG:NH1	2:D:3156:ASP:OD2	2.43	0.51
2:A:3515:LEU:HD23	2:A:3607:LEU:HD21	1.93	0.51
2:B:909:VAL:HG21	2:B:914:LEU:HA	1.93	0.51
2:B:4964:ASP:OD1	2:B:4965:TYR:N	2.44	0.51
2:D:1297:GLN:NE2	2:D:1546:ASN:OD1	2.44	0.51
2:D:3515:LEU:HD23	2:D:3607:LEU:HD21	1.93	0.51
2:D:4953:GLU:N	2:D:4953:GLU:OE2	2.44	0.51
2:A:885:LEU:HD12	2:A:960:TYR:HE2	1.76	0.51
2:A:979:THR:O	2:A:983:THR:HG23	2.10	0.51
2:B:2007:ILE:HD11	2:B:3642:LEU:HD21	1.93	0.51
2:B:3861:MET:N	2:B:3861:MET:SD	2.84	0.51
2:B:4953:GLU:N	2:B:4953:GLU:OE2	2.44	0.51
2:C:942:MET:HB2	2:C:1052:TYR:CD1	2.46	0.51
2:D:385:MET:HE1	2:A:168:ASP:OD1	2.11	0.51
2:A:3079:ARG:NH1	2:A:3156:ASP:OD2	2.43	0.51
2:A:4953:GLU:N	2:A:4953:GLU:OE2	2.44	0.51
2:B:868:LEU:HD13	2:B:930:LEU:HG	1.92	0.51
2:C:883:TRP:CH2	2:C:907:CYS:HB3	2.46	0.51
2:C:909:VAL:HG21	2:C:914:LEU:HA	1.93	0.51
2:D:887:ARG:HA	2:D:890:GLN:CD	2.36	0.51
2:D:3354:LEU:HA	2:D:3357:SER:OG	2.11	0.51
7:D:8005:PCW:H442	7:D:8005:PCW:H20	1.93	0.51
2:B:2882:ASN:O	2:B:2886:THR:HG23	2.11	0.51
2:C:885:LEU:HD12	2:C:960:TYR:HE2	1.76	0.51
2:C:887:ARG:HA	2:C:890:GLN:CD	2.36	0.51
2:C:898:ARG:O	2:C:898:ARG:HG2	2.11	0.51
2:C:909:VAL:HG23	2:C:914:LEU:HB2	1.93	0.51
2:C:1116:LEU:HD12	2:C:1194:SER:HB3	1.93	0.51
2:D:2873:GLN:O	2:D:2877:GLU:HG2	2.11	0.51
2:A:903:ARG:HA	2:A:903:ARG:NH2	2.21	0.51
2:A:3337:LYS:O	2:A:3341:VAL:HG23	2.11	0.51
2:A:4981:HIS:O	5:A:8003:ATP:N6	2.43	0.51
2:B:887:ARG:HA	2:B:890:GLN:CD	2.36	0.51
2:B:1063:GLN:OE1	2:B:1063:GLN:N	2.44	0.51
2:B:1645:GLU:OE1	2:B:1647:ARG:NH2	2.43	0.51
2:D:843:PRO:O	2:D:1198:GLY:N	2.38	0.50
2:A:887:ARG:HA	2:A:890:GLN:CD	2.36	0.50
2:A:942:MET:HB2	2:A:1052:TYR:CD1	2.46	0.50
2:A:3861:MET:N	2:A:3861:MET:SD	2.84	0.50
2:B:885:LEU:HD12	2:B:960:TYR:HE2	1.76	0.50
2:B:3354:LEU:HA	2:B:3357:SER:OG	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:883:TRP:CH2	2:D:907:CYS:HB3	2.46	0.50
2:D:3861:MET:N	2:D:3861:MET:SD	2.84	0.50
2:B:1116:LEU:HD12	2:B:1194:SER:HB3	1.93	0.50
2:C:868:LEU:HD13	2:C:930:LEU:HG	1.92	0.50
2:C:2863:LEU:HD22	2:C:2929:LYS:HB3	1.92	0.50
2:C:3861:MET:SD	2:C:3861:MET:N	2.84	0.50
2:D:885:LEU:HD12	2:D:960:TYR:HE2	1.76	0.50
2:A:103:LEU:HD23	2:A:163:LYS:HA	1.92	0.50
2:A:1116:LEU:HD12	2:A:1194:SER:HB3	1.92	0.50
2:B:953:LYS:HE3	2:B:969:ALA:HB1	1.93	0.50
2:C:2882:ASN:O	2:C:2886:THR:HG23	2.11	0.50
2:C:3337:LYS:O	2:C:3341:VAL:HG23	2.11	0.50
2:D:985:LEU:HD21	2:D:1057:PRO:CD	2.42	0.50
2:D:2961:LEU:HD21	2:D:3040:ILE:HD13	1.94	0.50
2:A:3645:LEU:HD21	2:A:3653:MET:HE3	1.93	0.50
2:B:2961:LEU:HD21	2:B:3040:ILE:HD13	1.94	0.50
2:B:3388:ALA:O	2:B:3392:GLU:N	2.39	0.50
2:D:71:GLU:OE1	2:D:111:ARG:NE	2.44	0.50
2:D:2882:ASN:O	2:D:2886:THR:HG23	2.11	0.50
2:D:3645:LEU:HD21	2:D:3653:MET:HE3	1.93	0.50
2:B:848:SER:N	2:B:851:ASP:OD1	2.43	0.50
2:B:898:ARG:HB2	2:B:905:HIS:CD2	2.47	0.50
2:B:902:LYS:HG3	2:B:904:LEU:HD11	1.93	0.50
2:B:3534:ILE:HG13	2:B:3597:VAL:HG23	1.94	0.50
7:C:8005:PCW:H442	7:C:8005:PCW:H20	1.93	0.50
2:D:2372:GLU:HG2	2:A:197:MET:CE	2.39	0.50
2:D:2600:GLN:O	2:D:2604:ILE:HG12	2.12	0.50
2:D:3584:GLU:OE1	2:D:3584:GLU:N	2.37	0.50
2:B:3515:LEU:HD23	2:B:3607:LEU:HD21	1.93	0.50
2:C:2600:GLN:O	2:C:2604:ILE:HG12	2.12	0.50
2:D:898:ARG:O	2:D:898:ARG:HG2	2.11	0.50
2:D:942:MET:HB2	2:D:1052:TYR:CD1	2.46	0.50
2:D:2863:LEU:HD22	2:D:2929:LYS:HB3	1.93	0.50
2:A:883:TRP:CH2	2:A:907:CYS:HB3	2.46	0.50
2:A:3354:LEU:HA	2:A:3357:SER:OG	2.11	0.50
2:B:2600:GLN:O	2:B:2604:ILE:HG12	2.12	0.50
2:B:2873:GLN:O	2:B:2877:GLU:HG2	2.11	0.50
2:B:2877:GLU:OE1	2:B:2909:TYR:OH	2.21	0.50
2:B:3025:VAL:HG23	2:B:3025:VAL:O	2.12	0.50
2:C:976:VAL:HG11	2:C:1045:ARG:O	2.12	0.50
2:C:1063:GLN:N	2:C:1063:GLN:OE1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3354:LEU:HA	2:C:3357:SER:OG	2.11	0.50
2:D:3025:VAL:HG23	2:D:3025:VAL:O	2.12	0.50
2:D:4875:ASP:O	2:C:4580:VAL:HG12	2.12	0.50
2:A:898:ARG:HB2	2:A:905:HIS:CD2	2.47	0.50
2:B:877:GLU:HG3	2:B:911:PHE:CG	2.47	0.50
2:C:953:LYS:HE3	2:C:969:ALA:HB1	1.93	0.50
2:C:985:LEU:HD21	2:C:1057:PRO:CD	2.42	0.50
2:C:2873:GLN:O	2:C:2877:GLU:HG2	2.11	0.50
2:C:3025:VAL:HG23	2:C:3025:VAL:O	2.12	0.50
2:C:3515:LEU:HD23	2:C:3607:LEU:HD21	1.93	0.50
2:D:953:LYS:HE3	2:D:969:ALA:HB1	1.93	0.50
2:A:909:VAL:HG21	2:A:914:LEU:HA	1.93	0.50
2:A:3534:ILE:HG13	2:A:3597:VAL:HG23	1.94	0.50
2:B:3337:LYS:O	2:B:3341:VAL:HG23	2.11	0.50
2:C:3645:LEU:HD21	2:C:3653:MET:HE3	1.93	0.50
2:C:3691:VAL:HG12	2:C:3693:GLU:H	1.77	0.50
2:D:909:VAL:HG23	2:D:914:LEU:HB2	1.93	0.49
2:A:1758:GLY:N	2:A:1759:PRO:HD2	2.27	0.49
7:A:8005:PCW:H442	7:A:8005:PCW:H20	1.93	0.49
2:B:258:ARG:O	2:B:285:HIS:NE2	2.42	0.49
2:B:976:VAL:HG11	2:B:1045:ARG:O	2.12	0.49
2:B:3591:GLU:O	2:B:3594:VAL:HG12	2.12	0.49
2:D:902:LYS:HG3	2:D:904:LEU:HD11	1.93	0.49
2:A:976:VAL:HG11	2:A:1045:ARG:O	2.12	0.49
2:A:985:LEU:HD21	2:A:1057:PRO:CD	2.42	0.49
2:A:2600:GLN:O	2:A:2604:ILE:HG12	2.12	0.49
2:A:2873:GLN:O	2:A:2877:GLU:HG2	2.12	0.49
2:A:2961:LEU:HD21	2:A:3040:ILE:HD13	1.94	0.49
2:A:3691:VAL:HG12	2:A:3693:GLU:H	1.77	0.49
2:C:898:ARG:HB2	2:C:905:HIS:CD2	2.47	0.49
2:C:1758:GLY:N	2:C:1759:PRO:HD2	2.27	0.49
2:D:898:ARG:HB2	2:D:905:HIS:CD2	2.47	0.49
2:D:976:VAL:HG11	2:D:1045:ARG:O	2.12	0.49
2:B:898:ARG:O	2:B:898:ARG:HG2	2.11	0.49
2:B:985:LEU:HD21	2:B:1057:PRO:CD	2.42	0.49
2:C:4122:GLU:OE1	2:C:4122:GLU:N	2.44	0.49
2:D:909:VAL:HG21	2:D:914:LEU:HA	1.93	0.49
2:A:608:CYS:SG	2:A:1673:SER:OG	2.69	0.49
2:A:877:GLU:HG3	2:A:911:PHE:CG	2.47	0.49
2:A:909:VAL:HG23	2:A:914:LEU:HB2	1.93	0.49
2:A:2882:ASN:O	2:A:2886:THR:HG23	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:909:VAL:HG23	2:B:914:LEU:HB2	1.93	0.49
2:B:2234:CYS:O	2:B:2237:LEU:N	2.46	0.49
2:B:2875:MET:HB3	2:B:2940:ARG:HB2	1.94	0.49
2:B:3220:TYR:CD1	2:B:3237:VAL:HG12	2.48	0.49
2:C:3591:GLU:O	2:C:3594:VAL:HG12	2.12	0.49
2:D:1758:GLY:N	2:D:1759:PRO:HD2	2.27	0.49
2:D:3534:ILE:HG13	2:D:3597:VAL:HG23	1.94	0.49
2:D:3691:VAL:HG12	2:D:3693:GLU:H	1.77	0.49
2:A:902:LYS:HG3	2:A:904:LEU:HD11	1.93	0.49
2:A:1645:GLU:OE1	2:A:1647:ARG:NH2	2.43	0.49
2:A:2875:MET:HB3	2:A:2940:ARG:HB2	1.94	0.49
2:C:103:LEU:HD23	2:C:163:LYS:HA	1.92	0.49
2:A:1297:GLN:NE2	2:A:1546:ASN:OD1	2.44	0.49
2:C:902:LYS:HG3	2:C:904:LEU:HD11	1.93	0.49
2:C:903:ARG:HA	2:C:903:ARG:NH2	2.21	0.49
2:C:2234:CYS:O	2:C:2237:LEU:N	2.46	0.49
2:C:3220:TYR:CD1	2:C:3237:VAL:HG12	2.48	0.49
2:D:500:THR:HG23	2:D:503:HIS:H	1.77	0.49
2:D:877:GLU:HG3	2:D:911:PHE:CG	2.47	0.49
2:D:3317:LEU:HD23	2:D:3354:LEU:CD2	2.43	0.49
2:A:71:GLU:OE1	2:A:111:ARG:NH2	2.42	0.49
2:A:3025:VAL:HG23	2:A:3025:VAL:O	2.12	0.49
2:A:3230:ILE:HG13	2:A:3231:LEU:HD12	1.95	0.49
2:C:848:SER:N	2:C:851:ASP:OD1	2.43	0.49
2:C:3230:ILE:HG13	2:C:3231:LEU:HD12	1.95	0.49
2:D:3176:LEU:HD23	2:D:3176:LEU:C	2.38	0.49
2:C:673:ALA:O	2:C:681:THR:OG1	2.31	0.49
2:C:877:GLU:HG3	2:C:911:PHE:CG	2.47	0.49
2:C:2961:LEU:HD21	2:C:3040:ILE:HD13	1.94	0.49
2:D:1536:GLU:OE1	2:D:1536:GLU:N	2.46	0.49
2:D:2246:GLN:NE2	2:D:3867:THR:O	2.46	0.49
2:D:3230:ILE:HG13	2:D:3231:LEU:HD12	1.95	0.49
2:A:940:VAL:HG23	2:A:1052:TYR:HB3	1.95	0.49
2:A:3317:LEU:HD23	2:A:3354:LEU:CD2	2.43	0.49
2:B:883:TRP:CH2	2:B:907:CYS:HB3	2.46	0.49
2:B:940:VAL:HG23	2:B:1052:TYR:HB3	1.95	0.49
7:B:8005:PCW:H442	7:B:8005:PCW:H20	1.93	0.49
2:C:258:ARG:O	2:C:285:HIS:NE2	2.42	0.49
2:C:500:THR:HG23	2:C:503:HIS:H	1.77	0.49
2:C:2415:ASN:O	2:C:2415:ASN:ND2	2.46	0.49
2:C:3176:LEU:HD23	2:C:3176:LEU:C	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:4747:GLU:OE2	2:A:4747:GLU:HA	2.13	0.49
2:B:295:THR:O	2:B:299:GLY:N	2.46	0.49
2:B:673:ALA:O	2:B:681:THR:OG1	2.30	0.49
2:B:957:PRO:HB2	2:B:959:THR:HG23	1.95	0.49
2:B:3230:ILE:HG13	2:B:3231:LEU:HD12	1.95	0.49
2:B:3317:LEU:HD23	2:B:3354:LEU:CD2	2.43	0.49
2:C:2246:GLN:NE2	2:C:3867:THR:O	2.46	0.49
2:C:3435:LEU:CD2	2:C:3518:MET:HE2	2.42	0.49
2:D:2583:MET:HE3	2:D:2611:LEU:HD23	1.95	0.48
2:A:953:LYS:HE3	2:A:969:ALA:HB1	1.93	0.48
2:A:2246:GLN:NE2	2:A:3867:THR:O	2.46	0.48
2:B:2394:ASP:OD2	2:B:2419:LEU:N	2.46	0.48
2:B:4054:SER:O	2:B:4056:SER:N	2.46	0.48
2:C:2875:MET:HB3	2:C:2940:ARG:HB2	1.94	0.48
2:C:3317:LEU:HD23	2:C:3354:LEU:CD2	2.43	0.48
2:C:3556:ASN:OD1	2:C:3557:ASN:N	2.46	0.48
2:D:1783:CYS:SG	2:D:1785:VAL:HG22	2.53	0.48
2:D:2746:VAL:HG22	2:D:2747:ILE:N	2.28	0.48
2:D:4855:ASN:CG	7:C:8006:PCW:H341	2.38	0.48
2:A:1536:GLU:OE1	2:A:1536:GLU:N	2.46	0.48
2:A:2895:LEU:HD22	2:A:2901:GLY:O	2.13	0.48
2:B:500:THR:HG23	2:B:503:HIS:H	1.77	0.48
2:B:1758:GLY:N	2:B:1759:PRO:HD2	2.27	0.48
2:B:2415:ASN:O	2:B:2415:ASN:ND2	2.46	0.48
2:B:3645:LEU:HD21	2:B:3653:MET:HE3	1.93	0.48
2:B:3691:VAL:HG12	2:B:3693:GLU:H	1.77	0.48
2:C:843:PRO:O	2:C:1198:GLY:N	2.38	0.48
2:C:4747:GLU:HA	2:C:4747:GLU:OE2	2.13	0.48
2:D:608:CYS:SG	2:D:1673:SER:OG	2.69	0.48
2:D:3556:ASN:OD1	2:D:3557:ASN:N	2.46	0.48
2:A:500:THR:HG23	2:A:503:HIS:H	1.77	0.48
2:A:1783:CYS:SG	2:A:1785:VAL:HG22	2.53	0.48
2:A:2234:CYS:O	2:A:2237:LEU:N	2.46	0.48
2:A:4054:SER:O	2:A:4056:SER:N	2.46	0.48
2:C:2394:ASP:OD2	2:C:2419:LEU:N	2.47	0.48
2:D:951:LEU:HD22	2:D:973:LEU:HB3	1.95	0.48
2:D:2007:ILE:CD1	2:D:3642:LEU:HD21	2.44	0.48
2:D:2415:ASN:ND2	2:D:2415:ASN:O	2.46	0.48
2:D:4054:SER:O	2:D:4056:SER:N	2.46	0.48
2:D:4122:GLU:OE1	2:D:4122:GLU:N	2.44	0.48
2:A:888:ILE:HG13	2:A:889:GLU:N	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:957:PRO:HB2	2:A:959:THR:HG23	1.95	0.48
2:A:2007:ILE:CD1	2:A:3642:LEU:HD21	2.44	0.48
2:A:2415:ASN:O	2:A:2415:ASN:ND2	2.46	0.48
2:A:3176:LEU:HD23	2:A:3176:LEU:C	2.38	0.48
2:A:3591:GLU:O	2:A:3594:VAL:HG12	2.12	0.48
2:B:71:GLU:OE1	2:B:111:ARG:NE	2.44	0.48
2:B:2372:GLU:HG2	2:C:197:MET:CE	2.41	0.48
2:C:1536:GLU:OE1	2:C:1536:GLU:N	2.46	0.48
2:C:4054:SER:O	2:C:4056:SER:N	2.46	0.48
2:D:872:ARG:CG	2:D:927:GLY:HA2	2.43	0.48
2:D:877:GLU:O	2:D:881:GLU:HG2	2.13	0.48
2:D:903:ARG:HA	2:D:903:ARG:NH2	2.21	0.48
2:D:3220:TYR:CD1	2:D:3237:VAL:HG12	2.48	0.48
2:D:4747:GLU:HA	2:D:4747:GLU:OE2	2.13	0.48
2:A:3246:VAL:HG12	2:A:3247:LEU:N	2.29	0.48
2:A:3435:LEU:CD2	2:A:3518:MET:HE2	2.42	0.48
2:A:3556:ASN:OD1	2:A:3557:ASN:N	2.46	0.48
2:B:3410:TYR:O	2:B:3413:LEU:N	2.47	0.48
2:C:2542:PHE:O	2:C:2545:THR:OG1	2.28	0.48
2:D:2234:CYS:O	2:D:2237:LEU:N	2.46	0.48
2:D:2394:ASP:OD2	2:D:2419:LEU:N	2.46	0.48
2:D:2875:MET:HB3	2:D:2940:ARG:HB2	1.94	0.48
2:A:3220:TYR:CD1	2:A:3237:VAL:HG12	2.48	0.48
2:B:890:GLN:HB2	2:B:892:TRP:HD1	1.79	0.48
2:B:2746:VAL:HG22	2:B:2747:ILE:N	2.28	0.48
2:B:3435:LEU:CD2	2:B:3518:MET:HE2	2.42	0.48
2:B:4747:GLU:HA	2:B:4747:GLU:OE2	2.13	0.48
2:C:888:ILE:HG13	2:C:889:GLU:N	2.26	0.48
2:C:957:PRO:HB2	2:C:959:THR:HG23	1.95	0.48
2:C:3246:VAL:HG12	2:C:3247:LEU:N	2.29	0.48
2:D:890:GLN:HB2	2:D:892:TRP:HD1	1.79	0.48
2:A:2746:VAL:HG22	2:A:2747:ILE:N	2.28	0.48
2:B:3176:LEU:C	2:B:3176:LEU:HD23	2.38	0.48
2:B:3246:VAL:HG12	2:B:3247:LEU:N	2.29	0.48
2:B:4122:GLU:OE1	2:B:4122:GLU:N	2.44	0.48
2:B:4580:VAL:HG12	2:C:4875:ASP:O	2.12	0.48
2:C:158:ARG:CZ	2:C:165:ARG:HH21	2.27	0.48
2:C:951:LEU:HD22	2:C:973:LEU:HB3	1.95	0.48
2:D:898:ARG:NH1	2:D:907:CYS:HB2	2.29	0.48
2:D:940:VAL:HG23	2:D:1052:TYR:HB3	1.95	0.48
2:D:1645:GLU:OE1	2:D:1647:ARG:NH2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3246:VAL:HG12	2:D:3247:LEU:N	2.29	0.48
2:A:877:GLU:O	2:A:881:GLU:HG2	2.14	0.48
2:A:940:VAL:HB	2:A:1054:ILE:CG1	2.43	0.48
2:B:1536:GLU:OE1	2:B:1536:GLU:N	2.46	0.48
2:B:2007:ILE:CD1	2:B:3642:LEU:HD21	2.44	0.48
2:B:2583:MET:HE3	2:B:2611:LEU:HD23	1.95	0.48
2:C:877:GLU:O	2:C:881:GLU:HG2	2.13	0.48
2:C:890:GLN:HB2	2:C:892:TRP:HD1	1.79	0.48
2:C:955:LYS:HE3	2:C:955:LYS:HB3	1.61	0.48
2:C:1783:CYS:SG	2:C:1785:VAL:HG22	2.53	0.48
2:C:3168:ARG:O	2:C:3172:SER:OG	2.27	0.48
2:D:158:ARG:CZ	2:D:165:ARG:HH21	2.27	0.48
2:D:295:THR:O	2:D:299:GLY:N	2.46	0.48
2:D:940:VAL:HB	2:D:1054:ILE:CG1	2.43	0.48
2:D:957:PRO:HB2	2:D:959:THR:HG23	1.95	0.48
2:D:2634:LEU:HD12	2:D:2686:SER:HB3	1.96	0.48
2:A:890:GLN:HB2	2:A:892:TRP:HD1	1.79	0.48
2:A:2372:GLU:HG2	2:B:197:MET:CE	2.41	0.48
2:A:3864:GLU:O	2:A:3868:VAL:HG23	2.14	0.48
2:B:902:LYS:HD2	2:B:902:LYS:HA	1.55	0.48
2:B:1783:CYS:SG	2:B:1785:VAL:HG22	2.53	0.48
2:B:2234:CYS:HB3	2:B:2238:CYS:HB3	1.55	0.48
2:B:3556:ASN:OD1	2:B:3557:ASN:N	2.46	0.48
2:C:2007:ILE:CD1	2:C:3642:LEU:HD21	2.44	0.48
2:C:3534:ILE:HG13	2:C:3597:VAL:HG23	1.94	0.48
1:E:2:GLY:N	1:E:78:SER:OG	2.42	0.48
2:A:258:ARG:O	2:A:285:HIS:NE2	2.42	0.48
2:A:295:THR:O	2:A:299:GLY:N	2.46	0.48
2:A:898:ARG:NH1	2:A:907:CYS:HB2	2.29	0.48
2:B:871:ILE:HG13	2:B:1050:TYR:CE2	2.49	0.48
2:B:872:ARG:CG	2:B:927:GLY:HA2	2.43	0.48
2:B:888:ILE:HG13	2:B:889:GLU:N	2.26	0.48
2:B:2863:LEU:HD13	2:B:2929:LYS:HB2	1.96	0.48
2:B:2895:LEU:HD22	2:B:2901:GLY:O	2.14	0.48
2:C:872:ARG:CG	2:C:927:GLY:HA2	2.43	0.48
2:C:3864:GLU:O	2:C:3868:VAL:HG23	2.14	0.48
2:D:859:THR:CG2	2:D:932:THR:HA	2.44	0.47
2:D:955:LYS:HB3	2:D:955:LYS:HE3	1.61	0.47
2:D:3435:LEU:CD2	2:D:3518:MET:HE2	2.42	0.47
2:D:3864:GLU:O	2:D:3868:VAL:HG23	2.14	0.47
2:A:158:ARG:CZ	2:A:165:ARG:HH21	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:859:THR:CG2	2:A:932:THR:HA	2.44	0.47
2:A:3388:ALA:O	2:A:3392:GLU:N	2.39	0.47
2:B:158:ARG:CZ	2:B:165:ARG:HH21	2.27	0.47
2:B:877:GLU:O	2:B:881:GLU:HG2	2.13	0.47
2:B:951:LEU:HD22	2:B:973:LEU:HB3	1.95	0.47
7:B:8006:PCW:H341	2:C:4855:ASN:CG	2.39	0.47
2:C:940:VAL:HG23	2:C:1052:TYR:HB3	1.95	0.47
2:C:2119:ARG:NH2	2:C:3720:ASP:OD1	2.47	0.47
2:C:2746:VAL:HG22	2:C:2747:ILE:N	2.28	0.47
2:C:3410:TYR:O	2:C:3413:LEU:N	2.47	0.47
2:C:4088:ARG:NH1	2:C:4090:LEU:HD12	2.29	0.47
1:F:33:ASP:OD2	1:F:35:LYS:HG3	2.14	0.47
2:A:920:ASN:HA	2:A:923:LEU:HD12	1.97	0.47
2:A:2265:GLY:O	2:A:2267:GLY:N	2.45	0.47
2:A:3410:TYR:O	2:A:3413:LEU:N	2.47	0.47
2:A:4122:GLU:OE1	2:A:4122:GLU:N	2.44	0.47
2:B:157:GLN:OE1	2:B:158:ARG:NH1	2.47	0.47
2:B:2246:GLN:NE2	2:B:3867:THR:O	2.46	0.47
2:B:3088:ILE:HD12	2:B:3088:ILE:H	1.79	0.47
2:C:295:THR:O	2:C:299:GLY:N	2.46	0.47
2:C:886:THR:O	2:C:890:GLN:HG3	2.14	0.47
2:C:898:ARG:NH1	2:C:907:CYS:HB2	2.29	0.47
2:C:2624:LEU:O	2:C:2628:VAL:HG23	2.14	0.47
2:C:4670:LYS:O	2:C:4674:GLU:HG2	2.15	0.47
2:D:871:ILE:HG13	2:D:1050:TYR:CE2	2.49	0.47
2:B:4670:LYS:O	2:B:4674:GLU:HG2	2.15	0.47
2:C:871:ILE:HG13	2:C:1050:TYR:CE2	2.49	0.47
2:C:2583:MET:HE3	2:C:2611:LEU:HD23	1.95	0.47
2:C:2863:LEU:HD13	2:C:2929:LYS:HB2	1.96	0.47
2:C:2889:ARG:O	2:C:2893:GLN:OE1	2.32	0.47
2:D:888:ILE:HG13	2:D:889:GLU:N	2.26	0.47
2:D:2895:LEU:HD22	2:D:2901:GLY:O	2.14	0.47
2:D:3088:ILE:H	2:D:3088:ILE:HD12	1.79	0.47
2:D:3591:GLU:O	2:D:3594:VAL:HG12	2.12	0.47
2:D:3859:LEU:C	2:D:3859:LEU:HD12	2.39	0.47
2:A:2394:ASP:OD2	2:A:2419:LEU:N	2.46	0.47
2:A:3182:PRO:O	2:A:3185:GLU:HG3	2.15	0.47
2:B:931:LYS:HA	2:B:934:LEU:HD22	1.95	0.47
2:C:1116:LEU:HD12	2:C:1194:SER:CB	2.45	0.47
2:D:2624:LEU:O	2:D:2628:VAL:HG23	2.14	0.47
2:D:3322:ARG:HA	2:D:3325:VAL:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:848:SER:N	2:A:851:ASP:OD1	2.43	0.47
2:A:971:LEU:CD1	2:A:973:LEU:HD21	2.45	0.47
2:A:2583:MET:HE3	2:A:2611:LEU:HD23	1.95	0.47
2:A:2624:LEU:O	2:A:2628:VAL:HG23	2.14	0.47
2:A:3088:ILE:H	2:A:3088:ILE:HD12	1.79	0.47
2:B:649:ILE:HD13	2:B:812:CYS:HB3	1.96	0.47
2:C:916:GLU:HA	2:C:919:ARG:CD	2.44	0.47
2:C:971:LEU:CD1	2:C:973:LEU:HD21	2.45	0.47
2:C:2634:LEU:HD12	2:C:2686:SER:HB3	1.96	0.47
2:C:2895:LEU:HD22	2:C:2901:GLY:O	2.14	0.47
2:D:157:GLN:OE1	2:D:158:ARG:NH1	2.47	0.47
2:D:916:GLU:HA	2:D:919:ARG:CD	2.44	0.47
2:D:1127:GLY:O	2:D:1128:HIS:C	2.58	0.47
2:D:2265:GLY:O	2:D:2267:GLY:N	2.45	0.47
2:A:157:GLN:OE1	2:A:158:ARG:NH1	2.47	0.47
2:A:942:MET:HG3	2:A:1052:TYR:CD2	2.50	0.47
2:A:2863:LEU:HD13	2:A:2929:LYS:HB2	1.96	0.47
2:A:2942:LEU:HD21	2:A:2945:MET:HB2	1.97	0.47
2:C:608:CYS:SG	2:C:1673:SER:OG	2.69	0.47
2:C:608:CYS:SG	2:C:1673:SER:C	2.98	0.47
2:C:859:THR:CG2	2:C:932:THR:HA	2.44	0.47
2:C:3088:ILE:H	2:C:3088:ILE:HD12	1.79	0.47
2:D:608:CYS:SG	2:D:1673:SER:C	2.98	0.47
2:D:673:ALA:O	2:D:681:THR:OG1	2.31	0.47
2:D:886:THR:O	2:D:890:GLN:HG3	2.14	0.47
2:D:942:MET:HG3	2:D:1052:TYR:CD2	2.50	0.47
2:D:2746:VAL:HG22	2:D:2747:ILE:H	1.79	0.47
2:D:3410:TYR:O	2:D:3413:LEU:N	2.47	0.47
2:D:4638:GLU:HB3	2:D:4639:PRO:HD3	1.97	0.47
2:D:4670:LYS:O	2:D:4674:GLU:HG2	2.15	0.47
2:A:885:LEU:HD12	2:A:960:TYR:CE2	2.50	0.47
2:A:951:LEU:HD22	2:A:973:LEU:HB3	1.95	0.47
2:A:1127:GLY:O	2:A:1128:HIS:C	2.58	0.47
2:A:2574:GLU:H	2:A:2619:MET:HE1	1.80	0.47
2:A:2746:VAL:HG22	2:A:2747:ILE:H	1.79	0.47
2:A:3220:TYR:CE1	2:A:3237:VAL:HG12	2.50	0.47
2:A:4088:ARG:NH1	2:A:4090:LEU:HD12	2.29	0.47
2:B:296:GLU:OE1	2:B:296:GLU:N	2.37	0.47
2:B:859:THR:CG2	2:B:932:THR:HA	2.44	0.47
2:B:916:GLU:HA	2:B:919:ARG:CD	2.44	0.47
2:B:940:VAL:HB	2:B:1054:ILE:CG1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:971:LEU:CD1	2:B:973:LEU:HD21	2.45	0.47
2:B:3062:ALA:HB3	2:B:3063:PRO:HD3	1.97	0.47
2:B:3182:PRO:O	2:B:3185:GLU:HG3	2.15	0.47
2:B:3864:GLU:O	2:B:3868:VAL:HG23	2.14	0.47
2:C:920:ASN:HA	2:C:923:LEU:HD12	1.97	0.47
2:C:940:VAL:HB	2:C:1054:ILE:CG1	2.43	0.47
2:C:985:LEU:HD11	2:C:1056:PRO:HB3	1.97	0.47
2:C:2942:LEU:HD21	2:C:2945:MET:HB2	1.97	0.47
2:C:3062:ALA:HB3	2:C:3063:PRO:HD3	1.97	0.47
2:C:3182:PRO:O	2:C:3185:GLU:HG3	2.15	0.47
2:C:3220:TYR:CE1	2:C:3237:VAL:HG12	2.50	0.47
2:C:3859:LEU:C	2:C:3859:LEU:HD12	2.39	0.47
2:D:931:LYS:HA	2:D:934:LEU:HD22	1.95	0.47
2:D:2574:GLU:H	2:D:2619:MET:HE1	1.80	0.47
2:A:608:CYS:SG	2:A:1673:SER:C	2.98	0.47
2:B:70:LEU:HD13	2:B:102:LEU:HD11	1.97	0.47
2:B:71:GLU:OE1	2:B:111:ARG:NH2	2.42	0.47
2:C:2179:MET:HE2	2:C:2211:VAL:HG11	1.97	0.47
2:D:885:LEU:HD12	2:D:960:TYR:CE2	2.50	0.47
2:D:1116:LEU:HD12	2:D:1194:SER:CB	2.45	0.47
2:D:2210:GLU:OE1	2:D:2210:GLU:HA	2.15	0.47
2:D:2942:LEU:HD21	2:D:2945:MET:HB2	1.97	0.47
2:D:3062:ALA:HB3	2:D:3063:PRO:HD3	1.97	0.47
2:A:896:PRO:HD2	2:A:904:LEU:HD13	1.97	0.47
2:A:916:GLU:HA	2:A:919:ARG:CD	2.45	0.47
2:A:3062:ALA:HB3	2:A:3063:PRO:HD3	1.97	0.47
2:B:920:ASN:HA	2:B:923:LEU:HD12	1.97	0.47
2:B:985:LEU:HD11	2:B:1056:PRO:HB3	1.97	0.47
2:B:2283:ASP:HA	2:B:2342:VAL:HG13	1.97	0.47
2:B:2624:LEU:O	2:B:2628:VAL:HG23	2.14	0.47
2:B:2634:LEU:HD12	2:B:2686:SER:HB3	1.96	0.47
2:B:3859:LEU:C	2:B:3859:LEU:HD12	2.39	0.47
2:B:4088:ARG:NH1	2:B:4090:LEU:HD12	2.29	0.47
2:C:157:GLN:OE1	2:C:158:ARG:NH1	2.47	0.47
2:C:942:MET:HG3	2:C:1052:TYR:CD2	2.50	0.47
2:C:2746:VAL:HG22	2:C:2747:ILE:H	1.79	0.47
2:C:3322:ARG:HA	2:C:3325:VAL:HG12	1.97	0.47
2:D:926:SER:O	2:D:930:LEU:HD22	2.15	0.47
2:D:952:LYS:O	2:D:972:ASP:HB3	2.15	0.47
2:D:2863:LEU:HD13	2:D:2929:LYS:HB2	1.96	0.47
2:A:71:GLU:OE1	2:A:111:ARG:NE	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:886:THR:O	2:A:890:GLN:HG3	2.14	0.47
2:A:952:LYS:O	2:A:972:ASP:HB3	2.15	0.47
2:A:2889:ARG:O	2:A:2893:GLN:OE1	2.32	0.47
2:B:886:THR:O	2:B:890:GLN:HG3	2.14	0.47
2:C:885:LEU:HD12	2:C:960:TYR:CE2	2.50	0.47
2:C:3434:GLU:O	2:C:3438:MET:HG3	2.15	0.47
1:H:33:ASP:OD2	1:H:35:LYS:HG3	2.14	0.46
2:D:649:ILE:HD13	2:D:812:CYS:HB3	1.96	0.46
2:A:843:PRO:O	2:A:1198:GLY:N	2.38	0.46
2:A:921:TYR:O	2:A:924:GLN:HG3	2.15	0.46
2:A:926:SER:O	2:A:930:LEU:HD22	2.15	0.46
2:A:2179:MET:HE2	2:A:2211:VAL:HG11	1.97	0.46
2:A:3322:ARG:HA	2:A:3325:VAL:HG12	1.97	0.46
2:B:608:CYS:SG	2:B:1673:SER:C	2.98	0.46
2:B:885:LEU:HD12	2:B:960:TYR:CE2	2.50	0.46
2:B:896:PRO:HD2	2:B:904:LEU:HD13	1.97	0.46
2:B:2179:MET:HE2	2:B:2211:VAL:HG11	1.97	0.46
2:B:2746:VAL:HG22	2:B:2747:ILE:H	1.79	0.46
2:B:2756:ILE:HG23	2:B:2810:ILE:HB	1.97	0.46
2:B:4638:GLU:HB3	2:B:4639:PRO:HD3	1.97	0.46
2:C:910:ASN:O	2:C:911:PHE:C	2.58	0.46
2:D:921:TYR:O	2:D:924:GLN:HG3	2.16	0.46
2:D:971:LEU:CD1	2:D:973:LEU:HD21	2.45	0.46
2:D:2756:ILE:HG23	2:D:2810:ILE:HB	1.97	0.46
2:D:3220:TYR:CE1	2:D:3237:VAL:HG12	2.50	0.46
2:D:4709:PHE:HB3	2:D:4710:PRO:HD3	1.98	0.46
2:A:2756:ILE:HG23	2:A:2810:ILE:HB	1.97	0.46
2:A:4638:GLU:HB3	2:A:4639:PRO:HD3	1.97	0.46
2:A:4670:LYS:O	2:A:4674:GLU:HG2	2.14	0.46
2:B:652:GLY:N	2:B:659:GLN:OE1	2.46	0.46
2:B:1297:GLN:NE2	2:B:1546:ASN:OD1	2.44	0.46
2:B:2334:ASP:O	2:B:2337:ARG:HG2	2.15	0.46
2:B:2942:LEU:HD21	2:B:2945:MET:HB2	1.97	0.46
2:B:3220:TYR:CE1	2:B:3237:VAL:HG12	2.50	0.46
2:C:1297:GLN:NE2	2:C:1546:ASN:OD1	2.44	0.46
2:C:1645:GLU:OE1	2:C:1647:ARG:NH2	2.43	0.46
1:E:33:ASP:OD2	1:E:35:LYS:HG3	2.14	0.46
2:D:2889:ARG:O	2:D:2893:GLN:OE1	2.32	0.46
2:A:649:ILE:HD13	2:A:812:CYS:HB3	1.96	0.46
2:A:871:ILE:HG13	2:A:1050:TYR:CE2	2.49	0.46
2:A:1116:LEU:HD12	2:A:1194:SER:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2210:GLU:OE1	2:A:2210:GLU:HA	2.15	0.46
2:A:3859:LEU:HD12	2:A:3859:LEU:C	2.39	0.46
2:B:2265:GLY:O	2:B:2267:GLY:N	2.45	0.46
2:B:3434:GLU:O	2:B:3438:MET:HG3	2.15	0.46
2:C:2334:ASP:O	2:C:2337:ARG:HG2	2.15	0.46
2:C:2756:ILE:HG23	2:C:2810:ILE:HB	1.97	0.46
2:D:2179:MET:HE2	2:D:2211:VAL:HG11	1.97	0.46
2:D:3182:PRO:O	2:D:3185:GLU:HG3	2.15	0.46
2:D:4088:ARG:NH1	2:D:4090:LEU:HD12	2.29	0.46
2:A:931:LYS:HA	2:A:934:LEU:HD22	1.96	0.46
2:A:2334:ASP:O	2:A:2337:ARG:HG2	2.15	0.46
2:A:2634:LEU:HD12	2:A:2686:SER:HB3	1.96	0.46
2:B:942:MET:HG3	2:B:1052:TYR:CD2	2.50	0.46
2:B:2210:GLU:OE1	2:B:2210:GLU:HA	2.15	0.46
2:C:931:LYS:HA	2:C:934:LEU:HD22	1.95	0.46
2:C:2210:GLU:OE1	2:C:2210:GLU:HA	2.15	0.46
2:C:4709:PHE:HB3	2:C:4710:PRO:HD3	1.98	0.46
2:D:896:PRO:HD2	2:D:904:LEU:HD13	1.97	0.46
2:D:2334:ASP:O	2:D:2337:ARG:HG2	2.15	0.46
2:A:872:ARG:CG	2:A:927:GLY:HA2	2.43	0.46
2:A:911:PHE:CE1	2:A:923:LEU:HG	2.51	0.46
2:B:898:ARG:NH1	2:B:907:CYS:HB2	2.29	0.46
2:B:1116:LEU:HD12	2:B:1194:SER:CB	2.45	0.46
2:C:649:ILE:HD13	2:C:812:CYS:HB3	1.96	0.46
2:C:652:GLY:N	2:C:659:GLN:OE1	2.46	0.46
2:C:911:PHE:CE1	2:C:923:LEU:HG	2.51	0.46
2:C:1127:GLY:O	2:C:1128:HIS:C	2.58	0.46
2:C:2234:CYS:C	2:C:2236:PHE:N	2.74	0.46
2:D:848:SER:N	2:D:851:ASP:OD1	2.43	0.46
2:D:911:PHE:CE1	2:D:923:LEU:HG	2.51	0.46
2:D:4096:PHE:CZ	2:D:4100:MET:HE2	2.51	0.46
2:A:673:ALA:O	2:A:681:THR:OG1	2.31	0.46
2:A:3672:ASP:OD1	2:A:3735:HIS:NE2	2.36	0.46
2:A:4096:PHE:CZ	2:A:4100:MET:HE2	2.51	0.46
2:B:914:LEU:HD11	2:B:918:GLU:C	2.41	0.46
2:B:952:LYS:O	2:B:972:ASP:HB3	2.15	0.46
2:B:2889:ARG:O	2:B:2893:GLN:OE1	2.32	0.46
2:B:3322:ARG:HA	2:B:3325:VAL:HG12	1.97	0.46
2:B:3373:VAL:HG12	2:B:3399:PHE:CZ	2.51	0.46
2:B:3645:LEU:HD21	2:B:3653:MET:CE	2.46	0.46
2:B:4220:PHE:CE1	2:B:4224:VAL:HG21	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:896:PRO:HD2	2:C:904:LEU:HD13	1.97	0.46
2:C:2283:ASP:HA	2:C:2342:VAL:HG13	1.97	0.46
2:C:3645:LEU:HD21	2:C:3653:MET:CE	2.46	0.46
1:E:43:ARG:HA	2:A:1692:GLN:HE21	1.81	0.46
2:D:70:LEU:HD13	2:D:102:LEU:HD11	1.97	0.46
2:D:914:LEU:HD11	2:D:918:GLU:C	2.41	0.46
2:D:931:LYS:O	2:D:934:LEU:HB2	2.16	0.46
2:D:1293:SER:OG	2:D:1294:LEU:HD12	2.16	0.46
2:D:3645:LEU:HD21	2:D:3653:MET:CE	2.46	0.46
2:A:70:LEU:HD13	2:A:102:LEU:HD11	1.97	0.46
2:B:183:LEU:HD12	2:B:191:GLN:O	2.16	0.46
2:B:910:ASN:O	2:B:911:PHE:C	2.58	0.46
2:C:70:LEU:HD13	2:C:102:LEU:HD11	1.97	0.46
2:C:183:LEU:HD12	2:C:191:GLN:O	2.16	0.46
2:C:470:ARG:NE	2:C:3713:GLU:OE1	2.42	0.46
2:C:952:LYS:O	2:C:972:ASP:HB3	2.15	0.46
2:C:2802:ASP:OD1	2:C:2802:ASP:C	2.59	0.46
2:C:3373:VAL:HG12	2:C:3399:PHE:CZ	2.51	0.46
2:C:4009:ASP:OD1	2:C:4010:SER:N	2.49	0.46
2:D:258:ARG:O	2:D:285:HIS:NE2	2.42	0.46
2:D:2799:SER:O	2:D:2802:ASP:OD1	2.34	0.46
2:D:3373:VAL:HG12	2:D:3399:PHE:CZ	2.51	0.46
2:D:3944:ASP:OD2	2:D:3945:VAL:N	2.49	0.46
2:A:365:PRO:O	2:A:366:LYS:HB3	2.16	0.46
2:A:868:LEU:CD1	2:A:930:LEU:HB3	2.45	0.46
2:A:911:PHE:O	2:A:914:LEU:HD23	2.16	0.46
2:A:2215:VAL:HG21	2:A:2229:MET:CE	2.46	0.46
2:A:2224:ILE:HD11	2:A:2268:MET:SD	2.56	0.46
2:A:2799:SER:O	2:A:2802:ASP:OD1	2.34	0.46
2:A:2871:GLU:HG2	2:A:2940:ARG:HB3	1.98	0.46
2:B:642:VAL:HG21	2:B:682:HIS:HD1	1.81	0.46
2:B:921:TYR:O	2:B:924:GLN:HG3	2.16	0.46
2:B:1426:GLU:OE1	2:B:1426:GLU:N	2.41	0.46
2:B:2215:VAL:HG21	2:B:2229:MET:CE	2.46	0.46
2:C:870:ARG:NH2	2:C:871:ILE:HB	2.31	0.46
2:C:911:PHE:O	2:C:914:LEU:HD23	2.16	0.46
2:C:914:LEU:HD11	2:C:918:GLU:C	2.41	0.46
2:C:921:TYR:O	2:C:924:GLN:HG3	2.16	0.46
2:C:3041:THR:OG1	2:C:3081:VAL:HG21	2.16	0.46
2:C:4220:PHE:CE1	2:C:4224:VAL:HG21	2.51	0.46
2:C:4638:GLU:HB3	2:C:4639:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:365:PRO:O	2:D:366:LYS:HB3	2.16	0.46
2:D:868:LEU:CD1	2:D:930:LEU:HB3	2.45	0.46
2:D:985:LEU:HD11	2:D:1056:PRO:HB3	1.97	0.46
2:D:2119:ARG:NH2	2:D:3720:ASP:OD1	2.47	0.46
2:D:2283:ASP:HA	2:D:2342:VAL:HG13	1.97	0.46
2:D:3004:LEU:HB2	2:D:3005:PRO:HD3	1.97	0.46
2:D:4009:ASP:OD1	2:D:4010:SER:N	2.49	0.46
2:D:4893:GLY:N	2:D:4897:ASP:OD2	2.47	0.46
2:A:931:LYS:O	2:A:934:LEU:HB2	2.16	0.46
2:A:2283:ASP:HA	2:A:2342:VAL:HG13	1.97	0.46
2:B:1127:GLY:O	2:B:1128:HIS:C	2.58	0.46
2:B:2574:GLU:H	2:B:2619:MET:HE1	1.80	0.46
2:B:4009:ASP:OD1	2:B:4010:SER:N	2.49	0.46
2:C:926:SER:O	2:C:930:LEU:HD22	2.15	0.46
2:C:2265:GLY:O	2:C:2267:GLY:N	2.45	0.46
2:C:4096:PHE:CZ	2:C:4100:MET:HE2	2.51	0.46
1:G:26:HIS:ND1	1:G:105:LEU:HD11	2.31	0.46
2:D:870:ARG:NH2	2:D:871:ILE:HB	2.31	0.46
2:D:2224:ILE:HD11	2:D:2268:MET:SD	2.56	0.46
2:D:3388:ALA:O	2:D:3392:GLU:N	2.39	0.46
2:D:3434:GLU:O	2:D:3438:MET:HG3	2.15	0.46
2:A:985:LEU:HD11	2:A:1056:PRO:HB3	1.97	0.46
2:A:2525:VAL:HG23	2:A:2526:GLY:N	2.31	0.46
2:A:3373:VAL:HG12	2:A:3399:PHE:CZ	2.51	0.46
2:A:3645:LEU:HD21	2:A:3653:MET:CE	2.46	0.46
2:A:3944:ASP:OD2	2:A:3945:VAL:N	2.49	0.46
2:B:926:SER:O	2:B:930:LEU:HD22	2.15	0.46
2:B:931:LYS:O	2:B:934:LEU:HB2	2.16	0.46
2:B:2224:ILE:HD11	2:B:2268:MET:SD	2.56	0.46
2:B:3181:ASN:OD1	2:B:3183:TYR:CD1	2.69	0.46
2:B:3324:ILE:CG2	2:B:3409:LEU:HD21	2.46	0.46
2:C:1293:SER:OG	2:C:1294:LEU:HD12	2.16	0.46
2:C:2907:VAL:HG23	2:C:2912:LEU:HG	1.98	0.46
2:C:3004:LEU:HB2	2:C:3005:PRO:HD3	1.97	0.46
2:D:197:MET:CE	2:C:2372:GLU:HG2	2.41	0.45
2:D:2907:VAL:HG23	2:D:2912:LEU:HG	1.98	0.45
2:D:3041:THR:OG1	2:D:3081:VAL:HG21	2.16	0.45
2:A:914:LEU:HD11	2:A:918:GLU:C	2.41	0.45
2:A:955:LYS:HE3	2:A:955:LYS:HB3	1.61	0.45
2:A:2119:ARG:NH2	2:A:3720:ASP:OD1	2.47	0.45
2:A:2645:LEU:HD13	2:A:2679:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3324:ILE:CG2	2:A:3409:LEU:HD21	2.46	0.45
2:B:870:ARG:NH2	2:B:874:LYS:HD3	2.31	0.45
2:B:911:PHE:CE1	2:B:923:LEU:HG	2.51	0.45
2:B:2119:ARG:NH2	2:B:3720:ASP:OD1	2.47	0.45
2:B:2871:GLU:HG2	2:B:2940:ARG:HB3	1.98	0.45
2:B:4054:SER:O	2:B:4055:SER:C	2.59	0.45
2:C:71:GLU:OE1	2:C:111:ARG:NE	2.44	0.45
2:C:2645:LEU:HD13	2:C:2679:LEU:HD21	1.99	0.45
2:C:2794:PRO:O	2:C:2798:PHE:N	2.41	0.45
2:C:3324:ILE:CG2	2:C:3409:LEU:HD21	2.46	0.45
2:D:920:ASN:HA	2:D:923:LEU:HD12	1.97	0.45
2:D:3894:LEU:HD13	2:D:3902:PHE:CZ	2.52	0.45
2:D:4054:SER:O	2:D:4055:SER:C	2.59	0.45
2:D:4248:MET:HE1	2:D:4987:MET:HE1	1.98	0.45
2:A:3894:LEU:HD13	2:A:3902:PHE:CZ	2.52	0.45
2:A:4709:PHE:HB3	2:A:4710:PRO:HD3	1.98	0.45
2:B:956:LEU:HD12	2:B:968:PRO:CD	2.44	0.45
2:B:2799:SER:O	2:B:2802:ASP:OD1	2.34	0.45
2:B:3584:GLU:OE1	2:B:3584:GLU:N	2.37	0.45
2:C:3203:PRO:HA	2:C:3284:ARG:NH2	2.31	0.45
2:C:3536:LEU:CD2	2:C:3560:LEU:HD13	2.46	0.45
2:D:893:THR:O	2:D:904:LEU:HA	2.16	0.45
2:D:2525:VAL:HG23	2:D:2526:GLY:N	2.31	0.45
2:D:2802:ASP:OD1	2:D:2802:ASP:C	2.59	0.45
2:A:642:VAL:HG21	2:A:682:HIS:HD1	1.81	0.45
2:A:870:ARG:NH2	2:A:871:ILE:HB	2.31	0.45
2:A:3181:ASN:OD1	2:A:3183:TYR:CD1	2.69	0.45
2:B:868:LEU:CD1	2:B:930:LEU:HB3	2.45	0.45
2:B:2525:VAL:HG23	2:B:2526:GLY:N	2.31	0.45
2:B:3004:LEU:HB2	2:B:3005:PRO:HD3	1.97	0.45
2:B:4096:PHE:CZ	2:B:4100:MET:HE2	2.51	0.45
2:B:4248:MET:HE1	2:B:4987:MET:HE1	1.98	0.45
2:C:2574:GLU:H	2:C:2619:MET:HE1	1.80	0.45
2:C:2799:SER:O	2:C:2802:ASP:OD1	2.34	0.45
1:H:26:HIS:ND1	1:H:105:LEU:HD11	2.31	0.45
2:D:911:PHE:O	2:D:914:LEU:HD23	2.16	0.45
2:D:2215:VAL:HG21	2:D:2229:MET:CE	2.46	0.45
2:D:2645:LEU:HD13	2:D:2679:LEU:HD21	1.99	0.45
2:A:2907:VAL:HG23	2:A:2912:LEU:HG	1.98	0.45
2:A:4054:SER:O	2:A:4055:SER:C	2.59	0.45
2:B:365:PRO:O	2:B:366:LYS:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:870:ARG:NH2	2:B:871:ILE:HB	2.31	0.45
2:B:879:ILE:CA	2:B:882:LEU:HD12	2.33	0.45
2:B:911:PHE:O	2:B:914:LEU:HD23	2.16	0.45
2:B:978:LEU:HD13	2:B:982:GLN:HB3	1.98	0.45
2:B:2234:CYS:C	2:B:2236:PHE:N	2.74	0.45
2:B:2645:LEU:HD13	2:B:2679:LEU:HD21	1.99	0.45
2:B:2816:ALA:HB1	2:B:2882:ASN:ND2	2.32	0.45
2:B:2907:VAL:HG23	2:B:2912:LEU:HG	1.98	0.45
2:B:3756:PHE:HA	2:B:3759:LYS:HZ2	1.82	0.45
2:C:642:VAL:HG21	2:C:682:HIS:HD1	1.81	0.45
2:C:3944:ASP:OD2	2:C:3945:VAL:N	2.49	0.45
2:C:4248:MET:HE1	2:C:4987:MET:HE1	1.98	0.45
2:A:183:LEU:HD12	2:A:191:GLN:O	2.16	0.45
2:A:4009:ASP:OD1	2:A:4010:SER:N	2.49	0.45
2:B:422:PHE:CD1	2:B:422:PHE:C	2.95	0.45
2:B:4709:PHE:HB3	2:B:4710:PRO:HD3	1.98	0.45
1:F:26:HIS:ND1	1:F:105:LEU:HD11	2.31	0.45
2:D:862:ILE:HG22	2:D:931:LYS:HG2	1.99	0.45
2:D:888:ILE:CG1	2:D:960:TYR:HA	2.47	0.45
2:D:954:THR:HG22	2:D:972:ASP:HB2	1.98	0.45
2:D:4220:PHE:CE1	2:D:4224:VAL:HG21	2.51	0.45
2:B:321:LYS:HZ1	2:B:357:TRP:CG	2.35	0.45
2:B:1293:SER:OG	2:B:1294:LEU:HD12	2.16	0.45
2:B:3203:PRO:HA	2:B:3284:ARG:NH2	2.31	0.45
2:B:4686:ILE:HD12	2:B:4735:ILE:CD1	2.47	0.45
2:C:843:PRO:O	2:C:1197:PRO:HA	2.17	0.45
2:C:2215:VAL:HG21	2:C:2229:MET:CE	2.46	0.45
2:C:2866:VAL:CG1	2:C:2933:MET:HE3	2.45	0.45
2:C:2875:MET:HB3	2:C:2940:ARG:HD2	1.99	0.45
2:D:183:LEU:HD12	2:D:191:GLN:O	2.16	0.45
2:D:2862:ASP:O	2:D:2865:VAL:HG12	2.17	0.45
2:D:2871:GLU:HG2	2:D:2940:ARG:HB3	1.98	0.45
2:D:4066:ASP:OD1	2:D:4172:SER:OG	2.26	0.45
2:A:910:ASN:O	2:A:911:PHE:C	2.58	0.45
2:A:954:THR:HG22	2:A:972:ASP:HB2	1.98	0.45
2:A:3434:GLU:O	2:A:3438:MET:HG3	2.15	0.45
2:A:3536:LEU:CD2	2:A:3560:LEU:HD13	2.46	0.45
2:A:4686:ILE:HD12	2:A:4735:ILE:CD1	2.47	0.45
2:B:843:PRO:O	2:B:1197:PRO:HA	2.17	0.45
2:B:893:THR:O	2:B:904:LEU:HA	2.16	0.45
2:B:2187:MET:HE2	2:B:2236:PHE:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:296:GLU:OE1	2:C:296:GLU:N	2.37	0.45
2:C:931:LYS:O	2:C:934:LEU:HB2	2.16	0.45
2:C:978:LEU:HD13	2:C:982:GLN:HB3	1.98	0.45
2:C:2187:MET:HE2	2:C:2236:PHE:HA	1.99	0.45
2:D:910:ASN:O	2:D:911:PHE:C	2.58	0.45
2:D:978:LEU:HD22	2:D:978:LEU:HA	1.78	0.45
2:D:3324:ILE:CG2	2:D:3409:LEU:HD21	2.46	0.45
2:A:898:ARG:HB2	2:A:905:HIS:HA	1.99	0.45
2:A:1293:SER:OG	2:A:1294:LEU:HD12	2.16	0.45
2:A:3004:LEU:HB2	2:A:3005:PRO:HD3	1.97	0.45
2:B:888:ILE:CG1	2:B:960:TYR:HA	2.47	0.45
2:B:898:ARG:HB2	2:B:905:HIS:HA	1.99	0.45
2:B:2753:ASP:HA	2:B:2756:ILE:HD12	1.99	0.45
2:B:3041:THR:OG1	2:B:3081:VAL:HG21	2.16	0.45
2:C:893:THR:O	2:C:904:LEU:HA	2.16	0.45
2:C:2224:ILE:HD11	2:C:2268:MET:SD	2.56	0.45
2:C:4054:SER:O	2:C:4055:SER:C	2.59	0.45
2:C:4686:ILE:HD12	2:C:4735:ILE:CD1	2.47	0.45
2:D:422:PHE:C	2:D:422:PHE:CD1	2.95	0.45
2:D:642:VAL:HG21	2:D:682:HIS:HD1	1.81	0.45
2:D:843:PRO:O	2:D:1197:PRO:HA	2.17	0.45
2:D:898:ARG:HB2	2:D:905:HIS:HA	1.99	0.45
2:D:978:LEU:HD13	2:D:982:GLN:HB3	1.98	0.45
2:D:3198:LEU:HD11	2:D:3202:MET:CE	2.47	0.45
2:D:4580:VAL:HG12	2:A:4875:ASP:O	2.17	0.45
2:A:956:LEU:HD12	2:A:968:PRO:CD	2.44	0.45
2:A:961:MET:CG	2:A:965:GLY:HA2	2.43	0.45
2:A:3203:PRO:HA	2:A:3284:ARG:NH2	2.31	0.45
2:A:4086:ASP:OD2	2:A:4088:ARG:NH2	2.50	0.45
2:A:4220:PHE:CE1	2:A:4224:VAL:HG21	2.51	0.45
2:B:2802:ASP:OD1	2:B:2802:ASP:C	2.59	0.45
2:B:3177:GLY:C	2:B:3269:HIS:ND1	2.75	0.45
2:B:3536:LEU:CD2	2:B:3560:LEU:HD13	2.46	0.45
2:C:459:GLU:H	2:C:459:GLU:CD	2.25	0.45
2:C:3177:GLY:C	2:C:3269:HIS:ND1	2.75	0.45
2:D:3108:VAL:HA	2:D:3176:LEU:HD12	1.99	0.45
2:D:3181:ASN:OD1	2:D:3183:TYR:CD1	2.69	0.45
2:D:3226:ARG:CZ	2:D:3226:ARG:HB3	2.47	0.45
2:A:879:ILE:CA	2:A:882:LEU:HD12	2.33	0.45
2:A:3177:GLY:C	2:A:3269:HIS:ND1	2.75	0.45
2:B:843:PRO:O	2:B:1198:GLY:N	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2255:LEU:C	2:B:2255:LEU:HD23	2.42	0.45
2:C:321:LYS:HZ1	2:C:357:TRP:CG	2.35	0.45
2:C:898:ARG:HB2	2:C:905:HIS:HA	1.99	0.45
2:C:2862:ASP:O	2:C:2865:VAL:HG12	2.17	0.45
2:C:2871:GLU:HG2	2:C:2940:ARG:HB3	1.98	0.45
2:C:3756:PHE:HA	2:C:3759:LYS:HZ2	1.81	0.45
2:C:4066:ASP:OD1	2:C:4172:SER:OG	2.26	0.45
2:D:1426:GLU:OE1	2:D:1426:GLU:N	2.41	0.44
2:D:3177:GLY:C	2:D:3269:HIS:ND1	2.75	0.44
2:D:3820:LEU:HD13	2:D:3902:PHE:HD1	1.81	0.44
2:A:470:ARG:NE	2:A:3713:GLU:OE1	2.42	0.44
2:A:862:ILE:HG22	2:A:931:LYS:HG2	1.99	0.44
2:A:893:THR:O	2:A:904:LEU:HA	2.16	0.44
2:C:899:ASP:CB	2:C:902:LYS:HB2	2.21	0.44
2:C:954:THR:HG22	2:C:972:ASP:HB2	1.98	0.44
2:D:459:GLU:CD	2:D:459:GLU:H	2.25	0.44
2:D:2816:ALA:HB1	2:D:2882:ASN:ND2	2.32	0.44
2:D:2866:VAL:CG1	2:D:2933:MET:HE3	2.45	0.44
2:D:4628:TYR:OH	2:A:4858:ARG:NH1	2.49	0.44
2:A:888:ILE:CG1	2:A:960:TYR:HA	2.47	0.44
2:A:978:LEU:HD22	2:A:978:LEU:HA	1.78	0.44
2:A:3108:VAL:HA	2:A:3176:LEU:HD12	1.99	0.44
2:B:723:TRP:CZ2	2:B:728:ALA:HB2	2.53	0.44
2:B:954:THR:HG22	2:B:972:ASP:HB2	1.98	0.44
2:B:3944:ASP:OD2	2:B:3945:VAL:N	2.49	0.44
2:B:4671:ARG:NH1	2:B:4700:ASP:OD1	2.51	0.44
2:C:3226:ARG:HB3	2:C:3226:ARG:CZ	2.47	0.44
2:C:3820:LEU:HD13	2:C:3902:PHE:HD1	1.81	0.44
2:C:4893:GLY:N	2:C:4897:ASP:OD2	2.47	0.44
2:D:947:ALA:HA	2:D:950:ASN:ND2	2.32	0.44
2:D:2753:ASP:HA	2:D:2756:ILE:HD12	1.99	0.44
2:D:2875:MET:HB3	2:D:2940:ARG:HD2	1.99	0.44
2:D:4024:LYS:N	2:D:4142:ILE:HD13	2.33	0.44
2:D:4088:ARG:HH12	2:D:4090:LEU:HD12	1.82	0.44
2:D:4686:ILE:HD12	2:D:4735:ILE:CD1	2.47	0.44
2:A:978:LEU:HD13	2:A:982:GLN:HB3	1.98	0.44
2:A:2237:LEU:O	2:A:2240:PHE:HB3	2.18	0.44
2:A:2802:ASP:OD1	2:A:2802:ASP:C	2.59	0.44
2:B:872:ARG:HH12	2:B:923:LEU:HB3	1.82	0.44
2:B:978:LEU:HD11	2:B:1044:VAL:HG11	1.99	0.44
2:B:978:LEU:HD21	2:B:1044:VAL:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2413:GLU:HG3	2:B:2413:GLU:O	2.17	0.44
2:C:422:PHE:CD1	2:C:422:PHE:C	2.95	0.44
2:C:978:LEU:HD21	2:C:1044:VAL:HG12	1.99	0.44
2:C:2255:LEU:HD23	2:C:2255:LEU:C	2.42	0.44
2:C:2816:ALA:HB1	2:C:2882:ASN:ND2	2.32	0.44
2:C:3181:ASN:OD1	2:C:3183:TYR:CD1	2.69	0.44
2:C:3198:LEU:HD11	2:C:3202:MET:CE	2.47	0.44
1:E:33:ASP:OD2	1:E:33:ASP:C	2.60	0.44
2:D:956:LEU:HD12	2:D:968:PRO:CD	2.44	0.44
2:D:1478:GLY:HA2	2:D:1485:HIS:H	1.83	0.44
2:D:2234:CYS:HB3	2:D:2238:CYS:HB3	1.55	0.44
2:D:3203:PRO:HA	2:D:3284:ARG:NH2	2.31	0.44
2:D:4671:ARG:NH1	2:D:4700:ASP:OD1	2.51	0.44
2:A:723:TRP:CZ2	2:A:728:ALA:HB2	2.53	0.44
2:A:1478:GLY:HA2	2:A:1485:HIS:H	1.83	0.44
2:A:2862:ASP:O	2:A:2865:VAL:HG12	2.17	0.44
2:A:3446:TRP:HZ3	2:A:3610:THR:HG22	1.83	0.44
2:A:4248:MET:HE1	2:A:4987:MET:HE1	1.99	0.44
2:A:4689:GLN:OE1	2:A:4701:ARG:NH2	2.51	0.44
2:B:34:LEU:HD23	2:B:35:LYS:N	2.33	0.44
2:B:2237:LEU:O	2:B:2240:PHE:HB3	2.18	0.44
2:B:3108:VAL:HA	2:B:3176:LEU:HD12	1.99	0.44
2:B:3294:PRO:HB2	2:B:3297:LEU:HB3	1.99	0.44
2:C:365:PRO:O	2:C:366:LYS:HB3	2.16	0.44
2:C:865:PRO:CD	2:C:868:LEU:HB2	2.44	0.44
2:C:2525:VAL:HG23	2:C:2526:GLY:N	2.31	0.44
2:C:2753:ASP:HA	2:C:2756:ILE:HD12	1.99	0.44
2:C:4086:ASP:OD2	2:C:4088:ARG:NH2	2.50	0.44
2:D:2237:LEU:O	2:D:2240:PHE:HB3	2.18	0.44
2:D:2413:GLU:HG3	2:D:2413:GLU:O	2.17	0.44
2:D:3859:LEU:HD11	2:D:3871:ARG:NH2	2.29	0.44
2:A:843:PRO:O	2:A:1197:PRO:HA	2.17	0.44
2:A:862:ILE:HD13	2:A:931:LYS:O	2.18	0.44
2:A:2255:LEU:HD23	2:A:2255:LEU:C	2.42	0.44
2:A:2816:ALA:HB1	2:A:2882:ASN:ND2	2.32	0.44
2:B:3226:ARG:HB3	2:B:3226:ARG:CZ	2.47	0.44
2:C:947:ALA:HA	2:C:950:ASN:ND2	2.32	0.44
2:C:2237:LEU:O	2:C:2240:PHE:HB3	2.18	0.44
2:C:3580:VAL:HB	2:C:3583:ARG:HD3	2.00	0.44
2:C:3894:LEU:HD13	2:C:3902:PHE:CZ	2.52	0.44
2:D:463:GLU:HG3	2:D:3711:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2255:LEU:HD23	2:D:2255:LEU:C	2.42	0.44
2:A:872:ARG:HH12	2:A:923:LEU:HB3	1.82	0.44
2:A:1426:GLU:OE1	2:A:1426:GLU:N	2.41	0.44
2:A:2972:GLN:O	2:A:2975:ILE:HG22	2.18	0.44
2:B:459:GLU:H	2:B:459:GLU:CD	2.25	0.44
2:B:2862:ASP:O	2:B:2865:VAL:HG12	2.17	0.44
2:B:3446:TRP:HZ3	2:B:3610:THR:HG22	1.83	0.44
2:B:4869:GLU:OE1	2:B:4869:GLU:HA	2.18	0.44
2:C:868:LEU:CD1	2:C:930:LEU:HB3	2.45	0.44
2:C:2972:GLN:O	2:C:2975:ILE:HG22	2.18	0.44
2:C:3108:VAL:HA	2:C:3176:LEU:HD12	1.99	0.44
2:C:4088:ARG:HH12	2:C:4090:LEU:HD12	1.82	0.44
2:C:4689:GLN:OE1	2:C:4701:ARG:NH2	2.51	0.44
2:D:321:LYS:HZ1	2:D:357:TRP:CG	2.35	0.44
2:D:932:THR:HG23	2:D:989:LEU:HD22	2.00	0.44
2:D:978:LEU:HD11	2:D:1044:VAL:HG11	1.99	0.44
2:D:3446:TRP:HZ3	2:D:3610:THR:HG22	1.83	0.44
2:D:3580:VAL:HB	2:D:3583:ARG:HD3	2.00	0.44
2:D:4543:GLU:O	2:D:4547:VAL:HG23	2.18	0.44
2:D:4869:GLU:OE1	2:D:4869:GLU:HA	2.18	0.44
2:A:422:PHE:C	2:A:422:PHE:CD1	2.95	0.44
2:A:947:ALA:HA	2:A:950:ASN:ND2	2.32	0.44
2:A:971:LEU:H	2:A:971:LEU:HG	1.58	0.44
2:A:3293:PRO:O	2:A:3295:PRO:CD	2.66	0.44
2:A:3546:THR:HG22	2:A:3547:ASP:N	2.33	0.44
2:A:4088:ARG:HH12	2:A:4090:LEU:HD12	1.82	0.44
2:B:973:LEU:CB	2:B:976:VAL:HG23	2.46	0.44
2:B:1047:LEU:HA	2:B:1050:TYR:CD2	2.53	0.44
2:B:2866:VAL:CG1	2:B:2933:MET:HE3	2.45	0.44
2:B:4086:ASP:OD2	2:B:4088:ARG:NH2	2.50	0.44
2:C:34:LEU:HD23	2:C:35:LYS:N	2.33	0.44
2:C:862:ILE:HG22	2:C:931:LYS:HG2	1.99	0.44
2:C:1478:GLY:HA2	2:C:1485:HIS:H	1.82	0.44
2:D:2254:HIS:O	2:D:2255:LEU:C	2.60	0.44
2:D:3536:LEU:CD2	2:D:3560:LEU:HD13	2.46	0.44
2:A:870:ARG:NH2	2:A:874:LYS:HD3	2.31	0.44
2:A:1047:LEU:HA	2:A:1050:TYR:CD2	2.53	0.44
2:A:2383:GLU:OE1	2:A:2386:ARG:NH2	2.51	0.44
2:A:3198:LEU:HD11	2:A:3202:MET:CE	2.47	0.44
2:B:470:ARG:NE	2:B:3713:GLU:OE1	2.42	0.44
2:B:862:ILE:HD13	2:B:931:LYS:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:884:ALA:HA	2:B:908:LEU:HD22	2.00	0.44
2:B:2314:LEU:HD12	2:B:2319:TYR:CG	2.53	0.44
2:B:3868:VAL:HG12	2:B:3870:ASN:H	1.83	0.44
2:B:4024:LYS:N	2:B:4142:ILE:HD13	2.33	0.44
2:C:723:TRP:CZ2	2:C:728:ALA:HB2	2.53	0.44
2:C:2413:GLU:O	2:C:2413:GLU:HG3	2.17	0.44
2:C:4543:GLU:O	2:C:4547:VAL:HG23	2.18	0.44
1:E:26:HIS:ND1	1:E:105:LEU:HD11	2.32	0.44
2:D:723:TRP:CZ2	2:D:728:ALA:HB2	2.53	0.44
2:D:862:ILE:HD13	2:D:931:LYS:O	2.18	0.44
2:D:1047:LEU:HA	2:D:1050:TYR:CD2	2.53	0.44
2:D:3377:GLU:O	2:D:3380:LEU:HG	2.18	0.44
2:D:3453:LYS:O	2:D:3456:GLU:HG3	2.18	0.44
2:D:4689:GLN:OE1	2:D:4701:ARG:NH2	2.51	0.44
7:D:8006:PCW:H341	2:A:4855:ASN:CG	2.43	0.44
2:A:321:LYS:HZ1	2:A:357:TRP:CG	2.35	0.44
2:A:2866:VAL:CG1	2:A:2933:MET:HE3	2.45	0.44
2:A:3868:VAL:HG12	2:A:3870:ASN:H	1.83	0.44
2:B:463:GLU:HG3	2:B:3711:LEU:HD13	2.00	0.44
2:B:933:LEU:HD22	2:B:1054:ILE:HG21	2.00	0.44
2:B:947:ALA:HA	2:B:950:ASN:ND2	2.32	0.44
2:B:3377:GLU:O	2:B:3380:LEU:HG	2.18	0.44
2:B:4689:GLN:OE1	2:B:4701:ARG:NH2	2.51	0.44
2:C:463:GLU:HG3	2:C:3711:LEU:HD13	2.00	0.44
2:C:884:ALA:HA	2:C:908:LEU:HD22	2.00	0.44
2:C:2383:GLU:OE1	2:C:2386:ARG:NH2	2.51	0.44
2:D:2972:GLN:O	2:D:2975:ILE:HG22	2.18	0.43
2:A:459:GLU:CD	2:A:459:GLU:H	2.25	0.43
2:A:463:GLU:HG3	2:A:3711:LEU:HD13	2.00	0.43
2:A:2187:MET:HE2	2:A:2236:PHE:HA	1.99	0.43
2:A:3041:THR:OG1	2:A:3081:VAL:HG21	2.16	0.43
2:A:4024:LYS:N	2:A:4142:ILE:HD13	2.33	0.43
2:B:862:ILE:HG22	2:B:931:LYS:HG2	1.99	0.43
2:B:865:PRO:CD	2:B:868:LEU:HB2	2.44	0.43
2:B:2972:GLN:O	2:B:2975:ILE:HG22	2.18	0.43
2:B:3105:GLU:HA	2:B:3108:VAL:HG22	2.00	0.43
2:B:3293:PRO:O	2:B:3295:PRO:CD	2.66	0.43
2:B:3894:LEU:HD13	2:B:3902:PHE:CZ	2.52	0.43
2:B:4543:GLU:O	2:B:4547:VAL:HG23	2.18	0.43
2:C:888:ILE:CG1	2:C:960:TYR:HA	2.47	0.43
2:C:973:LEU:CB	2:C:976:VAL:HG23	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1047:LEU:HA	2:C:1050:TYR:CD2	2.53	0.43
2:C:3267:MET:HG3	2:C:3267:MET:O	2.18	0.43
2:C:3294:PRO:HB2	2:C:3297:LEU:HB3	1.99	0.43
2:C:3868:VAL:HG12	2:C:3870:ASN:H	1.83	0.43
2:C:4869:GLU:OE1	2:C:4869:GLU:HA	2.18	0.43
2:D:34:LEU:HD23	2:D:35:LYS:N	2.33	0.43
2:D:902:LYS:HA	2:D:902:LYS:HD2	1.55	0.43
2:D:2187:MET:HE2	2:D:2236:PHE:HA	1.99	0.43
2:A:875:LEU:HD12	2:A:878:ASN:HD22	1.83	0.43
2:A:978:LEU:HD11	2:A:1044:VAL:HG11	1.99	0.43
2:A:1742:GLU:OE1	2:A:1742:GLU:N	2.45	0.43
2:A:3226:ARG:HB3	2:A:3226:ARG:CZ	2.48	0.43
2:A:3294:PRO:HB2	2:A:3297:LEU:HB3	1.99	0.43
2:A:3820:LEU:HD13	2:A:3902:PHE:HD1	1.81	0.43
2:B:308:ALA:HB1	2:B:313:THR:HG21	2.01	0.43
2:B:2782:ILE:O	2:B:2783:ASP:C	2.61	0.43
2:B:3546:THR:HG22	2:B:3547:ASP:N	2.33	0.43
2:B:3820:LEU:HD13	2:B:3902:PHE:HD1	1.81	0.43
2:B:4854:PHE:O	2:B:4858:ARG:NH1	2.50	0.43
2:C:707:GLY:N	2:C:710:ASP:OD2	2.44	0.43
2:C:930:LEU:O	2:C:934:LEU:HD22	2.18	0.43
2:C:2254:HIS:O	2:C:2255:LEU:C	2.60	0.43
2:C:3291:GLU:OE2	2:C:3310:SER:N	2.38	0.43
2:C:3546:THR:HG22	2:C:3547:ASP:N	2.33	0.43
2:C:3594:VAL:O	2:C:3597:VAL:HG12	2.19	0.43
2:D:884:ALA:HA	2:D:908:LEU:HD22	2.00	0.43
2:D:3267:MET:HG3	2:D:3267:MET:O	2.18	0.43
2:D:4086:ASP:OD2	2:D:4088:ARG:NH2	2.50	0.43
2:A:652:GLY:N	2:A:659:GLN:OE1	2.46	0.43
2:A:884:ALA:HA	2:A:908:LEU:HD22	2.00	0.43
2:A:2753:ASP:HA	2:A:2756:ILE:HD12	1.99	0.43
2:B:4214:LYS:O	2:B:4218:ARG:HG3	2.18	0.43
2:C:11:GLU:OE1	2:C:12:VAL:N	2.52	0.43
2:C:894:TYR:CB	2:C:964:ASN:HB3	2.48	0.43
2:C:2314:LEU:HD12	2:C:2319:TYR:CG	2.53	0.43
2:C:3377:GLU:O	2:C:3380:LEU:HG	2.18	0.43
2:C:3453:LYS:O	2:C:3456:GLU:HG3	2.18	0.43
2:D:3294:PRO:HB2	2:D:3297:LEU:HB3	1.99	0.43
2:A:296:GLU:OE1	2:A:296:GLU:N	2.37	0.43
2:A:308:ALA:HB1	2:A:313:THR:HG21	2.00	0.43
2:A:952:LYS:HZ3	2:A:952:LYS:HG2	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3130:LEU:O	2:A:3133:THR:OG1	2.36	0.43
7:A:8006:PCW:H341	2:B:4855:ASN:CG	2.44	0.43
2:B:3198:LEU:HD11	2:B:3202:MET:CE	2.47	0.43
2:B:4187:MET:HE3	2:B:4191:ARG:HA	2.00	0.43
2:C:605:CYS:HB2	2:C:608:CYS:H	1.84	0.43
2:C:2241:CYS:SG	2:C:2251:MET:HG3	2.59	0.43
2:C:4024:LYS:N	2:C:4142:ILE:HD13	2.33	0.43
2:D:470:ARG:NE	2:D:3713:GLU:OE1	2.42	0.43
2:D:875:LEU:HD12	2:D:878:ASN:HD22	1.83	0.43
2:D:877:GLU:HA	2:D:911:PHE:CE2	2.54	0.43
2:A:11:GLU:OE1	2:A:12:VAL:N	2.52	0.43
2:A:930:LEU:O	2:A:934:LEU:HD22	2.18	0.43
2:A:3267:MET:HG3	2:A:3267:MET:O	2.18	0.43
2:B:953:LYS:HE2	2:B:953:LYS:HB2	1.84	0.43
2:B:1478:GLY:HA2	2:B:1485:HIS:H	1.82	0.43
2:B:3267:MET:O	2:B:3267:MET:HG3	2.18	0.43
2:C:933:LEU:HD22	2:C:1054:ILE:HG21	2.00	0.43
2:C:2234:CYS:HB3	2:C:2238:CYS:HB3	1.55	0.43
2:C:3105:GLU:HA	2:C:3108:VAL:HG22	2.00	0.43
2:C:3446:TRP:HZ3	2:C:3610:THR:HG22	1.83	0.43
2:D:2241:CYS:SG	2:D:2251:MET:HG3	2.59	0.43
2:D:3868:VAL:HG12	2:D:3870:ASN:H	1.83	0.43
2:A:297:ASP:N	2:A:297:ASP:OD1	2.52	0.43
2:A:978:LEU:HD21	2:A:1044:VAL:HG12	1.99	0.43
2:A:2254:HIS:O	2:A:2255:LEU:C	2.60	0.43
2:A:2314:LEU:HD12	2:A:2319:TYR:CG	2.53	0.43
2:A:2413:GLU:HG3	2:A:2413:GLU:O	2.17	0.43
2:A:2875:MET:HB3	2:A:2940:ARG:HD2	1.99	0.43
2:A:3105:GLU:HA	2:A:3108:VAL:HG22	2.00	0.43
2:A:3319:ASN:O	2:A:3323:ILE:HG12	2.19	0.43
2:A:3546:THR:HG22	2:A:3547:ASP:H	1.83	0.43
2:A:3580:VAL:HB	2:A:3583:ARG:HD3	2.00	0.43
2:B:930:LEU:O	2:B:934:LEU:HD22	2.18	0.43
2:B:3108:VAL:HG12	2:B:3176:LEU:CD1	2.49	0.43
2:C:862:ILE:HD13	2:C:931:LYS:O	2.18	0.43
2:C:3293:PRO:O	2:C:3295:PRO:CD	2.66	0.43
2:C:4214:LYS:O	2:C:4218:ARG:HG3	2.18	0.43
2:D:916:GLU:N	2:D:917:PRO:CD	2.82	0.43
2:D:930:LEU:O	2:D:934:LEU:HD22	2.18	0.43
2:D:2782:ILE:O	2:D:2783:ASP:C	2.61	0.43
2:D:3587:ALA:O	2:D:3593:ILE:HD11	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:956:LEU:HD22	2:A:957:PRO:HD2	2.01	0.43
2:A:3377:GLU:O	2:A:3380:LEU:HG	2.18	0.43
2:A:3894:LEU:CB	2:A:3902:PHE:CE2	3.02	0.43
2:A:4671:ARG:NH1	2:A:4700:ASP:OD1	2.51	0.43
2:B:2914:ALA:O	2:B:2917:LYS:HB2	2.19	0.43
2:B:4543:GLU:OE1	2:B:4543:GLU:HA	2.19	0.43
2:C:2914:ALA:O	2:C:2917:LYS:HB2	2.19	0.43
2:C:3324:ILE:HG21	2:C:3409:LEU:HD21	2.01	0.43
2:C:4688:GLU:O	2:C:4689:GLN:NE2	2.52	0.43
2:D:870:ARG:NH2	2:D:874:LYS:HD3	2.31	0.43
2:D:2872:LEU:O	2:D:2875:MET:HG2	2.19	0.43
2:D:3546:THR:HG22	2:D:3547:ASP:N	2.33	0.43
2:D:3594:VAL:O	2:D:3597:VAL:HG12	2.19	0.43
2:D:3756:PHE:HA	2:D:3759:LYS:HZ2	1.83	0.43
2:A:872:ARG:HH22	2:A:923:LEU:HD23	1.84	0.43
2:A:877:GLU:HA	2:A:911:PHE:CE2	2.54	0.43
2:A:894:TYR:CB	2:A:964:ASN:HB3	2.48	0.43
2:A:916:GLU:N	2:A:917:PRO:CD	2.82	0.43
2:A:933:LEU:HD22	2:A:1054:ILE:HG21	2.00	0.43
2:A:2872:LEU:O	2:A:2875:MET:HG2	2.19	0.43
2:B:1273:LEU:HD22	2:B:1290:LEU:HD11	2.01	0.43
2:B:2875:MET:HB3	2:B:2940:ARG:HD2	1.99	0.43
2:B:3324:ILE:HG21	2:B:3409:LEU:HD21	2.01	0.43
2:B:4088:ARG:HH12	2:B:4090:LEU:HD12	1.82	0.43
2:C:952:LYS:HZ3	2:C:952:LYS:HG2	1.66	0.43
2:C:956:LEU:HD12	2:C:968:PRO:CD	2.44	0.43
1:H:33:ASP:OD2	1:H:33:ASP:C	2.60	0.43
2:D:11:GLU:OE1	2:D:12:VAL:N	2.52	0.43
2:D:605:CYS:HB2	2:D:608:CYS:H	1.84	0.43
2:D:916:GLU:HA	2:D:919:ARG:HD2	2.01	0.43
2:D:1031:ALA:O	2:D:1034:ARG:HG2	2.19	0.43
2:D:2269:GLN:HG3	2:D:2269:GLN:O	2.19	0.43
2:D:2314:LEU:HD12	2:D:2319:TYR:CG	2.53	0.43
2:D:2914:ALA:O	2:D:2917:LYS:HB2	2.19	0.43
2:D:3546:THR:HG22	2:D:3547:ASP:H	1.84	0.43
2:A:916:GLU:HA	2:A:919:ARG:HD2	2.01	0.43
2:A:2782:ILE:O	2:A:2783:ASP:C	2.61	0.43
2:A:3453:LYS:O	2:A:3456:GLU:HG3	2.18	0.43
2:A:4869:GLU:OE1	2:A:4869:GLU:HA	2.18	0.43
2:B:877:GLU:HA	2:B:911:PHE:CE2	2.54	0.43
2:B:881:GLU:HB3	2:B:970:PRO:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:308:ALA:HB1	2:C:313:THR:HG21	2.00	0.43
2:C:978:LEU:HD11	2:C:1044:VAL:HG11	1.99	0.43
2:C:2519:LEU:O	2:C:2523:LEU:HD13	2.19	0.43
2:C:2782:ILE:O	2:C:2783:ASP:C	2.61	0.43
2:C:4187:MET:HE3	2:C:4191:ARG:HA	2.00	0.43
1:G:77:ILE:O	1:G:97:THR:HG23	2.19	0.43
2:D:791:ARG:HA	2:D:1627:TRP:O	2.19	0.43
2:D:872:ARG:HH12	2:D:923:LEU:HB3	1.82	0.43
2:D:973:LEU:CB	2:D:976:VAL:HG23	2.46	0.43
2:D:2519:LEU:O	2:D:2523:LEU:HD13	2.19	0.43
2:D:3108:VAL:HG12	2:D:3176:LEU:CD1	2.49	0.43
2:D:3324:ILE:HG21	2:D:3409:LEU:HD21	2.01	0.43
2:D:3399:PHE:HB2	2:D:3455:GLU:HG3	2.01	0.43
2:A:3756:PHE:HA	2:A:3759:LYS:HZ2	1.83	0.43
2:B:952:LYS:HZ3	2:B:952:LYS:HG2	1.65	0.43
2:B:1155:ASP:OD1	2:B:1157:THR:OG1	2.32	0.43
2:B:2768:ALA:HA	2:B:2771:LYS:HE3	2.01	0.43
2:B:3556:ASN:OD1	2:B:3556:ASN:C	2.62	0.43
2:C:872:ARG:HH12	2:C:923:LEU:HB3	1.82	0.43
2:C:1273:LEU:HD22	2:C:1290:LEU:HD11	2.01	0.43
2:D:707:GLY:N	2:D:710:ASP:OD2	2.44	0.42
2:D:978:LEU:HD21	2:D:1044:VAL:HG12	1.99	0.42
2:D:3293:PRO:O	2:D:3295:PRO:CD	2.66	0.42
2:A:34:LEU:HD23	2:A:35:LYS:N	2.33	0.42
2:A:2241:CYS:SG	2:A:2251:MET:HG3	2.59	0.42
2:A:2519:LEU:O	2:A:2523:LEU:HD13	2.19	0.42
2:A:3285:TRP:HB3	2:A:3306:THR:HG21	2.01	0.42
2:A:4543:GLU:OE1	2:A:4543:GLU:HA	2.19	0.42
2:B:875:LEU:HD12	2:B:878:ASN:HD22	1.83	0.42
2:B:932:THR:HG23	2:B:989:LEU:HD22	2.00	0.42
2:B:2519:LEU:O	2:B:2523:LEU:HD13	2.19	0.42
2:B:2794:PRO:O	2:B:2798:PHE:N	2.41	0.42
2:B:3453:LYS:O	2:B:3456:GLU:HG3	2.18	0.42
2:B:4625:MET:HA	2:B:4625:MET:HE2	2.01	0.42
2:C:791:ARG:HA	2:C:1627:TRP:O	2.19	0.42
2:C:875:LEU:HD12	2:C:878:ASN:HD22	1.83	0.42
2:C:932:THR:HG23	2:C:989:LEU:HD22	2.00	0.42
2:C:1857:SER:OG	2:C:1860:ASP:OD1	2.35	0.42
2:C:4671:ARG:NH1	2:C:4700:ASP:OD1	2.51	0.42
1:F:33:ASP:OD2	1:F:33:ASP:C	2.60	0.42
2:D:3366:LEU:HD13	2:D:3406:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4214:LYS:O	2:D:4218:ARG:HG3	2.18	0.42
2:A:3110:ASN:ND2	2:A:3126:VAL:HG13	2.34	0.42
2:A:4214:LYS:O	2:A:4218:ARG:HG3	2.18	0.42
2:B:948:GLU:HG2	2:B:1050:TYR:HA	2.01	0.42
2:B:2563:ILE:HG22	2:B:2611:LEU:HD11	2.01	0.42
2:B:3110:ASN:ND2	2:B:3126:VAL:HG13	2.34	0.42
2:B:3160:ASP:O	2:B:3164:VAL:HG23	2.19	0.42
2:B:3594:VAL:O	2:B:3597:VAL:HG12	2.19	0.42
2:C:216:THR:OG1	2:C:219:HIS:CD2	2.73	0.42
2:C:877:GLU:HA	2:C:911:PHE:CE2	2.54	0.42
2:C:881:GLU:HB3	2:C:970:PRO:N	2.34	0.42
2:C:3108:VAL:HG12	2:C:3176:LEU:CD1	2.49	0.42
2:C:3110:ASN:ND2	2:C:3126:VAL:HG13	2.34	0.42
2:C:3410:TYR:N	2:C:3411:PRO:HD2	2.34	0.42
2:C:3962:LYS:HG3	2:C:4025:ASP:OD1	2.20	0.42
2:D:872:ARG:HH22	2:D:923:LEU:HD23	1.84	0.42
2:D:956:LEU:HD22	2:D:957:PRO:HD2	2.01	0.42
2:D:3055:VAL:HG23	2:D:3062:ALA:HB1	2.02	0.42
2:D:3105:GLU:HA	2:D:3108:VAL:HG22	2.00	0.42
2:D:3130:LEU:O	2:D:3133:THR:OG1	2.36	0.42
2:D:3894:LEU:CB	2:D:3902:PHE:CE2	3.02	0.42
2:D:4625:MET:HE2	2:D:4625:MET:HA	2.01	0.42
2:A:3587:ALA:O	2:A:3593:ILE:HD11	2.19	0.42
2:B:11:GLU:OE1	2:B:12:VAL:N	2.52	0.42
2:B:894:TYR:CB	2:B:964:ASN:HB3	2.48	0.42
2:B:2254:HIS:O	2:B:2255:LEU:C	2.60	0.42
2:B:2269:GLN:O	2:B:2269:GLN:HG3	2.19	0.42
2:B:3962:LYS:HG3	2:B:4025:ASP:OD1	2.20	0.42
2:C:859:THR:HG21	2:C:932:THR:HA	2.01	0.42
2:C:925:MET:O	2:C:929:THR:HG23	2.20	0.42
2:C:2768:ALA:HA	2:C:2771:LYS:HE3	2.01	0.42
2:C:3160:ASP:O	2:C:3164:VAL:HG23	2.19	0.42
2:C:3366:LEU:HD13	2:C:3406:LEU:HD23	2.01	0.42
2:D:652:GLY:N	2:D:659:GLN:OE1	2.46	0.42
2:D:881:GLU:HB3	2:D:970:PRO:N	2.34	0.42
2:D:894:TYR:CB	2:D:964:ASN:HB3	2.48	0.42
2:D:1480:GLU:OE1	2:D:1480:GLU:N	2.43	0.42
2:D:1742:GLU:OE1	2:D:1742:GLU:N	2.45	0.42
2:D:3110:ASN:ND2	2:D:3126:VAL:HG13	2.34	0.42
2:D:3285:TRP:HB3	2:D:3306:THR:HG21	2.02	0.42
2:D:3319:ASN:O	2:D:3323:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:875:LEU:HD12	2:A:875:LEU:O	2.19	0.42
2:A:2314:LEU:HD11	2:A:2417:VAL:CG1	2.50	0.42
2:A:3055:VAL:HG23	2:A:3062:ALA:HB1	2.01	0.42
2:A:3594:VAL:O	2:A:3597:VAL:HG12	2.19	0.42
2:A:4543:GLU:O	2:A:4547:VAL:HG23	2.18	0.42
2:B:605:CYS:HB2	2:B:608:CYS:H	1.84	0.42
2:B:875:LEU:HD12	2:B:875:LEU:O	2.19	0.42
2:B:951:LEU:H	2:B:951:LEU:HG	1.70	0.42
2:B:961:MET:CG	2:B:965:GLY:HA2	2.43	0.42
2:B:1031:ALA:O	2:B:1034:ARG:HG2	2.19	0.42
2:B:2241:CYS:SG	2:B:2251:MET:HG3	2.59	0.42
2:C:902:LYS:HA	2:C:902:LYS:HD2	1.55	0.42
2:C:916:GLU:N	2:C:917:PRO:CD	2.82	0.42
2:C:3285:TRP:HB3	2:C:3306:THR:HG21	2.02	0.42
2:C:3587:ALA:O	2:C:3593:ILE:HD11	2.19	0.42
1:G:57:ILE:CG1	1:G:60:TRP:HD1	2.32	0.42
2:D:308:ALA:HB1	2:D:313:THR:HG21	2.01	0.42
2:D:933:LEU:HD22	2:D:1054:ILE:HG21	2.00	0.42
2:D:4649:THR:OG1	2:D:4801:HIS:CD2	2.73	0.42
2:A:902:LYS:CE	2:A:904:LEU:HD21	2.39	0.42
2:A:2623:LEU:O	2:A:2627:LEU:HD13	2.19	0.42
2:A:4625:MET:HE2	2:A:4625:MET:HA	2.01	0.42
2:B:859:THR:HG21	2:B:932:THR:HA	2.01	0.42
2:B:872:ARG:HH22	2:B:923:LEU:HD23	1.84	0.42
2:B:3580:VAL:HB	2:B:3583:ARG:HD3	2.00	0.42
2:C:1031:ALA:O	2:C:1034:ARG:HG2	2.19	0.42
2:C:2269:GLN:HG3	2:C:2269:GLN:O	2.19	0.42
2:C:3319:ASN:O	2:C:3323:ILE:HG12	2.19	0.42
1:F:80:ASP:OD2	1:F:81:TYR:CD1	2.73	0.42
2:D:3410:TYR:N	2:D:3411:PRO:HD2	2.34	0.42
2:A:1153:MET:HE1	2:A:1164:THR:HG23	2.02	0.42
2:A:2269:GLN:HG3	2:A:2269:GLN:O	2.19	0.42
2:A:2768:ALA:HA	2:A:2771:LYS:HE3	2.01	0.42
2:A:2794:PRO:O	2:A:2798:PHE:N	2.41	0.42
2:A:3324:ILE:HG21	2:A:3409:LEU:HD21	2.01	0.42
2:A:4649:THR:OG1	2:A:4801:HIS:CD2	2.73	0.42
2:A:4893:GLY:N	2:A:4897:ASP:OD2	2.47	0.42
2:B:2383:GLU:OE1	2:B:2386:ARG:NH2	2.51	0.42
2:B:2623:LEU:O	2:B:2627:LEU:HD13	2.19	0.42
2:C:978:LEU:HD22	2:C:978:LEU:HA	1.78	0.42
2:C:2270:GLY:O	2:C:2272:THR:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:4543:GLU:OE1	2:C:4543:GLU:HA	2.19	0.42
1:E:77:ILE:O	1:E:97:THR:HG23	2.19	0.42
2:D:216:THR:OG1	2:D:219:HIS:CD2	2.73	0.42
2:D:1428:ILE:HG23	2:D:1429:LEU:HD22	2.01	0.42
2:D:2314:LEU:HD11	2:D:2417:VAL:CG1	2.50	0.42
2:D:3962:LYS:HG3	2:D:4025:ASP:OD1	2.20	0.42
2:A:791:ARG:HA	2:A:1627:TRP:O	2.19	0.42
2:A:881:GLU:HB3	2:A:970:PRO:N	2.34	0.42
2:A:948:GLU:HG2	2:A:1050:TYR:HA	2.02	0.42
2:A:973:LEU:CB	2:A:976:VAL:HG23	2.46	0.42
2:A:1031:ALA:O	2:A:1034:ARG:HG2	2.19	0.42
2:A:2563:ILE:HG22	2:A:2611:LEU:HD11	2.01	0.42
2:A:3108:VAL:HG12	2:A:3176:LEU:CD1	2.49	0.42
2:A:3160:ASP:O	2:A:3164:VAL:HG23	2.20	0.42
2:A:3366:LEU:HD13	2:A:3406:LEU:HD23	2.01	0.42
2:B:1153:MET:HE1	2:B:1164:THR:HG23	2.02	0.42
2:B:3285:TRP:HB3	2:B:3306:THR:HG21	2.02	0.42
2:B:3443:PHE:CD2	2:B:3515:LEU:HD22	2.55	0.42
2:B:4688:GLU:O	2:B:4689:GLN:NE2	2.52	0.42
2:C:872:ARG:HH22	2:C:923:LEU:HD23	1.84	0.42
2:C:956:LEU:HD22	2:C:957:PRO:HD2	2.01	0.42
2:C:3999:PHE:HD1	2:C:4019:LEU:HD11	1.85	0.42
2:D:925:MET:O	2:D:929:THR:HG23	2.20	0.42
2:D:2623:LEU:O	2:D:2627:LEU:HD13	2.19	0.42
2:D:3160:ASP:O	2:D:3164:VAL:HG23	2.19	0.42
2:D:3556:ASN:OD1	2:D:3556:ASN:C	2.62	0.42
2:D:4688:GLU:O	2:D:4689:GLN:NE2	2.52	0.42
2:A:859:THR:HG21	2:A:932:THR:HA	2.01	0.42
2:A:1273:LEU:HD22	2:A:1290:LEU:HD11	2.01	0.42
2:B:955:LYS:HB3	2:B:955:LYS:HE3	1.61	0.42
2:B:2270:GLY:O	2:B:2272:THR:HG23	2.20	0.42
2:B:2413:GLU:O	2:B:2416:ARG:N	2.53	0.42
2:B:2922:GLU:HA	2:B:2925:GLN:HG2	2.02	0.42
2:B:3410:TYR:N	2:B:3411:PRO:HD2	2.34	0.42
2:C:875:LEU:HD12	2:C:875:LEU:O	2.19	0.42
2:C:3055:VAL:HG23	2:C:3062:ALA:HB1	2.02	0.42
2:C:3360:ILE:HB	2:C:3361:PRO:HD3	2.02	0.42
2:C:3392:GLU:O	2:C:3396:ARG:HG2	2.20	0.42
2:C:3974:GLY:N	2:C:3975:PRO:HA	2.35	0.42
1:H:77:ILE:O	1:H:97:THR:HG23	2.20	0.42
1:H:80:ASP:OD2	1:H:81:TYR:CD1	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:784:PHE:CG	2:D:788:ILE:HD11	2.55	0.42
2:D:870:ARG:HD3	2:D:1052:TYR:OH	2.20	0.42
2:D:2270:GLY:O	2:D:2272:THR:HG23	2.20	0.42
2:D:2876:ALA:HB1	2:D:2921:ARG:NH1	2.35	0.42
2:A:784:PHE:CG	2:A:788:ILE:HD11	2.55	0.42
2:A:932:THR:HG23	2:A:989:LEU:HD22	2.00	0.42
2:A:1144:TRP:HB2	2:A:1148:ASP:HB2	2.02	0.42
2:A:1428:ILE:HG23	2:A:1429:LEU:HD22	2.01	0.42
2:A:2876:ALA:HB1	2:A:2921:ARG:NH1	2.35	0.42
2:A:2914:ALA:O	2:A:2917:LYS:HB2	2.19	0.42
2:A:3399:PHE:HB2	2:A:3455:GLU:HG3	2.01	0.42
2:A:3403:CYS:SG	2:A:3456:GLU:HA	2.60	0.42
2:A:3859:LEU:HD11	2:A:3871:ARG:NH2	2.29	0.42
2:A:3999:PHE:HD1	2:A:4019:LEU:HD11	1.85	0.42
2:A:4187:MET:HE3	2:A:4191:ARG:HA	2.00	0.42
2:B:784:PHE:CG	2:B:788:ILE:HD11	2.55	0.42
2:B:874:LYS:HE3	2:B:875:LEU:N	2.35	0.42
2:B:1064:VAL:HG13	2:B:1065:ASP:N	2.35	0.42
2:B:1546:ASN:OD1	2:B:1546:ASN:O	2.38	0.42
2:B:3130:LEU:O	2:B:3133:THR:OG1	2.36	0.42
2:B:3587:ALA:O	2:B:3593:ILE:HD11	2.19	0.42
2:C:2623:LEU:O	2:C:2627:LEU:HD13	2.19	0.42
2:C:3546:THR:HG22	2:C:3547:ASP:H	1.84	0.42
2:D:337:PRO:HA	2:D:338:PRO:HD3	1.92	0.42
2:D:859:THR:HG21	2:D:932:THR:HA	2.01	0.42
2:D:931:LYS:HB3	2:D:931:LYS:HE3	1.79	0.42
2:D:1127:GLY:HA3	2:D:1144:TRP:CE3	2.55	0.42
2:D:2635:ASN:OD1	2:D:2638:ALA:N	2.53	0.42
2:D:2762:TYR:CZ	2:D:2863:LEU:HG	2.55	0.42
2:D:2771:LYS:HB3	2:D:2776:TRP:HB2	2.02	0.42
2:D:4187:MET:HE3	2:D:4191:ARG:HA	2.00	0.42
2:D:4543:GLU:OE1	2:D:4543:GLU:HA	2.19	0.42
2:A:605:CYS:HB2	2:A:608:CYS:H	1.84	0.42
2:A:925:MET:O	2:A:929:THR:HG23	2.20	0.42
2:A:3198:LEU:HD12	2:A:3198:LEU:O	2.20	0.42
2:A:3556:ASN:OD1	2:A:3556:ASN:C	2.62	0.42
2:A:4703:VAL:O	2:A:4703:VAL:HG22	2.20	0.42
2:B:216:THR:OG1	2:B:219:HIS:CD2	2.73	0.42
2:B:297:ASP:OD1	2:B:297:ASP:N	2.52	0.42
2:B:791:ARG:HA	2:B:1627:TRP:O	2.19	0.42
2:B:3267:MET:O	2:B:3267:MET:CG	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3319:ASN:O	2:B:3323:ILE:HG12	2.19	0.42
2:B:3360:ILE:HB	2:B:3361:PRO:HD3	2.02	0.42
2:B:3974:GLY:N	2:B:3975:PRO:HA	2.35	0.42
2:B:3999:PHE:HD1	2:B:4019:LEU:HD11	1.85	0.42
2:B:4893:GLY:N	2:B:4897:ASP:OD2	2.47	0.42
2:C:784:PHE:CG	2:C:788:ILE:HD11	2.55	0.42
2:C:874:LYS:HE3	2:C:875:LEU:N	2.35	0.42
2:C:1064:VAL:HG13	2:C:1065:ASP:N	2.35	0.42
2:C:2563:ILE:HG22	2:C:2611:LEU:HD11	2.01	0.42
2:C:3367:ARG:NH1	2:C:3441:GLU:OE1	2.42	0.42
2:C:4625:MET:HE2	2:C:4625:MET:HA	2.01	0.42
1:E:91:ILE:N	1:E:91:ILE:HD12	2.35	0.41
2:D:1273:LEU:HD22	2:D:1290:LEU:HD11	2.01	0.41
2:D:3850:PHE:CZ	2:D:3940:TYR:OH	2.73	0.41
2:D:3999:PHE:HD1	2:D:4019:LEU:HD11	1.85	0.41
2:D:4854:PHE:O	2:D:4858:ARG:NH1	2.50	0.41
2:A:1546:ASN:OD1	2:A:1546:ASN:O	2.38	0.41
2:A:2779:GLY:HA3	2:A:2788:THR:HB	2.01	0.41
2:A:3392:GLU:O	2:A:3396:ARG:HG2	2.20	0.41
2:A:3443:PHE:CD2	2:A:3515:LEU:HD22	2.55	0.41
2:B:916:GLU:HA	2:B:919:ARG:HD2	2.01	0.41
2:B:916:GLU:N	2:B:917:PRO:CD	2.82	0.41
2:B:1127:GLY:HA3	2:B:1144:TRP:CE3	2.55	0.41
2:B:3177:GLY:HA3	2:B:3269:HIS:CE1	2.55	0.41
2:B:3198:LEU:HD12	2:B:3198:LEU:O	2.20	0.41
2:B:3366:LEU:HD13	2:B:3406:LEU:HD23	2.01	0.41
2:B:3399:PHE:HB2	2:B:3455:GLU:HG3	2.01	0.41
2:B:3403:CYS:SG	2:B:3456:GLU:HA	2.60	0.41
2:B:4578:TYR:HE1	2:B:4630:LEU:HD21	1.85	0.41
2:B:4909:LEU:HA	2:B:4912:VAL:HG22	2.02	0.41
2:C:843:PRO:HG2	2:C:1072:ARG:O	2.20	0.41
2:C:967:LYS:HZ1	2:C:969:ALA:HB2	1.84	0.41
2:C:1428:ILE:HG23	2:C:1429:LEU:HD22	2.01	0.41
2:C:3399:PHE:HB2	2:C:3455:GLU:HG3	2.01	0.41
2:C:4649:THR:OG1	2:C:4801:HIS:CD2	2.73	0.41
1:E:91:ILE:HD11	2:A:1685:ALA:HA	2.01	0.41
1:G:2:GLY:N	1:G:78:SER:OG	2.41	0.41
2:D:297:ASP:OD1	2:D:297:ASP:N	2.52	0.41
2:D:2334:ASP:HA	2:D:2337:ARG:HD3	2.02	0.41
2:D:2383:GLU:OE1	2:D:2386:ARG:NH2	2.51	0.41
2:D:3360:ILE:HB	2:D:3361:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1470:VAL:HG13	2:A:1493:CYS:HB3	2.03	0.41
2:A:3177:GLY:HA3	2:A:3269:HIS:CE1	2.55	0.41
2:A:3850:PHE:CZ	2:A:3940:TYR:OH	2.73	0.41
2:A:3962:LYS:HG3	2:A:4025:ASP:OD1	2.20	0.41
2:B:1996:THR:O	2:B:1997:ARG:C	2.63	0.41
2:B:2876:ALA:HB1	2:B:2921:ARG:NH1	2.35	0.41
2:B:3239:GLU:O	2:B:3240:MET:C	2.63	0.41
2:B:3546:THR:HG22	2:B:3547:ASP:H	1.84	0.41
2:B:4703:VAL:HG22	2:B:4703:VAL:O	2.20	0.41
8:B:8008:A1BYZ:O7	8:B:8008:A1BYZ:C10	2.68	0.41
2:C:1996:THR:O	2:C:1997:ARG:C	2.63	0.41
2:C:2234:CYS:O	2:C:2236:PHE:C	2.63	0.41
2:C:2746:VAL:O	2:C:2815:LYS:HE2	2.20	0.41
2:C:3202:MET:HG3	2:C:3204:VAL:H	1.85	0.41
2:D:2768:ALA:HA	2:D:2771:LYS:HE3	2.01	0.41
2:D:3198:LEU:HD12	2:D:3198:LEU:O	2.20	0.41
2:D:3443:PHE:CD2	2:D:3515:LEU:HD22	2.55	0.41
2:A:216:THR:OG1	2:A:219:HIS:CD2	2.73	0.41
2:A:870:ARG:HD3	2:A:1052:TYR:OH	2.20	0.41
2:A:2266:LEU:HD13	2:A:2327:CYS:HB3	2.02	0.41
2:A:2771:LYS:HB3	2:A:2776:TRP:HB2	2.02	0.41
2:A:3079:ARG:O	2:A:3083:LYS:HG2	2.21	0.41
2:A:3410:TYR:N	2:A:3411:PRO:HD2	2.34	0.41
2:B:956:LEU:HD22	2:B:957:PRO:HD2	2.01	0.41
2:B:1144:TRP:HB2	2:B:1148:ASP:HB2	2.02	0.41
2:B:2234:CYS:O	2:B:2236:PHE:C	2.63	0.41
2:B:2266:LEU:HD13	2:B:2327:CYS:HB3	2.03	0.41
2:B:2314:LEU:HD11	2:B:2417:VAL:CG1	2.50	0.41
2:B:2872:LEU:O	2:B:2875:MET:HG2	2.19	0.41
2:B:3850:PHE:CZ	2:B:3940:TYR:OH	2.73	0.41
2:C:2872:LEU:O	2:C:2875:MET:HG2	2.19	0.41
2:C:3894:LEU:CB	2:C:3902:PHE:CE2	3.02	0.41
2:C:4909:LEU:HA	2:C:4912:VAL:HG22	2.02	0.41
1:F:91:ILE:HD12	1:F:91:ILE:N	2.35	0.41
2:D:566:TYR:O	2:D:570:ILE:HG12	2.20	0.41
2:D:2234:CYS:O	2:D:2236:PHE:C	2.63	0.41
2:D:2563:ILE:HG22	2:D:2611:LEU:HD11	2.01	0.41
2:D:3008:ASN:OD1	2:D:3008:ASN:C	2.63	0.41
2:A:874:LYS:HE3	2:A:875:LEU:N	2.35	0.41
2:A:1996:THR:O	2:A:1997:ARG:C	2.63	0.41
2:A:4580:VAL:HG12	2:B:4875:ASP:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:4865:GLU:HA	2:A:4865:GLU:OE2	2.21	0.41
2:A:4899:ILE:HG13	2:A:4911:ARG:NH2	2.35	0.41
2:B:843:PRO:HG2	2:B:1072:ARG:O	2.20	0.41
2:B:967:LYS:HZ1	2:B:969:ALA:HB2	1.85	0.41
2:B:2975:ILE:HD11	2:B:3057:LEU:HD22	2.02	0.41
2:B:3055:VAL:HG23	2:B:3062:ALA:HB1	2.02	0.41
2:C:870:ARG:NH2	2:C:874:LYS:HD3	2.31	0.41
2:C:870:ARG:HD3	2:C:1052:TYR:OH	2.20	0.41
2:C:2334:ASP:HA	2:C:2337:ARG:HD3	2.03	0.41
2:C:2876:ALA:HB1	2:C:2921:ARG:NH1	2.35	0.41
2:C:2922:GLU:HA	2:C:2925:GLN:HG2	2.02	0.41
2:C:3008:ASN:OD1	2:C:3008:ASN:C	2.63	0.41
2:D:902:LYS:CE	2:D:904:LEU:HD21	2.39	0.41
2:D:1144:TRP:HB2	2:D:1148:ASP:HB2	2.02	0.41
2:D:1546:ASN:OD1	2:D:1546:ASN:O	2.38	0.41
2:D:3267:MET:O	2:D:3267:MET:CG	2.68	0.41
2:D:4703:VAL:HG22	2:D:4703:VAL:O	2.20	0.41
2:A:951:LEU:H	2:A:951:LEU:HG	1.70	0.41
2:A:1127:GLY:HA3	2:A:1144:TRP:CE3	2.55	0.41
2:A:4578:TYR:HE1	2:A:4630:LEU:HD21	1.85	0.41
2:B:925:MET:O	2:B:929:THR:HG23	2.20	0.41
2:B:1781:PRO:HA	2:B:1782:PRO:HD3	1.97	0.41
2:B:3567:SER:HB3	2:B:3570:LEU:HD13	2.03	0.41
2:B:4934:ILE:H	2:B:4934:ILE:HD12	1.86	0.41
2:C:916:GLU:HA	2:C:919:ARG:HD2	2.01	0.41
2:C:1127:GLY:H	2:C:1144:TRP:HZ3	1.68	0.41
2:C:3079:ARG:O	2:C:3083:LYS:HG2	2.21	0.41
2:C:3403:CYS:SG	2:C:3456:GLU:HA	2.60	0.41
2:C:3443:PHE:CD2	2:C:3515:LEU:HD22	2.55	0.41
2:C:4578:TYR:HE1	2:C:4630:LEU:HD21	1.85	0.41
8:C:8008:A1BYZ:O7	8:C:8008:A1BYZ:C10	2.68	0.41
1:G:91:ILE:HD12	1:G:91:ILE:N	2.35	0.41
2:D:875:LEU:HD12	2:D:875:LEU:O	2.19	0.41
2:D:1064:VAL:HG13	2:D:1065:ASP:N	2.35	0.41
2:D:2975:ILE:HD11	2:D:3057:LEU:HD22	2.02	0.41
2:D:3567:SER:HB3	2:D:3570:LEU:HD13	2.03	0.41
2:A:1064:VAL:HG13	2:A:1065:ASP:N	2.35	0.41
2:A:2029:ARG:O	2:A:2033:VAL:HG23	2.21	0.41
2:A:2234:CYS:O	2:A:2236:PHE:C	2.63	0.41
2:A:2874:ALA:O	2:A:2878:GLN:OE1	2.39	0.41
2:A:2978:LEU:HA	2:A:2981:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3360:ILE:HB	2:A:3361:PRO:HD3	2.02	0.41
2:A:3567:SER:HB3	2:A:3570:LEU:HD13	2.03	0.41
2:A:3896:GLU:HA	2:A:3970:GLU:OE1	2.21	0.41
2:B:566:TYR:O	2:B:570:ILE:HG12	2.20	0.41
2:B:859:THR:HG21	2:B:932:THR:CA	2.51	0.41
2:B:1428:ILE:HG23	2:B:1429:LEU:HD22	2.01	0.41
2:B:1470:VAL:HG13	2:B:1493:CYS:HB3	2.03	0.41
2:B:2635:ASN:OD1	2:B:2638:ALA:N	2.53	0.41
2:B:2762:TYR:CZ	2:B:2863:LEU:HG	2.55	0.41
2:C:859:THR:HG21	2:C:932:THR:CA	2.51	0.41
2:C:902:LYS:CE	2:C:904:LEU:HD21	2.39	0.41
2:C:948:GLU:HG2	2:C:1050:TYR:HA	2.01	0.41
2:C:1144:TRP:HB2	2:C:1148:ASP:HB2	2.02	0.41
2:C:2413:GLU:O	2:C:2416:ARG:N	2.53	0.41
2:C:3239:GLU:O	2:C:3240:MET:C	2.63	0.41
2:D:1153:MET:HE1	2:D:1164:THR:HG23	2.02	0.41
2:D:1470:VAL:HG13	2:D:1493:CYS:HB3	2.03	0.41
2:D:2413:GLU:O	2:D:2416:ARG:N	2.53	0.41
2:D:2779:GLY:HA3	2:D:2788:THR:HB	2.02	0.41
2:D:2782:ILE:O	2:D:2783:ASP:OD1	2.39	0.41
2:D:3177:GLY:HA3	2:D:3269:HIS:CE1	2.55	0.41
2:D:3202:MET:HG3	2:D:3204:VAL:H	1.85	0.41
2:D:3291:GLU:OE2	2:D:3310:SER:N	2.38	0.41
2:D:3392:GLU:O	2:D:3396:ARG:HG2	2.20	0.41
2:D:3403:CYS:SG	2:D:3456:GLU:HA	2.60	0.41
2:D:3936:PHE:CE2	2:D:3940:TYR:CE2	3.09	0.41
2:D:3974:GLY:N	2:D:3975:PRO:HA	2.35	0.41
2:A:2782:ILE:O	2:A:2783:ASP:OD1	2.39	0.41
2:A:2975:ILE:HD11	2:A:3057:LEU:HD22	2.02	0.41
2:A:3057:LEU:HD23	2:A:3057:LEU:C	2.45	0.41
2:B:2370:ARG:NH1	2:B:2373:GLY:O	2.54	0.41
2:B:2779:GLY:HA3	2:B:2788:THR:HB	2.02	0.41
2:B:3079:ARG:O	2:B:3083:LYS:HG2	2.21	0.41
2:B:3170:LEU:CD1	2:B:3195:LEU:HD11	2.50	0.41
2:B:4649:THR:OG1	2:B:4801:HIS:CD2	2.73	0.41
2:C:2779:GLY:HA3	2:C:2788:THR:HB	2.02	0.41
2:C:3556:ASN:OD1	2:C:3556:ASN:C	2.62	0.41
2:C:3687:GLU:O	2:C:3688:GLU:HB3	2.21	0.41
2:C:4934:ILE:H	2:C:4934:ILE:HD12	1.86	0.41
2:D:296:GLU:OE1	2:D:296:GLU:N	2.37	0.41
2:D:575:VAL:HA	2:D:578:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:874:LYS:HE3	2:D:875:LEU:N	2.35	0.41
2:D:1127:GLY:H	2:D:1144:TRP:HZ3	1.68	0.41
2:D:2922:GLU:HA	2:D:2925:GLN:HG2	2.02	0.41
2:D:3367:ARG:NH1	2:D:3441:GLU:OE1	2.42	0.41
2:D:4934:ILE:H	2:D:4934:ILE:HD12	1.86	0.41
2:A:865:PRO:CD	2:A:868:LEU:HB2	2.44	0.41
2:A:2635:ASN:OD1	2:A:2638:ALA:N	2.53	0.41
2:A:3239:GLU:O	2:A:3240:MET:C	2.63	0.41
2:A:3291:GLU:OE2	2:A:3310:SER:N	2.38	0.41
2:A:4173:ILE:H	2:A:4173:ILE:HD12	1.86	0.41
2:A:4688:GLU:O	2:A:4689:GLN:NE2	2.52	0.41
2:B:2186:ILE:HG21	2:B:2204:MET:HE1	2.03	0.41
2:B:3894:LEU:CB	2:B:3902:PHE:CE2	3.02	0.41
2:B:3896:GLU:HA	2:B:3970:GLU:OE1	2.21	0.41
2:B:5014:GLU:OE2	2:B:5014:GLU:HA	2.21	0.41
2:C:2771:LYS:HB3	2:C:2776:TRP:HB2	2.02	0.41
2:C:2874:ALA:O	2:C:2878:GLN:OE1	2.39	0.41
2:C:3177:GLY:HA3	2:C:3269:HIS:CE1	2.55	0.41
2:C:3567:SER:HB3	2:C:3570:LEU:HD13	2.03	0.41
2:C:4899:ILE:HG13	2:C:4911:ARG:NH2	2.35	0.41
1:H:91:ILE:N	1:H:91:ILE:HD12	2.35	0.41
2:D:892:TRP:CZ3	2:D:905:HIS:HD2	2.39	0.41
2:D:948:GLU:HG2	2:D:1050:TYR:HA	2.01	0.41
2:D:956:LEU:HD22	2:D:956:LEU:HA	1.84	0.41
2:D:2029:ARG:O	2:D:2033:VAL:HG23	2.21	0.41
2:D:2578:ILE:HG23	2:D:2579:MET:N	2.36	0.41
2:D:2746:VAL:O	2:D:2815:LYS:HE2	2.20	0.41
2:D:2978:LEU:O	2:D:2982:VAL:HG23	2.21	0.41
2:D:3057:LEU:HD23	2:D:3057:LEU:C	2.45	0.41
2:D:3170:LEU:CD1	2:D:3195:LEU:HD11	2.50	0.41
2:D:3553:PHE:O	2:D:3556:ASN:OD1	2.39	0.41
2:D:4173:ILE:H	2:D:4173:ILE:HD12	1.86	0.41
2:D:4800:GLY:HA2	2:D:4806:PHE:HB2	2.03	0.41
2:D:4865:GLU:HA	2:D:4865:GLU:OE2	2.21	0.41
2:A:276:ARG:HE	2:A:329:LYS:HD3	1.86	0.41
2:A:2270:GLY:O	2:A:2272:THR:HG23	2.20	0.41
2:A:2668:THR:HG21	2:A:2673:LEU:HD21	2.03	0.41
2:A:2798:PHE:O	2:A:2803:LYS:HD2	2.21	0.41
2:A:2922:GLU:HA	2:A:2925:GLN:HG2	2.02	0.41
2:A:3202:MET:HG3	2:A:3204:VAL:H	1.85	0.41
2:A:3534:ILE:CG1	2:A:3597:VAL:HG23	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3553:PHE:O	2:A:3556:ASN:OD1	2.39	0.41
2:A:3687:GLU:O	2:A:3688:GLU:HB3	2.21	0.41
2:A:3974:GLY:N	2:A:3975:PRO:HA	2.35	0.41
2:A:4894:GLY:HA2	2:A:4923:ILE:HD11	2.03	0.41
2:A:4902:PRO:HB3	2:A:4911:ARG:HG2	2.03	0.41
2:A:4909:LEU:HA	2:A:4912:VAL:HG22	2.02	0.41
2:A:4934:ILE:HD12	2:A:4934:ILE:H	1.86	0.41
2:B:575:VAL:HA	2:B:578:ILE:HG12	2.02	0.41
2:B:870:ARG:HD3	2:B:1052:TYR:OH	2.20	0.41
2:B:898:ARG:HH12	2:B:907:CYS:CB	2.34	0.41
2:B:971:LEU:H	2:B:971:LEU:HG	1.57	0.41
2:B:1127:GLY:H	2:B:1144:TRP:HZ3	1.68	0.41
2:B:1742:GLU:OE1	2:B:1742:GLU:N	2.45	0.41
2:B:2029:ARG:O	2:B:2033:VAL:HG23	2.21	0.41
2:B:2746:VAL:O	2:B:2815:LYS:HE2	2.20	0.41
2:B:3057:LEU:HD23	2:B:3057:LEU:C	2.45	0.41
2:B:3291:GLU:OE2	2:B:3310:SER:N	2.38	0.41
2:B:3553:PHE:O	2:B:3556:ASN:OD1	2.39	0.41
2:B:3987:ARG:NH2	2:C:162:GLU:HA	2.36	0.41
2:B:4723:LEU:HD22	2:B:4741:MET:HE2	2.03	0.41
2:B:4899:ILE:HG13	2:B:4911:ARG:NH2	2.35	0.41
2:C:505:ALA:HB2	2:C:513:ALA:HB2	2.03	0.41
2:C:1127:GLY:HA3	2:C:1144:TRP:CE3	2.55	0.41
2:C:1153:MET:HE1	2:C:1164:THR:HG23	2.02	0.41
2:C:1546:ASN:OD1	2:C:1546:ASN:O	2.38	0.41
2:C:2314:LEU:HD11	2:C:2417:VAL:CG1	2.50	0.41
2:C:2370:ARG:NH1	2:C:2373:GLY:O	2.54	0.41
2:C:2420:GLY:O	2:C:2424:MET:HE3	2.21	0.41
2:C:2578:ILE:HG23	2:C:2579:MET:N	2.36	0.41
2:C:2635:ASN:OD1	2:C:2638:ALA:N	2.53	0.41
2:C:2975:ILE:HD11	2:C:3057:LEU:HD22	2.02	0.41
2:C:3198:LEU:HD12	2:C:3198:LEU:O	2.20	0.41
2:C:3267:MET:O	2:C:3267:MET:CG	2.68	0.41
2:C:3553:PHE:O	2:C:3556:ASN:OD1	2.39	0.41
2:C:3894:LEU:HD13	2:C:3902:PHE:HZ	1.86	0.41
2:C:4703:VAL:HG22	2:C:4703:VAL:O	2.20	0.41
2:C:4806:PHE:HA	7:C:8006:PCW:H39	2.03	0.41
2:D:862:ILE:CG2	2:D:934:LEU:HD23	2.51	0.41
2:D:961:MET:CG	2:D:965:GLY:HA2	2.43	0.41
2:D:2266:LEU:HD13	2:D:2327:CYS:HB3	2.03	0.41
2:D:2420:GLY:O	2:D:2424:MET:HE3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2748:ILE:O	2:D:2748:ILE:HG23	2.21	0.41
2:D:2863:LEU:O	2:D:2929:LYS:HD2	2.21	0.41
2:D:2978:LEU:HA	2:D:2981:VAL:HG22	2.03	0.41
2:D:3837:ALA:O	2:D:3841:THR:HG23	2.21	0.41
2:A:958:LYS:HA	2:A:961:MET:HB3	2.03	0.41
2:A:2420:GLY:O	2:A:2424:MET:HE3	2.21	0.41
2:A:2762:TYR:CZ	2:A:2863:LEU:HG	2.55	0.41
2:A:2881:GLU:OE1	2:A:2909:TYR:HB2	2.21	0.41
2:A:4806:PHE:HA	7:A:8006:PCW:H39	2.03	0.41
2:B:459:GLU:OE2	2:B:459:GLU:N	2.54	0.41
2:B:2771:LYS:HB3	2:B:2776:TRP:HB2	2.02	0.41
2:B:2978:LEU:HA	2:B:2981:VAL:HG22	2.03	0.41
2:B:3540:ARG:HD2	2:B:3543:LEU:HD12	2.03	0.41
2:B:3687:GLU:O	2:B:3688:GLU:HB3	2.21	0.41
2:B:4806:PHE:HA	7:B:8006:PCW:H39	2.03	0.41
2:B:4865:GLU:HA	2:B:4865:GLU:OE2	2.21	0.41
2:C:566:TYR:O	2:C:570:ILE:HG12	2.20	0.41
2:C:899:ASP:HB3	2:C:902:LYS:CG	2.51	0.41
2:C:951:LEU:H	2:C:951:LEU:HG	1.70	0.41
2:C:2863:LEU:O	2:C:2929:LYS:HD2	2.21	0.41
2:C:4173:ILE:H	2:C:4173:ILE:HD12	1.86	0.41
2:C:4545:GLN:OE1	2:C:4545:GLN:HA	2.21	0.41
1:F:77:ILE:O	1:F:97:THR:HG23	2.20	0.40
1:G:33:ASP:OD1	1:G:33:ASP:N	2.55	0.40
1:H:2:GLY:N	1:H:78:SER:OG	2.35	0.40
2:D:951:LEU:HD21	2:D:1049:GLY:CA	2.51	0.40
2:D:985:LEU:HD11	2:D:1056:PRO:CB	2.51	0.40
2:D:2874:ALA:O	2:D:2878:GLN:OE1	2.39	0.40
2:D:3079:ARG:O	2:D:3083:LYS:HG2	2.21	0.40
2:D:4578:TYR:HE1	2:D:4630:LEU:HD21	1.85	0.40
2:D:4899:ILE:HG13	2:D:4911:ARG:NH2	2.35	0.40
2:A:575:VAL:HA	2:A:578:ILE:HG12	2.03	0.40
2:A:1127:GLY:H	2:A:1144:TRP:HZ3	1.68	0.40
2:A:2334:ASP:HA	2:A:2337:ARG:HD3	2.03	0.40
2:A:2413:GLU:O	2:A:2416:ARG:N	2.53	0.40
2:A:2746:VAL:O	2:A:2815:LYS:HE2	2.20	0.40
2:B:276:ARG:HE	2:B:329:LYS:HD3	1.86	0.40
2:B:898:ARG:NH1	2:B:906:PRO:HD2	2.36	0.40
2:B:958:LYS:HA	2:B:961:MET:HB3	2.03	0.40
2:B:985:LEU:HD11	2:B:1056:PRO:HA	2.03	0.40
2:B:2445:GLN:OE1	2:B:2445:GLN:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2668:THR:HG21	2:B:2673:LEU:HD21	2.02	0.40
2:B:3202:MET:HG3	2:B:3204:VAL:H	1.85	0.40
2:B:3710:ALA:HB2	2:B:3785:MET:HE2	2.03	0.40
2:B:3894:LEU:HD13	2:B:3902:PHE:HZ	1.86	0.40
2:B:4800:GLY:HA2	2:B:4806:PHE:HB2	2.03	0.40
2:C:1470:VAL:HG13	2:C:1493:CYS:HB3	2.03	0.40
2:C:2668:THR:HG21	2:C:2673:LEU:HD21	2.03	0.40
2:C:2762:TYR:CZ	2:C:2863:LEU:HG	2.55	0.40
2:C:2978:LEU:O	2:C:2982:VAL:HG23	2.21	0.40
2:C:3057:LEU:HD23	2:C:3057:LEU:C	2.45	0.40
1:F:80:ASP:OD2	1:F:80:ASP:C	2.65	0.40
2:D:843:PRO:HG2	2:D:1072:ARG:O	2.20	0.40
2:D:952:LYS:HZ3	2:D:952:LYS:HG2	1.57	0.40
2:D:2736:PHE:O	2:D:2738:PRO:HD3	2.21	0.40
2:D:2958:PHE:HE1	2:D:3035:LYS:HG2	1.86	0.40
2:D:3534:ILE:CG1	2:D:3597:VAL:HG23	2.51	0.40
2:D:4909:LEU:HA	2:D:4912:VAL:HG22	2.02	0.40
2:A:862:ILE:CG2	2:A:934:LEU:HD23	2.51	0.40
2:A:892:TRP:CZ3	2:A:905:HIS:HD2	2.39	0.40
2:A:2958:PHE:HE1	2:A:3035:LYS:HG2	1.87	0.40
2:A:2990:SER:O	2:A:2993:GLU:N	2.52	0.40
2:A:3170:LEU:CD1	2:A:3195:LEU:HD11	2.50	0.40
2:A:3683:GLU:HB3	2:A:3686:GLU:HB2	2.04	0.40
2:A:3837:ALA:O	2:A:3841:THR:HG23	2.22	0.40
2:A:4723:LEU:HD22	2:A:4741:MET:HE2	2.03	0.40
2:A:5014:GLU:OE2	2:A:5014:GLU:HA	2.21	0.40
2:B:2782:ILE:O	2:B:2783:ASP:OD1	2.39	0.40
2:B:2798:PHE:O	2:B:2803:LYS:HD2	2.21	0.40
2:B:3392:GLU:O	2:B:3396:ARG:HG2	2.20	0.40
2:B:3936:PHE:CE2	2:B:3940:TYR:CE2	3.09	0.40
2:B:4545:GLN:OE1	2:B:4545:GLN:HA	2.21	0.40
2:C:593:LYS:NZ	2:C:1584:GLU:OE2	2.39	0.40
2:C:879:ILE:CA	2:C:882:LEU:HD12	2.33	0.40
2:C:898:ARG:NH1	2:C:906:PRO:HD2	2.36	0.40
2:C:953:LYS:HE2	2:C:953:LYS:HB2	1.84	0.40
2:C:2266:LEU:HD13	2:C:2327:CYS:HB3	2.03	0.40
2:C:2445:GLN:OE1	2:C:2445:GLN:HA	2.22	0.40
2:C:2782:ILE:O	2:C:2783:ASP:OD1	2.39	0.40
2:C:3896:GLU:HA	2:C:3970:GLU:OE1	2.21	0.40
2:C:4894:GLY:HA2	2:C:4923:ILE:HD11	2.03	0.40
2:C:4902:PRO:HB3	2:C:4911:ARG:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:43:ARG:HA	2:C:1692:GLN:HE21	1.86	0.40
1:H:80:ASP:OD2	1:H:80:ASP:C	2.64	0.40
2:D:4806:PHE:HA	7:D:8006:PCW:H39	2.03	0.40
2:D:4894:GLY:HA2	2:D:4923:ILE:HD11	2.03	0.40
2:A:566:TYR:O	2:A:570:ILE:HG12	2.20	0.40
2:A:967:LYS:HZ1	2:A:969:ALA:HB2	1.86	0.40
2:A:4578:TYR:HD2	2:A:4805:PHE:CZ	2.40	0.40
2:B:862:ILE:CG2	2:B:934:LEU:HD23	2.51	0.40
2:B:2874:ALA:O	2:B:2878:GLN:OE1	2.39	0.40
2:B:2958:PHE:HE1	2:B:3035:LYS:HG2	1.86	0.40
2:B:4042:MET:HE2	2:B:4045:ARG:NH2	2.37	0.40
2:B:4894:GLY:HA2	2:B:4923:ILE:HD11	2.03	0.40
2:C:951:LEU:HD21	2:C:1049:GLY:CA	2.51	0.40
2:C:956:LEU:HD22	2:C:956:LEU:HA	1.84	0.40
2:C:985:LEU:HD11	2:C:1056:PRO:CB	2.51	0.40
2:C:985:LEU:HD11	2:C:1056:PRO:HA	2.03	0.40
2:C:2736:PHE:O	2:C:2738:PRO:HD3	2.21	0.40
2:C:2958:PHE:HE1	2:C:3035:LYS:HG2	1.86	0.40
2:C:3524:ASN:OD1	2:C:3583:ARG:NH1	2.54	0.40
2:C:3683:GLU:HB3	2:C:3686:GLU:HB2	2.04	0.40
2:C:3710:ALA:HB2	2:C:3785:MET:HE2	2.03	0.40
2:C:3936:PHE:CE2	2:C:3940:TYR:CE2	3.09	0.40
2:D:505:ALA:HB2	2:D:513:ALA:HB2	2.03	0.40
2:D:859:THR:HG21	2:D:932:THR:CA	2.51	0.40
2:D:899:ASP:HB3	2:D:902:LYS:CG	2.51	0.40
2:D:2668:THR:HG21	2:D:2673:LEU:HD21	2.03	0.40
2:D:3239:GLU:O	2:D:3240:MET:C	2.63	0.40
2:D:3894:LEU:HD13	2:D:3902:PHE:HZ	1.86	0.40
2:D:3896:GLU:HA	2:D:3970:GLU:OE1	2.21	0.40
2:D:4042:MET:HE2	2:D:4045:ARG:NH2	2.37	0.40
2:D:5014:GLU:OE2	2:D:5014:GLU:HA	2.21	0.40
2:A:859:THR:HG21	2:A:932:THR:CA	2.51	0.40
2:A:2445:GLN:OE1	2:A:2445:GLN:HA	2.22	0.40
2:A:3008:ASN:C	2:A:3008:ASN:OD1	2.63	0.40
2:A:3540:ARG:HD2	2:A:3543:LEU:HD12	2.04	0.40
2:A:4987:MET:O	2:A:4991:MET:HG3	2.22	0.40
2:B:593:LYS:NZ	2:B:1584:GLU:OE2	2.39	0.40
2:B:4173:ILE:HD12	2:B:4173:ILE:H	1.86	0.40
2:C:862:ILE:CG2	2:C:934:LEU:HD23	2.51	0.40
2:C:3909:GLN:O	2:C:3915:THR:HG22	2.22	0.40
2:D:216:THR:OG1	2:D:219:HIS:NE2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1181:ARG:HB2	2:D:1181:ARG:CZ	2.52	0.40
2:D:2881:GLU:OE1	2:D:2909:TYR:HB2	2.21	0.40
2:D:3687:GLU:O	2:D:3688:GLU:HB3	2.21	0.40
2:D:4578:TYR:HD2	2:D:4805:PHE:CZ	2.40	0.40
2:D:4987:MET:O	2:D:4991:MET:HG3	2.22	0.40
2:A:2578:ILE:HG23	2:A:2579:MET:N	2.36	0.40
2:A:2736:PHE:O	2:A:2738:PRO:HD3	2.21	0.40
2:A:3894:LEU:HD13	2:A:3902:PHE:HZ	1.86	0.40
2:A:4686:ILE:HD12	2:A:4735:ILE:HD13	2.04	0.40
2:B:985:LEU:HD11	2:B:1056:PRO:CB	2.51	0.40
2:B:2334:ASP:HA	2:B:2337:ARG:HD3	2.03	0.40
2:B:2736:PHE:O	2:B:2738:PRO:HD3	2.21	0.40
2:B:2875:MET:HE1	2:B:2938:VAL:HG22	2.04	0.40
2:C:874:LYS:H	2:C:874:LYS:HG3	1.57	0.40
2:C:2875:MET:HE1	2:C:2938:VAL:HG22	2.04	0.40
2:C:2881:GLU:OE1	2:C:2909:TYR:HB2	2.21	0.40
2:C:3534:ILE:CG1	2:C:3597:VAL:HG23	2.51	0.40
2:C:3837:ALA:O	2:C:3841:THR:HG23	2.21	0.40
2:C:4578:TYR:HD2	2:C:4805:PHE:CZ	2.40	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	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
1	F	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
1	G	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
1	H	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	A	4345/5035 (86%)	4228 (97%)	114 (3%)	3 (0%)	48	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	4345/5035 (86%)	4227 (97%)	115 (3%)	3 (0%)	48	78
2	C	4345/5035 (86%)	4227 (97%)	115 (3%)	3 (0%)	48	78
2	D	4345/5035 (86%)	4228 (97%)	114 (3%)	3 (0%)	48	78
All	All	17800/20572 (86%)	17318 (97%)	470 (3%)	12 (0%)	49	78

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	2574	GLU
2	D	4055	SER
2	A	2574	GLU
2	A	4055	SER
2	B	2574	GLU
2	B	4055	SER
2	C	2574	GLU
2	C	4055	SER
2	D	3357	SER
2	A	3357	SER
2	B	3357	SER
2	C	3357	SER

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	89/90 (99%)	89 (100%)	0	100	100
1	F	89/90 (99%)	89 (100%)	0	100	100
1	G	89/90 (99%)	89 (100%)	0	100	100
1	H	89/90 (99%)	89 (100%)	0	100	100
2	A	3806/4296 (89%)	3742 (98%)	64 (2%)	53	74
2	B	3806/4296 (89%)	3742 (98%)	64 (2%)	53	74
2	C	3806/4296 (89%)	3742 (98%)	64 (2%)	53	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	3806/4296 (89%)	3742 (98%)	64 (2%)	53	74
All	All	15580/17544 (89%)	15324 (98%)	256 (2%)	54	75

All (256) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	864	LEU
2	D	868	LEU
2	D	869	GLU
2	D	870	ARG
2	D	871	ILE
2	D	872	ARG
2	D	874	LYS
2	D	877	GLU
2	D	878	ASN
2	D	885	LEU
2	D	887	ARG
2	D	888	ILE
2	D	889	GLU
2	D	893	THR
2	D	897	VAL
2	D	898	ARG
2	D	900	ASP
2	D	902	LYS
2	D	904	LEU
2	D	905	HIS
2	D	907	CYS
2	D	909	VAL
2	D	910	ASN
2	D	914	LEU
2	D	918	GLU
2	D	919	ARG
2	D	925	MET
2	D	929	THR
2	D	930	LEU
2	D	931	LYS
2	D	933	LEU
2	D	934	LEU
2	D	938	CYS
2	D	939	HIS
2	D	940	VAL
2	D	945	GLU

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Mol	Chain	Res	Type
2	D	948	GLU
2	D	949	ASP
2	D	951	LEU
2	D	952	LYS
2	D	953	LYS
2	D	954	THR
2	D	955	LYS
2	D	956	LEU
2	D	959	THR
2	D	961	MET
2	D	962	MET
2	D	963	SER
2	D	964	ASN
2	D	966	TYR
2	D	967	LYS
2	D	971	LEU
2	D	972	ASP
2	D	973	LEU
2	D	975	HIS
2	D	977	ARG
2	D	978	LEU
2	D	979	THR
2	D	1047	LEU
2	D	1048	LEU
2	D	1053	ASN
2	D	1055	GLU
2	D	2282	ILE
2	D	2337	ARG
2	A	864	LEU
2	A	868	LEU
2	A	869	GLU
2	A	870	ARG
2	A	871	ILE
2	A	872	ARG
2	A	874	LYS
2	A	877	GLU
2	A	878	ASN
2	A	885	LEU
2	A	887	ARG
2	A	888	ILE
2	A	889	GLU
2	A	893	THR

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Mol	Chain	Res	Type
2	A	897	VAL
2	A	898	ARG
2	A	900	ASP
2	A	902	LYS
2	A	904	LEU
2	A	905	HIS
2	A	907	CYS
2	A	909	VAL
2	A	910	ASN
2	A	914	LEU
2	A	918	GLU
2	A	919	ARG
2	A	925	MET
2	A	929	THR
2	A	930	LEU
2	A	931	LYS
2	A	933	LEU
2	A	934	LEU
2	A	938	CYS
2	A	939	HIS
2	A	940	VAL
2	A	945	GLU
2	A	948	GLU
2	A	949	ASP
2	A	951	LEU
2	A	952	LYS
2	A	953	LYS
2	A	954	THR
2	A	955	LYS
2	A	956	LEU
2	A	959	THR
2	A	961	MET
2	A	962	MET
2	A	963	SER
2	A	964	ASN
2	A	966	TYR
2	A	967	LYS
2	A	971	LEU
2	A	972	ASP
2	A	973	LEU
2	A	975	HIS
2	A	977	ARG

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Mol	Chain	Res	Type
2	A	978	LEU
2	A	979	THR
2	A	1047	LEU
2	A	1048	LEU
2	A	1053	ASN
2	A	1055	GLU
2	A	2282	ILE
2	A	2337	ARG
2	B	864	LEU
2	B	868	LEU
2	B	869	GLU
2	B	870	ARG
2	B	871	ILE
2	B	872	ARG
2	B	874	LYS
2	B	877	GLU
2	B	878	ASN
2	B	885	LEU
2	B	887	ARG
2	B	888	ILE
2	B	889	GLU
2	B	893	THR
2	B	897	VAL
2	B	898	ARG
2	B	900	ASP
2	B	902	LYS
2	B	904	LEU
2	B	905	HIS
2	B	907	CYS
2	B	909	VAL
2	B	910	ASN
2	B	914	LEU
2	B	918	GLU
2	B	919	ARG
2	B	925	MET
2	B	929	THR
2	B	930	LEU
2	B	931	LYS
2	B	933	LEU
2	B	934	LEU
2	B	938	CYS
2	B	939	HIS

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Mol	Chain	Res	Type
2	B	940	VAL
2	B	945	GLU
2	B	948	GLU
2	B	949	ASP
2	B	951	LEU
2	B	952	LYS
2	B	953	LYS
2	B	954	THR
2	B	955	LYS
2	B	956	LEU
2	B	959	THR
2	B	961	MET
2	B	962	MET
2	B	963	SER
2	B	964	ASN
2	B	966	TYR
2	B	967	LYS
2	B	971	LEU
2	B	972	ASP
2	B	973	LEU
2	B	975	HIS
2	B	977	ARG
2	B	978	LEU
2	B	979	THR
2	B	1047	LEU
2	B	1048	LEU
2	B	1053	ASN
2	B	1055	GLU
2	B	2282	ILE
2	B	2337	ARG
2	C	864	LEU
2	C	868	LEU
2	C	869	GLU
2	C	870	ARG
2	C	871	ILE
2	C	872	ARG
2	C	874	LYS
2	C	877	GLU
2	C	878	ASN
2	C	885	LEU
2	C	887	ARG
2	C	888	ILE

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Mol	Chain	Res	Type
2	C	889	GLU
2	C	893	THR
2	C	897	VAL
2	C	898	ARG
2	C	900	ASP
2	C	902	LYS
2	C	904	LEU
2	C	905	HIS
2	C	907	CYS
2	C	909	VAL
2	C	910	ASN
2	C	914	LEU
2	C	918	GLU
2	C	919	ARG
2	C	925	MET
2	C	929	THR
2	C	930	LEU
2	C	931	LYS
2	C	933	LEU
2	C	934	LEU
2	C	938	CYS
2	C	939	HIS
2	C	940	VAL
2	C	945	GLU
2	C	948	GLU
2	C	949	ASP
2	C	951	LEU
2	C	952	LYS
2	C	953	LYS
2	C	954	THR
2	C	955	LYS
2	C	956	LEU
2	C	959	THR
2	C	961	MET
2	C	962	MET
2	C	963	SER
2	C	964	ASN
2	C	966	TYR
2	C	967	LYS
2	C	971	LEU
2	C	972	ASP
2	C	973	LEU

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Mol	Chain	Res	Type
2	C	975	HIS
2	C	977	ARG
2	C	978	LEU
2	C	979	THR
2	C	1047	LEU
2	C	1048	LEU
2	C	1053	ASN
2	C	1055	GLU
2	C	2282	ILE
2	C	2337	ARG

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

Mol	Chain	Res	Type
1	H	21	GLN
2	D	106	HIS
2	D	380	HIS
2	D	594	HIS
2	D	905	HIS
2	D	950	ASN
2	D	995	ASN
2	D	1085	GLN
2	D	1131	GLN
2	D	1202	HIS
2	D	1299	HIS
2	D	1485	HIS
2	D	1570	GLN
2	D	1591	GLN
2	D	1612	HIS
2	D	1632	GLN
2	D	1641	HIS
2	D	1762	HIS
2	D	2773	GLN
2	D	2774	ASN
2	D	2932	GLN
2	D	2992	HIS
2	D	3110	ASN
2	D	3423	HIS
2	D	3598	GLN
2	D	3612	HIS
2	D	3885	GLN
2	D	3917	ASN

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Mol	Chain	Res	Type
2	D	3930	GLN
2	D	4001	HIS
2	D	4156	HIS
2	D	4834	GLN
2	D	5004	GLN
2	A	380	HIS
2	A	594	HIS
2	A	905	HIS
2	A	950	ASN
2	A	995	ASN
2	A	1085	GLN
2	A	1131	GLN
2	A	1202	HIS
2	A	1299	HIS
2	A	1430	ASN
2	A	1485	HIS
2	A	1570	GLN
2	A	1591	GLN
2	A	1632	GLN
2	A	1641	HIS
2	A	1762	HIS
2	A	1939	GLN
2	A	1973	ASN
2	A	2004	GLN
2	A	2764	HIS
2	A	2773	GLN
2	A	2774	ASN
2	A	2992	HIS
2	A	3110	ASN
2	A	3423	HIS
2	A	3612	HIS
2	A	3885	GLN
2	A	3917	ASN
2	A	3930	GLN
2	A	4037	ASN
2	A	4057	ASN
2	A	4156	HIS
2	A	4834	GLN
2	B	380	HIS
2	B	594	HIS
2	B	905	HIS
2	B	950	ASN

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Mol	Chain	Res	Type
2	B	995	ASN
2	B	1085	GLN
2	B	1131	GLN
2	B	1202	HIS
2	B	1485	HIS
2	B	1570	GLN
2	B	1591	GLN
2	B	1612	HIS
2	B	1632	GLN
2	B	1641	HIS
2	B	1720	HIS
2	B	1762	HIS
2	B	2037	GLN
2	B	2773	GLN
2	B	2774	ASN
2	B	2932	GLN
2	B	2992	HIS
2	B	3110	ASN
2	B	3423	HIS
2	B	3612	HIS
2	B	3885	GLN
2	B	3917	ASN
2	B	3930	GLN
2	B	4156	HIS
2	B	4834	GLN
2	B	5004	GLN
2	C	106	HIS
2	C	380	HIS
2	C	594	HIS
2	C	905	HIS
2	C	950	ASN
2	C	995	ASN
2	C	1085	GLN
2	C	1131	GLN
2	C	1202	HIS
2	C	1485	HIS
2	C	1570	GLN
2	C	1591	GLN
2	C	1612	HIS
2	C	1632	GLN
2	C	1641	HIS
2	C	1720	HIS

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Mol	Chain	Res	Type
2	C	1762	HIS
2	C	1973	ASN
2	C	2004	GLN
2	C	2037	GLN
2	C	2773	GLN
2	C	2774	ASN
2	C	2932	GLN
2	C	2992	HIS
2	C	3110	ASN
2	C	3423	HIS
2	C	3612	HIS
2	C	3885	GLN
2	C	3917	ASN
2	C	3930	GLN
2	C	4156	HIS
2	C	4834	GLN
2	C	5004	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 8 are monoatomic - leaving 28 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
8	A1BYZ	A	8008	-	32,32,32	0.67	1 (3%)	40,47,47	0.85	1 (2%)
5	ATP	A	8003	-	32,33,33	0.32	0	48,52,52	0.70	1 (2%)
7	PCW	A	8005	-	53,53,53	1.26	7 (13%)	59,61,61	1.12	3 (5%)
5	ATP	B	8007	-	32,33,33	0.27	0	48,52,52	0.66	0
5	ATP	A	8007	-	32,33,33	0.27	0	48,52,52	0.66	0
5	ATP	D	8007	-	32,33,33	0.27	0	48,52,52	0.66	0
8	A1BYZ	D	8009	-	32,32,32	0.60	1 (3%)	40,47,47	1.19	4 (10%)
8	A1BYZ	A	8009	-	32,32,32	0.60	1 (3%)	40,47,47	1.19	4 (10%)
7	PCW	C	8005	-	53,53,53	1.25	7 (13%)	59,61,61	1.12	3 (5%)
5	ATP	C	8003	-	32,33,33	0.32	0	48,52,52	0.69	1 (2%)
7	PCW	C	8006	-	53,53,53	1.24	7 (13%)	59,61,61	1.19	4 (6%)
7	PCW	B	8006	-	53,53,53	1.24	7 (13%)	59,61,61	1.19	4 (6%)
8	A1BYZ	C	8008	-	32,32,32	0.68	1 (3%)	40,47,47	0.85	1 (2%)
7	PCW	B	8005	-	53,53,53	1.25	7 (13%)	59,61,61	1.12	3 (5%)
4	CFF	C	8002	-	15,15,15	1.86	6 (40%)	23,23,23	2.94	12 (52%)
7	PCW	D	8005	-	53,53,53	1.26	7 (13%)	59,61,61	1.12	3 (5%)
5	ATP	D	8003	-	32,33,33	0.32	0	48,52,52	0.69	1 (2%)
4	CFF	B	8002	-	15,15,15	1.87	6 (40%)	23,23,23	2.94	12 (52%)
7	PCW	A	8006	-	53,53,53	1.24	7 (13%)	59,61,61	1.19	4 (6%)
5	ATP	C	8007	-	32,33,33	0.27	0	48,52,52	0.66	0
7	PCW	D	8006	-	53,53,53	1.24	7 (13%)	59,61,61	1.19	4 (6%)
5	ATP	B	8003	-	32,33,33	0.32	0	48,52,52	0.69	1 (2%)
8	A1BYZ	D	8008	-	32,32,32	0.68	1 (3%)	40,47,47	0.85	1 (2%)
8	A1BYZ	B	8009	-	32,32,32	0.60	1 (3%)	40,47,47	1.19	4 (10%)
4	CFF	A	8002	-	15,15,15	1.87	6 (40%)	23,23,23	2.94	12 (52%)
8	A1BYZ	B	8008	-	32,32,32	0.68	1 (3%)	40,47,47	0.85	1 (2%)
4	CFF	D	8002	-	15,15,15	1.87	6 (40%)	23,23,23	2.94	12 (52%)
8	A1BYZ	C	8009	-	32,32,32	0.60	1 (3%)	40,47,47	1.19	4 (10%)

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
8	A1BYZ	A	8008	-	-	3/18/59/59	0/3/3/3
5	ATP	A	8003	-	-	11/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PCW	A	8005	-	-	25/57/57/57	-
5	ATP	B	8007	-	-	8/22/38/38	0/3/3/3
5	ATP	A	8007	-	-	8/22/38/38	0/3/3/3
5	ATP	D	8007	-	-	8/22/38/38	0/3/3/3
8	A1BYZ	D	8009	-	-	4/18/59/59	0/3/3/3
8	A1BYZ	A	8009	-	-	4/18/59/59	0/3/3/3
7	PCW	C	8005	-	-	25/57/57/57	-
5	ATP	C	8003	-	-	11/22/38/38	0/3/3/3
7	PCW	C	8006	-	-	29/57/57/57	-
7	PCW	B	8006	-	-	29/57/57/57	-
8	A1BYZ	C	8008	-	-	3/18/59/59	0/3/3/3
7	PCW	B	8005	-	-	25/57/57/57	-
4	CFF	C	8002	-	-	-	0/2/2/2
7	PCW	D	8005	-	-	25/57/57/57	-
5	ATP	D	8003	-	-	11/22/38/38	0/3/3/3
4	CFF	B	8002	-	-	-	0/2/2/2
7	PCW	A	8006	-	-	29/57/57/57	-
5	ATP	C	8007	-	-	8/22/38/38	0/3/3/3
7	PCW	D	8006	-	-	29/57/57/57	-
5	ATP	B	8003	-	-	11/22/38/38	0/3/3/3
8	A1BYZ	D	8008	-	-	3/18/59/59	0/3/3/3
8	A1BYZ	B	8009	-	-	4/18/59/59	0/3/3/3
4	CFF	A	8002	-	-	-	0/2/2/2
8	A1BYZ	B	8008	-	-	3/18/59/59	0/3/3/3
8	A1BYZ	C	8009	-	-	4/18/59/59	0/3/3/3
4	CFF	D	8002	-	-	-	0/2/2/2

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	8002	CFF	C6-N1	-3.80	1.32	1.40
4	A	8002	CFF	C6-N1	-3.80	1.32	1.40
4	B	8002	CFF	C6-N1	-3.80	1.32	1.40
4	C	8002	CFF	C6-N1	-3.80	1.32	1.40
8	D	8008	A1BYZ	C16-C15	-3.34	1.51	1.54
8	B	8008	A1BYZ	C16-C15	-3.34	1.51	1.54
8	C	8008	A1BYZ	C16-C15	-3.34	1.51	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	8008	A1BYZ	C16-C15	-3.32	1.51	1.54
7	D	8006	PCW	O3-C11	3.03	1.42	1.33
7	B	8006	PCW	O3-C11	3.03	1.42	1.33
7	C	8006	PCW	O3-C11	3.03	1.42	1.33
7	A	8006	PCW	O3-C11	3.02	1.42	1.33
7	A	8005	PCW	O3-C11	3.00	1.42	1.33
7	D	8005	PCW	O3-C11	3.00	1.42	1.33
7	B	8005	PCW	O3-C11	3.00	1.42	1.33
7	C	8005	PCW	O3-C11	3.00	1.42	1.33
8	D	8009	A1BYZ	C16-C15	-2.98	1.51	1.54
8	A	8009	A1BYZ	C16-C15	-2.98	1.51	1.54
8	B	8009	A1BYZ	C16-C15	-2.98	1.51	1.54
8	C	8009	A1BYZ	C16-C15	-2.98	1.51	1.54
7	A	8005	PCW	O2-C31	2.96	1.42	1.34
7	D	8005	PCW	O2-C31	2.96	1.42	1.34
7	C	8005	PCW	O2-C31	2.96	1.42	1.34
7	B	8005	PCW	O2-C31	2.94	1.42	1.34
7	A	8006	PCW	O2-C31	2.70	1.41	1.34
7	D	8006	PCW	O2-C31	2.69	1.41	1.34
7	B	8006	PCW	O2-C31	2.69	1.41	1.34
7	C	8006	PCW	O2-C31	2.69	1.41	1.34
4	D	8002	CFF	C5-N7	-2.64	1.33	1.38
4	A	8002	CFF	C5-N7	-2.64	1.33	1.38
4	B	8002	CFF	C5-N7	-2.64	1.33	1.38
7	D	8005	PCW	P-O4P	2.64	1.69	1.59
7	B	8005	PCW	P-O4P	2.64	1.69	1.59
7	C	8005	PCW	P-O4P	2.64	1.69	1.59
7	A	8005	PCW	P-O4P	2.63	1.69	1.59
4	C	8002	CFF	C5-N7	-2.60	1.33	1.38
7	A	8006	PCW	P-O4P	2.54	1.69	1.59
7	D	8006	PCW	P-O4P	2.52	1.69	1.59
7	B	8006	PCW	P-O4P	2.52	1.69	1.59
7	C	8006	PCW	P-O4P	2.52	1.69	1.59
7	A	8006	PCW	O2-C2	-2.39	1.41	1.46
7	D	8005	PCW	C5-C4	2.39	1.58	1.51
7	B	8005	PCW	C5-C4	2.39	1.58	1.51
7	C	8005	PCW	C5-C4	2.39	1.58	1.51
7	D	8006	PCW	O2-C2	-2.38	1.41	1.46
7	B	8006	PCW	O2-C2	-2.38	1.41	1.46
7	C	8006	PCW	O2-C2	-2.38	1.41	1.46
7	A	8005	PCW	C5-C4	2.37	1.58	1.51
7	D	8005	PCW	C32-C31	2.36	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	8005	PCW	C32-C31	2.36	1.57	1.50
7	C	8005	PCW	C32-C31	2.35	1.57	1.50
7	A	8005	PCW	C32-C31	2.33	1.57	1.50
7	A	8005	PCW	O2-C2	-2.30	1.41	1.46
7	A	8005	PCW	P-O3P	2.29	1.68	1.59
7	D	8005	PCW	P-O3P	2.29	1.68	1.59
7	B	8005	PCW	P-O3P	2.29	1.68	1.59
7	C	8005	PCW	P-O3P	2.29	1.68	1.59
4	C	8002	CFF	O13-C6	-2.28	1.18	1.23
4	D	8002	CFF	O13-C6	-2.28	1.18	1.23
4	A	8002	CFF	O13-C6	-2.28	1.18	1.23
4	B	8002	CFF	O13-C6	-2.28	1.18	1.23
7	D	8005	PCW	O2-C2	-2.28	1.41	1.46
7	B	8005	PCW	O2-C2	-2.28	1.41	1.46
7	C	8005	PCW	O2-C2	-2.28	1.41	1.46
7	A	8006	PCW	C5-C4	2.23	1.58	1.51
7	D	8006	PCW	C5-C4	2.23	1.58	1.51
7	B	8006	PCW	C5-C4	2.23	1.58	1.51
7	C	8006	PCW	C5-C4	2.21	1.58	1.51
7	A	8006	PCW	P-O3P	2.16	1.67	1.59
7	D	8006	PCW	P-O3P	2.15	1.67	1.59
7	B	8006	PCW	P-O3P	2.15	1.67	1.59
7	C	8006	PCW	P-O3P	2.15	1.67	1.59
4	D	8002	CFF	C4-N3	-2.15	1.34	1.38
4	A	8002	CFF	C4-N3	-2.15	1.34	1.38
4	B	8002	CFF	C4-N3	-2.15	1.34	1.38
4	C	8002	CFF	C4-N3	-2.15	1.34	1.38
4	A	8002	CFF	O11-C2	-2.07	1.18	1.22
4	A	8002	CFF	C5-C6	-2.06	1.37	1.43
7	A	8006	PCW	C32-C31	2.06	1.56	1.50
4	D	8002	CFF	C5-C6	-2.05	1.37	1.43
4	B	8002	CFF	C5-C6	-2.05	1.37	1.43
4	C	8002	CFF	C5-C6	-2.05	1.37	1.43
7	D	8006	PCW	C32-C31	2.04	1.56	1.50
7	B	8006	PCW	C32-C31	2.04	1.56	1.50
7	C	8006	PCW	C32-C31	2.04	1.56	1.50
4	D	8002	CFF	O11-C2	-2.04	1.18	1.22
4	B	8002	CFF	O11-C2	-2.04	1.18	1.22
4	C	8002	CFF	O11-C2	-2.04	1.18	1.22

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	8002	CFF	C14-N7-C8	-8.05	111.22	126.28
4	D	8002	CFF	C14-N7-C8	-8.03	111.25	126.28
4	A	8002	CFF	C14-N7-C8	-8.03	111.25	126.28
4	C	8002	CFF	C14-N7-C8	-8.02	111.28	126.28
4	D	8002	CFF	C14-N7-C5	5.48	140.80	127.77
4	A	8002	CFF	C14-N7-C5	5.48	140.80	127.77
4	B	8002	CFF	C14-N7-C5	5.48	140.80	127.77
4	C	8002	CFF	C14-N7-C5	5.47	140.79	127.77
4	D	8002	CFF	C5-C6-N1	4.37	120.06	112.06
4	B	8002	CFF	C5-C6-N1	4.37	120.06	112.06
4	C	8002	CFF	C5-C6-N1	4.37	120.06	112.06
4	A	8002	CFF	C5-C6-N1	4.37	120.06	112.06
7	D	8006	PCW	O2-C31-C32	4.14	120.43	111.48
7	B	8006	PCW	O2-C31-C32	4.14	120.43	111.48
7	C	8006	PCW	O2-C31-C32	4.14	120.43	111.48
7	A	8006	PCW	O2-C31-C32	4.13	120.41	111.48
7	C	8005	PCW	O2-C31-C32	3.98	120.09	111.48
7	D	8005	PCW	O2-C31-C32	3.98	120.09	111.48
7	A	8006	PCW	C21-C20-C19	3.97	154.60	124.83
7	A	8005	PCW	O2-C31-C32	3.97	120.08	111.48
7	D	8006	PCW	C21-C20-C19	3.97	154.60	124.83
7	B	8006	PCW	C21-C20-C19	3.97	154.60	124.83
7	C	8006	PCW	C21-C20-C19	3.97	154.60	124.83
7	B	8005	PCW	O2-C31-C32	3.97	120.06	111.48
4	A	8002	CFF	N3-C4-N9	3.83	132.29	126.27
4	D	8002	CFF	N3-C4-N9	3.83	132.29	126.27
4	B	8002	CFF	N3-C4-N9	3.83	132.29	126.27
4	C	8002	CFF	N3-C4-N9	3.83	132.29	126.27
7	A	8005	PCW	C21-C20-C19	3.78	153.19	124.83
7	D	8005	PCW	C21-C20-C19	3.78	153.15	124.83
7	B	8005	PCW	C21-C20-C19	3.78	153.15	124.83
7	C	8005	PCW	C21-C20-C19	3.78	153.15	124.83
4	D	8002	CFF	C6-N1-C2	-3.78	119.52	125.66
4	B	8002	CFF	C6-N1-C2	-3.78	119.52	125.66
4	C	8002	CFF	C6-N1-C2	-3.78	119.52	125.66
4	A	8002	CFF	C6-N1-C2	-3.78	119.52	125.66
8	A	8009	A1BYZ	C15-C16-C17	-3.57	108.70	110.88
8	D	8009	A1BYZ	C15-C16-C17	-3.56	108.70	110.88
8	B	8009	A1BYZ	C15-C16-C17	-3.56	108.70	110.88
8	D	8009	A1BYZ	C14-C15-C16	3.52	112.57	110.70
8	B	8009	A1BYZ	C14-C15-C16	3.52	112.57	110.70
8	C	8009	A1BYZ	C14-C15-C16	3.52	112.57	110.70
8	C	8009	A1BYZ	C15-C16-C17	-3.52	108.73	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	8009	A1BYZ	C14-C15-C16	3.50	112.56	110.70
4	C	8002	CFF	O13-C6-C5	-3.42	119.37	126.38
4	D	8002	CFF	O13-C6-C5	-3.40	119.41	126.38
4	B	8002	CFF	O13-C6-C5	-3.40	119.41	126.38
4	A	8002	CFF	O13-C6-C5	-3.40	119.41	126.38
4	B	8002	CFF	N7-C8-N9	-3.01	108.03	113.48
8	D	8008	A1BYZ	C24-C25-C26	-3.01	111.36	116.30
8	B	8008	A1BYZ	C24-C25-C26	-3.01	111.36	116.30
8	C	8008	A1BYZ	C24-C25-C26	-3.01	111.36	116.30
4	D	8002	CFF	N7-C8-N9	-2.99	108.06	113.48
8	A	8008	A1BYZ	C24-C25-C26	-2.98	111.41	116.30
4	C	8002	CFF	N7-C8-N9	-2.98	108.09	113.48
4	A	8002	CFF	N7-C8-N9	-2.97	108.09	113.48
8	A	8009	A1BYZ	C24-C25-C26	-2.94	111.48	116.30
8	D	8009	A1BYZ	C24-C25-C26	-2.93	111.49	116.30
8	B	8009	A1BYZ	C24-C25-C26	-2.93	111.49	116.30
8	C	8009	A1BYZ	C24-C25-C26	-2.93	111.49	116.30
7	A	8005	PCW	O3-C11-C12	2.81	120.41	111.83
7	D	8005	PCW	O3-C11-C12	2.81	120.40	111.83
7	B	8005	PCW	O3-C11-C12	2.81	120.40	111.83
7	C	8005	PCW	O3-C11-C12	2.81	120.40	111.83
7	A	8006	PCW	C18-C19-C20	2.71	145.15	124.83
7	C	8006	PCW	C18-C19-C20	2.71	145.15	124.83
7	D	8006	PCW	C18-C19-C20	2.71	145.14	124.83
7	B	8006	PCW	C18-C19-C20	2.71	145.11	124.83
4	D	8002	CFF	N3-C2-N1	2.68	120.48	117.14
4	C	8002	CFF	N3-C2-N1	2.68	120.48	117.14
4	A	8002	CFF	N3-C2-N1	2.67	120.48	117.14
4	B	8002	CFF	N3-C2-N1	2.65	120.45	117.14
7	A	8006	PCW	O3-C11-C12	2.59	119.74	111.83
7	D	8006	PCW	O3-C11-C12	2.59	119.72	111.83
7	B	8006	PCW	O3-C11-C12	2.59	119.72	111.83
7	C	8006	PCW	O3-C11-C12	2.59	119.72	111.83
8	C	8009	A1BYZ	C16-C17-C18	-2.29	121.23	123.59
8	A	8009	A1BYZ	C16-C17-C18	-2.29	121.23	123.59
8	D	8009	A1BYZ	C16-C17-C18	-2.26	121.26	123.59
8	B	8009	A1BYZ	C16-C17-C18	-2.26	121.26	123.59
4	A	8002	CFF	C10-N1-C6	2.14	120.96	117.64
4	D	8002	CFF	C10-N1-C6	2.12	120.93	117.64
4	B	8002	CFF	C10-N1-C6	2.12	120.93	117.64
4	C	8002	CFF	C10-N1-C6	2.12	120.93	117.64
4	A	8002	CFF	C6-C5-C4	-2.11	120.26	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	8002	CFF	C6-C5-C4	-2.10	120.27	122.92
4	C	8002	CFF	C6-C5-C4	-2.10	120.27	122.92
4	B	8002	CFF	C6-C5-C4	-2.08	120.29	122.92
4	A	8002	CFF	C5-C4-N9	-2.03	108.07	112.10
4	D	8002	CFF	C8-N9-C4	2.03	107.85	102.98
4	B	8002	CFF	C8-N9-C4	2.03	107.85	102.98
4	C	8002	CFF	C8-N9-C4	2.03	107.85	102.98
4	D	8002	CFF	C5-C4-N9	-2.03	108.08	112.10
4	C	8002	CFF	C5-C4-N9	-2.03	108.08	112.10
4	A	8002	CFF	C8-N9-C4	2.02	107.83	102.98
4	B	8002	CFF	C5-C4-N9	-2.02	108.10	112.10
5	D	8003	ATP	O3'-C3'-C2'	-2.01	105.36	111.82
5	B	8003	ATP	O3'-C3'-C2'	-2.01	105.36	111.82
5	C	8003	ATP	O3'-C3'-C2'	-2.01	105.36	111.82
5	A	8003	ATP	O3'-C3'-C2'	-2.01	105.38	111.82

There are no chirality outliers.

All (320) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	8003	ATP	C5'-O5'-PA-O1A
5	D	8003	ATP	C5'-O5'-PA-O2A
5	D	8003	ATP	C5'-O5'-PA-O3A
5	D	8007	ATP	PB-O3B-PG-O3G
5	D	8007	ATP	C5'-O5'-PA-O2A
5	A	8003	ATP	C5'-O5'-PA-O1A
5	A	8003	ATP	C5'-O5'-PA-O2A
5	A	8003	ATP	C5'-O5'-PA-O3A
5	A	8007	ATP	PB-O3B-PG-O3G
5	A	8007	ATP	C5'-O5'-PA-O2A
5	B	8003	ATP	C5'-O5'-PA-O1A
5	B	8003	ATP	C5'-O5'-PA-O2A
5	B	8003	ATP	C5'-O5'-PA-O3A
5	B	8007	ATP	PB-O3B-PG-O3G
5	B	8007	ATP	C5'-O5'-PA-O2A
5	C	8003	ATP	C5'-O5'-PA-O1A
5	C	8003	ATP	C5'-O5'-PA-O2A
5	C	8003	ATP	C5'-O5'-PA-O3A
5	C	8007	ATP	PB-O3B-PG-O3G
5	C	8007	ATP	C5'-O5'-PA-O2A
7	D	8005	PCW	C32-C31-O2-C2
7	D	8005	PCW	O31-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
7	D	8005	PCW	C1-O3P-P-O2P
7	D	8005	PCW	C1-O3P-P-O4P
7	D	8005	PCW	C4-O4P-P-O2P
7	D	8006	PCW	C1-O3P-P-O2P
7	A	8005	PCW	C32-C31-O2-C2
7	A	8005	PCW	O31-C31-O2-C2
7	A	8005	PCW	C1-O3P-P-O2P
7	A	8005	PCW	C1-O3P-P-O4P
7	A	8005	PCW	C4-O4P-P-O2P
7	A	8006	PCW	C1-O3P-P-O2P
7	B	8005	PCW	C32-C31-O2-C2
7	B	8005	PCW	O31-C31-O2-C2
7	B	8005	PCW	C1-O3P-P-O2P
7	B	8005	PCW	C1-O3P-P-O4P
7	B	8005	PCW	C4-O4P-P-O2P
7	B	8006	PCW	C1-O3P-P-O2P
7	C	8005	PCW	C32-C31-O2-C2
7	C	8005	PCW	O31-C31-O2-C2
7	C	8005	PCW	C1-O3P-P-O2P
7	C	8005	PCW	C1-O3P-P-O4P
7	C	8005	PCW	C4-O4P-P-O2P
7	C	8006	PCW	C1-O3P-P-O2P
8	D	8009	A1BYZ	C3-C6-O8-C9
8	D	8009	A1BYZ	O7-C6-O8-C9
8	A	8009	A1BYZ	C3-C6-O8-C9
8	A	8009	A1BYZ	O7-C6-O8-C9
8	B	8009	A1BYZ	C3-C6-O8-C9
8	B	8009	A1BYZ	O7-C6-O8-C9
8	C	8009	A1BYZ	C3-C6-O8-C9
8	C	8009	A1BYZ	O7-C6-O8-C9
8	D	8008	A1BYZ	C10-C9-O8-C6
8	A	8008	A1BYZ	C10-C9-O8-C6
8	B	8008	A1BYZ	C10-C9-O8-C6
8	C	8008	A1BYZ	C10-C9-O8-C6
7	D	8006	PCW	O11-C11-O3-C3
7	A	8006	PCW	O11-C11-O3-C3
7	B	8006	PCW	O11-C11-O3-C3
7	C	8006	PCW	O11-C11-O3-C3
7	D	8006	PCW	C32-C31-O2-C2
7	A	8006	PCW	C32-C31-O2-C2
7	B	8006	PCW	C32-C31-O2-C2
7	C	8006	PCW	C32-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
7	D	8006	PCW	C12-C11-O3-C3
7	A	8006	PCW	C12-C11-O3-C3
7	B	8006	PCW	C12-C11-O3-C3
7	C	8006	PCW	C12-C11-O3-C3
7	D	8006	PCW	O31-C31-O2-C2
7	A	8006	PCW	O31-C31-O2-C2
7	B	8006	PCW	O31-C31-O2-C2
7	C	8006	PCW	O31-C31-O2-C2
7	D	8006	PCW	C21-C22-C23-C24
7	A	8006	PCW	C21-C22-C23-C24
7	B	8006	PCW	C21-C22-C23-C24
7	C	8006	PCW	C21-C22-C23-C24
7	D	8005	PCW	C22-C23-C24-C25
7	B	8005	PCW	C22-C23-C24-C25
7	C	8005	PCW	C22-C23-C24-C25
7	A	8005	PCW	C22-C23-C24-C25
8	D	8009	A1BYZ	C15-C20-C21-C22
8	A	8009	A1BYZ	C15-C20-C21-C22
8	B	8009	A1BYZ	C15-C20-C21-C22
8	C	8009	A1BYZ	C15-C20-C21-C22
7	D	8005	PCW	C4-C5-N-C6
7	A	8005	PCW	C4-C5-N-C6
7	B	8005	PCW	C4-C5-N-C6
7	C	8005	PCW	C4-C5-N-C6
7	D	8005	PCW	C31-C32-C33-C34
7	A	8005	PCW	C31-C32-C33-C34
7	B	8005	PCW	C31-C32-C33-C34
7	C	8005	PCW	C31-C32-C33-C34
7	D	8005	PCW	C4-C5-N-C8
7	A	8005	PCW	C4-C5-N-C8
7	B	8005	PCW	C4-C5-N-C8
7	C	8005	PCW	C4-C5-N-C8
7	A	8006	PCW	C35-C36-C37-C38
7	D	8006	PCW	C35-C36-C37-C38
7	B	8006	PCW	C35-C36-C37-C38
7	C	8006	PCW	C35-C36-C37-C38
7	D	8005	PCW	C33-C34-C35-C36
7	A	8005	PCW	C33-C34-C35-C36
7	B	8005	PCW	C33-C34-C35-C36
7	C	8005	PCW	C33-C34-C35-C36
7	D	8006	PCW	C11-C12-C13-C14
7	A	8006	PCW	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
7	B	8006	PCW	C11-C12-C13-C14
7	C	8006	PCW	C11-C12-C13-C14
7	D	8005	PCW	C11-C12-C13-C14
7	A	8005	PCW	C11-C12-C13-C14
7	B	8005	PCW	C11-C12-C13-C14
7	C	8005	PCW	C11-C12-C13-C14
7	D	8006	PCW	C22-C23-C24-C25
7	D	8006	PCW	C34-C35-C36-C37
7	A	8006	PCW	C22-C23-C24-C25
7	A	8006	PCW	C34-C35-C36-C37
7	B	8006	PCW	C22-C23-C24-C25
7	B	8006	PCW	C34-C35-C36-C37
7	C	8006	PCW	C22-C23-C24-C25
7	C	8006	PCW	C34-C35-C36-C37
7	D	8005	PCW	C12-C11-O3-C3
7	A	8005	PCW	C12-C11-O3-C3
7	B	8005	PCW	C12-C11-O3-C3
7	C	8005	PCW	C12-C11-O3-C3
7	D	8005	PCW	C4-C5-N-C7
7	A	8005	PCW	C4-C5-N-C7
7	B	8005	PCW	C4-C5-N-C7
7	C	8005	PCW	C4-C5-N-C7
7	D	8005	PCW	C13-C14-C15-C16
7	B	8005	PCW	C13-C14-C15-C16
7	A	8005	PCW	C13-C14-C15-C16
7	C	8005	PCW	C13-C14-C15-C16
7	D	8005	PCW	C20-C21-C22-C23
7	A	8005	PCW	C20-C21-C22-C23
7	B	8005	PCW	C20-C21-C22-C23
7	C	8005	PCW	C20-C21-C22-C23
7	A	8005	PCW	C44-C45-C46-C47
7	C	8005	PCW	C44-C45-C46-C47
7	D	8005	PCW	C44-C45-C46-C47
7	B	8005	PCW	C44-C45-C46-C47
7	D	8005	PCW	C2-C3-O3-C11
7	A	8005	PCW	C2-C3-O3-C11
7	B	8005	PCW	C2-C3-O3-C11
7	C	8005	PCW	C2-C3-O3-C11
7	A	8005	PCW	O11-C11-O3-C3
7	D	8005	PCW	O11-C11-O3-C3
7	B	8005	PCW	O11-C11-O3-C3
7	C	8005	PCW	O11-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
7	D	8006	PCW	C15-C16-C17-C18
7	A	8006	PCW	C15-C16-C17-C18
7	B	8006	PCW	C15-C16-C17-C18
7	C	8006	PCW	C15-C16-C17-C18
5	D	8003	ATP	PB-O3B-PG-O1G
5	A	8003	ATP	PB-O3B-PG-O1G
5	B	8003	ATP	PB-O3B-PG-O1G
5	C	8003	ATP	PB-O3B-PG-O1G
8	D	8008	A1BYZ	C20-C21-C22-C23
8	A	8008	A1BYZ	C20-C21-C22-C23
8	B	8008	A1BYZ	C20-C21-C22-C23
8	C	8008	A1BYZ	C20-C21-C22-C23
7	D	8006	PCW	C20-C21-C22-C23
7	A	8006	PCW	C20-C21-C22-C23
7	B	8006	PCW	C20-C21-C22-C23
7	C	8006	PCW	C20-C21-C22-C23
7	D	8006	PCW	C42-C43-C44-C45
7	A	8006	PCW	C42-C43-C44-C45
7	B	8006	PCW	C42-C43-C44-C45
7	C	8006	PCW	C42-C43-C44-C45
5	D	8003	ATP	PA-O3A-PB-O1B
5	A	8003	ATP	PA-O3A-PB-O1B
5	B	8003	ATP	PA-O3A-PB-O1B
5	C	8003	ATP	PA-O3A-PB-O1B
5	D	8003	ATP	C4'-C5'-O5'-PA
5	A	8003	ATP	C4'-C5'-O5'-PA
5	B	8003	ATP	C4'-C5'-O5'-PA
5	C	8003	ATP	C4'-C5'-O5'-PA
7	D	8005	PCW	C12-C13-C14-C15
7	A	8005	PCW	C12-C13-C14-C15
7	B	8005	PCW	C12-C13-C14-C15
7	C	8005	PCW	C12-C13-C14-C15
7	D	8006	PCW	C31-C32-C33-C34
7	A	8006	PCW	C31-C32-C33-C34
7	B	8006	PCW	C31-C32-C33-C34
7	C	8006	PCW	C31-C32-C33-C34
7	D	8006	PCW	O3P-C1-C2-O2
7	A	8006	PCW	O3P-C1-C2-O2
7	B	8006	PCW	O3P-C1-C2-O2
7	C	8006	PCW	O3P-C1-C2-O2
8	D	8008	A1BYZ	C16-C15-C20-C21
8	A	8008	A1BYZ	C16-C15-C20-C21

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Mol	Chain	Res	Type	Atoms
8	B	8008	A1BYZ	C16-C15-C20-C21
8	C	8008	A1BYZ	C16-C15-C20-C21
7	B	8006	PCW	C44-C45-C46-C47
7	D	8006	PCW	C44-C45-C46-C47
7	A	8006	PCW	C44-C45-C46-C47
7	C	8006	PCW	C44-C45-C46-C47
7	D	8006	PCW	C40-C41-C42-C43
7	A	8006	PCW	C40-C41-C42-C43
7	B	8006	PCW	C40-C41-C42-C43
7	C	8006	PCW	C40-C41-C42-C43
7	D	8006	PCW	O3P-C1-C2-C3
7	A	8006	PCW	O3P-C1-C2-C3
7	B	8006	PCW	O3P-C1-C2-C3
7	C	8006	PCW	O3P-C1-C2-C3
5	D	8003	ATP	PB-O3B-PG-O3G
5	A	8003	ATP	PB-O3B-PG-O3G
5	B	8003	ATP	PB-O3B-PG-O3G
5	C	8003	ATP	PB-O3B-PG-O3G
7	D	8006	PCW	C41-C42-C43-C44
7	A	8006	PCW	C41-C42-C43-C44
7	B	8006	PCW	C41-C42-C43-C44
7	C	8006	PCW	C41-C42-C43-C44
7	C	8005	PCW	C45-C46-C47-C48
7	D	8005	PCW	C45-C46-C47-C48
7	A	8005	PCW	C45-C46-C47-C48
7	B	8005	PCW	C45-C46-C47-C48
7	D	8006	PCW	O4P-C4-C5-N
7	A	8006	PCW	O4P-C4-C5-N
7	B	8006	PCW	O4P-C4-C5-N
7	C	8006	PCW	O4P-C4-C5-N
5	D	8007	ATP	C5'-O5'-PA-O1A
5	D	8007	ATP	C5'-O5'-PA-O3A
5	A	8007	ATP	C5'-O5'-PA-O1A
5	A	8007	ATP	C5'-O5'-PA-O3A
5	B	8007	ATP	C5'-O5'-PA-O1A
5	B	8007	ATP	C5'-O5'-PA-O3A
5	C	8007	ATP	C5'-O5'-PA-O1A
5	C	8007	ATP	C5'-O5'-PA-O3A
7	D	8005	PCW	C1-O3P-P-O1P
7	D	8005	PCW	C4-O4P-P-O1P
7	D	8005	PCW	C4-O4P-P-O3P
7	D	8006	PCW	C4-O4P-P-O2P

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Mol	Chain	Res	Type	Atoms
7	A	8005	PCW	C1-O3P-P-O1P
7	A	8005	PCW	C4-O4P-P-O1P
7	A	8005	PCW	C4-O4P-P-O3P
7	A	8006	PCW	C4-O4P-P-O2P
7	B	8005	PCW	C1-O3P-P-O1P
7	B	8005	PCW	C4-O4P-P-O1P
7	B	8005	PCW	C4-O4P-P-O3P
7	B	8006	PCW	C4-O4P-P-O2P
7	C	8005	PCW	C1-O3P-P-O1P
7	C	8005	PCW	C4-O4P-P-O1P
7	C	8005	PCW	C4-O4P-P-O3P
7	C	8006	PCW	C4-O4P-P-O2P
7	D	8005	PCW	C19-C20-C21-C22
7	A	8005	PCW	C19-C20-C21-C22
7	B	8005	PCW	C19-C20-C21-C22
7	C	8005	PCW	C19-C20-C21-C22
7	D	8006	PCW	C37-C38-C39-C40
7	A	8006	PCW	C37-C38-C39-C40
7	B	8006	PCW	C37-C38-C39-C40
7	C	8006	PCW	C37-C38-C39-C40
7	D	8006	PCW	C19-C20-C21-C22
7	A	8006	PCW	C19-C20-C21-C22
7	B	8006	PCW	C19-C20-C21-C22
7	C	8006	PCW	C19-C20-C21-C22
7	D	8006	PCW	C36-C37-C38-C39
7	B	8006	PCW	C36-C37-C38-C39
7	C	8006	PCW	C36-C37-C38-C39
8	D	8009	A1BYZ	C2-C3-C6-O7
8	A	8009	A1BYZ	C2-C3-C6-O7
8	B	8009	A1BYZ	C2-C3-C6-O7
8	C	8009	A1BYZ	C2-C3-C6-O7
5	D	8007	ATP	PB-O3A-PA-O1A
5	A	8007	ATP	PB-O3A-PA-O1A
5	B	8007	ATP	PB-O3A-PA-O1A
5	C	8007	ATP	PB-O3A-PA-O1A
7	A	8006	PCW	C36-C37-C38-C39
7	A	8006	PCW	C25-C26-C27-C28
5	D	8007	ATP	C4'-C5'-O5'-PA
5	A	8007	ATP	C4'-C5'-O5'-PA
5	B	8007	ATP	C4'-C5'-O5'-PA
5	C	8007	ATP	C4'-C5'-O5'-PA
7	D	8006	PCW	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
7	B	8006	PCW	C25-C26-C27-C28
7	C	8006	PCW	C25-C26-C27-C28
5	D	8003	ATP	O4'-C1'-N9-C8
5	A	8003	ATP	O4'-C1'-N9-C8
5	B	8003	ATP	O4'-C1'-N9-C8
5	C	8003	ATP	O4'-C1'-N9-C8
7	D	8005	PCW	C39-C40-C41-C42
7	D	8006	PCW	C17-C18-C19-C20
7	A	8005	PCW	C39-C40-C41-C42
7	A	8006	PCW	C17-C18-C19-C20
7	B	8005	PCW	C39-C40-C41-C42
7	B	8006	PCW	C17-C18-C19-C20
7	C	8005	PCW	C39-C40-C41-C42
7	C	8006	PCW	C17-C18-C19-C20
5	D	8007	ATP	PB-O3B-PG-O1G
5	A	8007	ATP	PB-O3B-PG-O1G
5	B	8007	ATP	PB-O3B-PG-O1G
5	C	8007	ATP	PB-O3B-PG-O1G
5	D	8003	ATP	O4'-C1'-N9-C4
5	A	8003	ATP	O4'-C1'-N9-C4
5	B	8003	ATP	O4'-C1'-N9-C4
5	C	8003	ATP	O4'-C1'-N9-C4
5	D	8003	ATP	PG-O3B-PB-O1B
5	D	8003	ATP	PG-O3B-PB-O2B
5	A	8003	ATP	PG-O3B-PB-O1B
5	A	8003	ATP	PG-O3B-PB-O2B
5	B	8003	ATP	PG-O3B-PB-O1B
5	B	8003	ATP	PG-O3B-PB-O2B
5	C	8003	ATP	PG-O3B-PB-O1B
5	C	8003	ATP	PG-O3B-PB-O2B
7	D	8006	PCW	O2-C31-C32-C33
7	A	8006	PCW	O2-C31-C32-C33
7	B	8006	PCW	O2-C31-C32-C33
7	C	8006	PCW	O2-C31-C32-C33
7	D	8006	PCW	C16-C17-C18-C19
7	A	8006	PCW	C16-C17-C18-C19
7	B	8006	PCW	C16-C17-C18-C19
7	C	8006	PCW	C16-C17-C18-C19
7	D	8006	PCW	O31-C31-C32-C33
7	B	8006	PCW	O31-C31-C32-C33
7	A	8006	PCW	O31-C31-C32-C33
7	C	8006	PCW	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
5	D	8007	ATP	PB-O3A-PA-O2A
5	A	8007	ATP	PB-O3A-PA-O2A
5	B	8007	ATP	PB-O3A-PA-O2A
5	C	8007	ATP	PB-O3A-PA-O2A

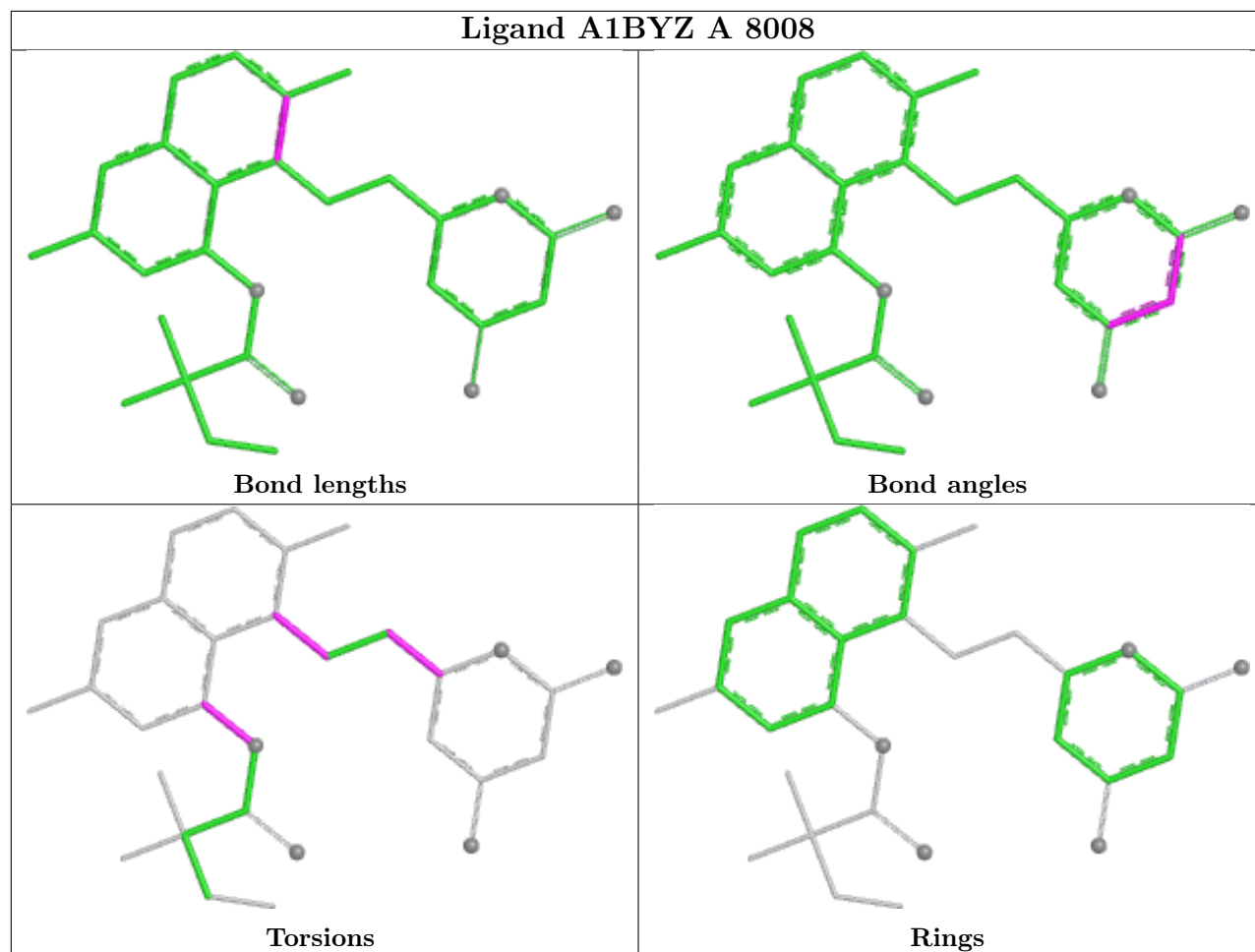
There are no ring outliers.

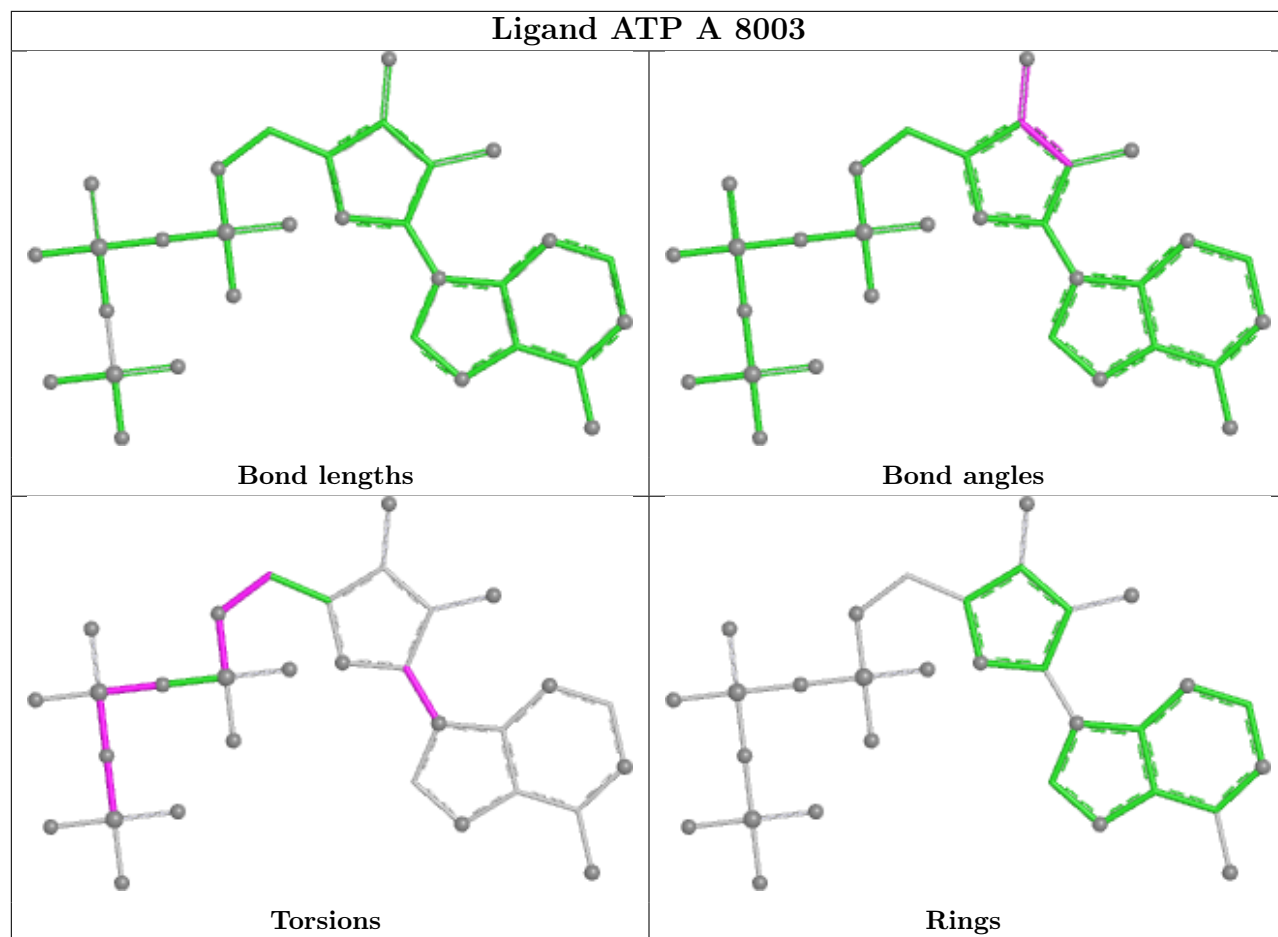
18 monomers are involved in 30 short contacts:

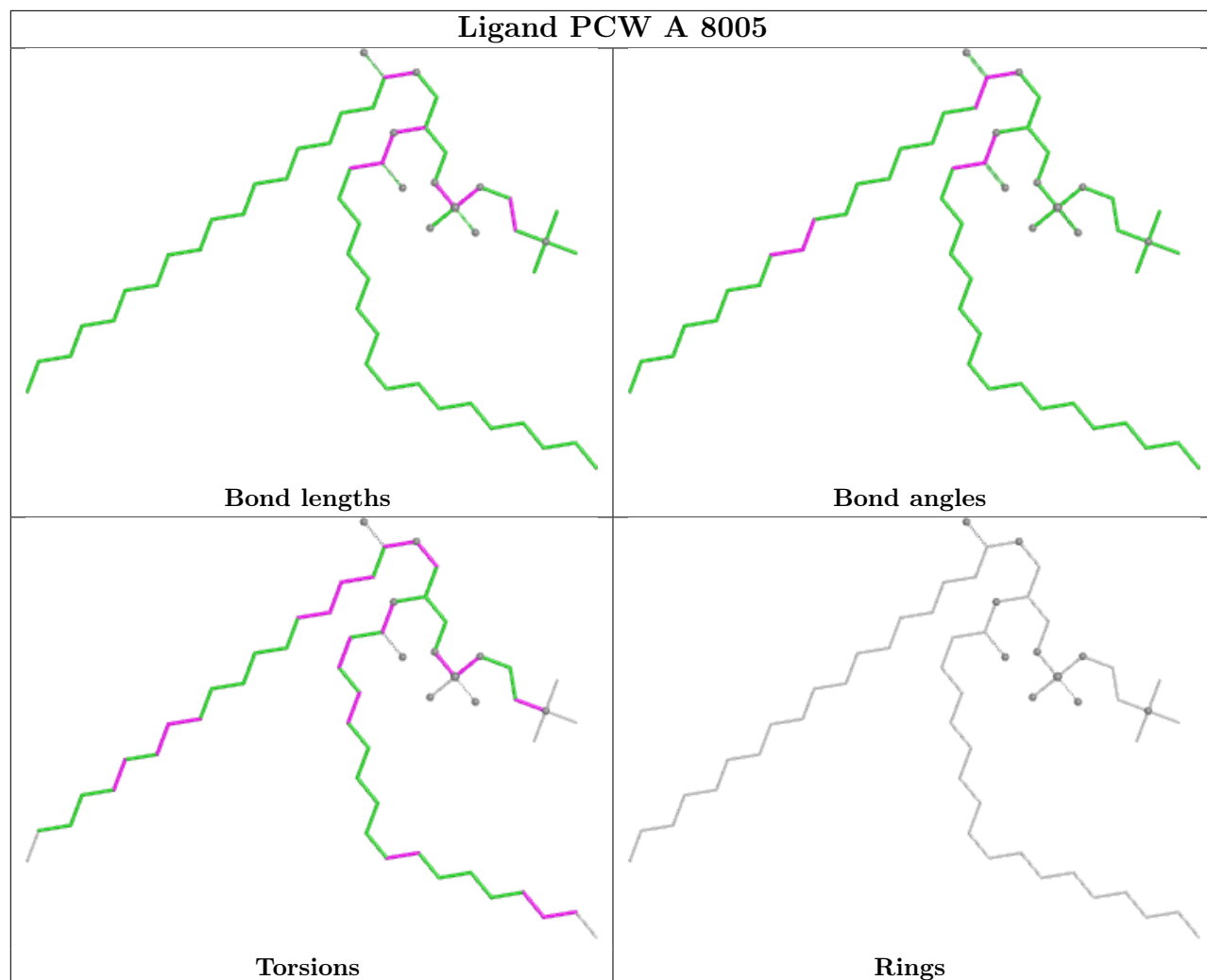
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	8003	ATP	1	0
7	A	8005	PCW	2	0
8	D	8009	A1BYZ	2	0
8	A	8009	A1BYZ	2	0
7	C	8005	PCW	2	0
5	C	8003	ATP	1	0
7	C	8006	PCW	3	0
7	B	8006	PCW	3	0
8	C	8008	A1BYZ	1	0
7	B	8005	PCW	2	0
7	D	8005	PCW	2	0
5	D	8003	ATP	1	0
7	A	8006	PCW	3	0
7	D	8006	PCW	3	0
5	B	8003	ATP	1	0
8	B	8009	A1BYZ	2	0
8	B	8008	A1BYZ	1	0
8	C	8009	A1BYZ	2	0

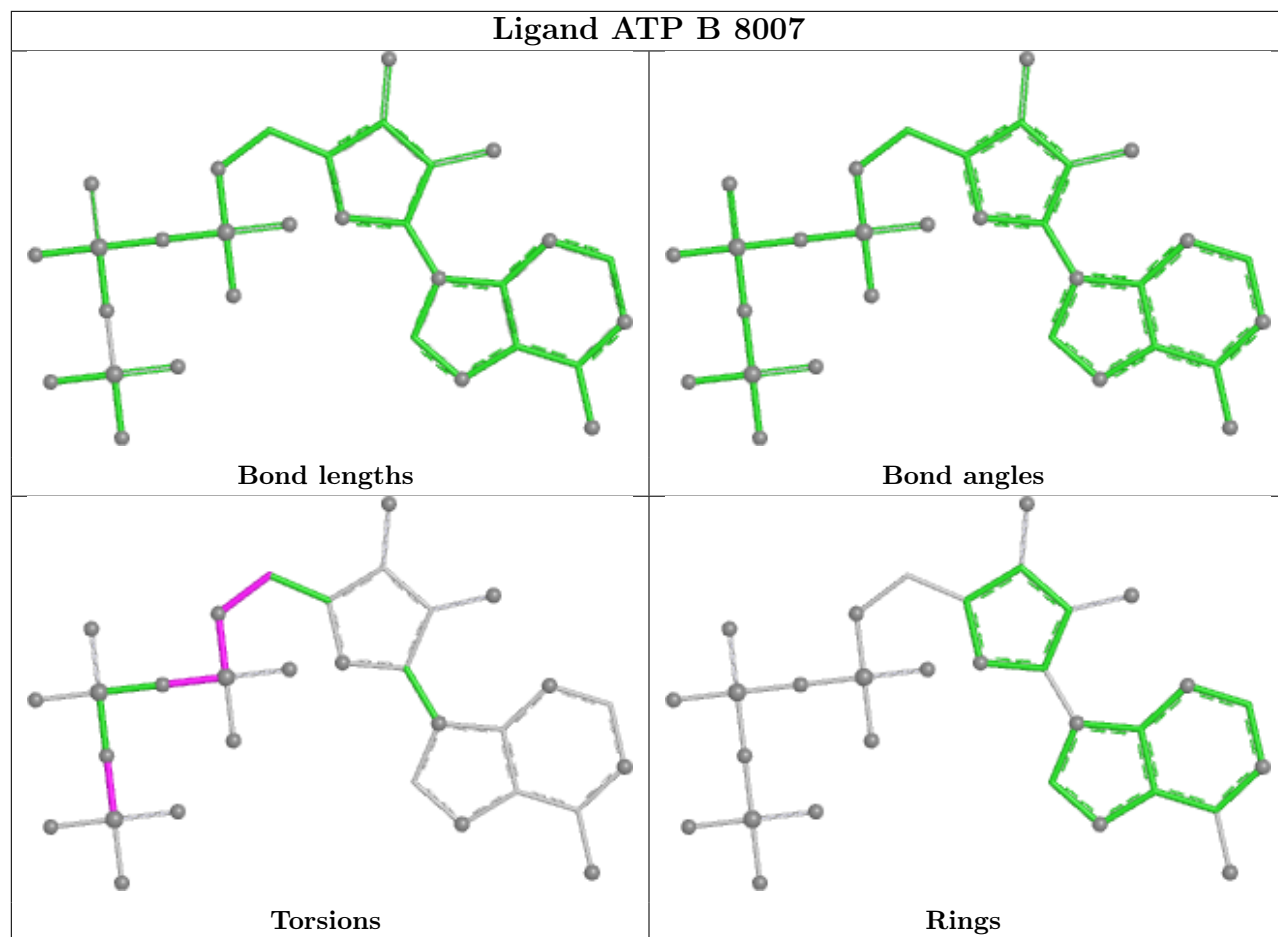
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

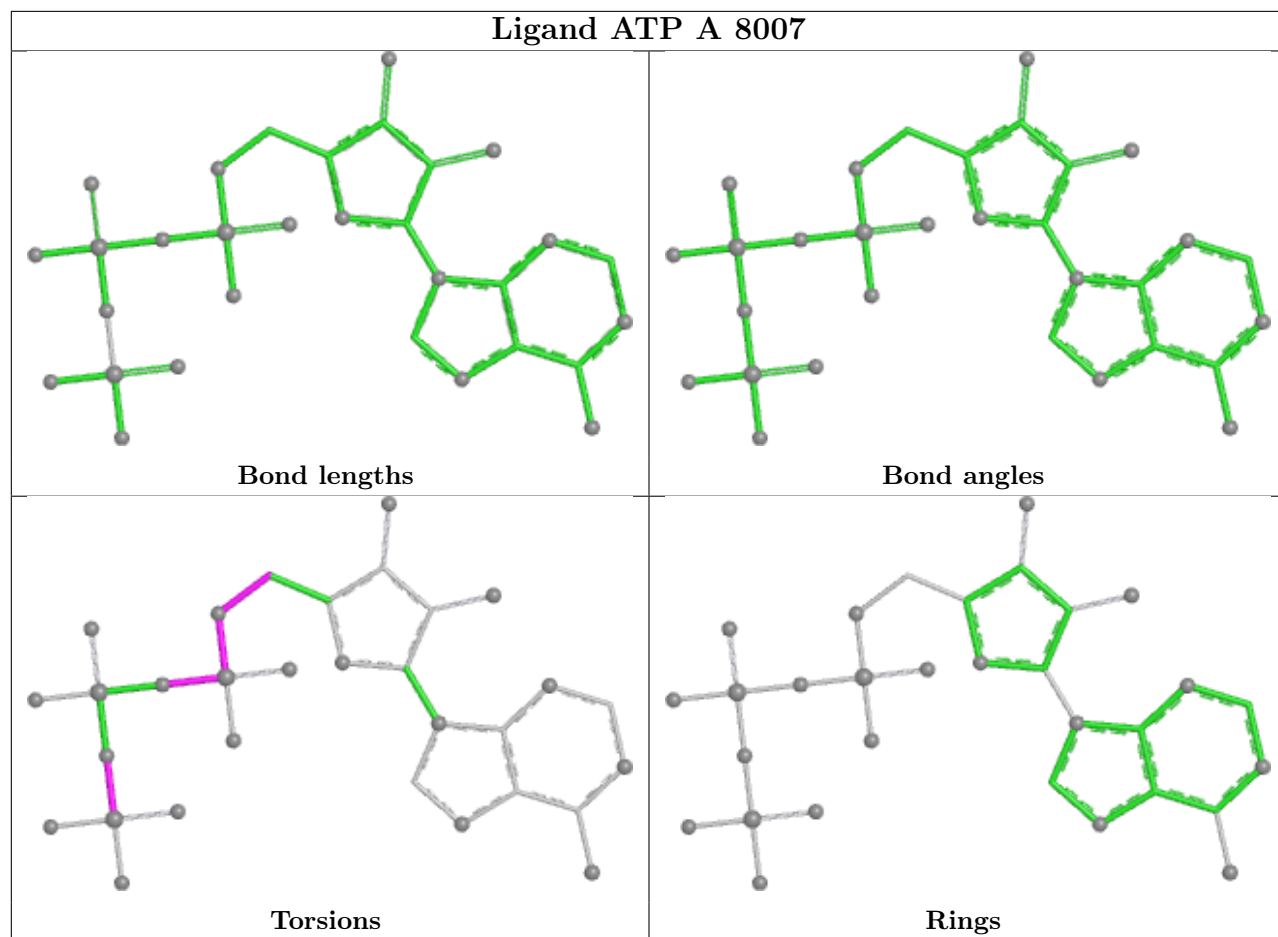
Ligand A1BYZ A 8008

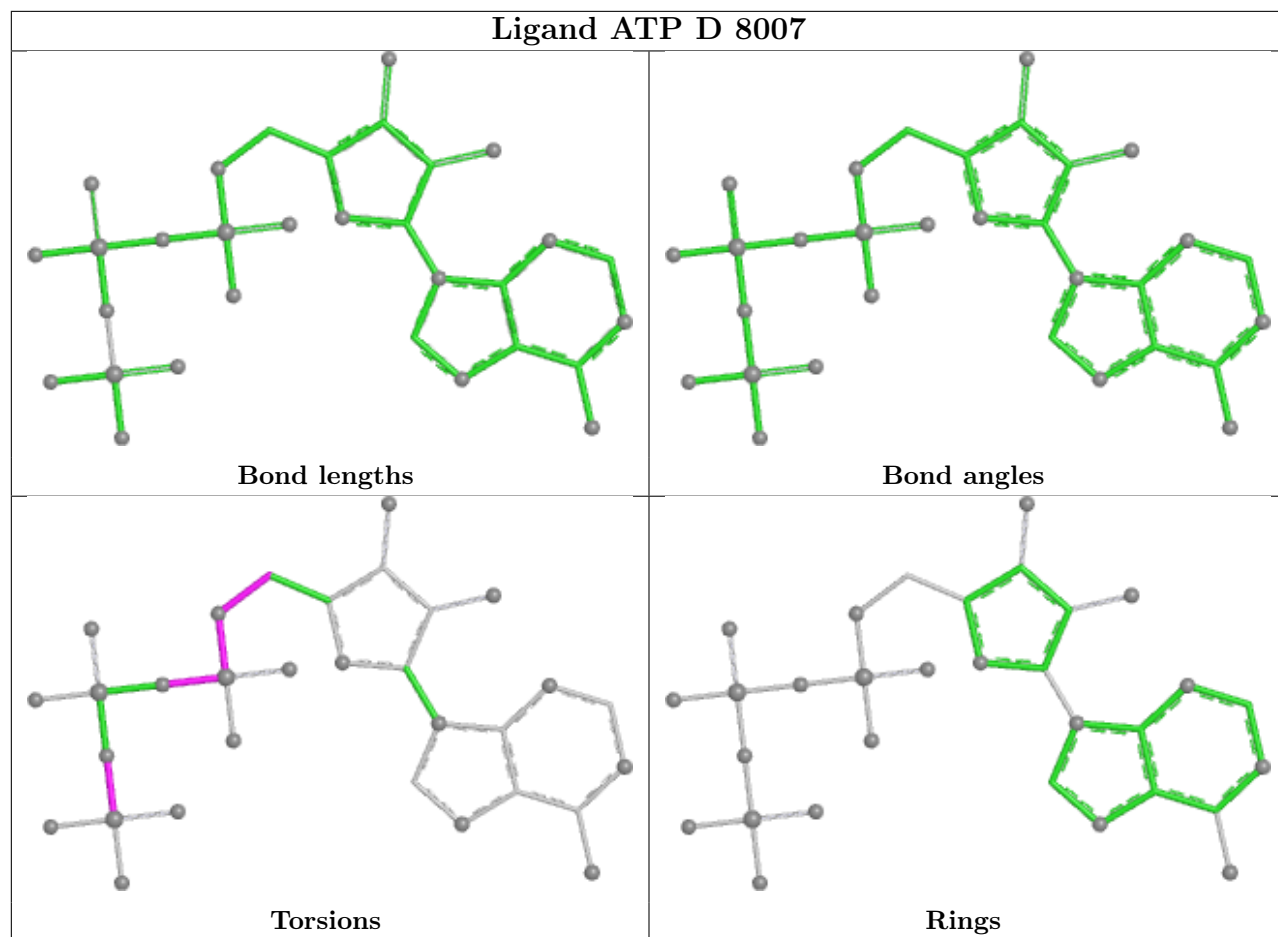




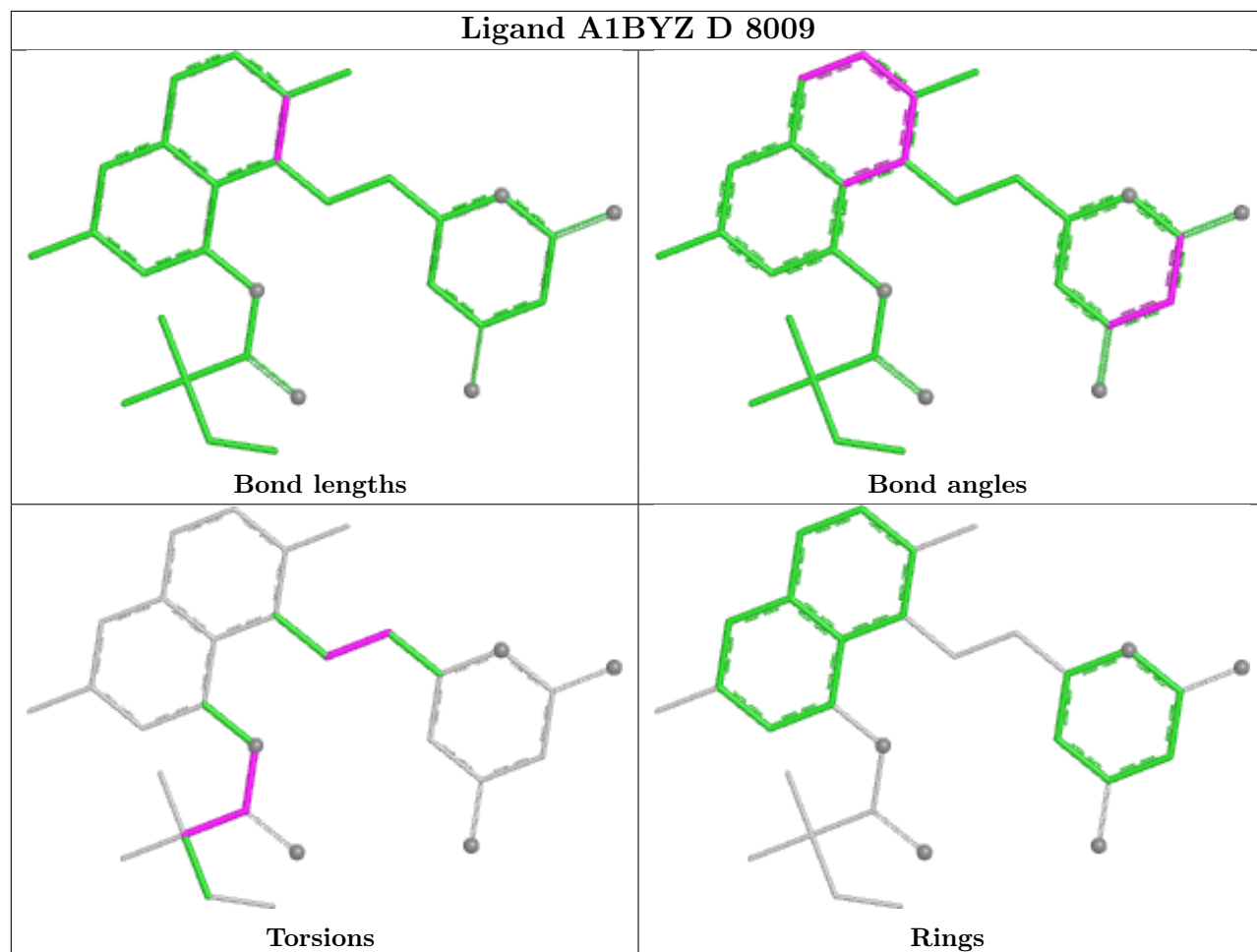




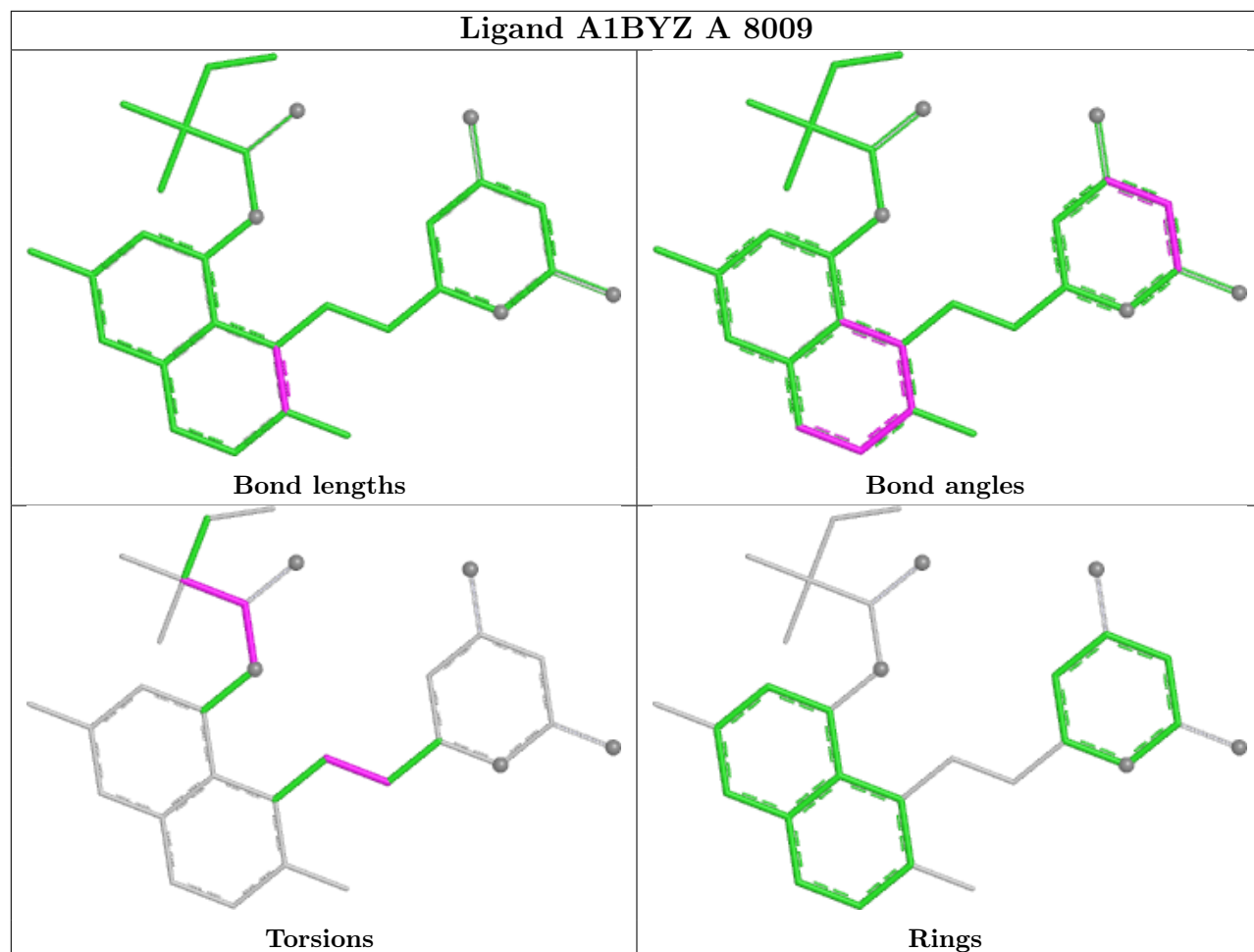


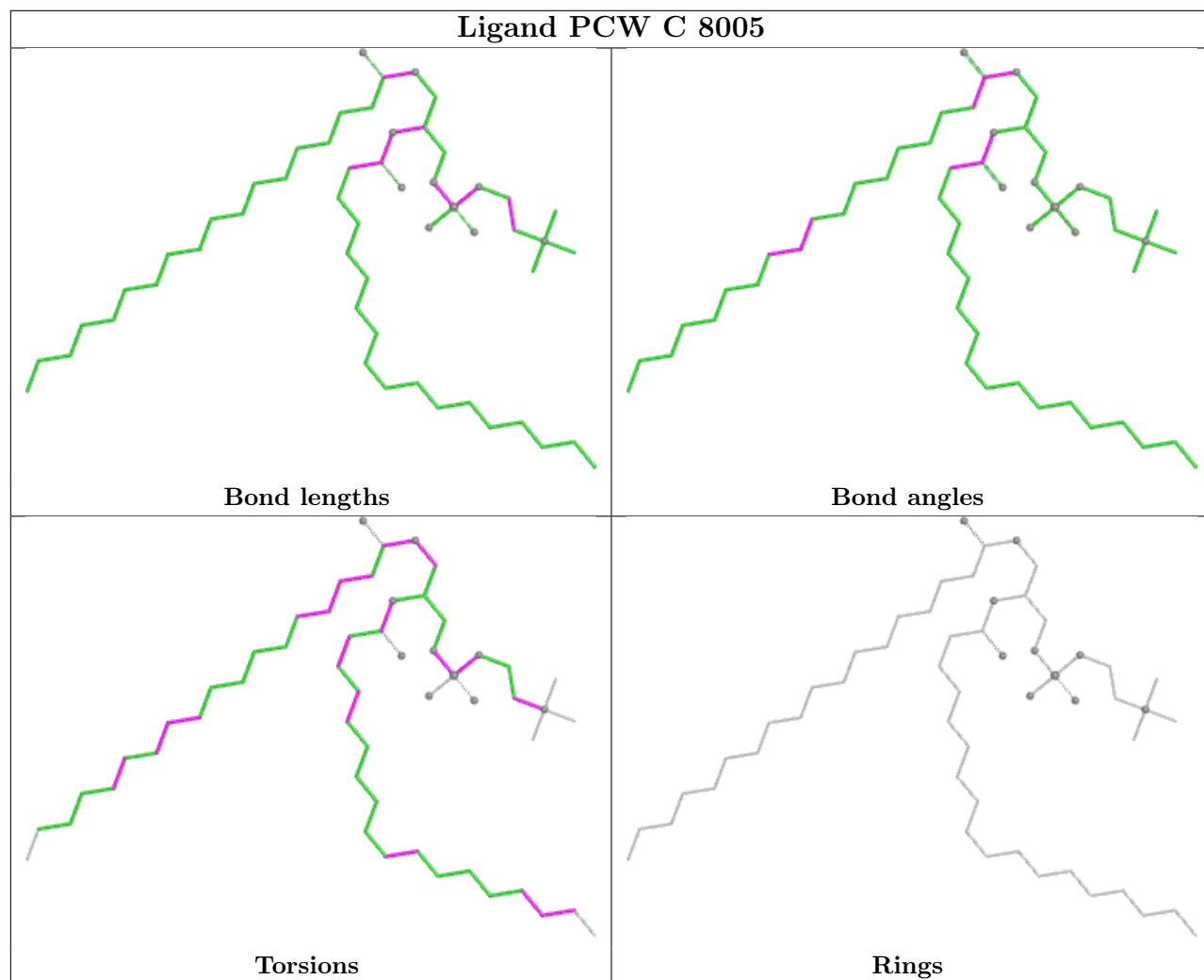


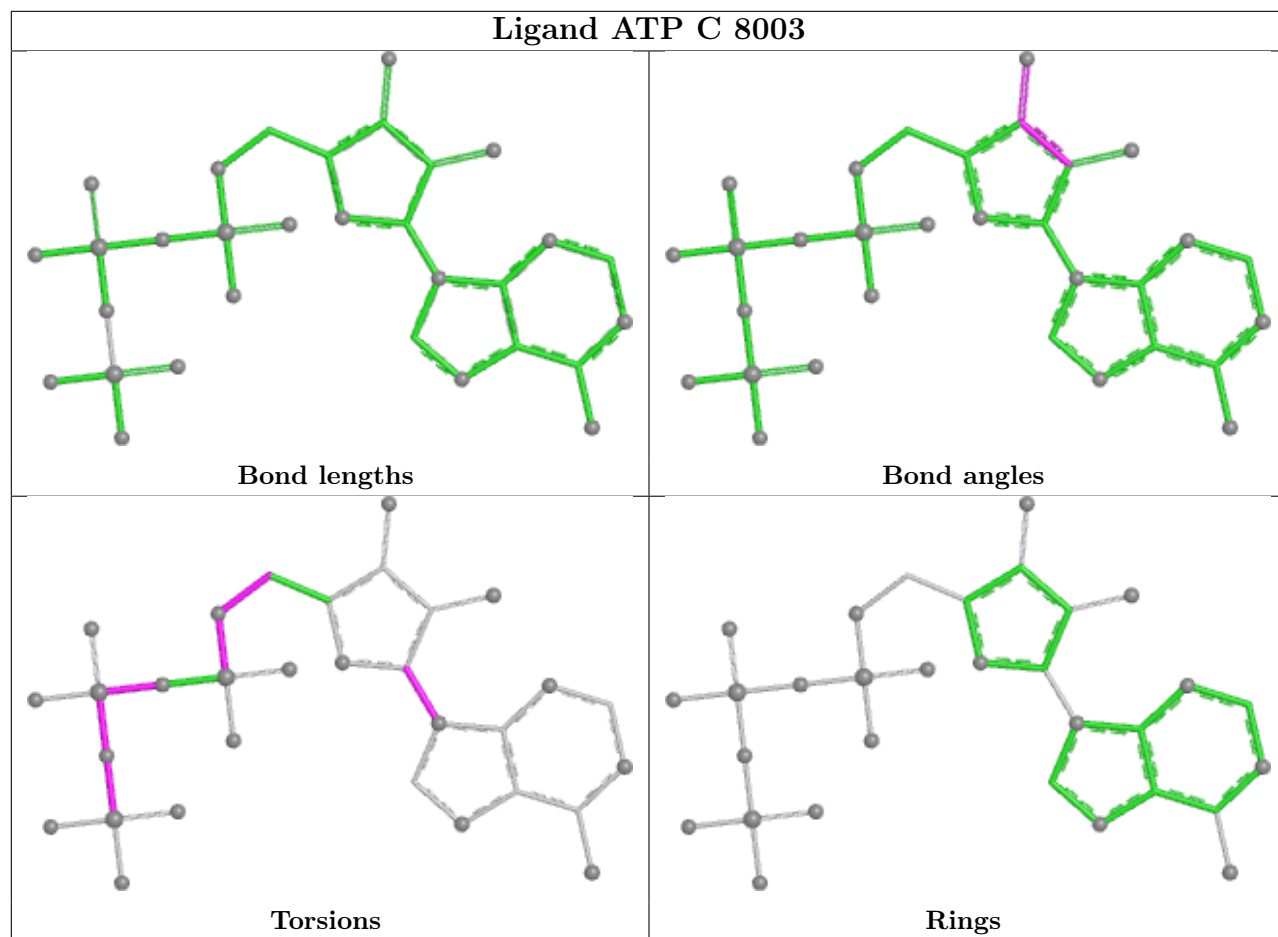
Ligand A1BYZ D 8009

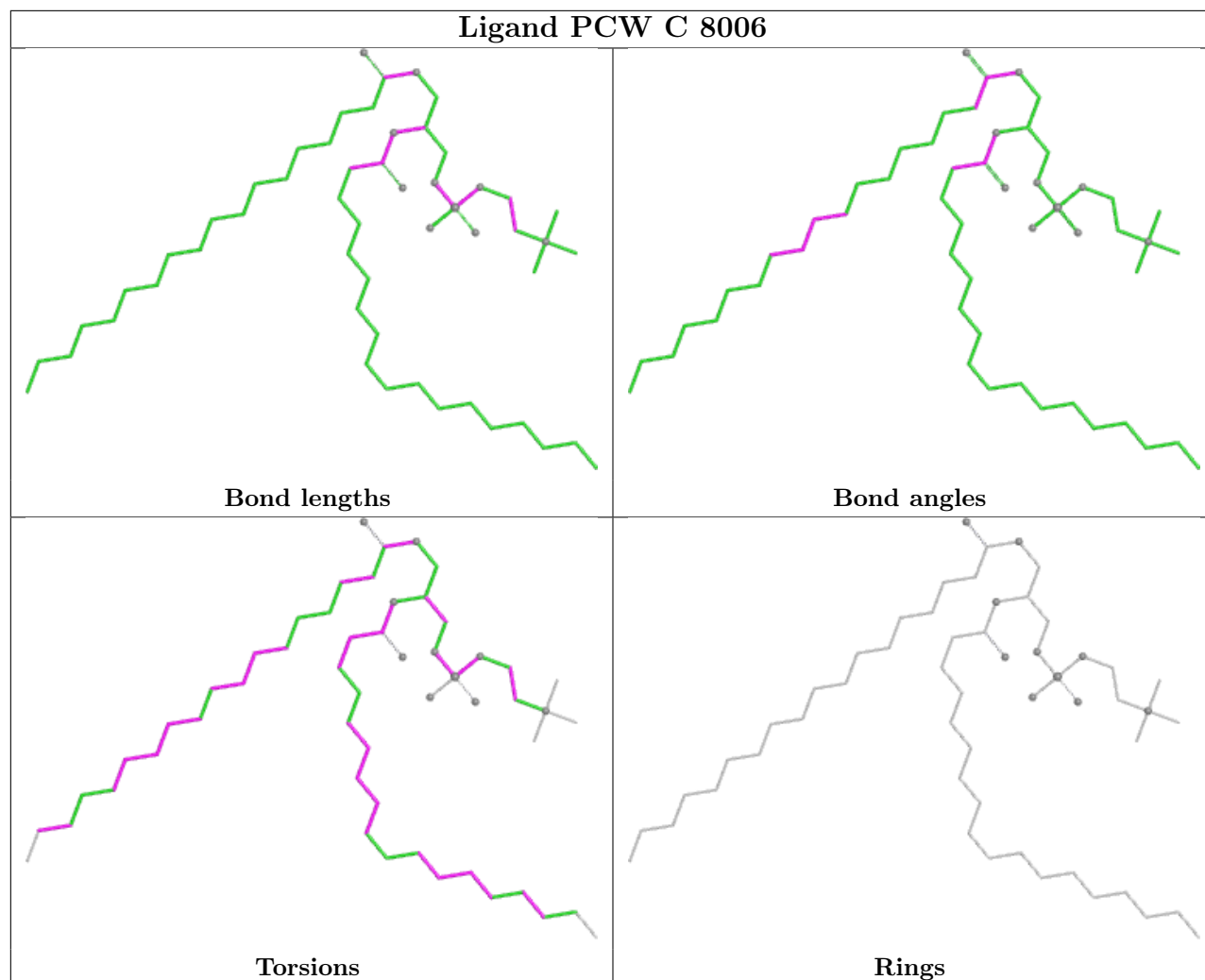


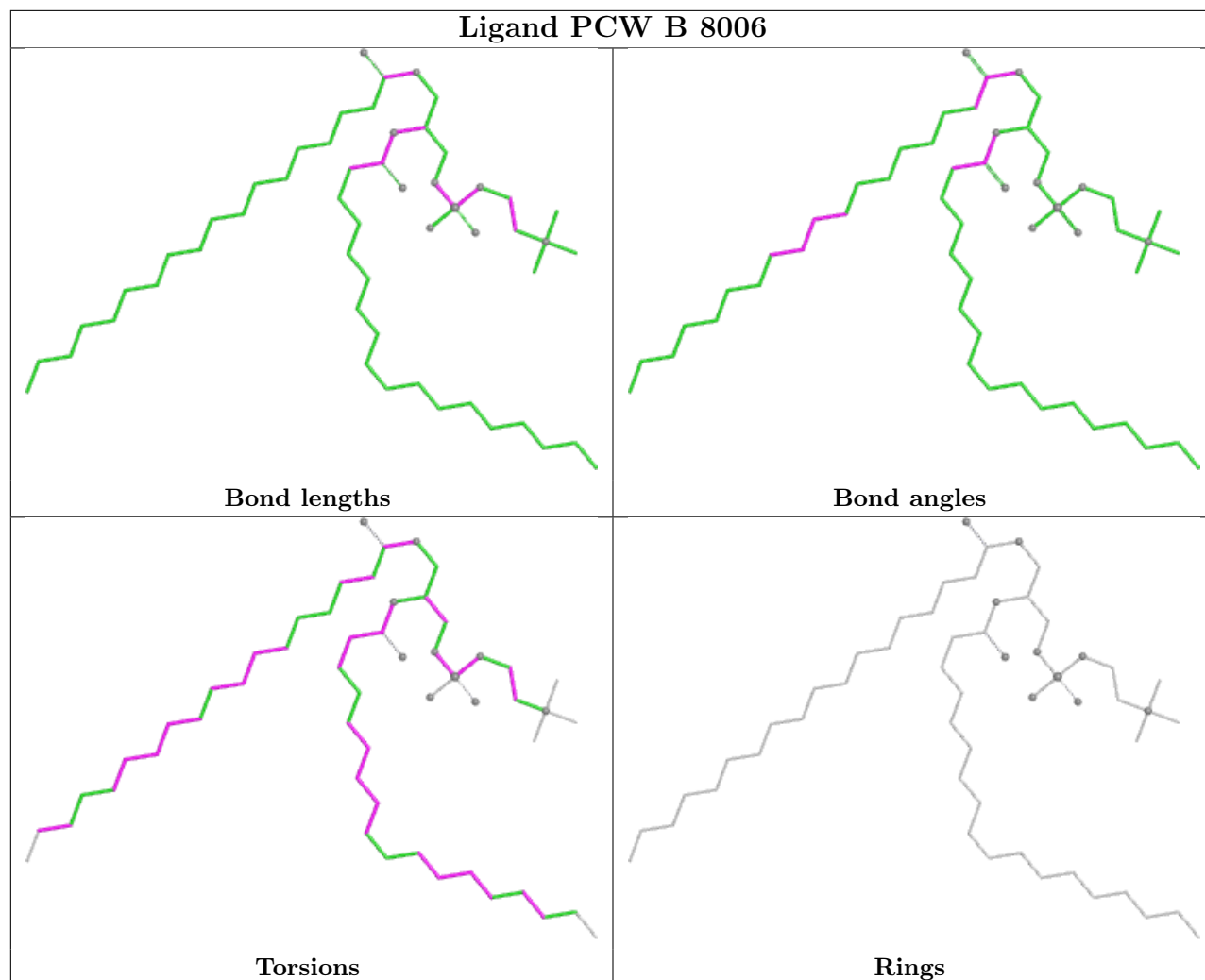
Ligand A1BYZ A 8009



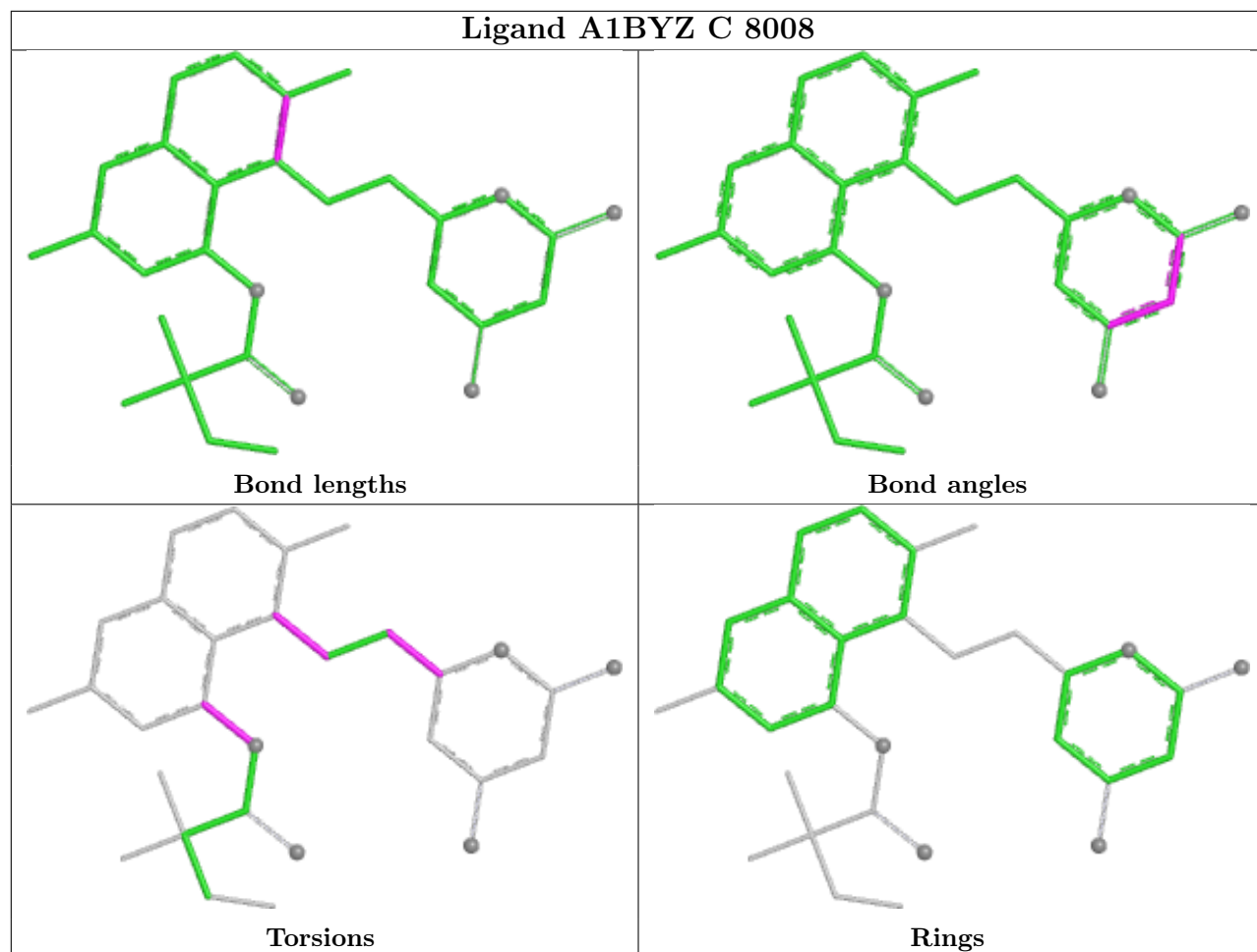


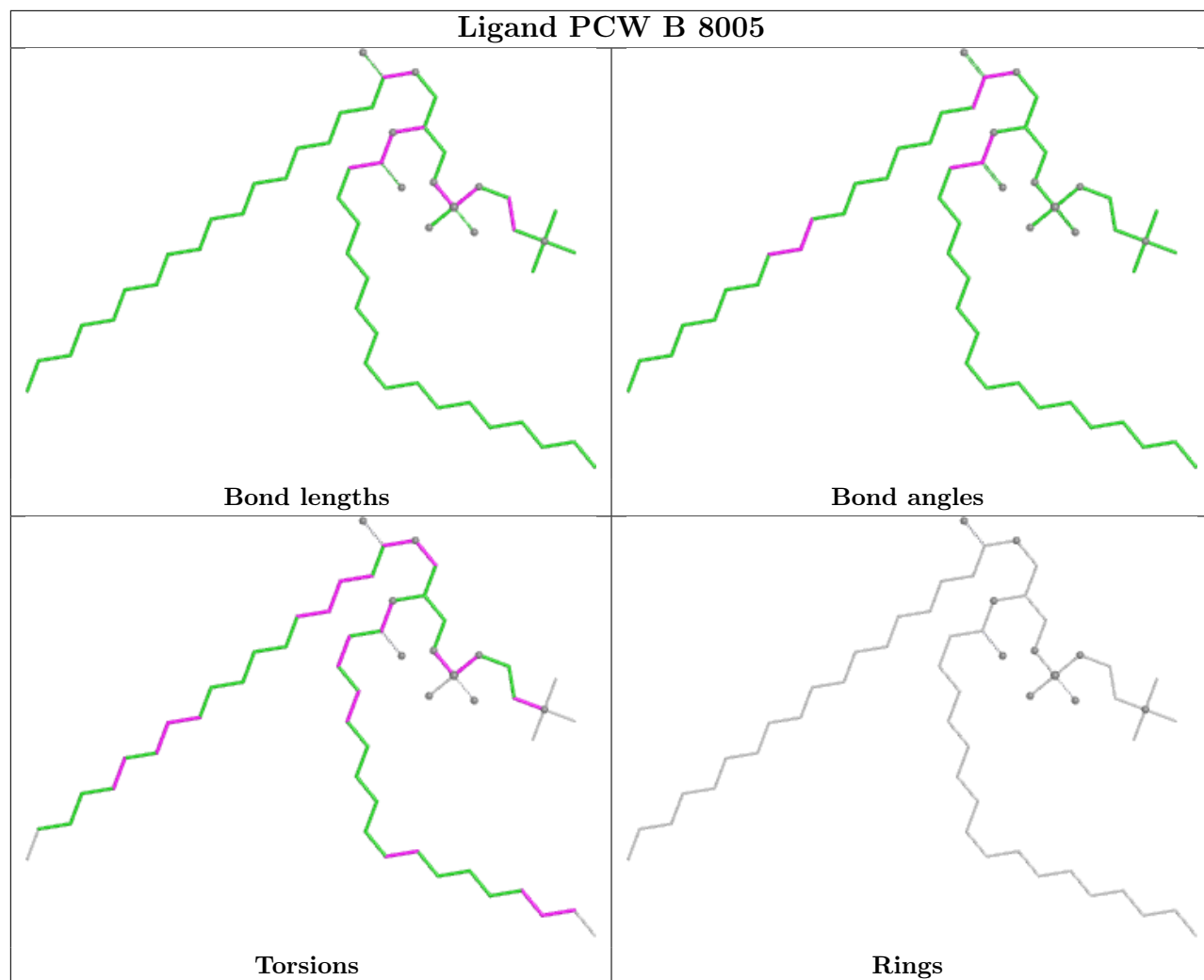


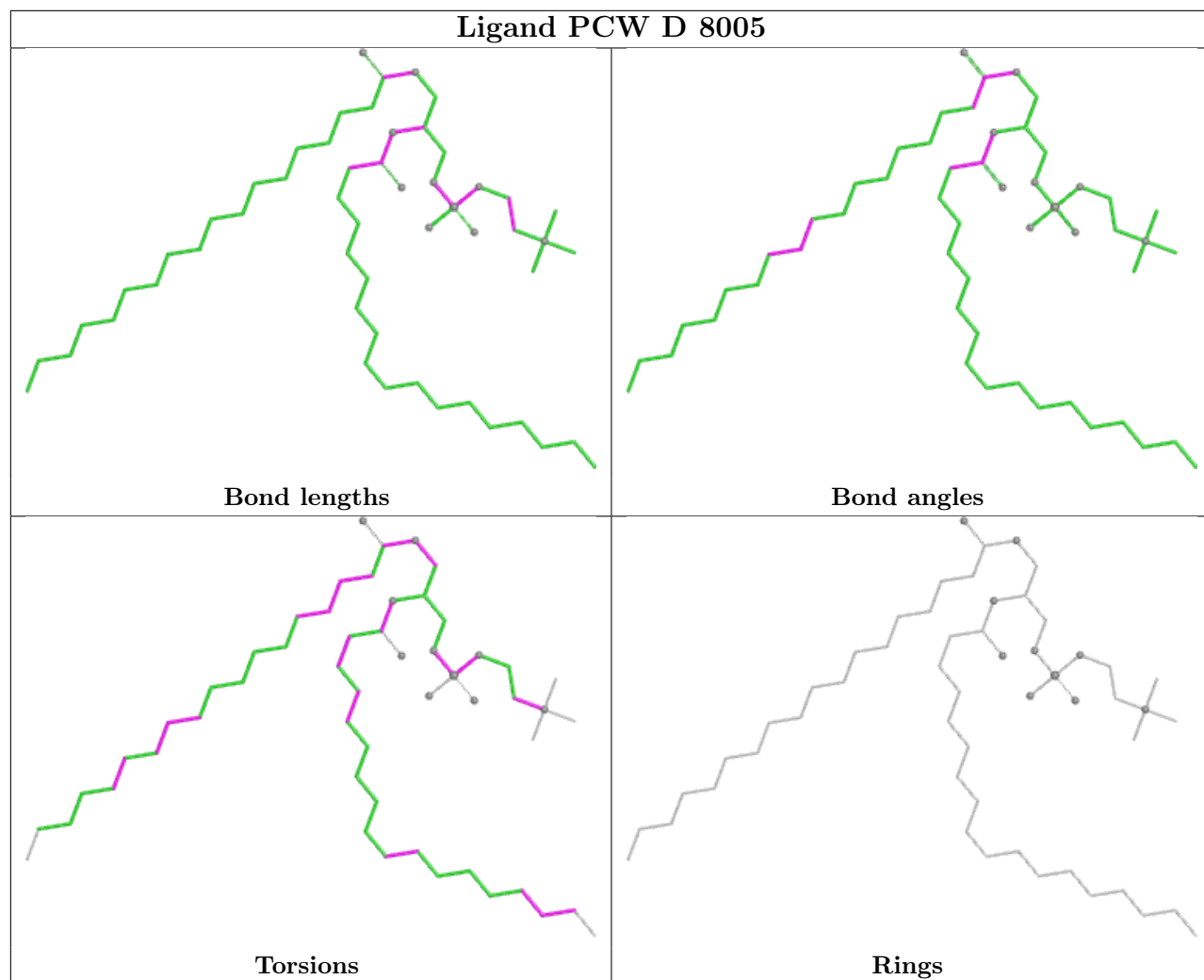


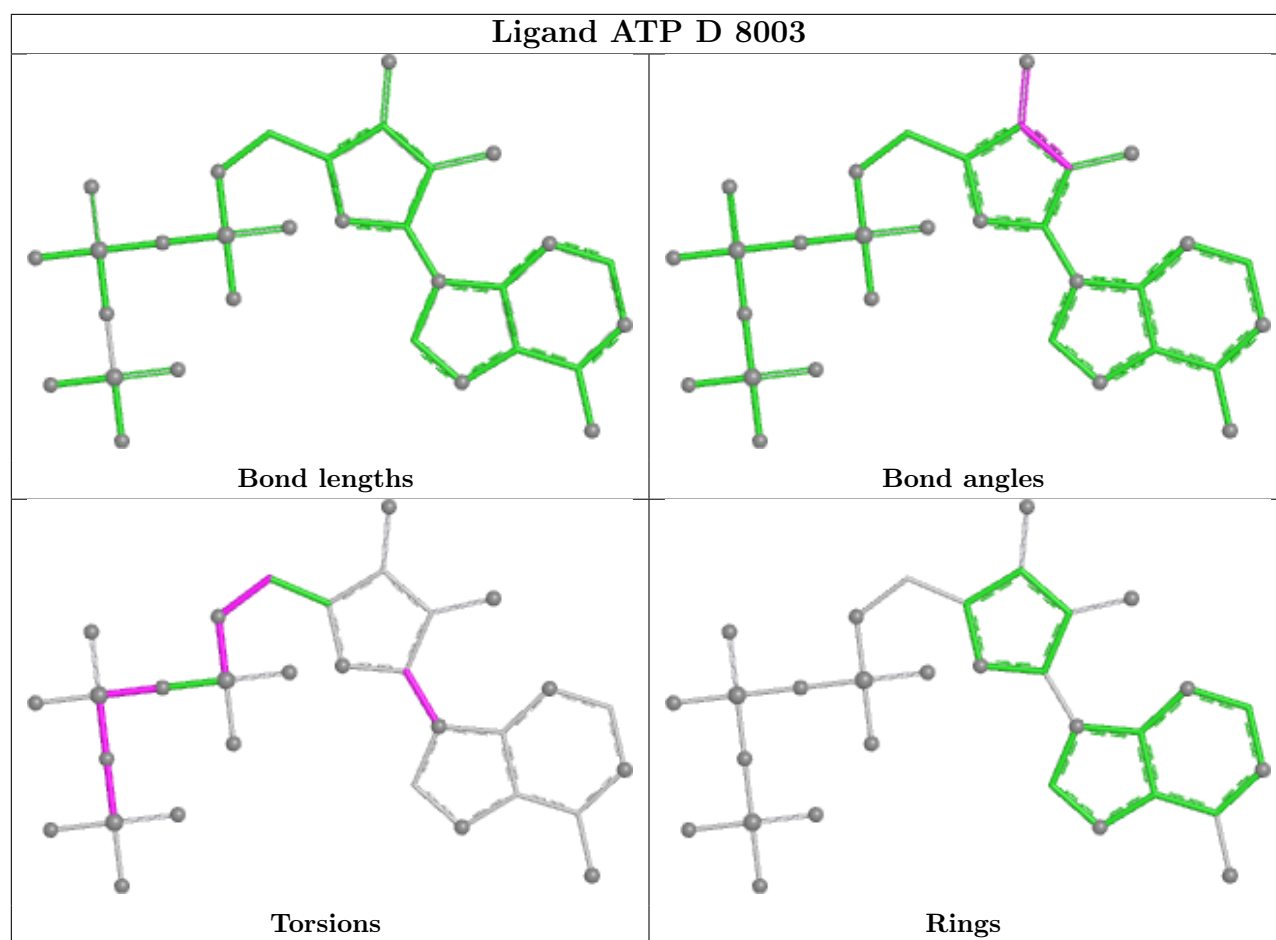


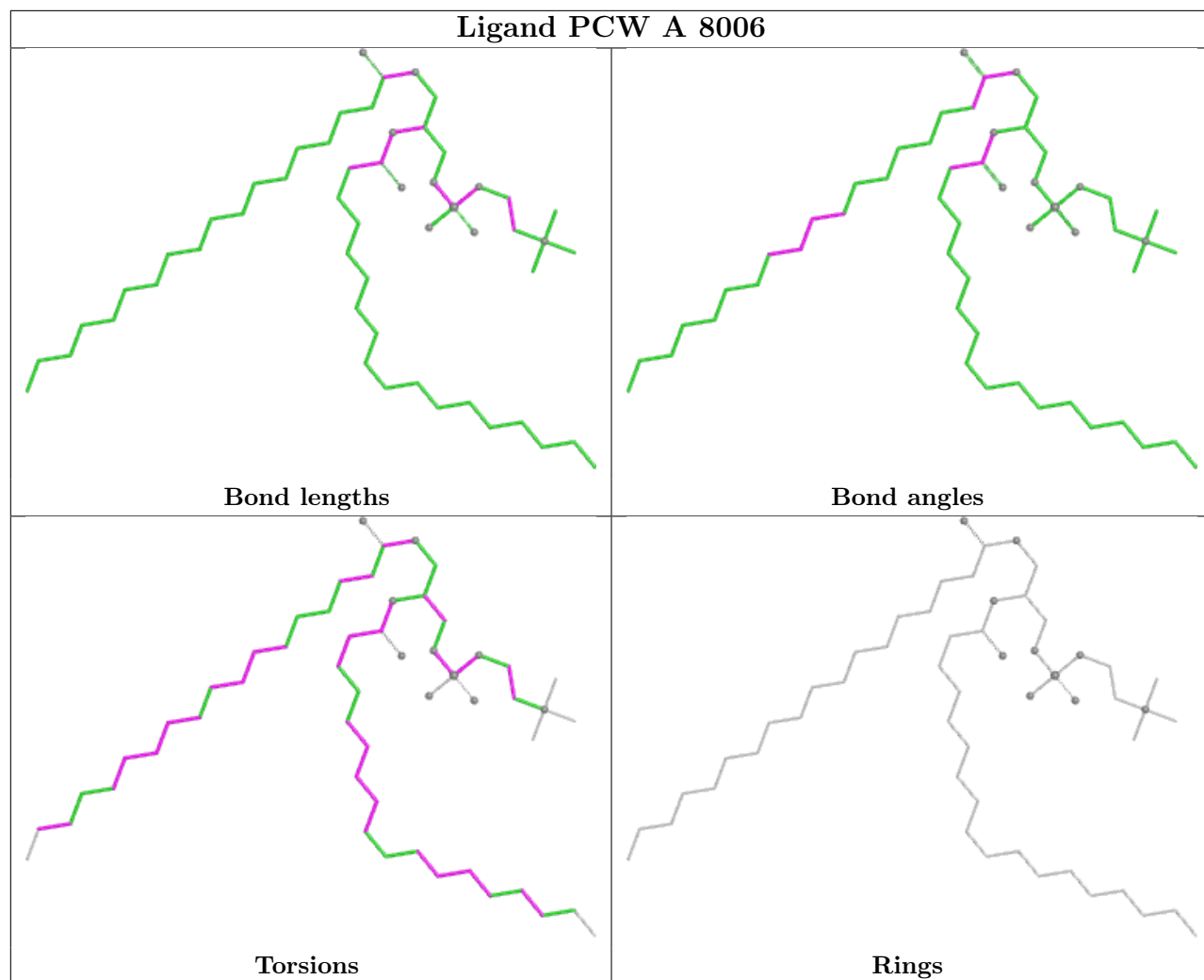
Ligand A1BYZ C 8008

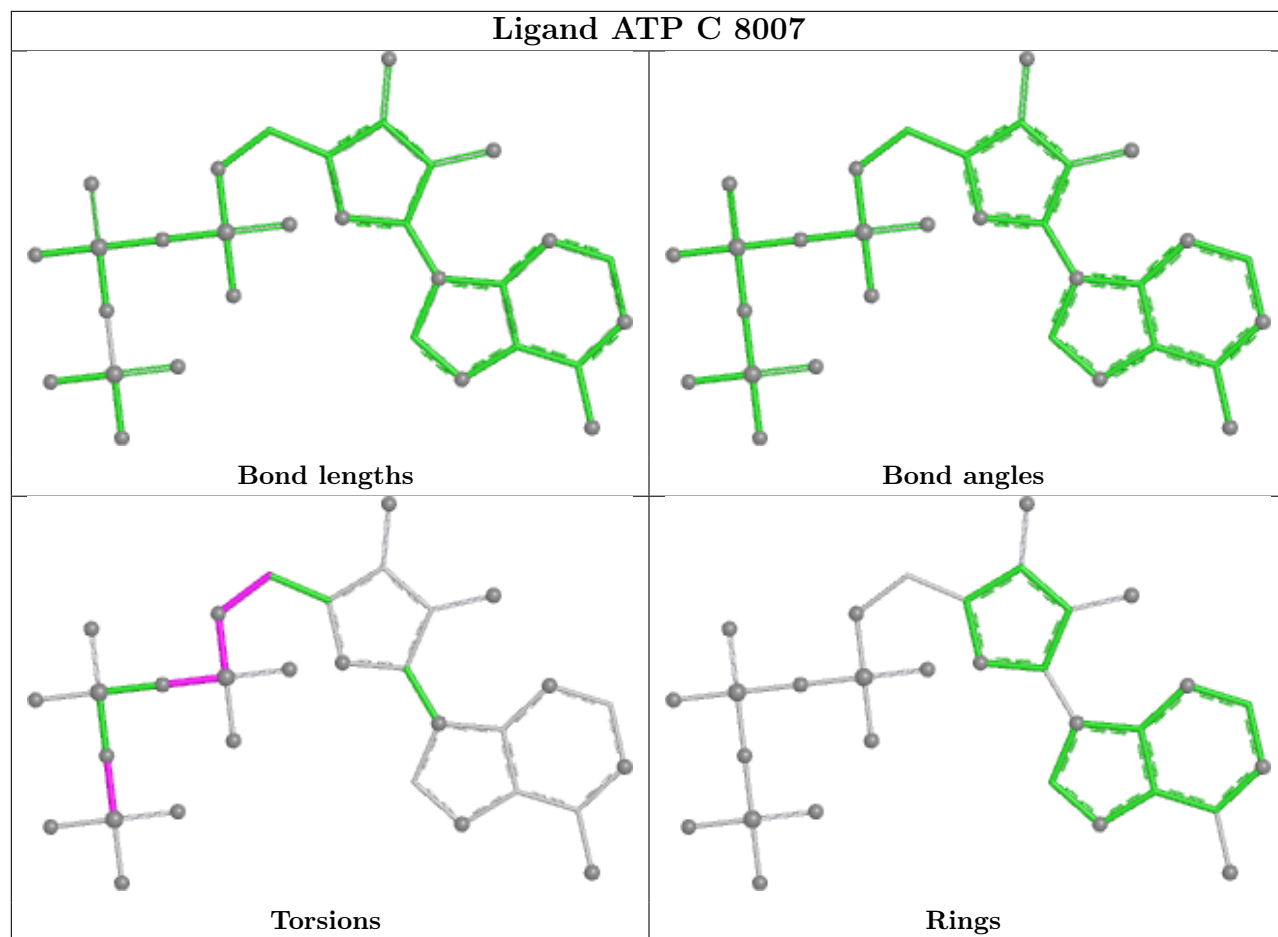


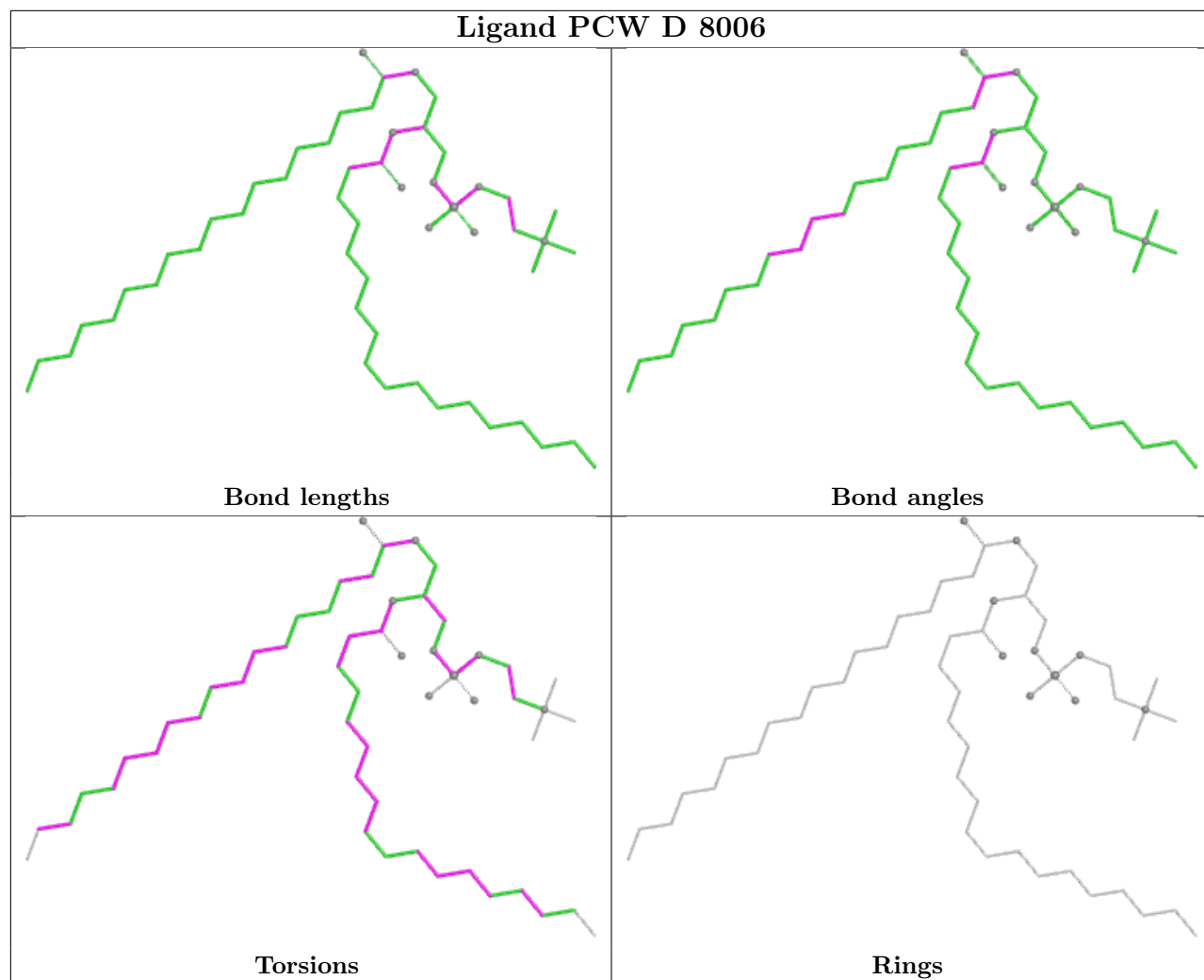


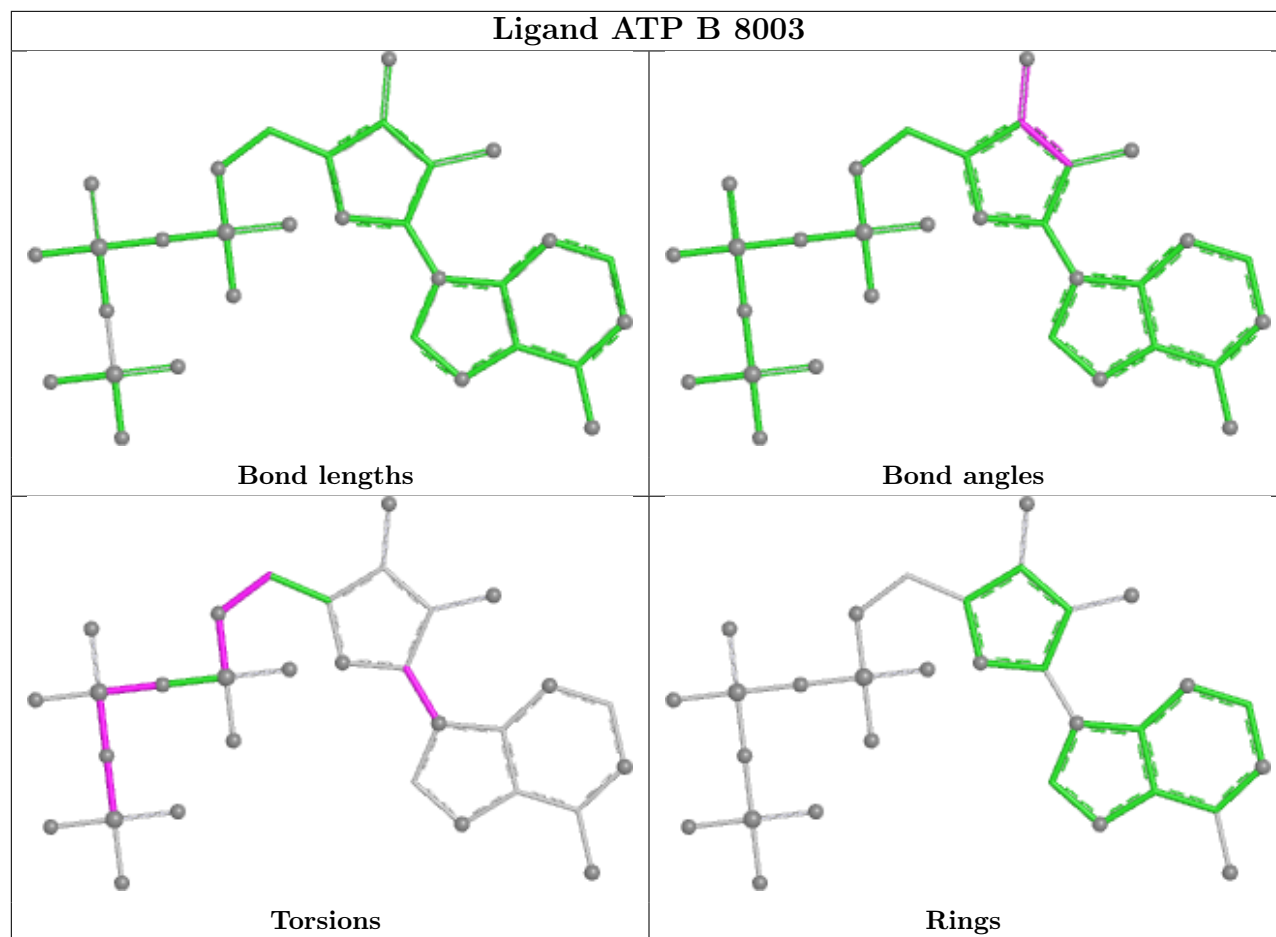




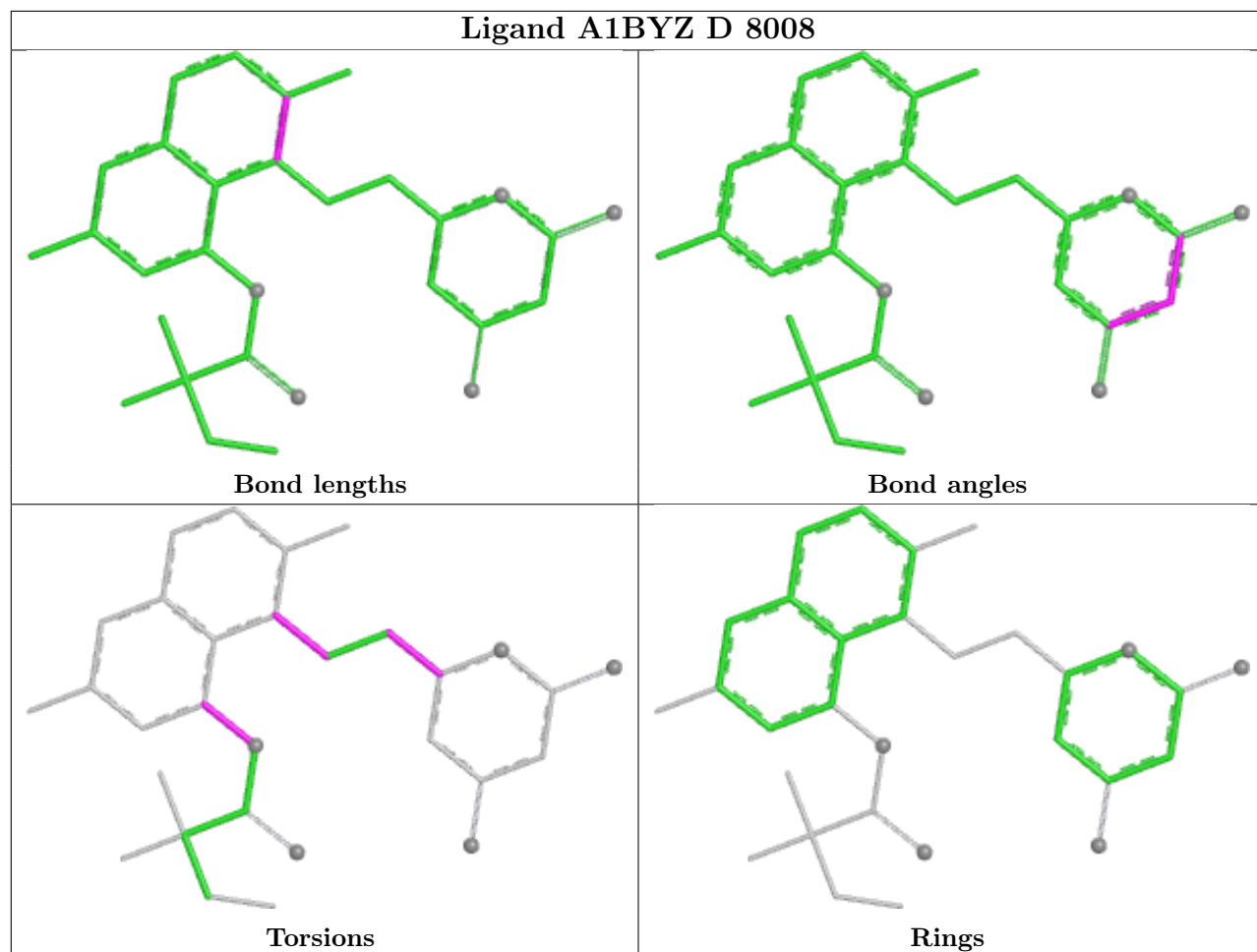




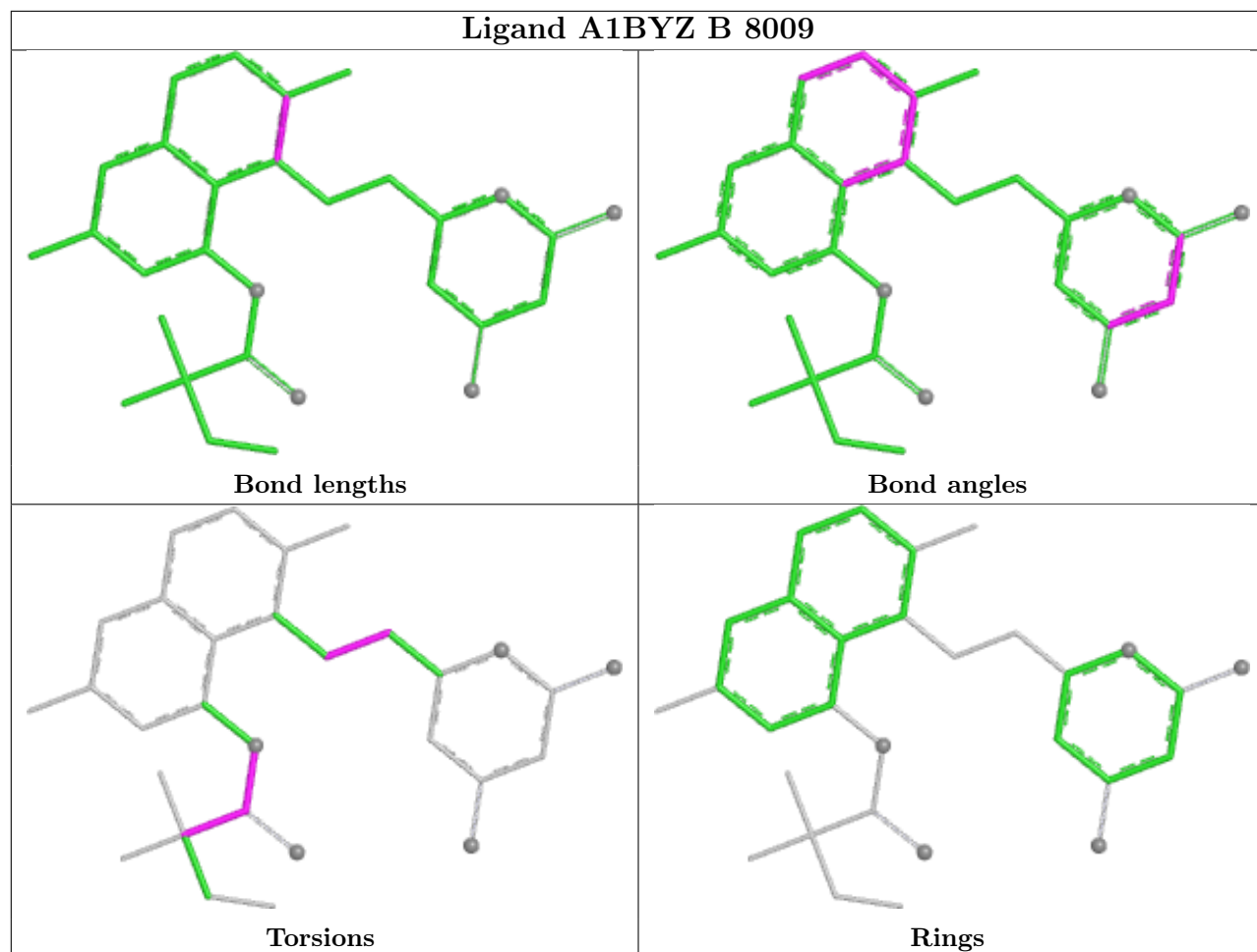




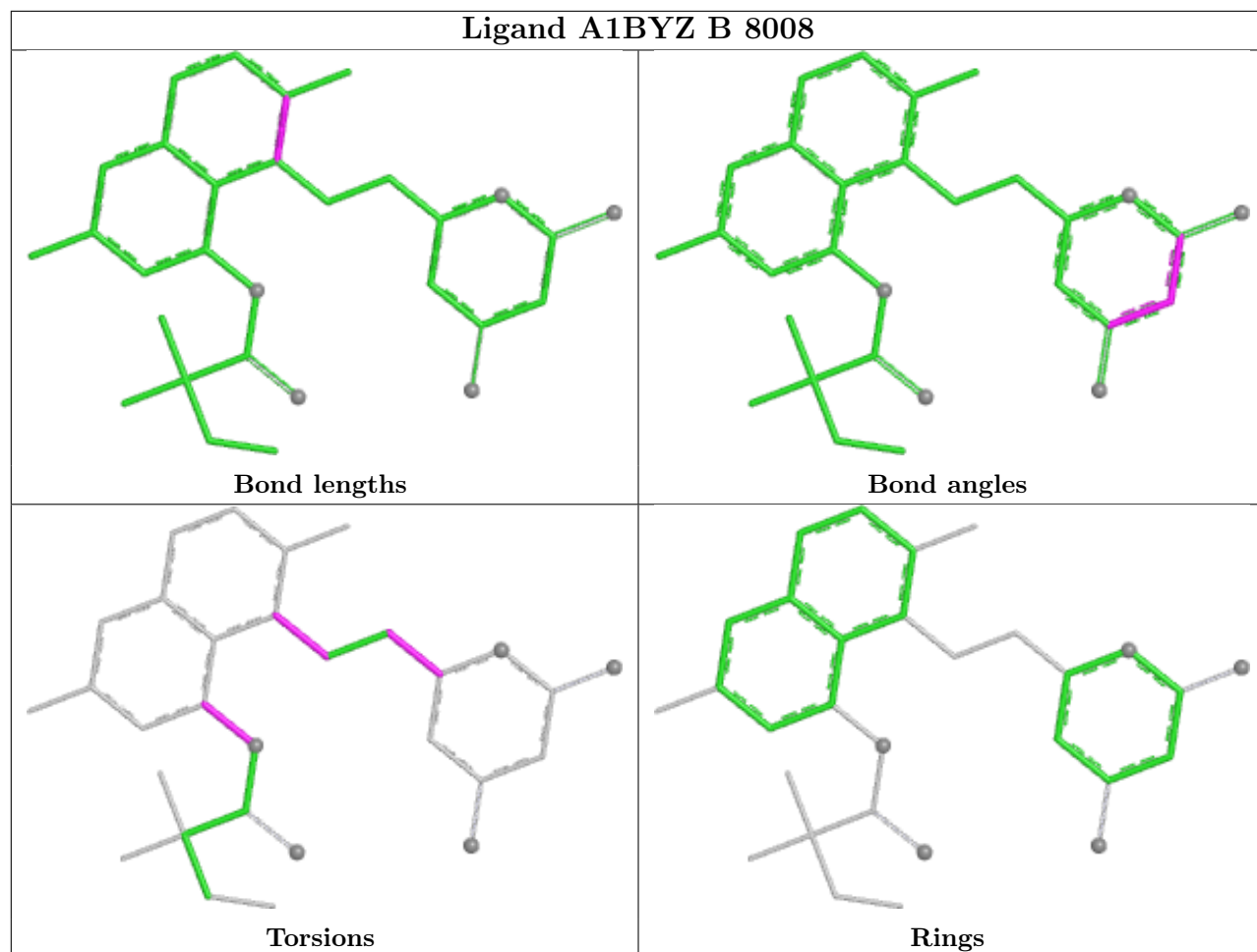
Ligand A1BYZ D 8008

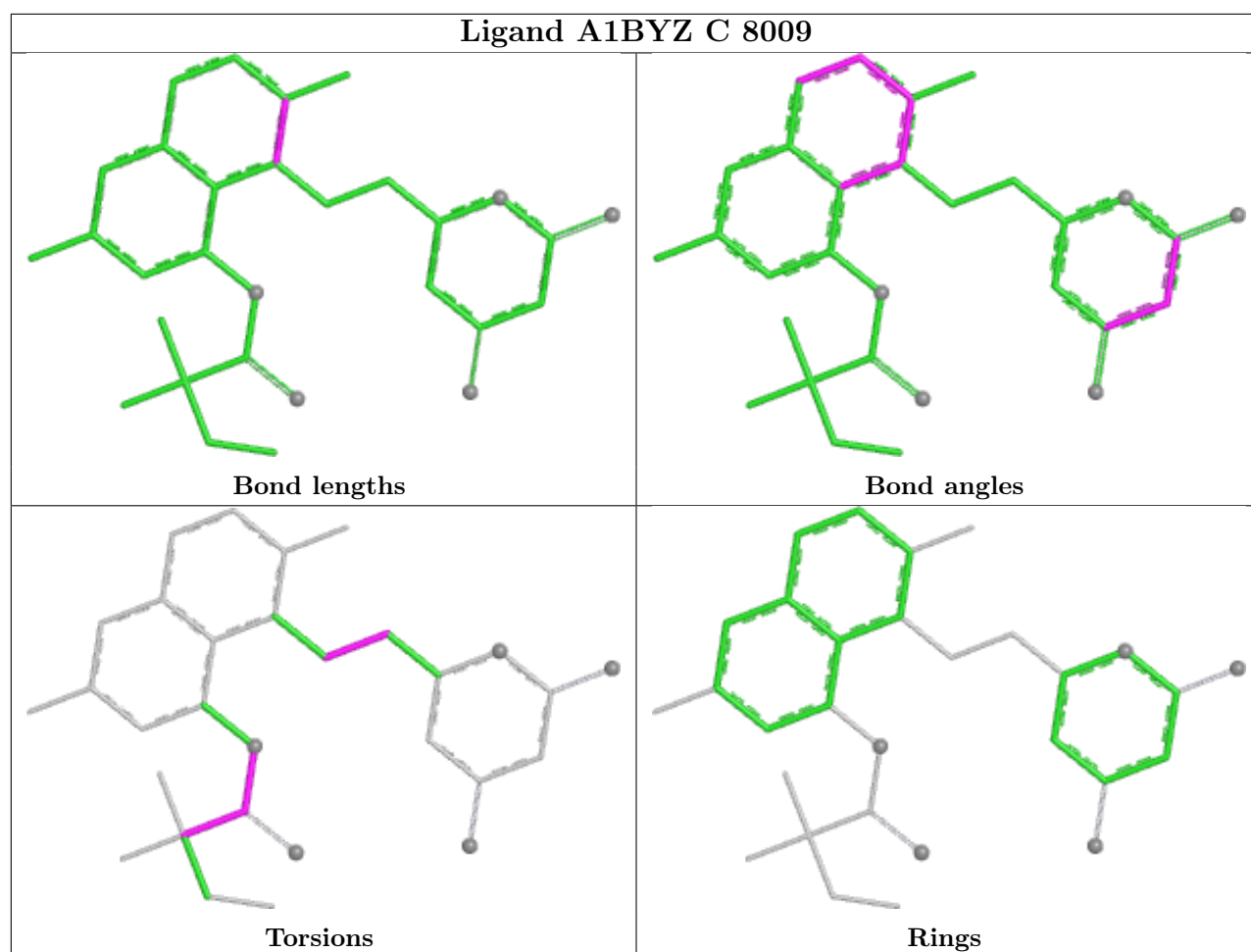


Ligand A1BYZ B 8009



Ligand A1BYZ B 8008





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

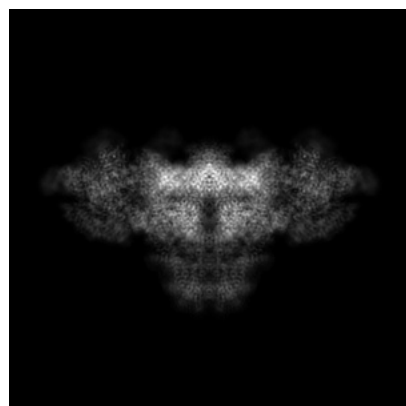
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49536. These allow visual inspection of the internal detail of the map and identification of artifacts.

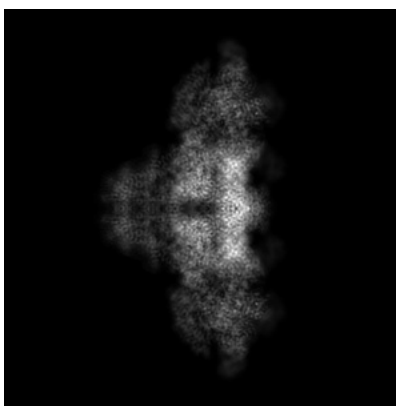
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

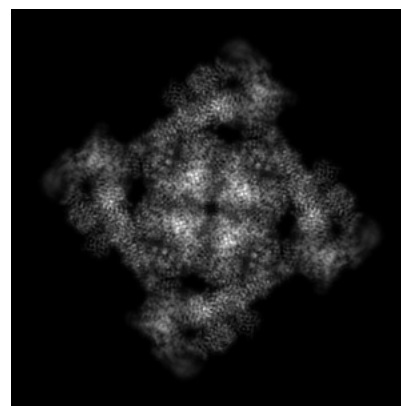
6.1.1 Primary map



X

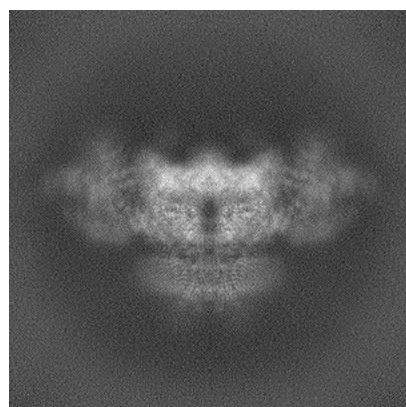


Y

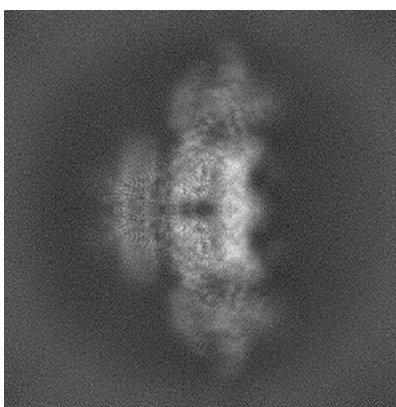


Z

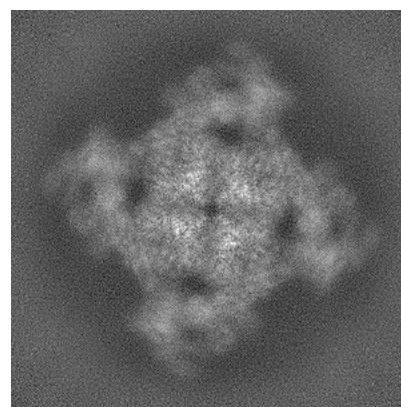
6.1.2 Raw map



X



Y



Z

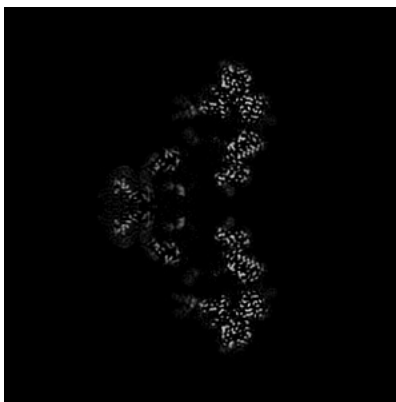
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

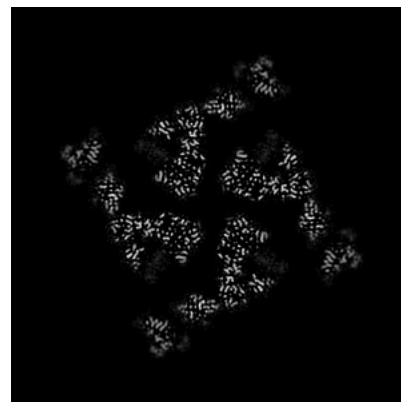
6.2.1 Primary map



X Index: 256



Y Index: 256

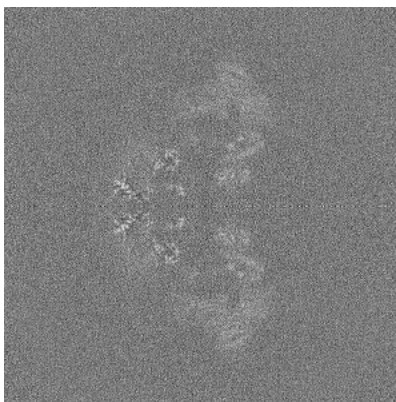


Z Index: 256

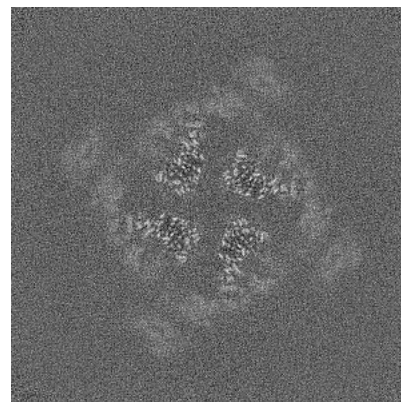
6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

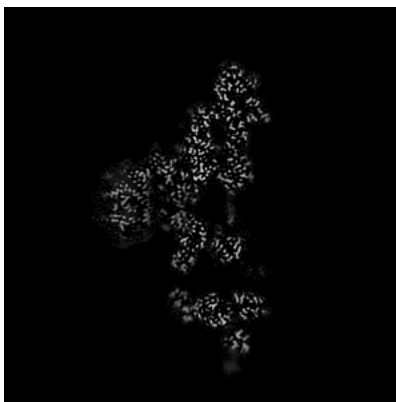
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

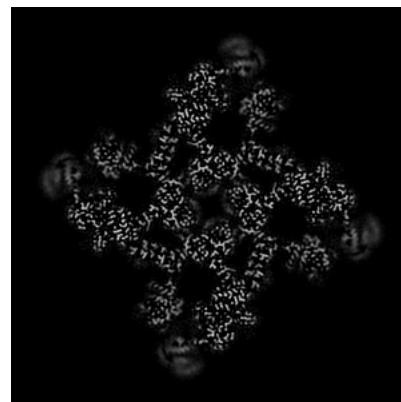
6.3.1 Primary map



X Index: 238

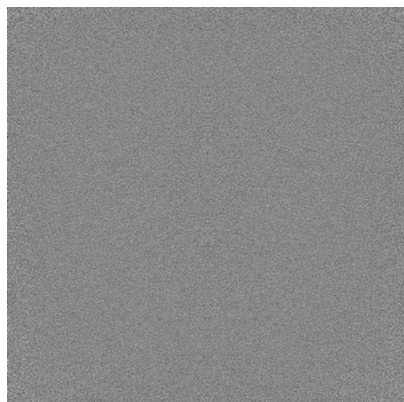


Y Index: 274

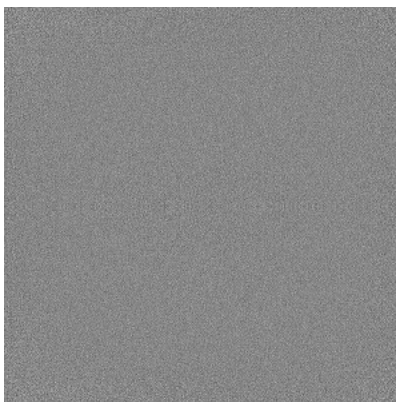


Z Index: 287

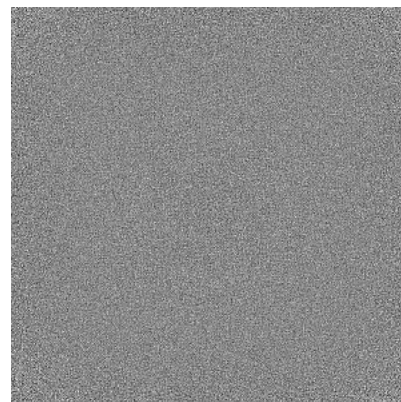
6.3.2 Raw map



X Index: 0



Y Index: 0

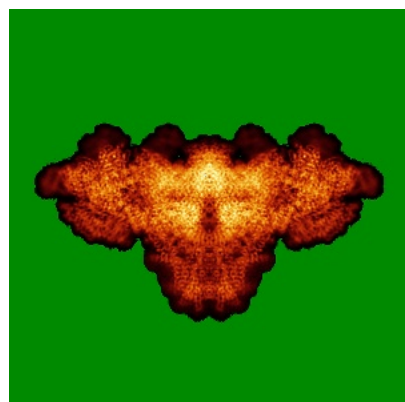


Z Index: 0

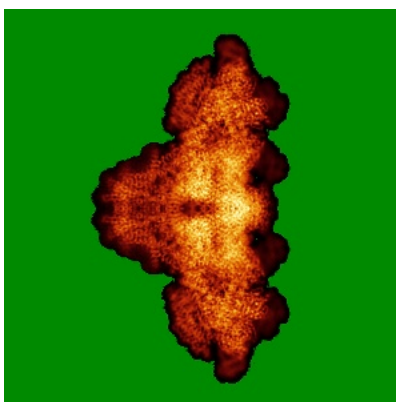
The images above show the largest variance slices of the map in three orthogonal directions.

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

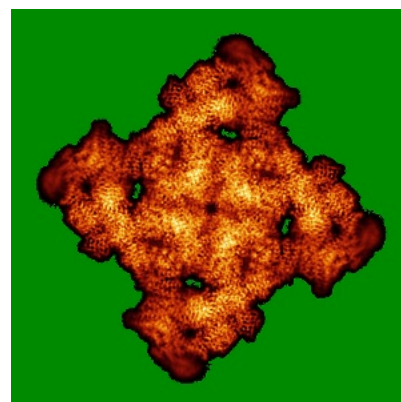
6.4.1 Primary map



X

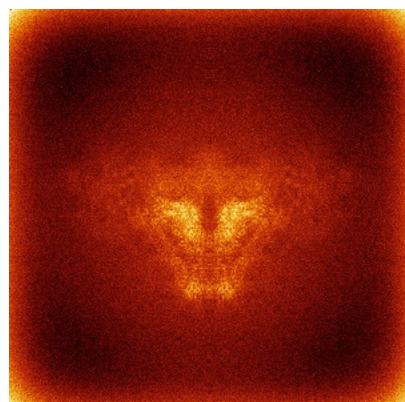


Y

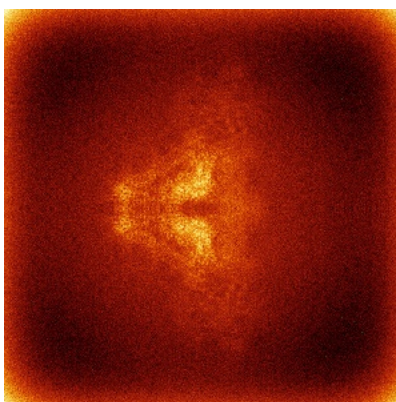


Z

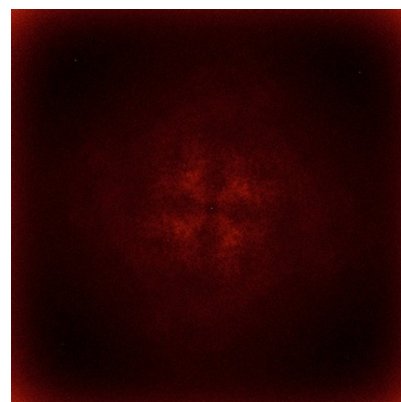
6.4.2 Raw map



X



Y

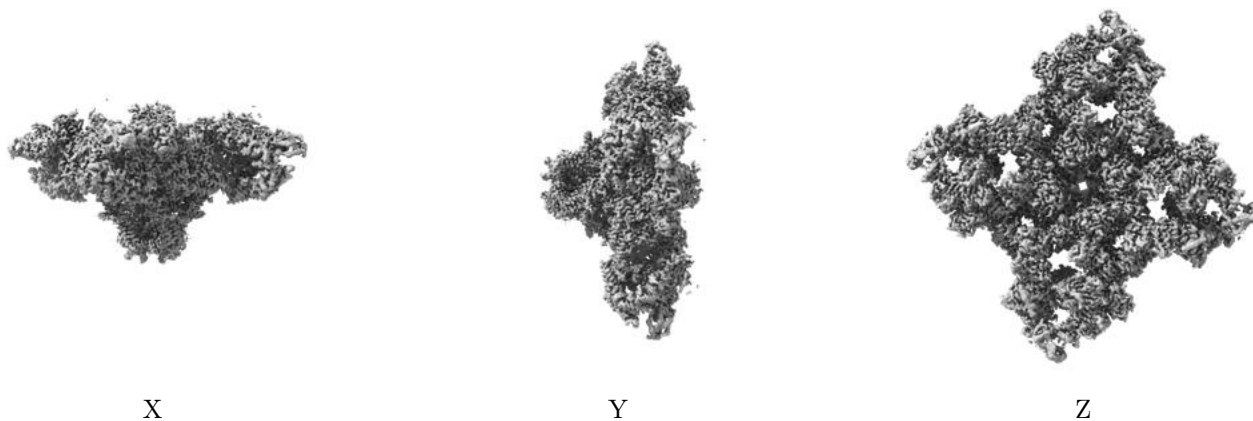


Z

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

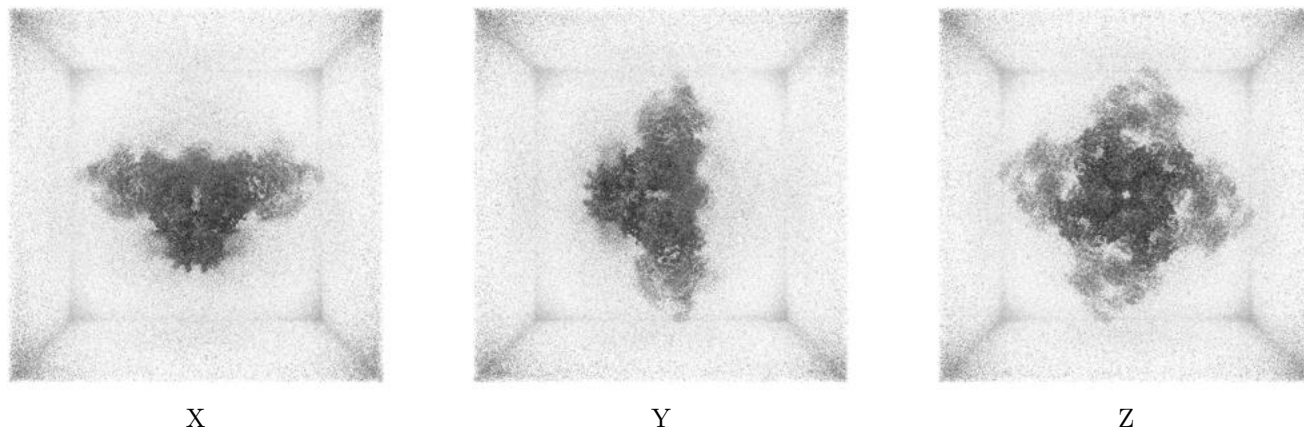
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

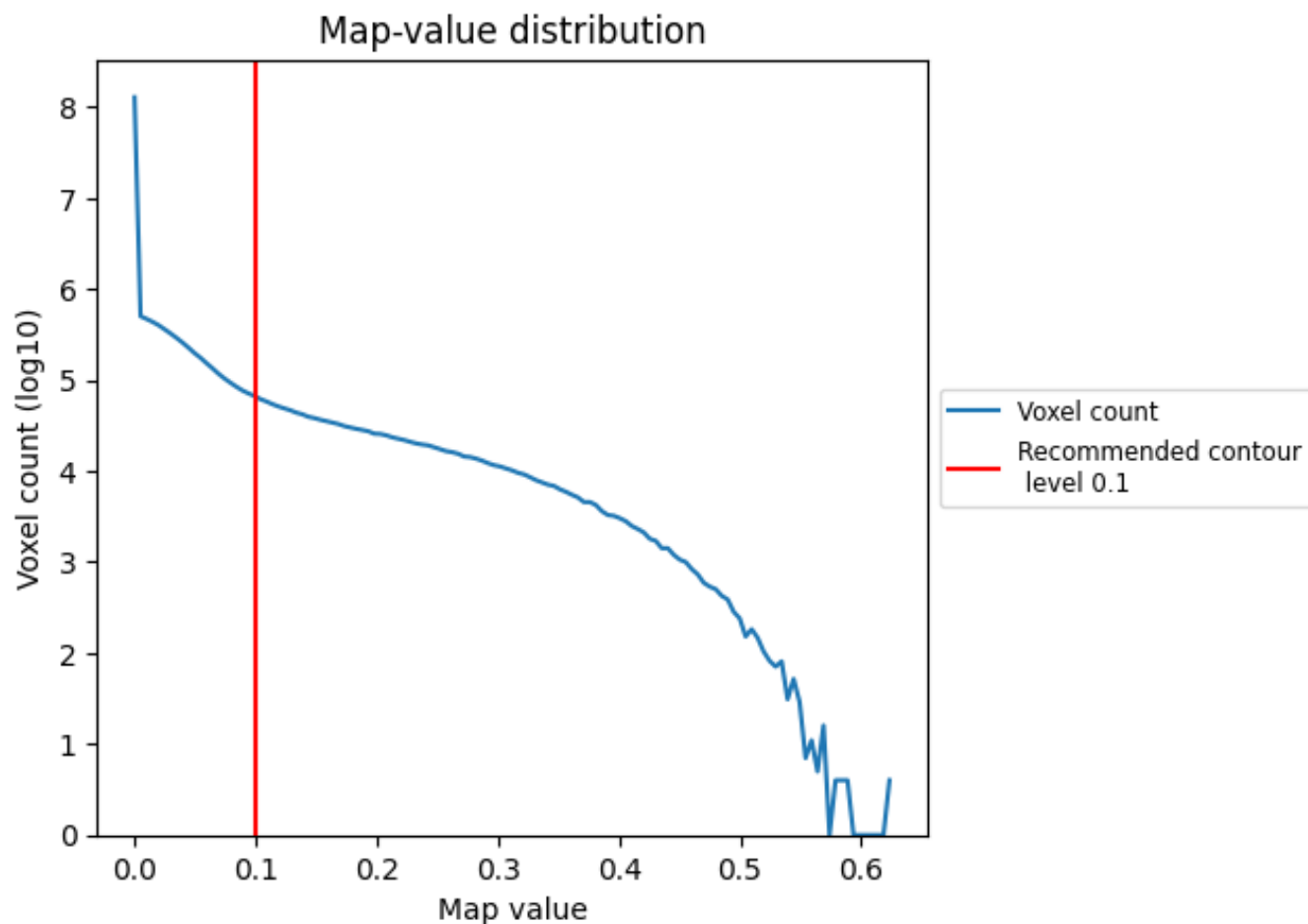
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

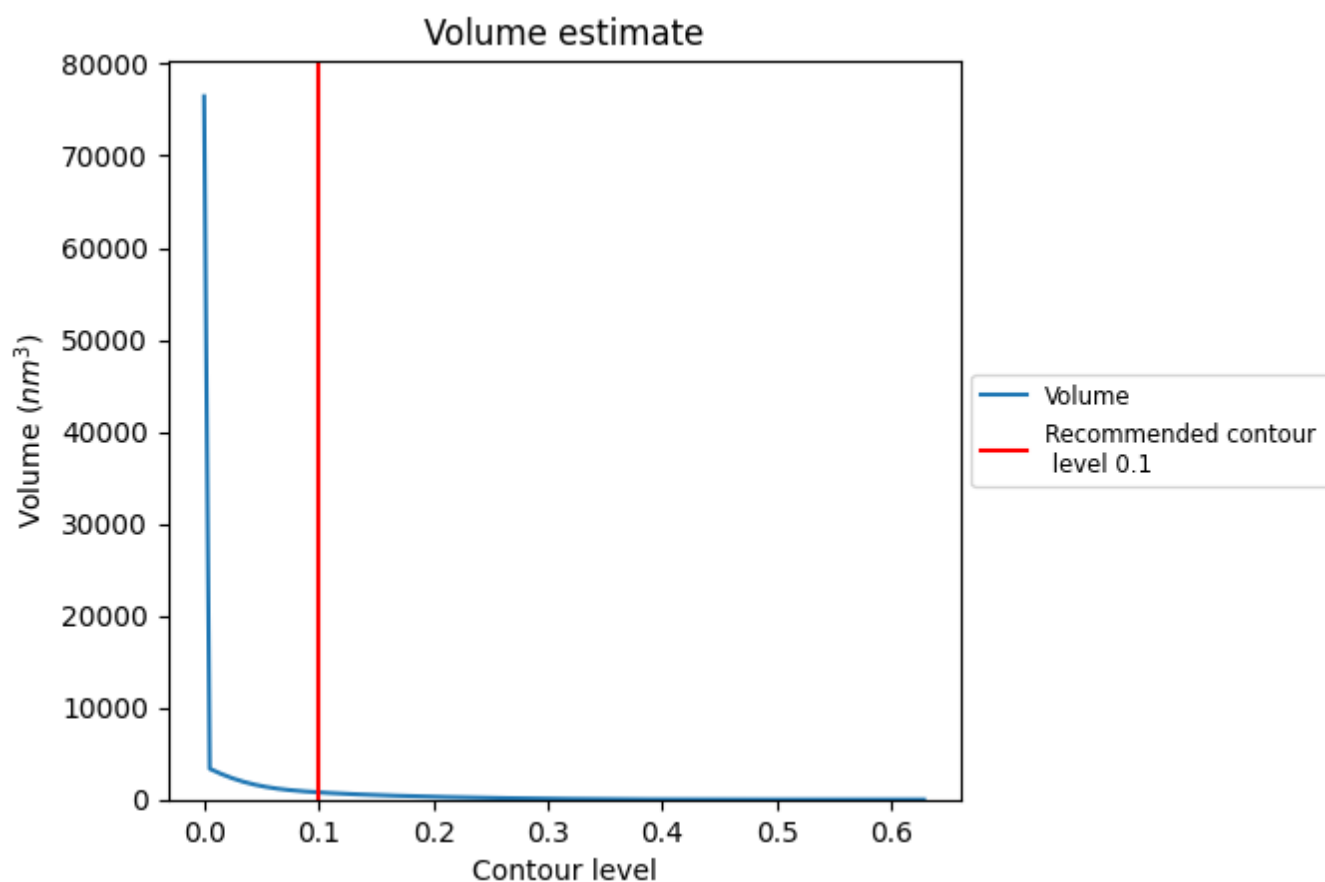
This section contains the results of statistical analysis of the map.

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.

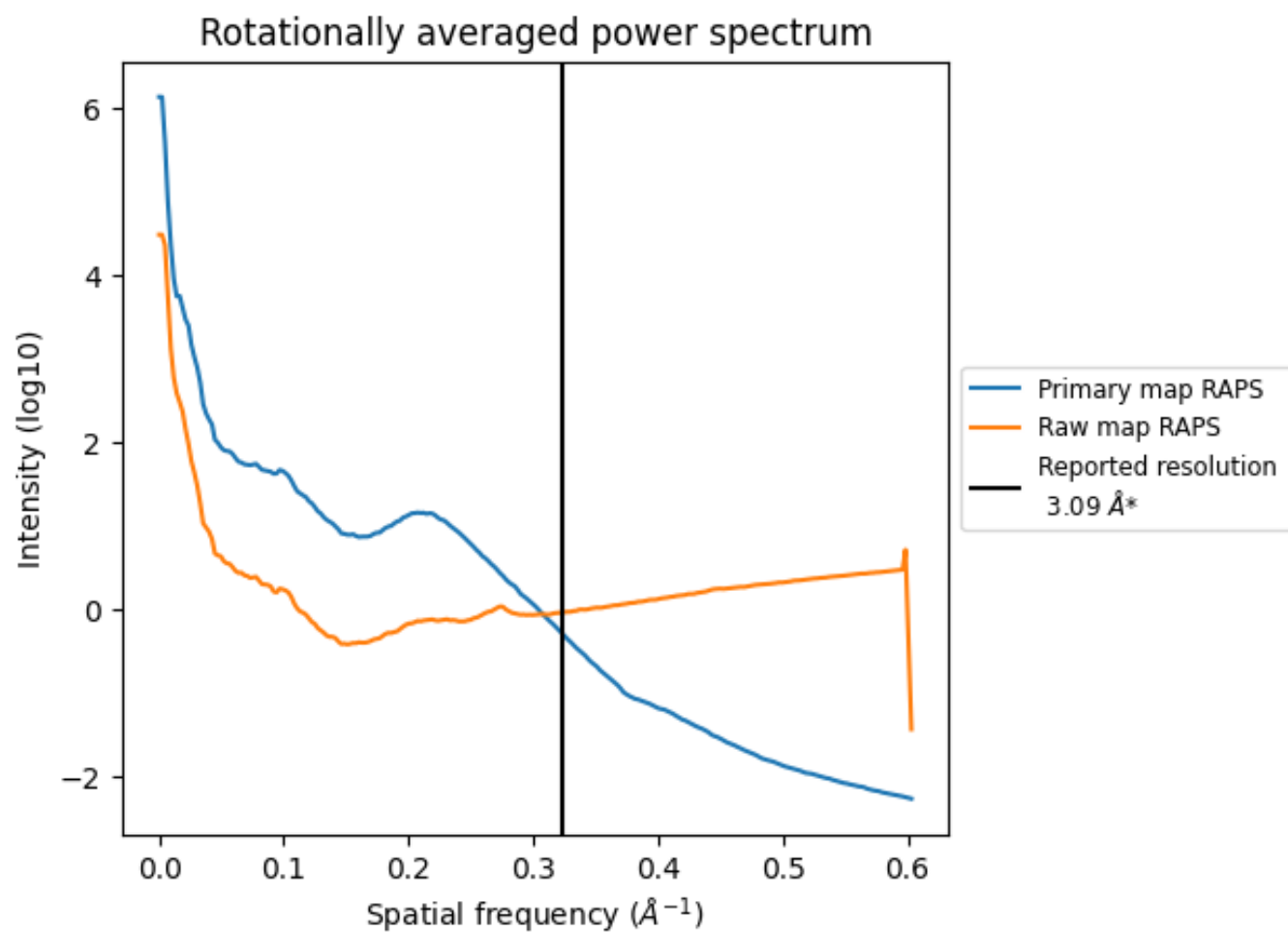
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 783 nm³; this corresponds to an approximate mass of 707 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 ⓘ

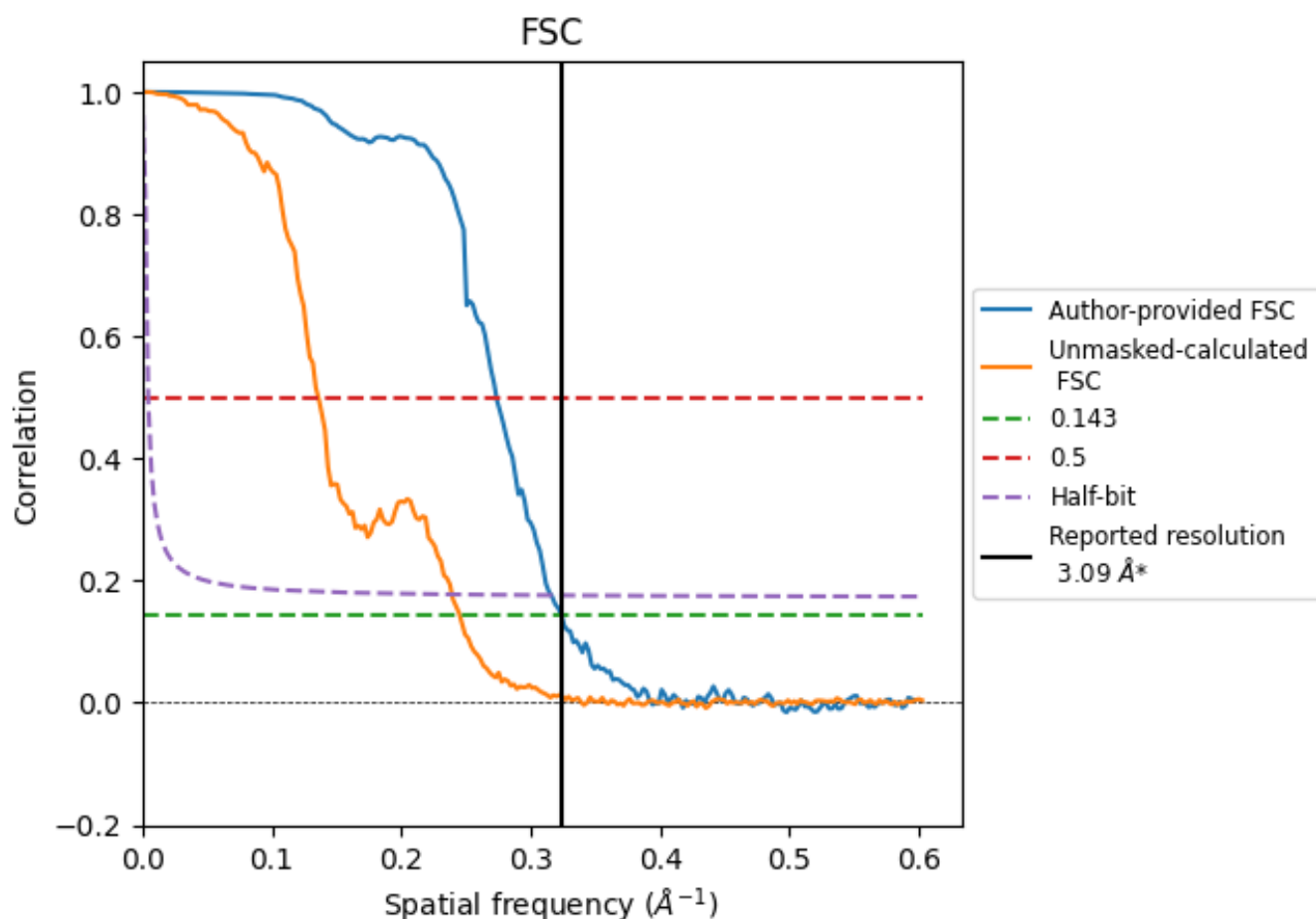


*Reported resolution corresponds to spatial frequency of 0.324 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.324 \text{ \AA}^{-1}$

8.2 Resolution estimates

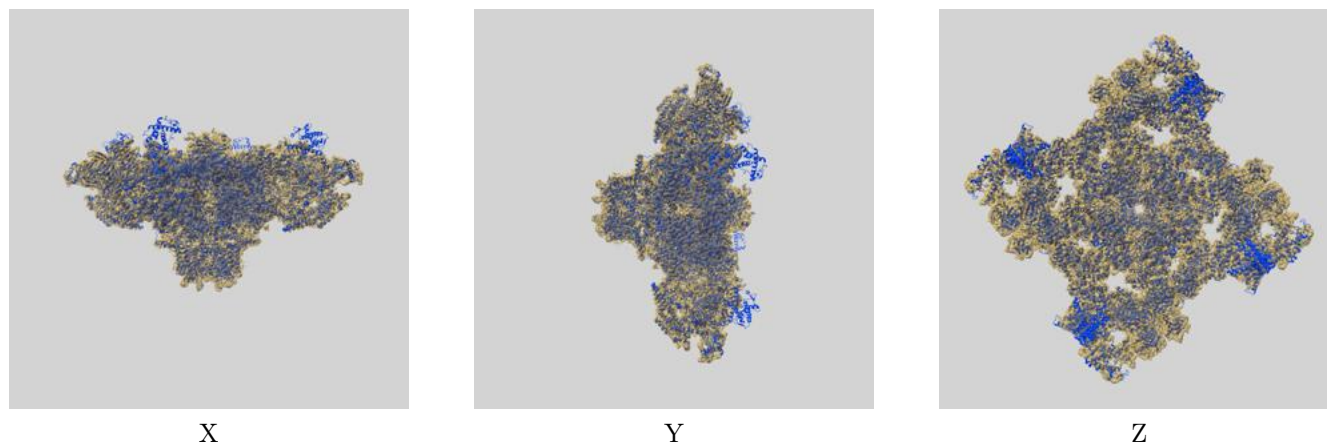
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.09	-	-
Author-provided FSC curve	3.09	3.65	3.16
Unmasked-calculated*	4.08	7.35	4.18

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.08 differs from the reported value 3.09 by more than 10 %

9 Map-model fit [i](#)

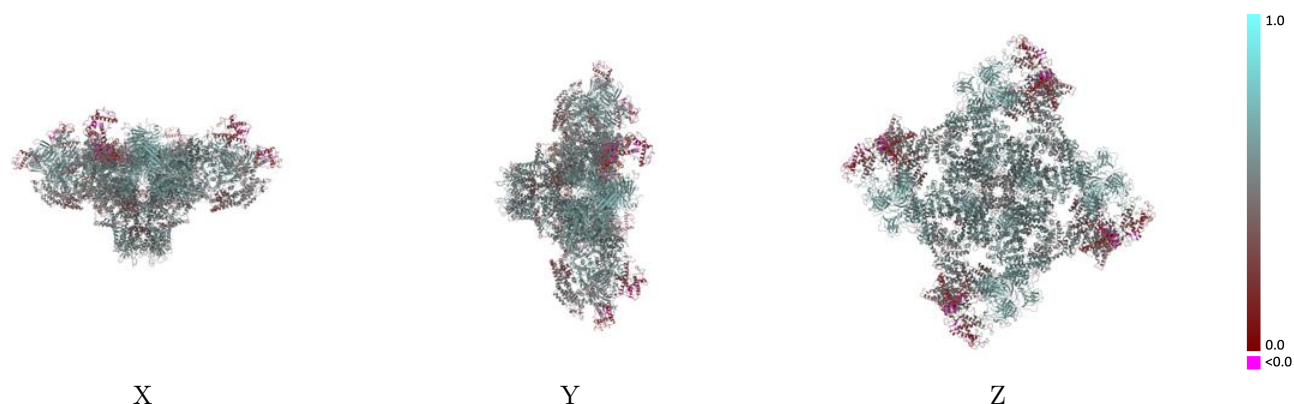
This section contains information regarding the fit between EMDB map EMD-49536 and PDB model 9NMP. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



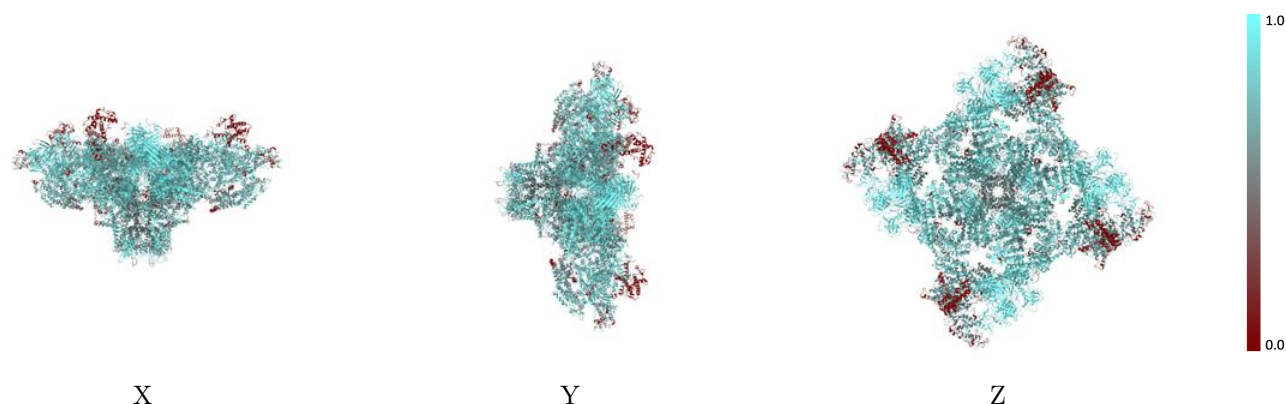
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



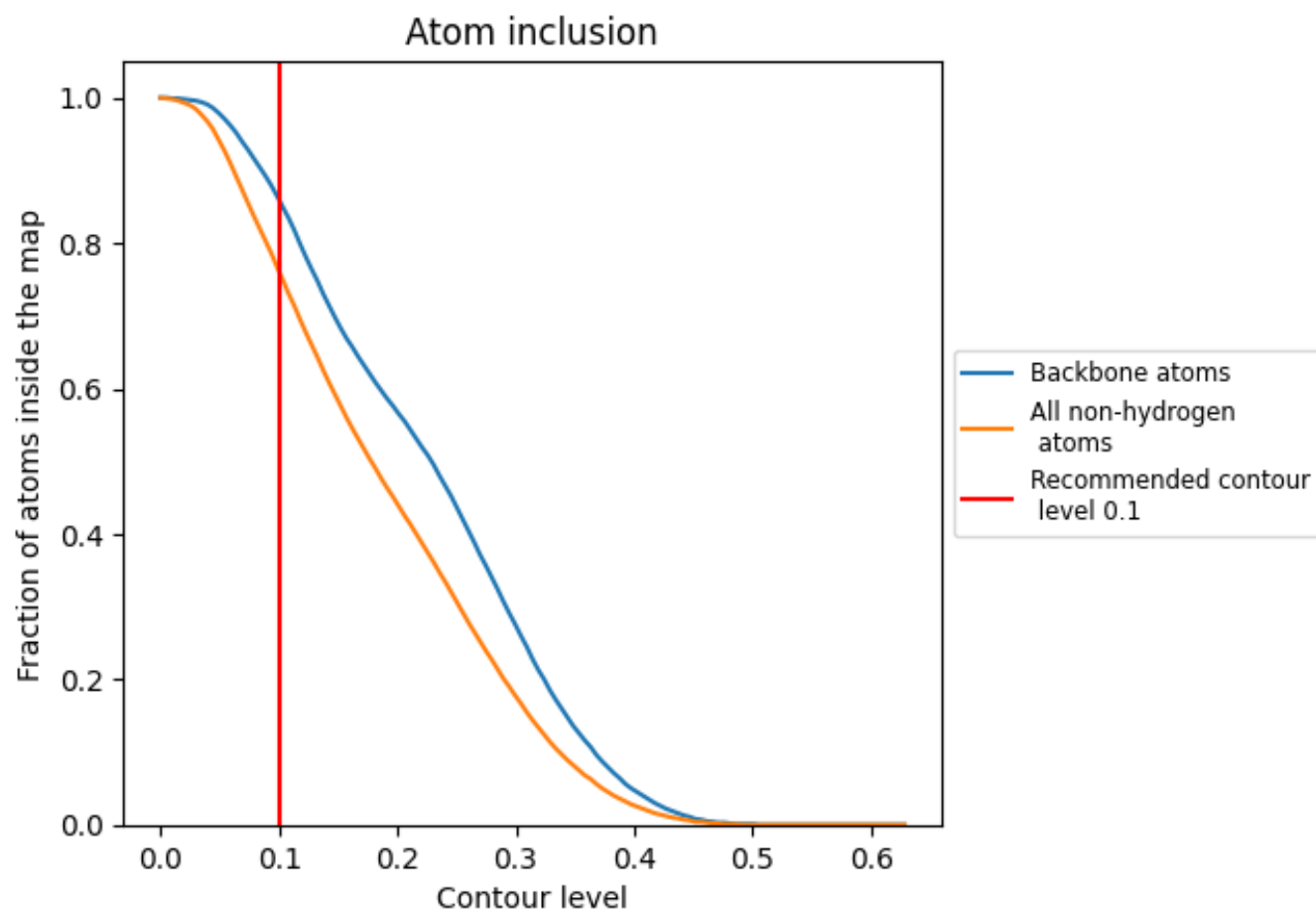
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 76% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7610	0.5090
A	0.7600	0.5080
B	0.7580	0.5070
C	0.7580	0.5070
D	0.7580	0.5070
E	0.8810	0.5870
F	0.8840	0.5890
G	0.8770	0.5850
H	0.8840	0.5910

1.0

0.0

<0.0