



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 04:25 AM UTC

PDB ID : 8XLH / pdb_00008xlh
EMDB ID : EMD-38448
Title : Structure of chimeric RyR-I4657M/G4819E
Authors : Lin, L.; Wang, C.; Wang, W.; Jiang, H.; Yuchi, Z.
Deposited on : 2023-12-26
Resolution : 3.62 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:

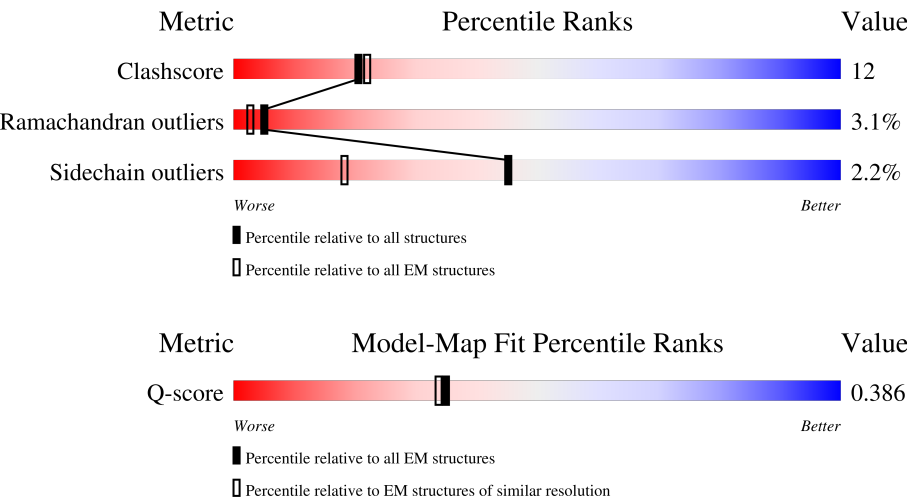
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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

The reported resolution of this entry is 3.62 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.



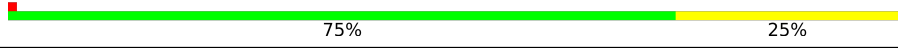
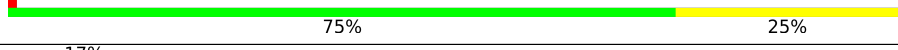
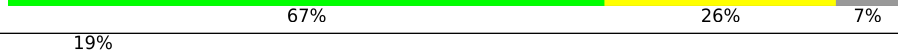
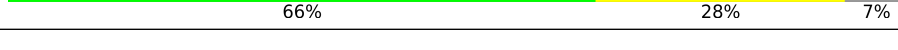
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11773 (3.12 - 4.12)

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

Mol	Chain	Length	Quality of chain
1	A	5037	6% 61% 18% • 18%
1	B	5037	6% 61% 18% • 18%
1	C	5037	6% 61% 18% • 18%
1	D	5037	7% 61% 18% • 18%

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Mol	Chain	Length	Quality of chain
2	E	107	 77%23%
2	F	107	 75%25%
2	G	107	 75%25%
2	H	107	 75%25%
3	I	149	 17%67%26%7%
3	J	149	 17%66%27%7%
3	K	149	 17%67%26%7%
3	L	149	 19%66%28%7%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 124364 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4135	Total	C	N	O	S	0	0
			29207	18536	5163	5346	162		
1	D	4135	Total	C	N	O	S	0	0
			29207	18536	5163	5346	162		
1	C	4135	Total	C	N	O	S	0	0
			29207	18536	5163	5346	162		
1	B	4135	Total	C	N	O	S	0	0
			29207	18536	5163	5346	162		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4563	LYS	ARG	engineered mutation	UNP P11716
A	4564	TYR	PHE	engineered mutation	UNP P11716
A	4657	MET	CYS	engineered mutation	UNP P11716
A	4792	SER	LEU	engineered mutation	UNP P11716
A	4819	GLU	GLY	engineered mutation	UNP P11716
D	4563	LYS	ARG	engineered mutation	UNP P11716
D	4564	TYR	PHE	engineered mutation	UNP P11716
D	4657	MET	CYS	engineered mutation	UNP P11716
D	4792	SER	LEU	engineered mutation	UNP P11716
D	4819	GLU	GLY	engineered mutation	UNP P11716
C	4563	LYS	ARG	engineered mutation	UNP P11716
C	4564	TYR	PHE	engineered mutation	UNP P11716
C	4657	MET	CYS	engineered mutation	UNP P11716
C	4792	SER	LEU	engineered mutation	UNP P11716
C	4819	GLU	GLY	engineered mutation	UNP P11716
B	4563	LYS	ARG	engineered mutation	UNP P11716
B	4564	TYR	PHE	engineered mutation	UNP P11716
B	4657	MET	CYS	engineered mutation	UNP P11716
B	4792	SER	LEU	engineered mutation	UNP P11716
B	4819	GLU	GLY	engineered mutation	UNP P11716

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total	C	N	O	S	0	0
			804	510	144	146	4		
2	H	107	Total	C	N	O	S	0	0
			804	510	144	146	4		
2	G	107	Total	C	N	O	S	0	0
			804	510	144	146	4		
2	F	107	Total	C	N	O	S	0	0
			804	510	144	146	4		

- Molecule 3 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	139	Total	C	N	O	S	0	0
			1033	638	174	212	9		
3	L	139	Total	C	N	O	S	0	0
			1033	638	174	212	9		
3	K	139	Total	C	N	O	S	0	0
			1033	638	174	212	9		
3	J	139	Total	C	N	O	S	0	0
			1033	638	174	212	9		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	32	ALA	GLU	engineered mutation	UNP P0DP23
I	68	ALA	GLU	engineered mutation	UNP P0DP23
I	105	ALA	GLU	engineered mutation	UNP P0DP23
I	141	ALA	GLU	engineered mutation	UNP P0DP23
L	32	ALA	GLU	engineered mutation	UNP P0DP23
L	68	ALA	GLU	engineered mutation	UNP P0DP23
L	105	ALA	GLU	engineered mutation	UNP P0DP23
L	141	ALA	GLU	engineered mutation	UNP P0DP23
K	32	ALA	GLU	engineered mutation	UNP P0DP23
K	68	ALA	GLU	engineered mutation	UNP P0DP23
K	105	ALA	GLU	engineered mutation	UNP P0DP23
K	141	ALA	GLU	engineered mutation	UNP P0DP23
J	32	ALA	GLU	engineered mutation	UNP P0DP23
J	68	ALA	GLU	engineered mutation	UNP P0DP23
J	105	ALA	GLU	engineered mutation	UNP P0DP23
J	141	ALA	GLU	engineered mutation	UNP P0DP23

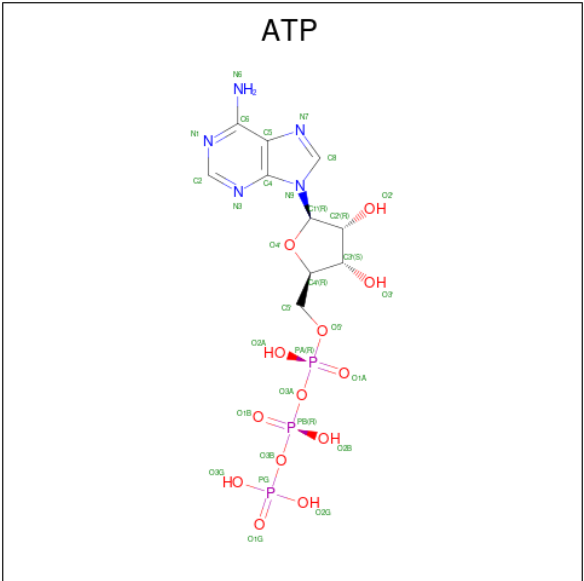
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



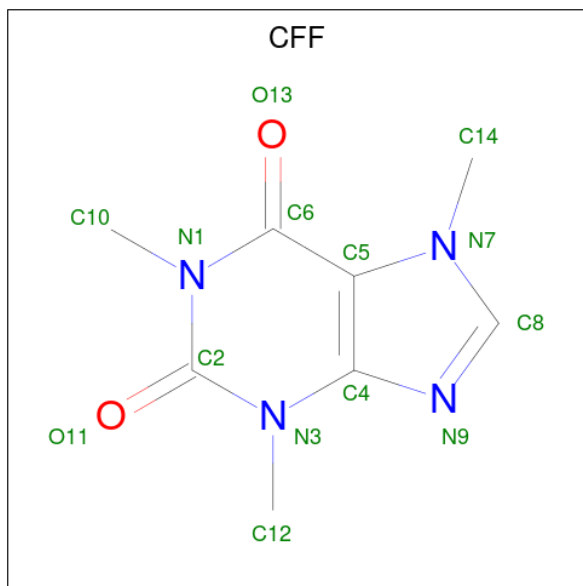
Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

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

- Molecule 7 is CAFFEINE (CCD ID: CFF) (formula: $C_8H_{10}N_4O_2$) (labeled as "Ligand of Interest" by depositor).

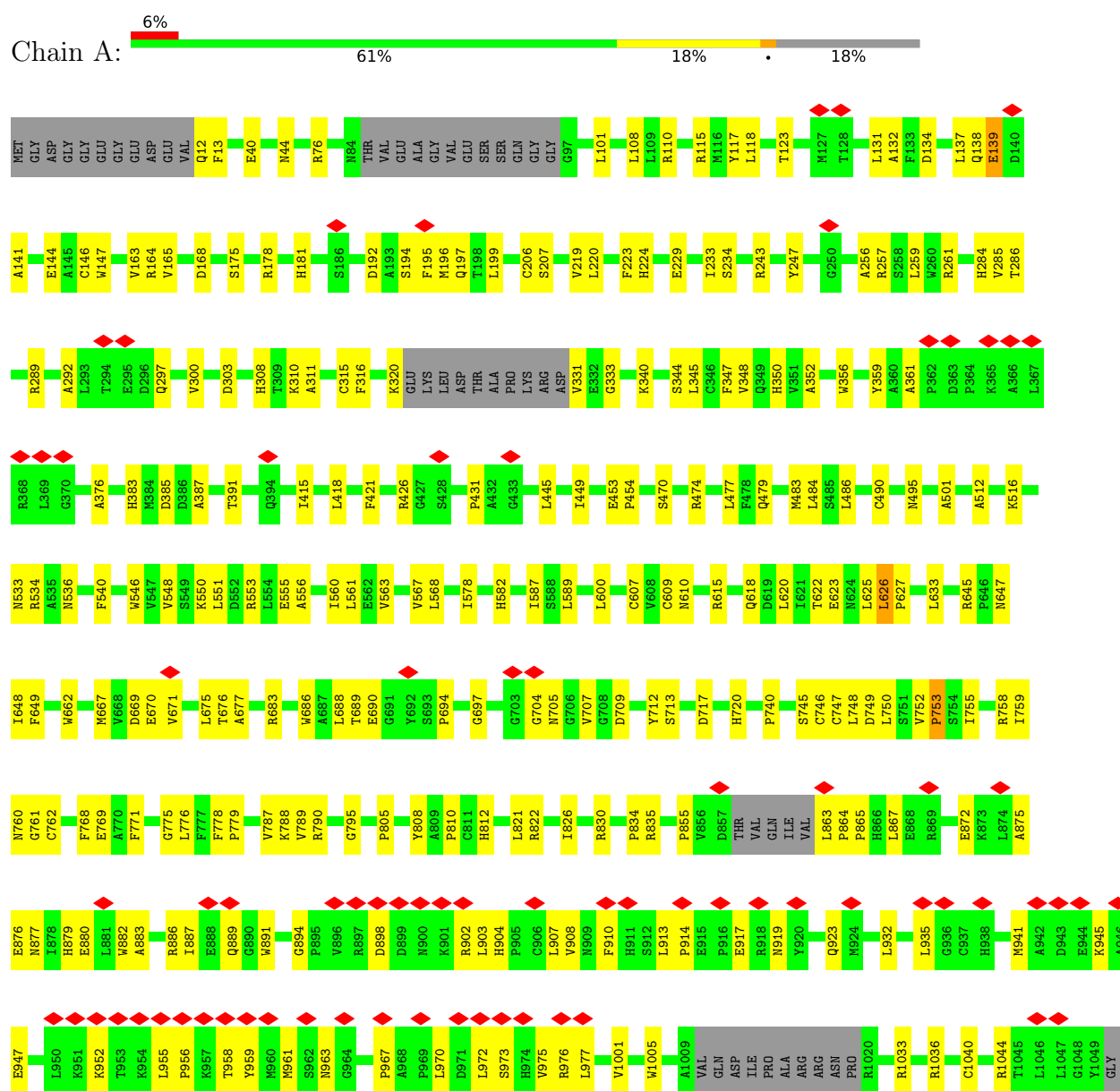


Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			14	8	4	2	
7	D	1	Total	C	N	O	0
			14	8	4	2	
7	C	1	Total	C	N	O	0
			14	8	4	2	
7	B	1	Total	C	N	O	0
			14	8	4	2	

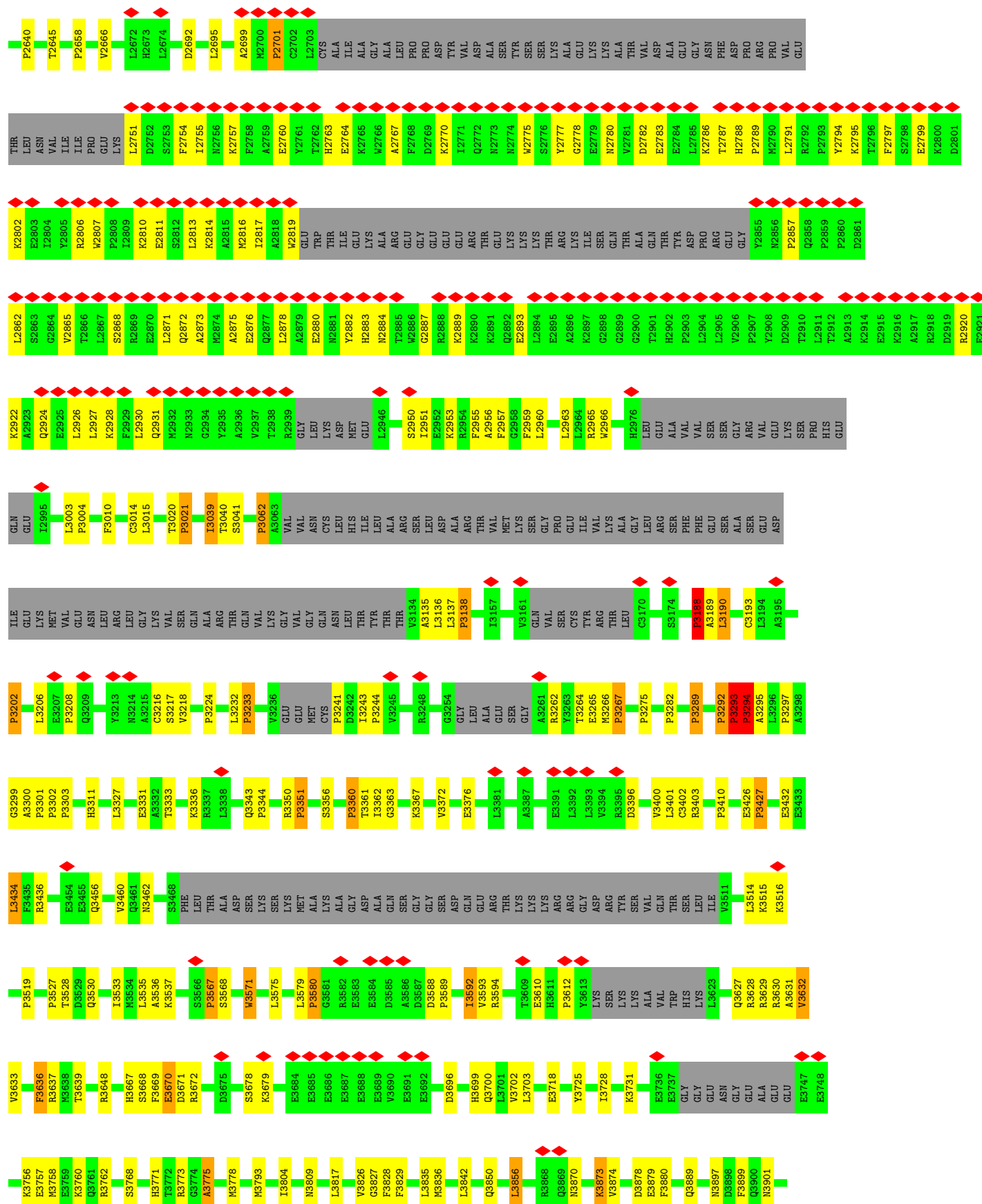
3 Residue-property plots

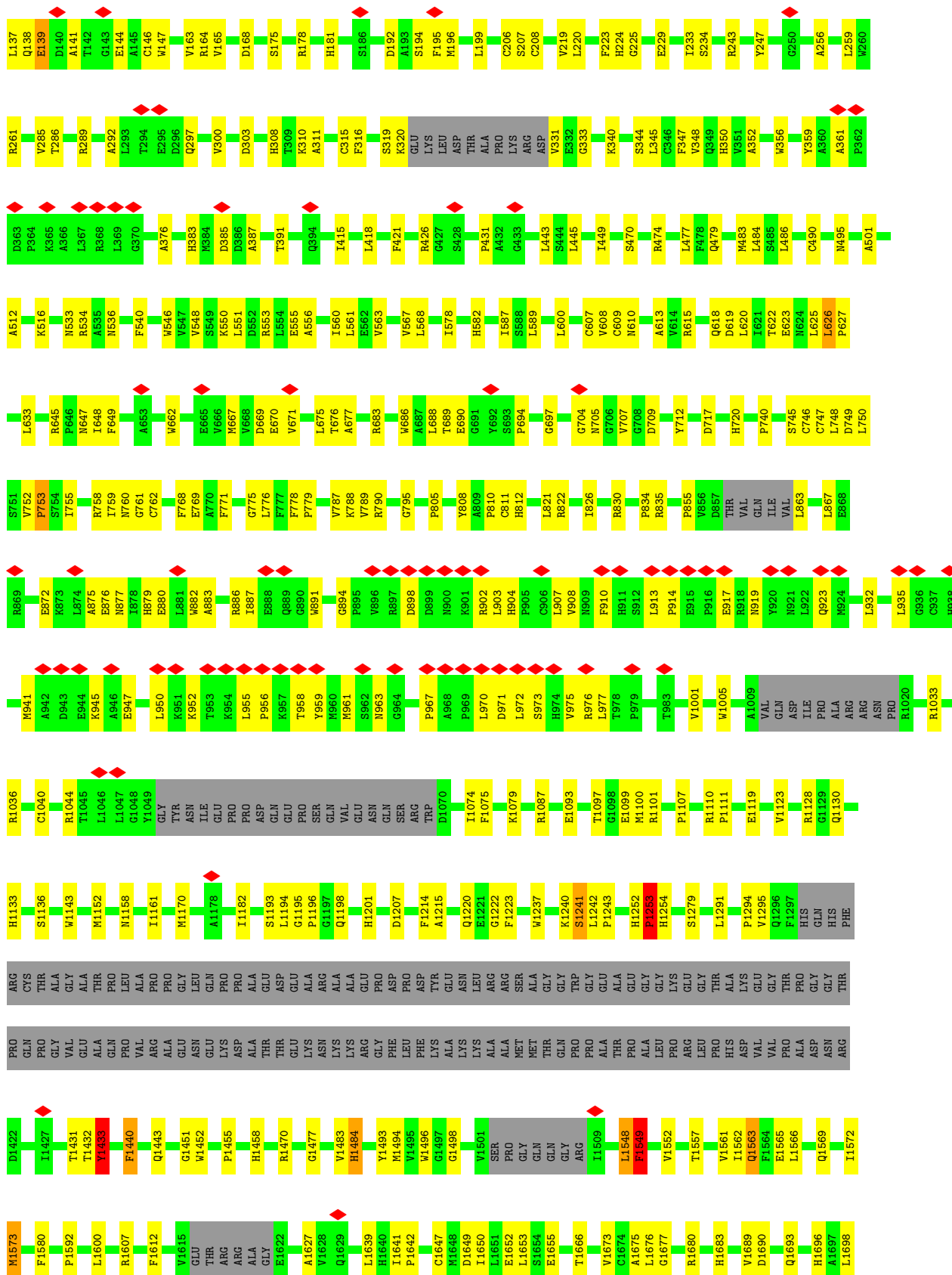
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Ryanodine receptor 1



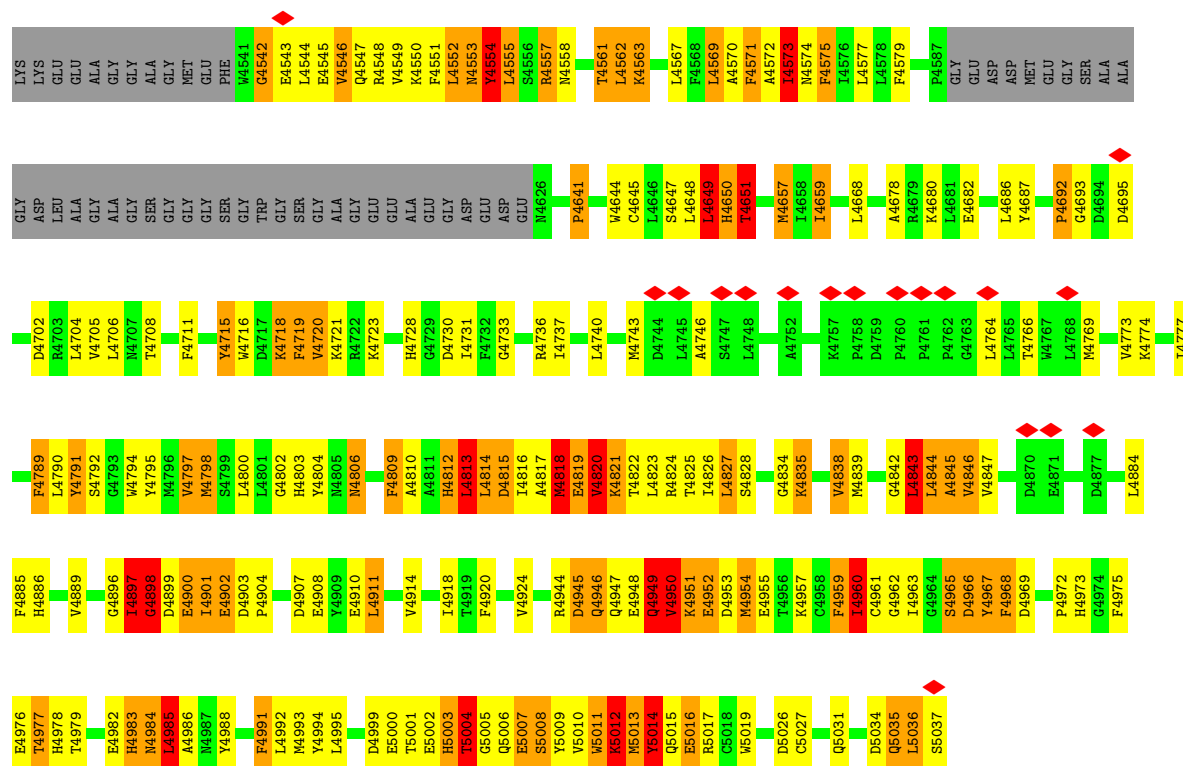




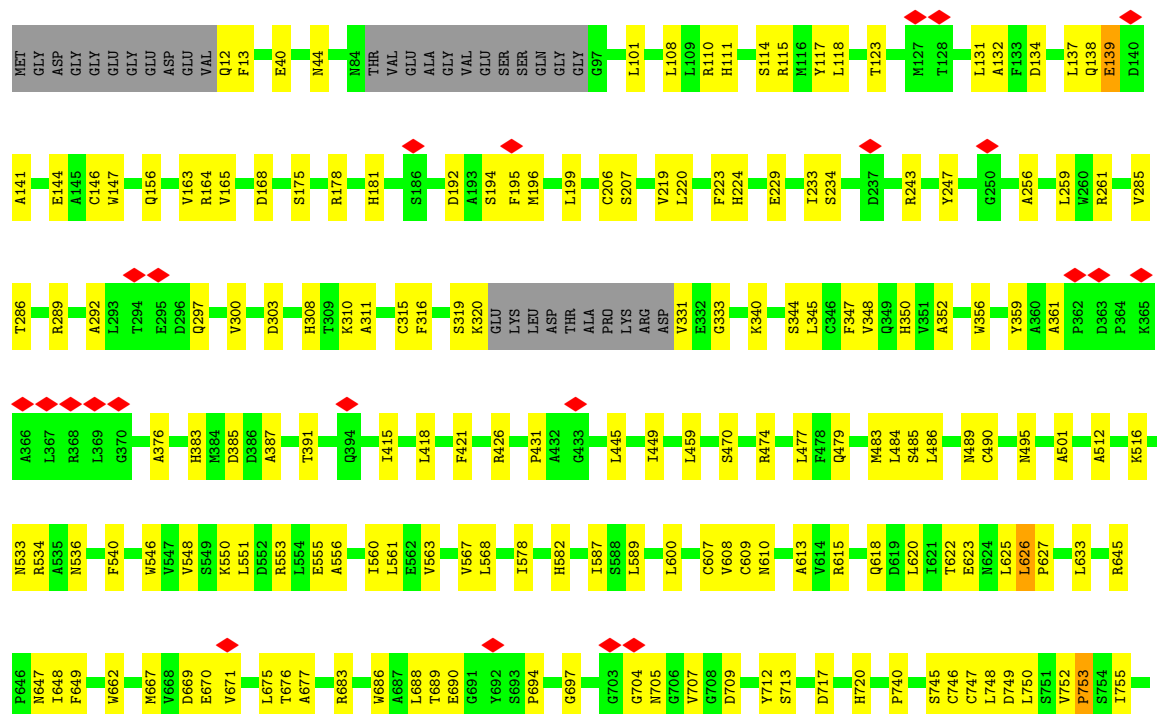








• Molecule 1: Ryanodine receptor 1



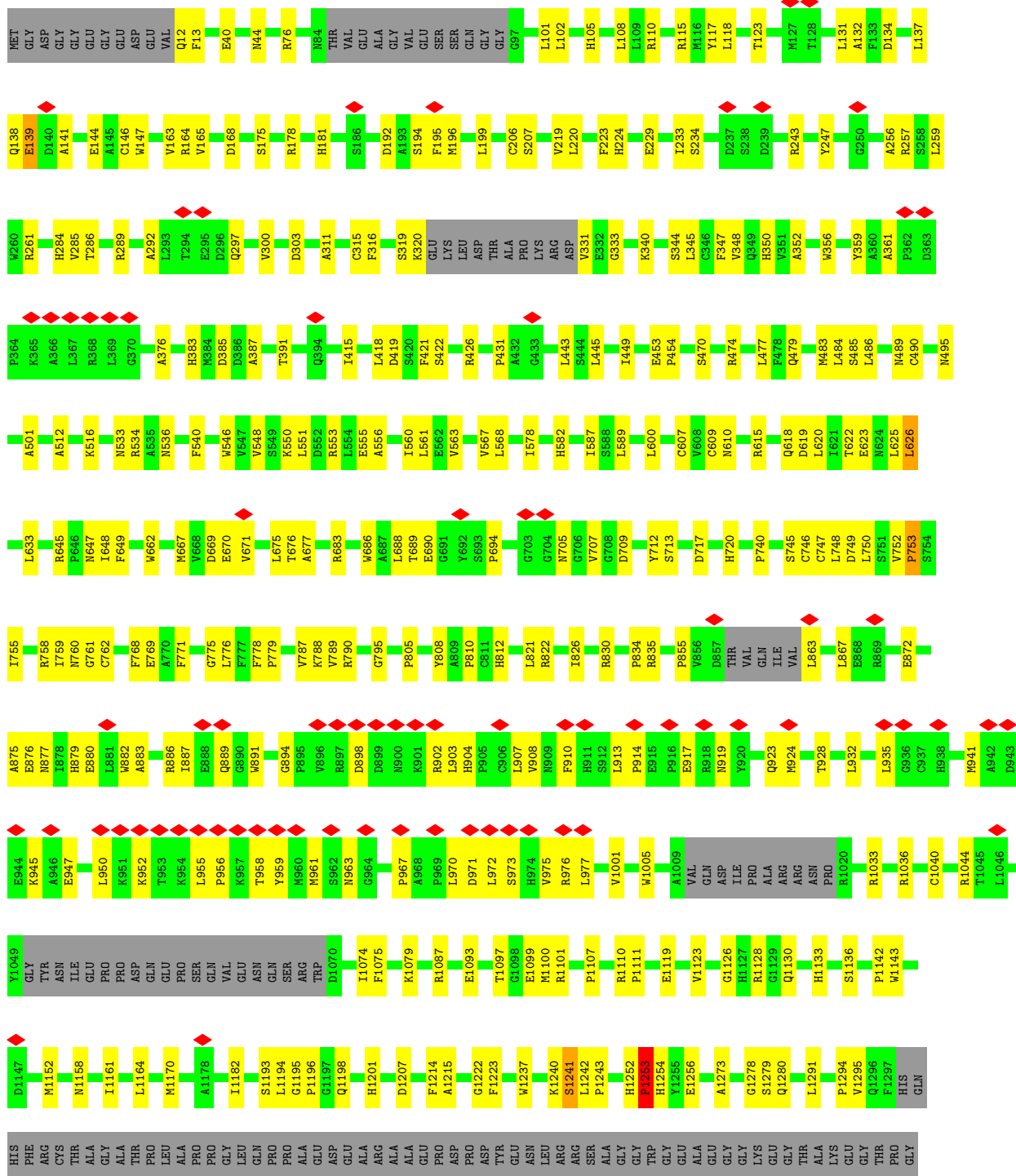




G4936	G4793	V4705	ALA	THR	M4207	V4035	N3901	E3748	M3638	K3534
T4897	W4794	L4706	GLY	ALA	M4216	G4038	R3904	K3756	T3639	L3535
D4898	Y4795	M4707	ARG	ARG	Q4217	G4038	R3904	E3757	T3639	A3536
D4899	Y4796	T4708	GLY	LEU	F4218	R4042	N3909	M3758	R3648	K3537
E4900	W4797	G4711	GLY	ALA	F4219	S4051	T3910	E3759	M3652	S3566
E4901	M4798	G4711	VAL	ALA	F4220	S4051	T3910	K3760	M3652	P3567
E4902	S4799	G4711	ASP	ALA	G4225	L4066	T3913	K3761	S3656	L3569
D4903	L4801	G4716	GLY	ALA	G4226	L4066	T3913	R3762	S3656	S3568
P4904	G4802	G4717	GLY	ARG	E4227	L4071	T3919	R3762	S3656	R3570
D4907	H4803	K4718	GLY	ARG	E4228	E4075	D3921	S3768	S3668	K3571
E4908	Y4804	W4719	ALA	LEU	A4228	Q4078	D3922	H3771	F3669	D3671
Y4909	M4805	W4720	GLY	GLY	Y4235	Q4078	L3923	T3772	D3670	R3672
E4910	M4806	K4721	HIS	GLY	Y4236	Q4078	L3924	R3773	L3575	L3575
L4911	ALA	K4722	LEU	LEU	Y4236	Q4078	L3924	G3774	L3579	L3579
F4809	GLY	K4723	VAL	LEU	Y4236	Q4078	L3924	A3775	P3580	P3580
A4810	GLY	K4723	GLY	TYR	Y4242	R4086	S3929	M3778	G3581	G3581
A4811	ASP	H4728	GLY	ARG	Y4242	R4086	S3929	M3778	R3582	R3582
H4812	GLY	G4729	GLY	ARG	Y4251	L4087	D3932	M3793	E3583	E3583
L4813	ASP	D4730	GLY	LEU	S4252	L4087	D3932	M3793	E3584	E3584
L4814	ASP	L4731	GLY	LEU	GLU	M4097	D3941	M3793	D3585	D3585
D4815	ASP	F4732	ALA	ARG	GLU	Q4102	D3942	M3793	A3586	A3586
I4816	ASP	Y4554	VAL	ARG	GLU	F4103	V3942	M3793	D3587	D3587
I4817	ASP	L4555	VAL	ARG	GLU	T4104	V3942	M3793	P3589	P3589
M4818	ASP	S4556	VAL	ARG	GLU	G4105	K3955	M3793	E3684	E3684
E4819	ASP	R4557	VAL	ARG	GLU	E4107	D3942	M3793	E3685	E3685
E4820	ASP	R4558	VAL	ARG	GLU	E4107	D3942	M3793	E3686	E3686
K4821	ASP	T4561	VAL	ARG	GLU	E4107	D3942	M3793	E3687	E3687
L4822	ASP	K4563	VAL	ARG	GLU	E4107	D3942	M3793	E3688	E3688
L4823	ASP	K4563	VAL	ARG	GLU	E4107	D3942	M3793	E3689	E3689
L4824	ASP	K4563	VAL	ARG	GLU	E4107	D3942	M3793	E3691	E3691
R4824	ASP	K4563	VAL	ARG	GLU	E4107	D3942	M3793	E3692	E3692
L4825	ASP	K4563	VAL	ARG	GLU	E4107	D3942	M3793	E3693	E3693
L4826	ASP	K4563	VAL	ARG	GLU	E4107	D3942	M3793	E3694	E3694
L4827	ASP	K4563	VAL	ARG	GLU	E4107	D3942	M3793	E3695	E3695
S4828	ASP	K4563	VAL	ARG	GLU	E4107	D3942	M3793	E3696	E3696
G4834	ASP	K4563	VAL	ARG	GLU	E4107	D3942	M3793	E3697	E3697
K4835	ASP	K4563	VAL	ARG	GLU	E4107	D3942	M3793	E3698	E3698
V4838	ASP	K4563	VAL	ARG	GLU	E4107	D3942	M3793	E3699	E3699
M4839	ASP	K4563	VAL	ARG	GLU	E4107	D3942	M3793	E3700	E3700
G4842	ASP	K4563	VAL	ARG	GLU	E4107	D3942	M3793	E3701	E3701
L4843	ASP	K4563	VAL	ARG	GLU	E4107	D3942	M3793	E3702	E3702
L4844	ASP	K4563	VAL	ARG	GLU	E4107	D3942	M3793	E3703	E3703
A4845	ASP	K4563	VAL	ARG	GLU	E4107	D3942	M3793	E3704	E3704
V4846	ASP	K4563	VAL	ARG	GLU	E4107	D3942	M3793	E3705	E3705
V4847	ASP	K4563	VAL	ARG	GLU	E4107	D3942	M3793	E3706	E3706
L4848	ASP	K4563	VAL	ARG	GLU	E4107	D3942	M3793	E3707	E3707
D4870	ASP	K4563	VAL	ARG	GLU	E4107	D3942	M3793	E3708	E3708
E4871	ASP	K4563	VAL	ARG	GLU	E4107	D3942	M3793	E3709	E3709
D4877	ASP	K4563	VAL	ARG	GLU	E4107	D3942	M3793	E3710	E3710
L4884	ASP	K4563	VAL	ARG	GLU	E4107	D3942	M3793	E3711	E3711
F4885	ASP	K4563	VAL	ARG	GLU	E4107	D3942	M3793	E3712	E3712
Y4888	ASP	K4563	VAL	ARG	GLU	E4107	D3942	M3793	E3713	E3713
H4878	ASP	K4563	VAL	ARG	GLU	E4107	D3942	M3793	E3714	E3714
L4790	ASP	K4563	VAL	ARG	GLU	E4107	D3942	M3793	E3715	E3715
Y4791	ASP	K4563	VAL	ARG	GLU	E4107	D3942	M3793	E3716	E3716
S4792	ASP	K4563	VAL	ARG	GLU	E4107	D3942	M3793	E3717	E3717



• Molecule 1: Ryanodine receptor 1

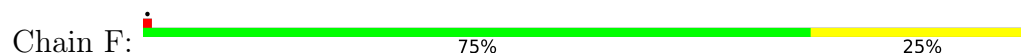




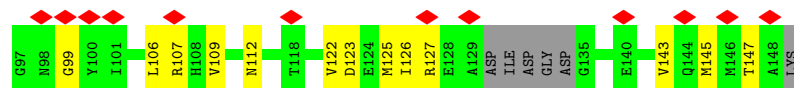
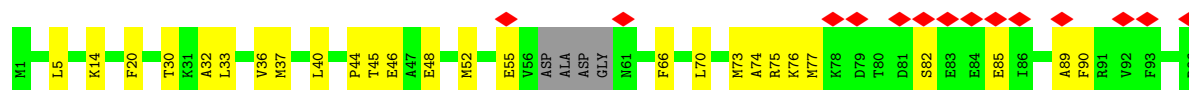
E4168	E4015	K3873	K3731	THR	C3402	P3282	C3170	GLY	VAL	A2913	GLY	GLY
S4169	L4016	V3874	E3736	HIS	R3403	P3289	S3174	LEU	SER	K2914	ARG	GLY
R4175	L4017	D3878	E3737	LYS	P3410	P3292	P3188	ARG	SER	E2915	PHE	N2856
L4181	Q4020	F3879	L3514	Q3627	E3426	P3293	P3189	GLY	VAL	K2916	GLY	P2857
N4194	K4021	F3880	K3515	R3628	P3427	P3294	L3190	VAL	GLY	A2917	GLY	Q2858
N4194	S4029	Q3889	K3516	R3629	E3432	A3295	C3193	VAL	LYS	R2918	SER	P2859
R4189	E4032	N3897	P3519	R3630	E3433	L3296	L3194	VAL	LYS	D2919	SER	P2860
R4190	G4033	D3898	P3527	A3631	L3434	P3297	A3195	VAL	PRO	R2920	HIS	D2861
N4034	N4034	F3899	P3530	V3632	E3454	A3298	P3202	GLY	GLY	E2921	ASP	L2862
V4035	V4035	Q3900	Q3530	V3633	E3455	A3300	P3206	GLY	GLY	Q2924	GLY	S2863
Q4038	Q4038	N3901	P3533	F3637	Q3456	P3301	L3206	GLY	GLY	E2925	GLY	G2864
R4042	R4042	R3904	L3533	M3638	V3460	P3302	P3207	LYS	GLY	L2926	VAL	V2865
S4051	S4051	N3909	M3534	T3639	Q3461	P3303	P3208	VAL	VAL	L2927	GLY	T2866
L4218	L4218	T3910	L3535	R3648	N3462	H3311	Q3209	ASN	ASN	K2928	GLY	L2867
F4219	L4066	M3652	K3537	M3652	S3468	L3327	Y3213	LEU	ARG	F2929	GLY	S2868
D4220	L4071	S3656	S3566	S3656	PHE	E3331	N3214	ARG	ARG	L2930	GLY	R2869
G4225	T3919	P3567	P3567	S3656	THR	A3332	A3215	LEU	GLY	Q2931	GLY	E2870
E4227	N3921	S3568	S3568	S3658	ALA	T3333	C3216	LYS	LYS	M2932	VAL	L2871
A4228	Y3922	F3659	V3571	F3659	ASP	K3336	S3217	VAL	SER	N2933	VAL	Q2872
V4235	L3923	O3670	L3575	O3670	SER	R3337	V3218	SER	GLN	G2934	GLY	A2873
L4242	L3924	R3672	L3576	R3672	LYS	L3338	P3224	ALA	ALA	Y2935	GLY	N2874
I4251	S3929	D3675	L3579	D3675	LYS	Q3343	L3232	THR	THR	A2936	GLY	A2875
S4252	D3932	S3678	P3580	S3678	ALA	P3344	P3233	GLN	GLN	V2937	GLY	E2876
GLY	D3941	K3679	G3581	K3679	ALA	R3350	V3236	VAL	VAL	T2938	LEU	Q2877
PRD	V3942	K3679	R3582	K3679	ALA	P3351	GLY	VAL	VAL	R2939	GLY	L2878
GLY	F3951	E3684	E3583	E3684	GLY	S3556	GLY	VAL	VAL	GLY	LYS	A2879
GLY	N3955	E3685	E3584	E3685	ASP	S3556	GLY	VAL	ASN	LEU	LYS	E2880
PRD	M3955	E3686	E3585	E3686	GLN	P3360	GLY	VAL	ASN	ASP	GLY	N2881
ALA	V3961	E3687	D3587	E3687	SER	T3361	GLY	GLY	CYS	GLY	GLY	Y2882
ASP	E3967	E3688	P3589	E3688	GLY	I3362	P3241	THR	THR	GLY	THR	H2883
ASP	G3971	E3689	L3592	E3689	SER	G3363	P3244	THR	THR	L2946	THR	N2884
GLY	P3972	V3690	V3593	V3690	ASP	K3367	V3246	THR	ALA	S2950	THR	T2885
GLY	T3974	E3691	R3594	E3691	GLN	V3372	R3248	THR	ALA	I2951	ALA	W2886
GLY	N3976	E3692	E3598	E3692	THR	E3376	G3254	THR	ARG	E2952	ARG	G2887
GLY	Q3978	D3696	A3601	D3696	LYS	L3381	GLY	THR	ARG	K2953	LEU	R2888
ALA	V3990	H3699	T3609	H3699	LYS	A3387	ALA	THR	THR	R2954	ALA	K2889
ALA	L4003	L3701	E3610	L3701	ARG	E3391	ALA	THR	THR	F2955	ARG	K2890
GLY	L4012	V3702	H3611	V3702	GLY	L3392	GLY	THR	VAL	F2957	VAL	Q2891
GLY	L4012	L3703	P3612	L3703	ASP	L3393	SER	THR	VAL	G2958	LYS	E2892
ALA	L4012	K3713	Y3613	K3713	ARG	V3394	GLY	THR	LYS	F2959	GLY	E2893
ALA	L4012	E3718	LYS	E3718	THR	R3395	GLY	THR	GLY	L2960	SER	L2894
ALA	L4012	Y3725	SER	Y3725	THR	L3401	GLY	THR	GLY	L2963	GLY	E2895
ALA	L4012	N3870	LYS	N3870	THR	L3401	GLY	THR	GLY	L2964	PRO	A2896
ALA	L4012	N3870	LYS	N3870	THR	L3401	GLY	THR	GLY	L2965	GLY	A2897
ALA	L4012	N3870	LYS	N3870	THR	L3401	GLY	THR	GLY	W2966	ILE	K2897
ALA	L4012	N3870	LYS	N3870	THR	L3401	GLY	THR	GLY	W2966	VAL	G2898
ALA	L4012	N3870	LYS	N3870	THR	L3401	GLY	THR	GLY	S2970	LYS	G2899
ALA	L4012	N3870	LYS	N3870	THR	L3401	GLY	THR	GLY	A2975	ALA	G2900
ALA	L4012	N3870	LYS	N3870	THR	L3401	GLY	THR	GLY	H2976	ALA	T2901
ALA	L4012	N3870	LYS	N3870	THR	L3401	GLY	THR	GLY	LEU	GLY	H2902
ALA	L4012	N3870	LYS	N3870	THR	L3401	GLY	THR	GLY	LEU	GLY	P2903
ALA	L4012	N3870	LYS	N3870	THR	L3401	GLY	THR	GLY	ALA	ALA	L2904
ALA	L4012	N3870	LYS	N3870	THR	L3401	GLY	THR	GLY	ALA	ALA	L2905
ALA	L4012	N3870	LYS	N3870	THR	L3401	GLY	THR	GLY	ALA	ALA	V2906
ALA	L4012	N3870	LYS	N3870	THR	L3401	GLY	THR	GLY	ALA	ALA	P2907
ALA	L4012	N3870	LYS	N3870	THR	L3401	GLY	THR	GLY	ALA	ALA	Y2908
ALA	L4012	N3870	LYS	N3870	THR	L3401	GLY	THR	GLY	ALA	ALA	D2909
ALA	L4012	N3870	LYS	N3870	THR	L3401	GLY	THR	GLY	ALA	ALA	T2910
ALA	L4012	N3870	LYS	N3870	THR	L3401	GLY	THR	GLY	ALA	ALA	L2911
ALA	L4012	N3870	LYS	N3870	THR	L3401	GLY	THR	GLY	ALA	ALA	T2912



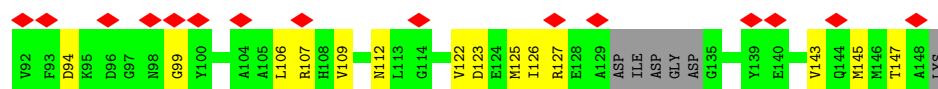
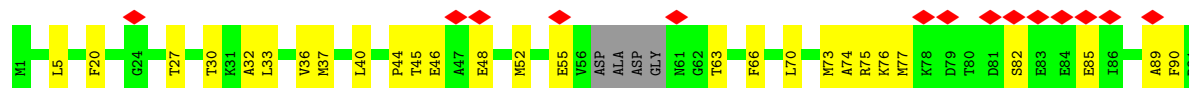
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



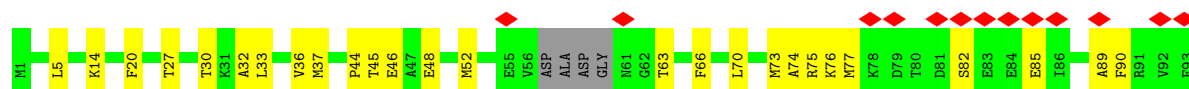
- Molecule 3: Calmodulin-1



- Molecule 3: Calmodulin-1

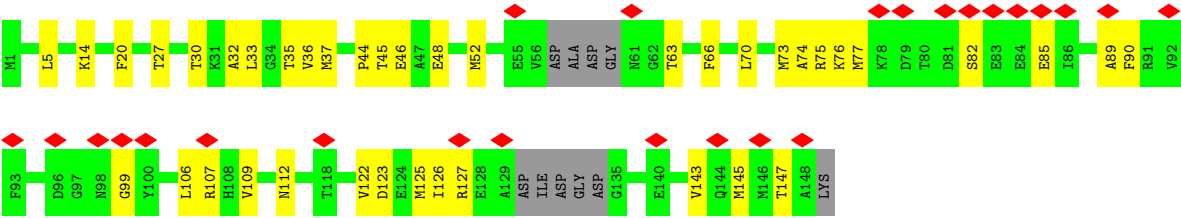


- Molecule 3: Calmodulin-1



- Molecule 3: Calmodulin-1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28189	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.354	Depositor
Minimum map value	-0.808	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.135	Depositor
Map size (Å)	502.80002, 502.80002, 502.80002	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0475, 1.0475, 1.0475	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.44	17/29778 (0.1%)	0.77	106/40610 (0.3%)
1	B	0.45	17/29778 (0.1%)	0.77	106/40610 (0.3%)
1	C	0.45	17/29778 (0.1%)	0.77	109/40610 (0.3%)
1	D	0.45	17/29778 (0.1%)	0.77	109/40610 (0.3%)
2	E	0.15	0/820	0.43	0/1105
2	F	0.15	0/820	0.43	0/1105
2	G	0.15	0/820	0.43	0/1105
2	H	0.15	0/820	0.43	0/1105
3	I	0.16	0/1042	0.42	0/1404
3	J	0.16	0/1042	0.42	0/1404
3	K	0.16	0/1042	0.42	0/1404
3	L	0.16	0/1042	0.42	0/1404
All	All	0.43	68/126560 (0.1%)	0.76	430/172476 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	8
1	C	0	7
1	D	0	7
All	All	0	29

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	4910	GLU	CA-C	-8.54	1.45	1.52
1	C	4910	GLU	CA-C	-8.54	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	855	PRO	CG-CD	-7.94	1.23	1.50
1	C	855	PRO	CG-CD	-7.94	1.23	1.50
1	A	855	PRO	CG-CD	-7.93	1.23	1.50
1	B	855	PRO	CG-CD	-7.93	1.23	1.50
1	A	4910	GLU	CA-C	-7.23	1.45	1.53
1	D	4910	GLU	CA-C	-7.20	1.45	1.53
1	B	4897	ILE	CA-C	-6.59	1.44	1.52
1	A	4897	ILE	CA-C	-6.58	1.44	1.52
1	D	4897	ILE	CA-C	-6.57	1.44	1.52
1	C	4897	ILE	CA-C	-6.54	1.44	1.52
1	C	5012	LYS	CA-C	-6.47	1.44	1.52
1	A	1563	GLN	C-O	-6.47	1.15	1.24
1	C	1563	GLN	C-O	-6.47	1.15	1.24
1	B	1563	GLN	C-O	-6.47	1.15	1.24
1	A	5012	LYS	CA-C	-6.45	1.44	1.52
1	D	1563	GLN	C-O	-6.44	1.15	1.24
1	D	5012	LYS	CA-C	-6.44	1.44	1.52
1	B	5012	LYS	CA-C	-6.38	1.44	1.52
1	D	1484	HIS	N-CA	-6.32	1.36	1.45
1	C	1484	HIS	N-CA	-6.31	1.36	1.45
1	A	1484	HIS	N-CA	-6.28	1.36	1.45
1	B	1484	HIS	N-CA	-6.28	1.36	1.45
1	A	5004	THR	CA-C	-6.21	1.44	1.52
1	B	5004	THR	CA-C	-6.21	1.44	1.52
1	D	5004	THR	CA-C	-6.20	1.44	1.52
1	C	5004	THR	CA-C	-6.18	1.44	1.52
1	A	4791	TYR	CA-C	-6.02	1.44	1.52
1	D	4791	TYR	CA-C	-6.02	1.44	1.52
1	C	4791	TYR	CA-C	-6.01	1.44	1.52
1	B	4791	TYR	CA-C	-6.01	1.44	1.52
1	D	1484	HIS	CA-CB	-6.01	1.45	1.54
1	A	1484	HIS	CA-CB	-6.01	1.45	1.54
1	C	1484	HIS	CA-CB	-6.01	1.45	1.54
1	B	1484	HIS	CA-CB	-6.01	1.45	1.54
1	D	1549	PHE	C-O	-5.89	1.16	1.24
1	A	1549	PHE	C-O	-5.85	1.16	1.24
1	C	1549	PHE	C-O	-5.85	1.16	1.24
1	B	1549	PHE	C-O	-5.85	1.16	1.24
1	D	4824	ARG	N-CA	-5.67	1.39	1.46
1	A	4824	ARG	N-CA	-5.59	1.39	1.46
1	C	4824	ARG	N-CA	-5.59	1.39	1.46
1	B	4824	ARG	N-CA	-5.59	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4812	HIS	C-O	5.43	1.31	1.24
1	B	4812	HIS	C-O	5.43	1.31	1.24
1	C	4812	HIS	C-O	5.42	1.31	1.24
1	D	4812	HIS	C-O	5.38	1.31	1.24
1	A	5011	TRP	CA-C	-5.37	1.46	1.52
1	C	5011	TRP	CA-C	-5.37	1.46	1.52
1	B	5011	TRP	CA-C	-5.37	1.46	1.52
1	D	5011	TRP	CA-C	-5.37	1.46	1.52
1	D	4994	TYR	CA-C	-5.32	1.46	1.53
1	C	4994	TYR	CA-C	-5.31	1.46	1.53
1	A	4994	TYR	CA-C	-5.29	1.46	1.53
1	B	4994	TYR	CA-C	-5.29	1.46	1.53
1	D	1573	MET	CA-C	-5.29	1.46	1.52
1	C	1573	MET	CA-C	-5.27	1.46	1.52
1	A	1573	MET	CA-C	-5.22	1.46	1.52
1	B	1573	MET	CA-C	-5.22	1.46	1.52
1	A	4651	THR	N-CA	5.19	1.52	1.46
1	C	4651	THR	N-CA	5.19	1.52	1.46
1	B	4651	THR	N-CA	5.19	1.52	1.46
1	D	4651	THR	N-CA	5.18	1.52	1.46
1	A	4824	ARG	C-O	-5.11	1.18	1.24
1	C	4824	ARG	C-O	-5.11	1.18	1.24
1	B	4824	ARG	C-O	-5.11	1.18	1.24
1	D	4824	ARG	C-O	-5.03	1.18	1.24

All (430) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4791	TYR	N-CA-C	-14.66	93.74	114.12
1	D	4791	TYR	N-CA-C	-14.65	93.75	114.12
1	C	4791	TYR	N-CA-C	-14.65	93.75	114.12
1	B	4791	TYR	N-CA-C	-14.65	93.75	114.12
1	D	4949	GLN	N-CA-C	-12.57	96.63	112.72
1	A	4949	GLN	N-CA-C	-12.56	96.64	112.72
1	C	4949	GLN	N-CA-C	-12.56	96.64	112.72
1	B	4949	GLN	N-CA-C	-12.56	96.64	112.72
1	A	4954	MET	N-CA-C	-11.65	96.05	110.61
1	B	4954	MET	N-CA-C	-11.65	96.05	110.61
1	C	4954	MET	N-CA-C	-11.64	96.06	110.61
1	D	4954	MET	N-CA-C	-11.62	96.08	110.61
1	D	3244	PRO	N-CA-CB	11.49	110.51	102.35
1	A	3244	PRO	N-CA-CB	11.49	110.51	102.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3244	PRO	N-CA-CB	11.49	110.51	102.35
1	B	3244	PRO	N-CA-CB	11.45	110.48	102.35
1	D	4557	ARG	N-CA-C	-10.66	99.01	113.18
1	C	4557	ARG	N-CA-C	-10.64	99.03	113.18
1	B	4557	ARG	N-CA-C	-10.64	99.03	113.18
1	A	4557	ARG	N-CA-C	-10.64	99.03	113.18
1	C	4542	GLY	N-CA-C	-10.57	100.04	112.73
1	A	4542	GLY	N-CA-C	-10.55	100.07	112.73
1	D	4542	GLY	N-CA-C	-10.54	100.08	112.73
1	B	4542	GLY	N-CA-C	-10.53	100.09	112.73
1	A	855	PRO	N-CD-CG	-10.06	88.11	103.20
1	B	855	PRO	N-CD-CG	-10.06	88.11	103.20
1	D	855	PRO	N-CD-CG	-10.04	88.14	103.20
1	C	855	PRO	N-CD-CG	-10.04	88.15	103.20
1	D	4795	TYR	N-CA-C	-9.88	99.54	112.68
1	A	4795	TYR	N-CA-C	-9.86	99.56	112.68
1	B	4795	TYR	N-CA-C	-9.86	99.56	112.68
1	C	4795	TYR	N-CA-C	-9.86	99.57	112.68
1	A	4798	MET	N-CA-C	-9.28	101.52	113.12
1	C	4798	MET	N-CA-C	-9.27	101.53	113.12
1	D	4798	MET	N-CA-C	-9.26	101.54	113.12
1	B	4798	MET	N-CA-C	-9.24	101.57	113.12
1	D	5012	LYS	N-CA-C	-9.23	100.41	112.41
1	B	5012	LYS	N-CA-C	-9.23	100.41	112.41
1	A	5012	LYS	N-CA-C	-9.22	100.43	112.41
1	C	5012	LYS	N-CA-C	-9.19	100.47	112.41
1	B	1549	PHE	CB-CA-C	-8.96	95.44	108.88
1	A	1549	PHE	CB-CA-C	-8.94	95.47	108.88
1	C	1549	PHE	CB-CA-C	-8.94	95.47	108.88
1	D	1549	PHE	CB-CA-C	-8.94	95.48	108.88
1	A	4994	TYR	N-CA-C	-8.93	99.19	112.04
1	B	4994	TYR	N-CA-C	-8.93	99.19	112.04
1	C	4994	TYR	N-CA-C	-8.91	99.21	112.04
1	D	4994	TYR	N-CA-C	-8.90	99.22	112.04
1	B	4813	LEU	N-CA-C	-8.86	101.57	112.38
1	C	4813	LEU	N-CA-C	-8.84	101.60	112.38
1	A	4813	LEU	N-CA-C	-8.78	101.67	112.38
1	D	4813	LEU	N-CA-C	-8.40	102.79	112.87
1	C	5016	GLU	N-CA-C	-8.34	99.57	110.33
1	A	5016	GLU	N-CA-C	-8.33	99.58	110.33
1	D	5016	GLU	N-CA-C	-8.33	99.58	110.33
1	B	5016	GLU	N-CA-C	-8.33	99.58	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	5014	TYR	N-CA-C	-8.22	93.29	110.80
1	A	5014	TYR	N-CA-C	-8.21	93.30	110.80
1	B	5014	TYR	N-CA-C	-8.20	93.34	110.80
1	C	5014	TYR	N-CA-C	-8.20	93.34	110.80
1	A	5016	GLU	CA-C-N	-8.13	111.24	122.95
1	A	5016	GLU	C-N-CA	-8.13	111.24	122.95
1	C	5016	GLU	CA-C-N	-8.13	111.24	122.95
1	C	5016	GLU	C-N-CA	-8.13	111.24	122.95
1	D	5016	GLU	CA-C-N	-8.13	111.25	122.95
1	D	5016	GLU	C-N-CA	-8.13	111.25	122.95
1	B	5016	GLU	CA-C-N	-8.11	111.28	122.95
1	B	5016	GLU	C-N-CA	-8.11	111.28	122.95
1	D	3301	PRO	N-CA-CB	8.10	110.94	103.08
1	A	3301	PRO	N-CA-CB	8.07	110.91	103.08
1	B	3301	PRO	N-CA-CB	8.07	110.91	103.08
1	C	3301	PRO	N-CA-CB	8.03	110.87	103.08
1	A	3293	PRO	N-CA-CB	8.00	110.84	103.08
1	C	3293	PRO	N-CA-CB	8.00	110.84	103.08
1	B	3293	PRO	N-CA-CB	8.00	110.84	103.08
1	D	3293	PRO	N-CA-CB	7.99	110.83	103.08
1	D	4657	MET	N-CA-C	-7.93	102.71	111.36
1	D	3292	PRO	N-CA-CB	7.93	110.77	103.08
1	A	4657	MET	N-CA-C	-7.91	102.74	111.36
1	C	4657	MET	N-CA-C	-7.91	102.74	111.36
1	B	4815	ASP	N-CA-C	-7.90	104.12	114.31
1	B	4657	MET	N-CA-C	-7.90	102.75	111.36
1	B	3302	PRO	N-CA-CB	7.89	110.74	103.08
1	B	3292	PRO	N-CA-CB	7.89	110.74	103.08
1	A	3292	PRO	N-CA-CB	7.88	110.72	103.08
1	A	3302	PRO	N-CA-CB	7.88	110.72	103.08
1	C	3302	PRO	N-CA-CB	7.88	110.72	103.08
1	D	3302	PRO	N-CA-CB	7.87	110.72	103.08
1	A	4815	ASP	N-CA-C	-7.87	104.16	114.31
1	C	3527	PRO	N-CA-CB	7.87	110.67	103.20
1	B	3527	PRO	N-CA-CB	7.87	110.67	103.20
1	C	3292	PRO	N-CA-CB	7.86	110.70	103.08
1	C	4815	ASP	N-CA-C	-7.85	104.18	114.31
1	A	3527	PRO	N-CA-CB	7.83	110.64	103.20
1	A	4898	GLY	N-CA-C	-7.82	94.65	113.18
1	D	4991	PHE	N-CA-C	-7.82	102.35	111.03
1	C	4898	GLY	N-CA-C	-7.82	94.65	113.18
1	D	4898	GLY	N-CA-C	-7.81	94.67	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4898	GLY	N-CA-C	-7.81	94.67	113.18
1	A	4991	PHE	N-CA-C	-7.80	102.37	111.03
1	C	4991	PHE	N-CA-C	-7.80	102.37	111.03
1	B	4991	PHE	N-CA-C	-7.80	102.38	111.03
1	D	3527	PRO	N-CA-CB	7.80	110.61	103.20
1	C	3303	PRO	N-CA-CB	7.73	110.54	103.20
1	A	3303	PRO	N-CA-CB	7.72	110.53	103.20
1	B	3303	PRO	N-CA-CB	7.72	110.53	103.20
1	D	3303	PRO	N-CA-CB	7.67	110.49	103.20
1	C	1549	PHE	CA-C-N	7.64	127.63	119.76
1	C	1549	PHE	C-N-CA	7.64	127.63	119.76
1	D	3612	PRO	N-CA-CB	7.63	110.55	103.46
1	C	3612	PRO	N-CA-CB	7.61	110.54	103.46
1	D	1549	PHE	CA-C-N	7.61	127.60	119.76
1	D	1549	PHE	C-N-CA	7.61	127.60	119.76
1	A	1549	PHE	CA-C-N	7.61	127.59	119.76
1	A	1549	PHE	C-N-CA	7.61	127.59	119.76
1	A	3612	PRO	N-CA-CB	7.60	110.53	103.46
1	B	1549	PHE	CA-C-N	7.58	127.56	119.76
1	B	1549	PHE	C-N-CA	7.58	127.56	119.76
1	B	3612	PRO	N-CA-CB	7.58	110.51	103.46
1	D	3297	PRO	N-CA-CB	7.57	110.52	103.41
1	D	3589	PRO	N-CA-CB	7.54	110.75	103.51
1	D	5007	GLU	N-CA-C	-7.54	103.93	113.43
1	C	5007	GLU	N-CA-C	-7.54	103.94	113.43
1	A	3589	PRO	N-CA-CB	7.53	110.74	103.51
1	C	3589	PRO	N-CA-CB	7.53	110.74	103.51
1	B	3589	PRO	N-CA-CB	7.53	110.74	103.51
1	A	2567	PRO	N-CA-CB	7.52	110.73	103.51
1	C	2567	PRO	N-CA-CB	7.52	110.73	103.51
1	D	2567	PRO	N-CA-CB	7.52	110.73	103.51
1	A	5007	GLU	N-CA-C	-7.51	103.97	113.43
1	B	5007	GLU	N-CA-C	-7.51	103.97	113.43
1	A	3297	PRO	N-CA-CB	7.50	110.47	103.41
1	C	3297	PRO	N-CA-CB	7.50	110.47	103.41
1	D	2640	PRO	N-CA-CB	7.50	110.44	103.46
1	B	2567	PRO	N-CA-CB	7.50	110.71	103.51
1	B	3297	PRO	N-CA-CB	7.49	110.45	103.41
1	A	2640	PRO	N-CA-CB	7.49	110.42	103.46
1	B	2640	PRO	N-CA-CB	7.47	110.40	103.46
1	A	3224	PRO	N-CA-CB	7.46	110.67	103.51
1	C	3224	PRO	N-CA-CB	7.46	110.67	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3224	PRO	N-CA-CB	7.46	110.67	103.51
1	B	3224	PRO	N-CA-CB	7.45	110.66	103.51
1	C	2640	PRO	N-CA-CB	7.43	110.37	103.46
1	B	2528	PRO	N-CA-CB	7.34	110.56	103.51
1	D	2616	PRO	N-CA-CB	7.34	110.96	103.25
1	A	4824	ARG	N-CA-C	-7.34	103.36	111.36
1	B	4824	ARG	N-CA-C	-7.34	103.36	111.36
1	C	2528	PRO	N-CA-CB	7.33	110.54	103.51
1	C	4824	ARG	N-CA-C	-7.33	103.38	111.36
1	D	4824	ARG	N-CA-C	-7.32	103.38	111.36
1	A	2528	PRO	N-CA-CB	7.32	110.54	103.51
1	C	2616	PRO	N-CA-CB	7.31	110.92	103.25
1	A	2616	PRO	N-CA-CB	7.30	110.91	103.25
1	B	2616	PRO	N-CA-CB	7.30	110.91	103.25
1	B	3188	PRO	N-CA-CB	7.29	110.90	103.25
1	D	3188	PRO	N-CA-CB	7.28	110.89	103.25
1	C	3188	PRO	N-CA-CB	7.28	110.89	103.25
1	C	3267	PRO	N-CA-CB	7.27	110.88	103.25
1	D	2528	PRO	N-CA-CB	7.26	110.48	103.51
1	A	3188	PRO	N-CA-CB	7.25	110.86	103.25
1	B	3267	PRO	N-CA-CB	7.25	110.86	103.25
1	D	3267	PRO	N-CA-CB	7.24	110.86	103.25
1	A	3267	PRO	N-CA-CB	7.24	110.85	103.25
1	C	3360	PRO	N-CA-CB	7.20	110.81	103.25
1	A	3360	PRO	N-CA-CB	7.17	110.78	103.25
1	B	3360	PRO	N-CA-CB	7.17	110.78	103.25
1	A	3202	PRO	N-CA-CB	7.15	110.76	103.25
1	B	3202	PRO	N-CA-CB	7.15	110.76	103.25
1	D	3202	PRO	N-CA-CB	7.15	110.75	103.25
1	B	3351	PRO	N-CA-CB	7.15	110.75	103.25
1	A	3351	PRO	N-CA-CB	7.14	110.75	103.25
1	C	3351	PRO	N-CA-CB	7.14	110.75	103.25
1	D	3360	PRO	N-CA-CB	7.13	110.73	103.25
1	C	3202	PRO	N-CA-CB	7.12	110.73	103.25
1	D	3275	PRO	N-CA-CB	7.12	111.07	103.52
1	C	3275	PRO	N-CA-CB	7.12	111.07	103.52
1	A	3275	PRO	N-CA-CB	7.12	111.06	103.52
1	D	3351	PRO	N-CA-CB	7.11	110.71	103.25
1	B	3062	PRO	N-CA-CB	7.11	110.71	103.25
1	B	3344	PRO	N-CA-CB	7.11	110.63	102.88
1	A	3344	PRO	N-CA-CB	7.10	110.62	102.88
1	D	3138	PRO	N-CA-CB	7.09	110.69	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3062	PRO	N-CA-CB	7.09	110.69	103.25
1	C	3344	PRO	N-CA-CB	7.09	110.60	102.88
1	B	3275	PRO	N-CA-CB	7.08	111.03	103.52
1	D	3062	PRO	N-CA-CB	7.08	110.69	103.25
1	D	3344	PRO	N-CA-CB	7.08	110.60	102.88
1	A	3138	PRO	N-CA-CB	7.07	110.67	103.25
1	C	3138	PRO	N-CA-CB	7.07	110.67	103.25
1	C	3062	PRO	N-CA-CB	7.05	110.65	103.25
1	B	3138	PRO	N-CA-CB	7.04	110.64	103.25
1	D	2701	PRO	N-CA-CB	7.03	110.64	103.25
1	D	3004	PRO	N-CA-CB	7.03	110.64	103.25
1	A	3233	PRO	N-CA-CB	7.03	110.63	103.25
1	B	3233	PRO	N-CA-CB	7.03	110.63	103.25
1	B	3580	PRO	N-CA-CB	7.03	110.63	103.25
1	B	4910	GLU	N-CA-C	-7.01	102.52	112.13
1	A	2701	PRO	N-CA-CB	7.01	110.61	103.25
1	D	3233	PRO	N-CA-CB	7.00	110.60	103.25
1	C	3233	PRO	N-CA-CB	7.00	110.60	103.25
1	A	2560	PRO	N-CA-CB	7.00	110.60	103.25
1	C	2560	PRO	N-CA-CB	7.00	110.60	103.25
1	B	2560	PRO	N-CA-CB	7.00	110.59	103.25
1	C	3580	PRO	N-CA-CB	7.00	110.59	103.25
1	B	2701	PRO	N-CA-CB	7.00	110.59	103.25
1	A	3580	PRO	N-CA-CB	6.99	110.59	103.25
1	C	3567	PRO	N-CA-CB	6.99	110.59	103.25
1	C	4910	GLU	N-CA-C	-6.99	102.55	112.13
1	A	3004	PRO	N-CA-CB	6.99	110.59	103.25
1	A	3427	PRO	N-CA-CB	6.99	110.59	103.25
1	C	3004	PRO	N-CA-CB	6.99	110.59	103.25
1	C	3427	PRO	N-CA-CB	6.99	110.59	103.25
1	B	3004	PRO	N-CA-CB	6.99	110.59	103.25
1	D	3427	PRO	N-CA-CB	6.98	110.58	103.25
1	C	2701	PRO	N-CA-CB	6.98	110.58	103.25
1	A	3294	PRO	N-CA-CB	6.98	110.58	103.25
1	B	3294	PRO	N-CA-CB	6.98	110.58	103.25
1	D	3294	PRO	N-CA-CB	6.97	110.57	103.25
1	A	3567	PRO	N-CA-CB	6.97	110.57	103.25
1	B	3567	PRO	N-CA-CB	6.97	110.57	103.25
1	D	2560	PRO	N-CA-CB	6.97	110.56	103.25
1	C	3294	PRO	N-CA-CB	6.97	110.57	103.25
1	A	2496	PRO	N-CA-CB	6.96	110.56	103.25
1	C	2496	PRO	N-CA-CB	6.96	110.56	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2496	PRO	N-CA-CB	6.96	110.56	103.25
1	B	3427	PRO	N-CA-CB	6.95	110.55	103.25
1	C	4885	PHE	N-CA-C	-6.95	104.67	113.43
1	D	3580	PRO	N-CA-CB	6.95	110.55	103.25
1	D	3567	PRO	N-CA-CB	6.94	110.54	103.25
1	B	2496	PRO	N-CA-CB	6.94	110.54	103.25
1	D	4835	LYS	N-CA-C	-6.94	102.05	112.04
1	D	4903	ASP	CA-C-N	-6.92	111.19	119.84
1	D	4903	ASP	C-N-CA	-6.92	111.19	119.84
1	A	4835	LYS	N-CA-C	-6.92	102.08	112.04
1	C	4903	ASP	CA-C-N	-6.92	111.19	119.84
1	C	4903	ASP	C-N-CA	-6.92	111.19	119.84
1	A	4903	ASP	CA-C-N	-6.92	111.20	119.84
1	A	4903	ASP	C-N-CA	-6.92	111.20	119.84
1	B	4835	LYS	N-CA-C	-6.91	102.09	112.04
1	D	3289	PRO	N-CA-CB	6.91	110.50	103.25
1	C	4835	LYS	N-CA-C	-6.90	102.10	112.04
1	D	5006	GLN	N-CA-C	-6.89	104.18	112.59
1	B	4903	ASP	CA-C-N	-6.89	111.23	119.84
1	B	4903	ASP	C-N-CA	-6.89	111.23	119.84
1	A	3289	PRO	N-CA-CB	6.88	110.48	103.25
1	C	3289	PRO	N-CA-CB	6.88	110.48	103.25
1	B	3289	PRO	N-CA-CB	6.88	110.48	103.25
1	B	5006	GLN	N-CA-C	-6.87	104.21	112.59
1	D	4885	PHE	N-CA-C	-6.87	104.78	113.43
1	C	2658	PRO	N-CA-CB	6.86	110.79	103.52
1	B	3241	PRO	N-CA-CB	6.85	110.53	103.00
1	C	3021	PRO	N-CA-CB	6.83	110.43	103.25
1	A	3241	PRO	N-CA-CB	6.83	110.51	103.00
1	D	3241	PRO	N-CA-CB	6.83	110.51	103.00
1	D	2658	PRO	N-CA-CB	6.83	110.75	103.52
1	A	2658	PRO	N-CA-CB	6.82	110.75	103.52
1	B	2658	PRO	N-CA-CB	6.82	110.75	103.52
1	C	3282	PRO	N-CA-CB	6.80	111.06	103.44
1	C	3241	PRO	N-CA-CB	6.80	110.48	103.00
1	A	3021	PRO	N-CA-CB	6.79	110.38	103.25
1	B	3021	PRO	N-CA-CB	6.78	110.37	103.25
1	D	3021	PRO	N-CA-CB	6.77	110.36	103.25
1	D	3282	PRO	N-CA-CB	6.77	111.03	103.44
1	A	3282	PRO	N-CA-CB	6.77	111.02	103.44
1	D	4815	ASP	N-CA-C	-6.77	105.18	113.50
1	B	3282	PRO	N-CA-CB	6.74	110.99	103.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5006	GLN	N-CA-C	-6.74	104.19	112.88
1	C	5006	GLN	N-CA-C	-6.71	104.22	112.88
1	D	4910	GLU	N-CA-C	-6.71	102.50	111.96
1	A	4910	GLU	N-CA-C	-6.69	102.52	111.96
1	D	3519	PRO	N-CA-CB	6.69	110.61	103.52
1	A	2488	PRO	N-CA-CB	6.67	110.46	102.72
1	B	2488	PRO	N-CA-CB	6.67	110.46	102.72
1	A	3519	PRO	N-CA-CB	6.67	110.59	103.52
1	B	3519	PRO	N-CA-CB	6.67	110.59	103.52
1	C	2488	PRO	N-CA-CB	6.66	110.45	102.72
1	C	3519	PRO	N-CA-CB	6.66	110.58	103.52
1	D	2488	PRO	N-CA-CB	6.64	110.42	102.72
1	A	3410	PRO	N-CA-CB	6.61	110.85	103.44
1	C	3410	PRO	N-CA-CB	6.61	110.85	103.44
1	D	3410	PRO	N-CA-CB	6.60	110.83	103.44
1	B	4960	ILE	N-CA-C	-6.60	105.89	111.56
1	B	3410	PRO	N-CA-CB	6.59	110.82	103.44
1	C	3208	PRO	N-CA-CB	6.56	110.79	103.44
1	A	5001	THR	O-C-N	6.56	132.01	122.43
1	A	4960	ILE	N-CA-C	-6.56	105.92	111.56
1	C	4960	ILE	N-CA-C	-6.56	105.92	111.56
1	B	5001	THR	O-C-N	6.56	132.00	122.43
1	D	5001	THR	O-C-N	6.54	131.98	122.43
1	C	5001	THR	O-C-N	6.54	131.97	122.43
1	A	3208	PRO	N-CA-CB	6.53	110.76	103.44
1	B	3208	PRO	N-CA-CB	6.53	110.76	103.44
1	D	4960	ILE	N-CA-C	-6.53	105.94	111.56
1	C	4554	TYR	N-CA-C	-6.50	103.41	112.45
1	D	3208	PRO	N-CA-CB	6.50	110.72	103.44
1	B	4554	TYR	N-CA-C	-6.49	103.43	112.45
1	A	4554	TYR	N-CA-C	-6.48	103.44	112.45
1	D	4554	TYR	N-CA-C	-6.47	103.45	112.45
1	B	4885	PHE	N-CA-C	-6.44	104.47	112.72
1	A	4885	PHE	N-CA-C	-6.39	104.54	112.72
1	C	2631	PRO	N-CA-CB	6.39	110.59	103.44
1	D	855	PRO	CA-N-CD	-6.37	103.08	112.00
1	A	855	PRO	CA-N-CD	-6.36	103.09	112.00
1	C	855	PRO	CA-N-CD	-6.36	103.09	112.00
1	B	855	PRO	CA-N-CD	-6.36	103.09	112.00
1	A	2631	PRO	N-CA-CB	6.36	110.56	103.44
1	B	2631	PRO	N-CA-CB	6.34	110.54	103.44
1	D	2631	PRO	N-CA-CB	6.33	110.53	103.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4573	ILE	O-C-N	-6.25	114.75	122.57
1	C	1483	VAL	O-C-N	6.25	128.98	122.54
1	A	4573	ILE	O-C-N	-6.25	114.76	122.57
1	C	4573	ILE	O-C-N	-6.25	114.76	122.57
1	B	4573	ILE	O-C-N	-6.25	114.76	122.57
1	D	4649	LEU	N-CA-C	-6.22	104.12	111.03
1	A	4649	LEU	N-CA-C	-6.22	104.13	111.03
1	B	4649	LEU	N-CA-C	-6.22	104.13	111.03
1	D	4965	SER	N-CA-C	-6.21	105.19	112.89
1	C	4965	SER	N-CA-C	-6.21	105.18	112.89
1	D	1483	VAL	O-C-N	6.21	128.94	122.54
1	A	1483	VAL	O-C-N	6.21	128.93	122.54
1	B	1483	VAL	O-C-N	6.21	128.93	122.54
1	A	4791	TYR	O-C-N	-6.20	115.08	122.27
1	A	4965	SER	N-CA-C	-6.20	105.20	112.89
1	D	4791	TYR	O-C-N	-6.20	115.08	122.27
1	C	4791	TYR	O-C-N	-6.20	115.08	122.27
1	B	4791	TYR	O-C-N	-6.20	115.08	122.27
1	B	4965	SER	N-CA-C	-6.20	105.20	112.89
1	C	4649	LEU	N-CA-C	-6.19	104.16	111.03
1	C	1294	PRO	N-CA-CB	6.17	109.73	103.25
1	B	1294	PRO	N-CA-CB	6.17	109.72	103.25
1	A	1294	PRO	N-CA-CB	6.15	109.70	103.25
1	D	1294	PRO	N-CA-CB	6.12	109.68	103.25
1	C	1484	HIS	N-CA-CB	-6.12	102.90	110.98
1	D	1484	HIS	N-CA-CB	-6.11	102.91	110.98
1	D	5035	GLN	N-CA-C	-6.11	104.93	112.38
1	A	5035	GLN	N-CA-C	-6.10	104.93	112.38
1	B	5035	GLN	N-CA-C	-6.10	104.93	112.38
1	C	5035	GLN	N-CA-C	-6.10	104.94	112.38
1	A	1484	HIS	N-CA-CB	-6.10	102.93	110.98
1	B	1484	HIS	N-CA-CB	-6.10	102.93	110.98
1	D	4719	PHE	N-CA-C	-6.02	104.78	113.21
1	C	4719	PHE	N-CA-C	-6.01	104.80	113.21
1	A	4719	PHE	N-CA-C	-6.00	104.81	113.21
1	B	4719	PHE	N-CA-C	-5.98	104.84	113.21
1	D	1207	ASP	CA-CB-CG	5.96	118.56	112.60
1	C	5003	HIS	N-CA-C	-5.94	101.62	110.23
1	A	5003	HIS	N-CA-C	-5.93	101.63	110.23
1	D	5003	HIS	N-CA-C	-5.91	101.66	110.23
1	B	5003	HIS	N-CA-C	-5.90	101.67	110.23
1	C	4953	ASP	N-CA-C	-5.83	103.60	112.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4953	ASP	N-CA-C	-5.83	103.61	112.99
1	A	4953	ASP	N-CA-C	-5.82	103.62	112.99
1	D	4953	ASP	N-CA-C	-5.78	103.68	112.99
1	D	4789	PHE	N-CA-C	-5.76	104.88	112.72
1	C	1207	ASP	CA-CB-CG	5.76	118.36	112.60
1	A	4789	PHE	N-CA-C	-5.75	104.90	112.72
1	C	4789	PHE	N-CA-C	-5.75	104.90	112.72
1	B	4789	PHE	N-CA-C	-5.75	104.90	112.72
1	A	1207	ASP	CA-CB-CG	5.73	118.33	112.60
1	B	4897	ILE	N-CA-C	-5.71	97.47	109.34
1	C	4897	ILE	N-CA-C	-5.70	97.48	109.34
1	A	5011	TRP	N-CA-C	-5.70	104.19	113.19
1	C	5011	TRP	N-CA-C	-5.70	104.19	113.19
1	B	5011	TRP	N-CA-C	-5.70	104.19	113.19
1	D	4897	ILE	N-CA-C	-5.69	97.50	109.34
1	A	4897	ILE	N-CA-C	-5.69	97.50	109.34
1	D	5011	TRP	N-CA-C	-5.69	104.20	113.19
1	C	1433	TYR	CA-C-N	5.65	130.96	122.99
1	C	1433	TYR	C-N-CA	5.65	130.96	122.99
1	D	4571	PHE	N-CA-C	-5.65	105.65	112.54
1	B	1440	PHE	CB-CA-C	-5.64	99.12	111.71
1	D	1440	PHE	CB-CA-C	-5.64	99.12	111.71
1	A	4571	PHE	N-CA-C	-5.64	105.66	112.54
1	B	4571	PHE	N-CA-C	-5.64	105.66	112.54
1	C	4571	PHE	N-CA-C	-5.64	105.66	112.54
1	A	1440	PHE	CB-CA-C	-5.63	99.15	111.71
1	A	4809	PHE	N-CA-C	-5.63	106.39	113.20
1	C	1440	PHE	CB-CA-C	-5.63	99.15	111.71
1	C	4809	PHE	N-CA-C	-5.63	106.39	113.20
1	B	4809	PHE	N-CA-C	-5.63	106.39	113.20
1	B	1433	TYR	CA-C-N	5.63	130.93	122.99
1	B	1433	TYR	C-N-CA	5.63	130.93	122.99
1	A	1433	TYR	CA-C-N	5.62	130.92	122.99
1	A	1433	TYR	C-N-CA	5.62	130.92	122.99
1	A	855	PRO	CA-CB-CG	-5.62	93.82	104.50
1	B	855	PRO	CA-CB-CG	-5.62	93.82	104.50
1	A	4810	ALA	N-CA-C	5.62	118.17	111.71
1	D	4809	PHE	N-CA-C	-5.61	106.41	113.20
1	D	855	PRO	CA-CB-CG	-5.61	93.84	104.50
1	C	855	PRO	CA-CB-CG	-5.61	93.84	104.50
1	A	1548	LEU	O-C-N	-5.58	116.88	123.41
1	C	1548	LEU	O-C-N	-5.58	116.88	123.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1548	LEU	O-C-N	-5.58	116.88	123.41
1	D	1433	TYR	CA-C-N	5.58	130.86	122.99
1	D	1433	TYR	C-N-CA	5.58	130.86	122.99
1	D	1548	LEU	O-C-N	-5.58	116.89	123.41
1	D	4561	THR	N-CA-C	-5.48	105.22	111.14
1	D	4810	ALA	N-CA-C	5.47	118.00	111.71
1	B	4810	ALA	N-CA-C	5.47	118.00	111.71
1	C	4810	ALA	N-CA-C	5.46	117.99	111.71
1	A	4561	THR	N-CA-C	-5.46	105.25	111.14
1	C	4561	THR	N-CA-C	-5.46	105.25	111.14
1	B	4561	THR	N-CA-C	-5.46	105.25	111.14
1	B	3311	HIS	CB-CA-C	-5.41	110.32	116.54
1	A	3311	HIS	CB-CA-C	-5.41	110.32	116.54
1	C	3311	HIS	CB-CA-C	-5.41	110.32	116.54
1	C	4790	LEU	N-CA-C	-5.40	104.60	113.50
1	B	4790	LEU	N-CA-C	-5.40	104.60	113.50
1	A	4790	LEU	N-CA-C	-5.39	104.60	113.50
1	D	4790	LEU	N-CA-C	-5.39	104.60	113.50
1	B	1207	ASP	CA-CB-CG	5.38	117.98	112.60
1	D	3311	HIS	CB-CA-C	-5.37	110.37	116.54
1	C	4959	PHE	CA-C-N	-5.35	117.67	123.08
1	C	4959	PHE	C-N-CA	-5.35	117.67	123.08
1	A	4959	PHE	CA-C-N	-5.35	117.68	123.08
1	A	4959	PHE	C-N-CA	-5.35	117.68	123.08
1	B	4959	PHE	CA-C-N	-5.34	117.68	123.08
1	B	4959	PHE	C-N-CA	-5.34	117.68	123.08
1	D	4959	PHE	CA-C-N	-5.33	117.69	123.08
1	D	4959	PHE	C-N-CA	-5.33	117.69	123.08
1	D	3570	ARG	CB-CA-C	-5.10	110.67	116.54
1	A	1253	PRO	CB-CA-C	-5.09	103.17	111.56
1	D	1253	PRO	CB-CA-C	-5.08	103.17	111.56
1	C	1253	PRO	CB-CA-C	-5.08	103.17	111.56
1	B	1253	PRO	CB-CA-C	-5.08	103.17	111.56
1	C	3570	ARG	CB-CA-C	-5.08	110.70	116.54
1	D	4886	HIS	CA-C-O	-5.05	113.29	120.51
1	C	4825	THR	CA-C-N	5.05	126.92	120.56
1	C	4825	THR	C-N-CA	5.05	126.92	120.56
1	D	4827	LEU	N-CA-C	-5.01	105.89	111.36

There are no chirality outliers.

All (29) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	GLU	Peptide
1	A	1432	THR	Mainchain
1	A	1796	ALA	Peptide
1	A	4553	ASN	Mainchain
1	A	4791	TYR	Mainchain
1	A	4831	THR	Mainchain
1	A	752	VAL	Peptide
1	B	139	GLU	Peptide
1	B	1432	THR	Mainchain
1	B	1796	ALA	Peptide
1	B	4553	ASN	Mainchain
1	B	4715	TYR	Sidechain
1	B	4791	TYR	Mainchain
1	B	4831	THR	Mainchain
1	B	752	VAL	Peptide
1	C	139	GLU	Peptide
1	C	1432	THR	Mainchain
1	C	1796	ALA	Peptide
1	C	4553	ASN	Mainchain
1	C	4715	TYR	Sidechain
1	C	4791	TYR	Mainchain
1	C	752	VAL	Peptide
1	D	139	GLU	Peptide
1	D	1432	THR	Mainchain
1	D	1796	ALA	Peptide
1	D	4553	ASN	Mainchain
1	D	4791	TYR	Mainchain
1	D	4944	ARG	Sidechain
1	D	752	VAL	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	29207	0	25765	674	0
1	B	29207	0	25765	678	0
1	C	29207	0	25765	678	0
1	D	29207	0	25765	677	0
2	E	804	0	812	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	804	0	812	16	0
2	G	804	0	812	16	0
2	H	804	0	812	16	0
3	I	1033	0	958	31	0
3	J	1033	0	958	31	0
3	K	1033	0	958	30	0
3	L	1033	0	958	32	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	31	0	12	1	0
6	B	31	0	12	1	0
6	C	31	0	12	1	0
6	D	31	0	12	1	0
7	A	14	0	10	0	0
7	B	14	0	10	0	0
7	C	14	0	10	0	0
7	D	14	0	10	0	0
All	All	124364	0	110228	2849	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 12.

All (2849) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1698:LEU:HD12	1:B:1814:MET:HE1	1.53	0.90
1:C:1698:LEU:HD12	1:C:1814:MET:HE1	1.53	0.89
1:A:1698:LEU:HD12	1:A:1814:MET:HE1	1.53	0.89
1:D:1698:LEU:HD12	1:D:1814:MET:HE1	1.53	0.88
1:D:1484:HIS:ND1	1:D:1484:HIS:O	2.07	0.86
1:B:1484:HIS:ND1	1:B:1484:HIS:O	2.07	0.86
1:A:1484:HIS:ND1	1:A:1484:HIS:O	2.07	0.86
1:C:1484:HIS:ND1	1:C:1484:HIS:O	2.07	0.84
1:C:4954:MET:HE1	1:C:4959:PHE:CD1	2.13	0.84
1:D:4954:MET:HE1	1:D:4959:PHE:CD1	2.13	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4954:MET:HE1	1:B:4959:PHE:CD1	2.13	0.84
2:E:82:TYR:HB3	2:E:86:GLY:HA2	1.60	0.83
2:F:82:TYR:HB3	2:F:86:GLY:HA2	1.60	0.83
1:A:1703:LEU:HD21	1:A:1709:ALA:HB2	1.61	0.82
1:A:4954:MET:HE1	1:A:4959:PHE:CD1	2.13	0.82
2:H:82:TYR:HB3	2:H:86:GLY:HA2	1.60	0.82
2:G:82:TYR:HB3	2:G:86:GLY:HA2	1.60	0.82
1:D:1703:LEU:HD21	1:D:1709:ALA:HB2	1.61	0.81
1:C:1703:LEU:HD21	1:C:1709:ALA:HB2	1.61	0.81
1:B:1703:LEU:HD21	1:B:1709:ALA:HB2	1.61	0.81
1:A:1680:ARG:HB2	1:A:1796:ALA:HB1	1.63	0.79
1:B:1680:ARG:HB2	1:B:1796:ALA:HB1	1.63	0.79
1:A:2802:LYS:HG3	1:A:2806:ARG:HG3	1.64	0.79
1:A:4888:TYR:HD2	1:D:4914:VAL:HG23	1.48	0.79
1:D:1680:ARG:HB2	1:D:1796:ALA:HB1	1.63	0.79
1:C:1680:ARG:HB2	1:C:1796:ALA:HB1	1.64	0.78
1:C:2802:LYS:HG3	1:C:2806:ARG:HG3	1.64	0.78
3:L:107:ARG:NH1	3:L:123:ASP:OD1	2.17	0.78
3:K:107:ARG:NH1	3:K:123:ASP:OD1	2.17	0.78
1:D:2802:LYS:HG3	1:D:2806:ARG:HG3	1.64	0.78
1:B:2802:LYS:HG3	1:B:2806:ARG:HG3	1.64	0.78
3:J:107:ARG:NH1	3:J:123:ASP:OD1	2.17	0.77
3:I:107:ARG:NH1	3:I:123:ASP:OD1	2.17	0.77
1:D:2813:LEU:HD21	1:D:2926:LEU:HD11	1.68	0.76
3:L:37:MET:HE1	3:L:52:MET:HE1	1.67	0.76
3:K:37:MET:HE1	3:K:52:MET:HE1	1.67	0.76
1:C:2813:LEU:HD21	1:C:2926:LEU:HD11	1.68	0.76
1:D:3870:ASN:O	1:D:3873:LYS:NZ	2.18	0.76
1:C:1639:LEU:HD21	1:C:1650:ILE:HD13	1.67	0.76
1:A:3870:ASN:O	1:A:3873:LYS:NZ	2.18	0.76
1:D:1639:LEU:HD21	1:D:1650:ILE:HD13	1.68	0.75
3:J:37:MET:HE1	3:J:52:MET:HE1	1.67	0.75
1:B:2813:LEU:HD21	1:B:2926:LEU:HD11	1.68	0.75
1:C:3636:PHE:HB3	3:K:89:ALA:HB1	1.68	0.75
1:B:578:ILE:HG23	1:B:582:HIS:HB2	1.69	0.75
1:A:2813:LEU:HD21	1:A:2926:LEU:HD11	1.68	0.75
1:D:894:GLY:HA3	1:D:903:LEU:HB3	1.69	0.75
1:C:3870:ASN:O	1:C:3873:LYS:NZ	2.18	0.75
1:A:894:GLY:HA3	1:A:903:LEU:HB3	1.69	0.75
1:C:578:ILE:HG23	1:C:582:HIS:HB2	1.69	0.75
1:A:4104:THR:HG22	1:A:4106:PRO:HD2	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1639:LEU:HD21	1:B:1650:ILE:HD13	1.67	0.75
1:A:578:ILE:HG23	1:A:582:HIS:HB2	1.68	0.74
1:B:4104:THR:HG22	1:B:4106:PRO:HD2	1.69	0.74
1:B:3870:ASN:O	1:B:3873:LYS:NZ	2.18	0.74
1:D:578:ILE:HG23	1:D:582:HIS:HB2	1.69	0.74
1:B:3636:PHE:HB3	3:J:89:ALA:HB1	1.68	0.74
1:A:1639:LEU:HD21	1:A:1650:ILE:HD13	1.67	0.74
3:I:37:MET:HE1	3:I:52:MET:HE1	1.67	0.74
1:D:3636:PHE:HB3	3:L:89:ALA:HB1	1.68	0.74
1:A:4844:LEU:O	1:A:4846:VAL:N	2.21	0.73
1:B:4103:PHE:HB3	1:B:4108:ILE:HD11	1.70	0.73
1:C:4104:THR:HG22	1:C:4106:PRO:HD2	1.69	0.73
1:A:3528:THR:HA	1:D:1220:GLN:HG2	1.71	0.73
3:I:75:ARG:HH22	3:I:76:LYS:HZ2	1.35	0.73
1:C:4844:LEU:O	1:C:4846:VAL:N	2.21	0.73
1:A:3636:PHE:HB3	3:I:89:ALA:HB1	1.68	0.73
1:C:4103:PHE:HB3	1:C:4108:ILE:HD11	1.70	0.73
1:B:4844:LEU:O	1:B:4846:VAL:N	2.21	0.73
1:A:4103:PHE:HB3	1:A:4108:ILE:HD11	1.70	0.72
1:D:4104:THR:HG22	1:D:4106:PRO:HD2	1.69	0.72
1:B:894:GLY:HA3	1:B:903:LEU:HB3	1.69	0.72
1:A:1770:SER:OG	1:A:1772:ARG:NH2	2.22	0.72
1:D:883:ALA:HB3	1:D:967:PRO:HG3	1.72	0.72
1:D:4844:LEU:O	1:D:4846:VAL:N	2.21	0.72
1:C:894:GLY:HA3	1:C:903:LEU:HB3	1.69	0.72
1:C:973:SER:O	1:C:976:ARG:NH1	2.22	0.72
1:D:4552:LEU:HA	1:D:4555:LEU:HD22	1.72	0.72
1:B:1707:LEU:HG	1:B:1708:ARG:H	1.54	0.72
1:C:1770:SER:OG	1:C:1772:ARG:NH2	2.22	0.72
1:A:973:SER:O	1:A:976:ARG:NH1	2.22	0.72
1:C:1707:LEU:HG	1:C:1708:ARG:H	1.54	0.72
1:C:4552:LEU:HA	1:C:4555:LEU:HD22	1.72	0.72
1:B:1770:SER:OG	1:B:1772:ARG:NH2	2.22	0.72
1:A:1707:LEU:HG	1:A:1708:ARG:H	1.54	0.72
1:D:4103:PHE:HB3	1:D:4108:ILE:HD11	1.70	0.71
1:B:883:ALA:HB3	1:B:967:PRO:HG3	1.72	0.71
1:B:973:SER:O	1:B:976:ARG:NH1	2.22	0.71
1:D:898:ASP:HB2	1:D:903:LEU:HB2	1.72	0.71
1:B:4552:LEU:HA	1:B:4555:LEU:HD22	1.72	0.71
1:D:973:SER:O	1:D:976:ARG:NH1	2.22	0.71
1:D:1770:SER:OG	1:D:1772:ARG:NH2	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:898:ASP:HB2	1:A:903:LEU:HB2	1.72	0.71
1:B:898:ASP:HB2	1:B:903:LEU:HB2	1.72	0.71
1:A:4552:LEU:HA	1:A:4555:LEU:HD22	1.72	0.71
1:C:2336:ARG:HE	1:C:2435:ARG:HD3	1.56	0.71
1:C:883:ALA:HB3	1:C:967:PRO:HG3	1.72	0.71
1:A:883:ALA:HB3	1:A:967:PRO:HG3	1.72	0.71
1:A:1995:THR:OG1	3:I:112:ASN:O	2.09	0.70
1:D:1707:LEU:HG	1:D:1708:ARG:H	1.54	0.70
1:C:607:CYS:SG	1:C:618:GLN:NE2	2.61	0.70
1:A:2336:ARG:HE	1:A:2435:ARG:HD3	1.56	0.70
1:C:898:ASP:HB2	1:C:903:LEU:HB2	1.72	0.70
1:C:1833:SER:O	1:C:1835:GLU:N	2.25	0.70
1:B:2799:GLU:HA	1:B:2802:LYS:HD3	1.73	0.70
1:D:1833:SER:O	1:D:1835:GLU:N	2.25	0.70
1:A:1833:SER:O	1:A:1835:GLU:N	2.25	0.70
1:A:3932:ASP:OD1	1:D:76:ARG:HG3	1.92	0.70
1:C:4812:HIS:O	1:C:4813:LEU:C	2.34	0.70
1:D:2799:GLU:HA	1:D:2802:LYS:HD3	1.73	0.69
1:A:2799:GLU:HA	1:A:2802:LYS:HD3	1.73	0.69
1:D:4021:LYS:NZ	1:D:4142:ASN:OD1	2.26	0.69
1:B:607:CYS:SG	1:B:618:GLN:NE2	2.61	0.69
1:B:1833:SER:O	1:B:1835:GLU:N	2.25	0.69
1:B:2336:ARG:HE	1:B:2435:ARG:HD3	1.56	0.69
1:A:2209:GLU:O	1:A:2213:ASN:ND2	2.25	0.69
1:A:4812:HIS:O	1:A:4813:LEU:C	2.33	0.69
1:D:1995:THR:OG1	3:L:112:ASN:O	2.09	0.69
1:D:2209:GLU:O	1:D:2213:ASN:ND2	2.25	0.69
1:B:1704:PRO:HG2	1:B:1707:LEU:HD23	1.74	0.69
1:B:2209:GLU:O	1:B:2213:ASN:ND2	2.25	0.69
1:D:2336:ARG:HE	1:D:2435:ARG:HD3	1.56	0.69
1:C:2203:MET:HE3	1:C:2235:PHE:HZ	1.58	0.69
1:D:2770:LYS:HB3	1:D:2775:TRP:HB2	1.75	0.69
1:D:4017:LEU:HD12	1:D:4139:ILE:HG13	1.74	0.69
1:C:1704:PRO:HG2	1:C:1707:LEU:HD23	1.74	0.69
1:C:2209:GLU:O	1:C:2213:ASN:ND2	2.25	0.69
1:C:4021:LYS:NZ	1:C:4142:ASN:OD1	2.26	0.69
1:C:138:GLN:N	1:C:138:GLN:OE1	2.26	0.69
1:B:1995:THR:OG1	3:J:112:ASN:O	2.09	0.69
1:D:1704:PRO:HG2	1:D:1707:LEU:HD23	1.74	0.69
1:B:745:SER:HB2	1:B:758:ARG:HB3	1.75	0.69
1:B:4017:LEU:HD12	1:B:4139:ILE:HG13	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2203:MET:HE3	1:D:2235:PHE:HZ	1.58	0.68
3:L:75:ARG:HH22	3:L:76:LYS:HZ2	1.40	0.68
1:A:2117:VAL:HA	1:A:2120:MET:HE3	1.76	0.68
1:C:2770:LYS:HB3	1:C:2775:TRP:HB2	1.75	0.68
1:C:2799:GLU:HA	1:C:2802:LYS:HD3	1.73	0.68
1:C:4017:LEU:HD12	1:C:4139:ILE:HG13	1.74	0.68
1:B:4021:LYS:NZ	1:B:4142:ASN:OD1	2.26	0.68
1:A:745:SER:HB2	1:A:758:ARG:HB3	1.75	0.68
1:A:3636:PHE:C	3:I:89:ALA:HB1	2.19	0.68
1:B:2117:VAL:HA	1:B:2120:MET:HE3	1.76	0.68
1:A:4017:LEU:HD12	1:A:4139:ILE:HG13	1.74	0.68
1:C:1995:THR:OG1	3:K:112:ASN:O	2.09	0.68
1:B:138:GLN:OE1	1:B:138:GLN:N	2.26	0.68
1:A:4021:LYS:NZ	1:A:4142:ASN:OD1	2.26	0.68
1:C:3636:PHE:C	3:K:89:ALA:HB1	2.19	0.68
1:B:2770:LYS:HB3	1:B:2775:TRP:HB2	1.75	0.68
1:A:1704:PRO:HG2	1:A:1707:LEU:HD23	1.74	0.68
1:D:4812:HIS:O	1:D:4813:LEU:C	2.33	0.68
1:D:138:GLN:OE1	1:D:138:GLN:N	2.26	0.68
1:D:3636:PHE:C	3:L:89:ALA:HB1	2.19	0.68
1:B:2203:MET:HE3	1:B:2235:PHE:HZ	1.58	0.68
1:A:2770:LYS:HB3	1:A:2775:TRP:HB2	1.75	0.67
1:C:745:SER:HB2	1:C:758:ARG:HB3	1.75	0.67
1:A:138:GLN:OE1	1:A:138:GLN:N	2.26	0.67
1:B:3636:PHE:C	3:J:89:ALA:HB1	2.19	0.67
1:B:4812:HIS:O	1:B:4813:LEU:C	2.34	0.67
1:A:2203:MET:HE3	1:A:2235:PHE:HZ	1.58	0.67
1:D:2117:VAL:HA	1:D:2120:MET:HE3	1.76	0.67
1:A:1433:TYR:HB3	1:A:1573:MET:O	1.94	0.67
1:D:745:SER:HB2	1:D:758:ARG:HB3	1.75	0.67
1:C:2117:VAL:HA	1:C:2120:MET:HE3	1.76	0.67
1:C:1433:TYR:HB3	1:C:1573:MET:O	1.94	0.67
1:B:1433:TYR:HB3	1:B:1573:MET:O	1.94	0.67
1:C:810:PRO:HB2	1:C:812:HIS:CD2	2.31	0.66
1:A:4966:ASP:O	1:A:4967:TYR:C	2.39	0.66
1:B:2321:ILE:HG13	1:B:2322:GLY:H	1.60	0.66
1:D:2321:ILE:HG13	1:D:2322:GLY:H	1.60	0.66
1:D:607:CYS:SG	1:D:618:GLN:NE2	2.61	0.66
1:D:1433:TYR:HB3	1:D:1573:MET:O	1.94	0.66
1:B:810:PRO:HB2	1:B:812:HIS:CD2	2.31	0.66
1:C:2321:ILE:HG13	1:C:2322:GLY:H	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4966:ASP:O	1:C:4967:TYR:C	2.39	0.66
1:A:810:PRO:HB2	1:A:812:HIS:CD2	2.31	0.66
1:A:2321:ILE:HG13	1:A:2322:GLY:H	1.60	0.66
1:A:495:ASN:OD1	1:A:553:ARG:NH2	2.29	0.65
1:A:4896:GLY:O	1:A:4898:GLY:N	2.30	0.65
1:D:4966:ASP:O	1:D:4967:TYR:C	2.39	0.65
1:D:810:PRO:HB2	1:D:812:HIS:CD2	2.31	0.65
1:C:4896:GLY:O	1:C:4898:GLY:N	2.29	0.65
1:B:587:ILE:HG23	1:B:625:LEU:HD12	1.78	0.65
1:D:4945:ASP:O	1:D:4947:GLN:N	2.29	0.65
1:B:882:TRP:HA	1:B:886:ARG:HH11	1.61	0.65
1:D:587:ILE:HG23	1:D:625:LEU:HD12	1.78	0.65
1:B:4945:ASP:O	1:B:4947:GLN:N	2.29	0.65
1:A:4945:ASP:O	1:A:4947:GLN:N	2.29	0.65
1:D:4984:ASN:O	1:D:4985:LEU:C	2.40	0.65
1:C:3702:VAL:HG11	1:C:3775:ALA:HA	1.79	0.65
1:B:4896:GLY:O	1:B:4898:GLY:N	2.29	0.65
1:A:3637:ARG:CB	3:I:89:ALA:HB2	2.27	0.65
1:D:4896:GLY:O	1:D:4898:GLY:N	2.30	0.65
1:D:3637:ARG:CB	3:L:89:ALA:HB2	2.27	0.65
1:D:4945:ASP:O	1:D:4948:GLU:N	2.30	0.65
1:C:495:ASN:OD1	1:C:553:ARG:NH2	2.29	0.65
1:A:958:THR:HG23	1:A:959:TYR:H	1.62	0.65
1:A:4218:ILE:HG23	1:A:4954:MET:HE2	1.79	0.65
1:D:3702:VAL:HG11	1:D:3775:ALA:HA	1.79	0.65
2:H:29:MET:HA	2:H:35:LYS:HA	1.78	0.65
1:C:4945:ASP:O	1:C:4947:GLN:N	2.29	0.65
1:B:495:ASN:OD1	1:B:553:ARG:NH2	2.29	0.65
1:C:3637:ARG:CB	3:K:89:ALA:HB2	2.27	0.65
1:C:4984:ASN:O	1:C:4985:LEU:C	2.40	0.65
1:B:795:GLY:H	1:B:812:HIS:CD2	2.15	0.65
1:A:795:GLY:H	1:A:812:HIS:CD2	2.15	0.64
1:B:1693:GLN:HA	1:B:1696:HIS:HB3	1.79	0.64
1:B:4984:ASN:O	1:B:4985:LEU:C	2.40	0.64
2:F:29:MET:HA	2:F:35:LYS:HA	1.78	0.64
1:C:4945:ASP:O	1:C:4948:GLU:N	2.30	0.64
1:A:4812:HIS:C	1:A:4814:LEU:N	2.53	0.64
2:H:24:VAL:HG12	2:H:26:TYR:HB3	1.79	0.64
1:B:2780:ASN:HA	1:B:2789:PRO:HB3	1.79	0.64
1:B:3702:VAL:HG11	1:B:3775:ALA:HA	1.79	0.64
1:A:882:TRP:HA	1:A:886:ARG:HH11	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:29:MET:HA	2:E:35:LYS:HA	1.78	0.64
1:D:495:ASN:OD1	1:D:553:ARG:NH2	2.29	0.64
1:B:958:THR:HG23	1:B:959:TYR:H	1.62	0.64
1:B:3637:ARG:CB	3:J:89:ALA:HB2	2.27	0.64
1:C:795:GLY:H	1:C:812:HIS:CD2	2.15	0.64
1:A:4819:GLU:O	1:A:4820:VAL:C	2.41	0.64
1:D:4218:ILE:HG23	1:D:4954:MET:HE2	1.79	0.64
1:C:4819:GLU:O	1:C:4820:VAL:C	2.41	0.64
2:G:29:MET:HA	2:G:35:LYS:HA	1.78	0.64
1:A:4945:ASP:O	1:A:4948:GLU:N	2.30	0.64
1:D:795:GLY:H	1:D:812:HIS:CD2	2.15	0.64
1:D:958:THR:HG23	1:D:959:TYR:H	1.62	0.64
1:C:587:ILE:HG23	1:C:625:LEU:HD12	1.78	0.64
1:C:882:TRP:HA	1:C:886:ARG:HH11	1.61	0.64
1:C:1693:GLN:HA	1:C:1696:HIS:HB3	1.79	0.64
1:B:4218:ILE:HG23	1:B:4954:MET:HE2	1.79	0.64
1:B:1738:LEU:HB3	1:B:2146:PRO:HD3	1.80	0.64
1:A:3702:VAL:HG11	1:A:3775:ALA:HA	1.79	0.64
1:A:587:ILE:HG23	1:A:625:LEU:HD12	1.78	0.63
1:A:2780:ASN:HA	1:A:2789:PRO:HB3	1.79	0.63
1:A:4844:LEU:O	1:A:4845:ALA:C	2.41	0.63
1:D:4819:GLU:O	1:D:4820:VAL:C	2.41	0.63
1:B:4844:LEU:O	1:B:4845:ALA:C	2.41	0.63
1:B:4945:ASP:O	1:B:4948:GLU:N	2.30	0.63
2:F:24:VAL:HG12	2:F:26:TYR:HB3	1.79	0.63
1:A:551:LEU:HD12	1:A:589:LEU:HD22	1.81	0.63
2:E:24:VAL:HG12	2:E:26:TYR:HB3	1.79	0.63
3:I:143:VAL:O	3:I:147:THR:OG1	2.13	0.63
1:D:2816:MET:HE1	1:D:2930:LEU:HD11	1.81	0.63
1:C:132:ALA:HA	1:C:194:SER:HB2	1.81	0.63
1:C:2780:ASN:O	1:C:2787:THR:OG1	2.17	0.63
1:D:2780:ASN:HA	1:D:2789:PRO:HB3	1.79	0.63
1:D:4991:PHE:O	1:D:4993:MET:N	2.31	0.63
1:B:2780:ASN:O	1:B:2787:THR:OG1	2.17	0.63
1:A:4950:VAL:C	1:A:4952:GLU:H	2.07	0.63
1:B:4966:ASP:O	1:B:4967:TYR:C	2.39	0.63
1:A:1693:GLN:HA	1:A:1696:HIS:HB3	1.79	0.63
1:A:2816:MET:HE1	1:A:2930:LEU:HD11	1.81	0.63
1:D:132:ALA:HA	1:D:194:SER:HB2	1.81	0.63
1:D:882:TRP:HA	1:D:886:ARG:HH11	1.61	0.63
1:D:4820:VAL:HG11	1:C:4839:MET:HE1	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1738:LEU:HB3	1:C:2146:PRO:HD3	1.80	0.63
1:C:671:VAL:HG12	1:C:740:PRO:HG3	1.81	0.63
1:C:2780:ASN:HA	1:C:2789:PRO:HB3	1.79	0.63
1:C:4950:VAL:C	1:C:4952:GLU:H	2.07	0.63
1:B:4819:GLU:O	1:B:4820:VAL:C	2.41	0.63
1:B:4950:VAL:C	1:B:4952:GLU:H	2.07	0.63
1:D:2780:ASN:O	1:D:2787:THR:OG1	2.17	0.62
1:C:256:ALA:HB2	1:C:477:LEU:HD11	1.81	0.62
1:C:958:THR:HG23	1:C:959:TYR:H	1.62	0.62
2:G:24:VAL:HG12	2:G:26:TYR:HB3	1.79	0.62
1:B:551:LEU:HD12	1:B:589:LEU:HD22	1.81	0.62
1:A:1738:LEU:HB3	1:A:2146:PRO:HD3	1.80	0.62
1:D:1739:THR:HG1	1:D:1742:THR:HG1	1.47	0.62
1:C:910:PHE:HA	1:C:913:LEU:HD12	1.81	0.62
1:C:4991:PHE:O	1:C:4993:MET:N	2.32	0.62
1:A:4991:PHE:O	1:A:4993:MET:N	2.31	0.62
1:D:1693:GLN:HA	1:D:1696:HIS:HB3	1.79	0.62
1:D:4999:ASP:OD1	1:D:5000:GLU:N	2.32	0.62
1:C:4218:ILE:HG23	1:C:4954:MET:HE2	1.79	0.62
1:B:2816:MET:HE1	1:B:2930:LEU:HD11	1.81	0.62
1:D:910:PHE:HA	1:D:913:LEU:HD12	1.81	0.62
1:D:3990:VAL:HG23	1:D:4051:SER:HB3	1.82	0.62
1:D:4844:LEU:O	1:D:4845:ALA:C	2.41	0.62
1:C:2764:GLU:HG2	1:C:2857:PRO:HB2	1.82	0.62
1:C:4844:LEU:O	1:C:4845:ALA:C	2.41	0.62
1:C:4999:ASP:OD1	1:C:5000:GLU:N	2.32	0.62
1:B:910:PHE:HA	1:B:913:LEU:HD12	1.81	0.62
1:B:2764:GLU:HG2	1:B:2857:PRO:HB2	1.82	0.62
1:A:132:ALA:HA	1:A:194:SER:HB2	1.81	0.62
1:A:675:LEU:HD23	1:A:676:THR:HG23	1.82	0.62
1:D:256:ALA:HB2	1:D:477:LEU:HD11	1.81	0.62
1:D:675:LEU:HD23	1:D:676:THR:HG23	1.82	0.62
1:A:2764:GLU:HG2	1:A:2857:PRO:HB2	1.82	0.62
1:A:4984:ASN:O	1:A:4985:LEU:C	2.40	0.62
1:D:2764:GLU:HG2	1:D:2857:PRO:HB2	1.82	0.62
1:D:4812:HIS:C	1:D:4814:LEU:N	2.53	0.62
1:C:551:LEU:HD12	1:C:589:LEU:HD22	1.81	0.62
1:A:607:CYS:SG	1:A:618:GLN:NE2	2.61	0.62
1:D:551:LEU:HD12	1:D:589:LEU:HD22	1.81	0.62
1:D:4950:VAL:C	1:D:4952:GLU:H	2.07	0.62
1:C:3990:VAL:HG23	1:C:4051:SER:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4812:HIS:C	1:C:4814:LEU:N	2.52	0.62
1:B:132:ALA:HA	1:B:194:SER:HB2	1.81	0.62
1:B:671:VAL:HG12	1:B:740:PRO:HG3	1.81	0.62
1:A:910:PHE:HA	1:A:913:LEU:HD12	1.81	0.62
1:C:4687:TYR:HE1	1:C:4692:PRO:HG3	1.65	0.62
1:B:675:LEU:HD23	1:B:676:THR:HG23	1.82	0.62
1:D:1738:LEU:HB3	1:D:2146:PRO:HD3	1.80	0.62
1:D:3826:VAL:O	1:D:3828:PHE:N	2.33	0.62
1:D:4687:TYR:HE1	1:D:4692:PRO:HG3	1.65	0.62
1:C:2816:MET:HE1	1:C:2930:LEU:HD11	1.81	0.62
1:B:4812:HIS:C	1:B:4814:LEU:N	2.51	0.62
1:B:4991:PHE:O	1:B:4993:MET:N	2.32	0.62
1:B:3990:VAL:HG23	1:B:4051:SER:HB3	1.82	0.62
1:D:662:TRP:HD1	1:D:748:LEU:HD22	1.65	0.61
1:A:4999:ASP:OD1	1:A:5000:GLU:N	2.32	0.61
1:D:647:ASN:OD1	1:D:822:ARG:N	2.33	0.61
3:J:75:ARG:HH22	3:J:76:LYS:HZ2	1.48	0.61
1:A:1455:PRO:HG3	1:A:1549:PHE:CE1	2.36	0.61
1:A:4687:TYR:HE1	1:A:4692:PRO:HG3	1.65	0.61
1:D:671:VAL:HG12	1:D:740:PRO:HG3	1.81	0.61
1:C:662:TRP:HD1	1:C:748:LEU:HD22	1.65	0.61
1:D:1455:PRO:HG3	1:D:1549:PHE:CE1	2.36	0.61
1:C:790:ARG:HG2	1:C:1627:ALA:HB2	1.82	0.61
1:C:1455:PRO:HG3	1:C:1549:PHE:CE1	2.36	0.61
1:B:662:TRP:HD1	1:B:748:LEU:HD22	1.65	0.61
1:B:1703:LEU:HD11	1:B:1709:ALA:H	1.66	0.61
1:A:790:ARG:HG2	1:A:1627:ALA:HB2	1.82	0.61
1:C:675:LEU:HD23	1:C:676:THR:HG23	1.82	0.61
1:C:749:ASP:O	1:C:753:PRO:HA	2.01	0.61
1:C:1703:LEU:HD11	1:C:1709:ALA:H	1.66	0.61
1:B:1455:PRO:HG3	1:B:1549:PHE:CE1	2.36	0.61
1:B:4999:ASP:OD1	1:B:5000:GLU:N	2.32	0.61
1:A:749:ASP:O	1:A:753:PRO:HA	2.01	0.61
1:A:3990:VAL:HG23	1:A:4051:SER:HB3	1.82	0.61
1:B:4687:TYR:HE1	1:B:4692:PRO:HG3	1.65	0.61
1:B:256:ALA:HB2	1:B:477:LEU:HD11	1.81	0.61
1:A:256:ALA:HB2	1:A:477:LEU:HD11	1.81	0.61
1:A:647:ASN:OD1	1:A:822:ARG:N	2.33	0.61
1:A:2780:ASN:O	1:A:2787:THR:OG1	2.17	0.61
1:A:4950:VAL:O	1:A:4952:GLU:N	2.34	0.61
1:D:4950:VAL:O	1:D:4952:GLU:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:647:ASN:OD1	1:C:822:ARG:N	2.33	0.61
1:B:4950:VAL:O	1:B:4952:GLU:N	2.34	0.61
1:B:609:CYS:SG	1:B:610:ASN:N	2.73	0.61
1:A:662:TRP:HD1	1:A:748:LEU:HD22	1.65	0.60
1:C:4950:VAL:O	1:C:4952:GLU:N	2.34	0.60
1:B:219:VAL:HG12	1:B:259:LEU:HD12	1.83	0.60
1:B:790:ARG:HG2	1:B:1627:ALA:HB2	1.82	0.60
1:D:4235:VAL:HG13	1:D:5014:TYR:HE1	1.67	0.60
1:B:749:ASP:O	1:B:753:PRO:HA	2.01	0.60
1:B:3826:VAL:O	1:B:3828:PHE:N	2.33	0.60
1:B:4743:MET:HE2	1:B:4746:ALA:HB2	1.84	0.60
1:A:913:LEU:HD13	1:A:917:GLU:HB3	1.84	0.60
1:D:749:ASP:O	1:D:753:PRO:HA	2.01	0.60
1:D:913:LEU:HD13	1:D:917:GLU:HB3	1.84	0.60
1:D:3678:SER:OG	1:D:3679:LYS:N	2.34	0.60
1:D:4743:MET:HE2	1:D:4746:ALA:HB2	1.83	0.60
1:A:671:VAL:HG12	1:A:740:PRO:HG3	1.81	0.60
1:A:1128:ARG:HB2	1:A:1130:GLN:HE21	1.67	0.60
1:A:1703:LEU:HD11	1:A:1709:ALA:H	1.66	0.60
1:A:609:CYS:SG	1:A:610:ASN:N	2.73	0.60
1:C:4743:MET:HE2	1:C:4746:ALA:HB2	1.84	0.60
1:C:4235:VAL:HG13	1:C:5014:TYR:HE1	1.66	0.60
1:B:1128:ARG:HB2	1:B:1130:GLN:HE21	1.67	0.60
1:D:219:VAL:HG12	1:D:259:LEU:HD12	1.83	0.60
1:C:1128:ARG:HB2	1:C:1130:GLN:HE21	1.67	0.60
1:B:647:ASN:OD1	1:B:822:ARG:N	2.33	0.60
3:J:143:VAL:O	3:J:147:THR:OG1	2.13	0.60
1:D:1703:LEU:HD11	1:D:1709:ALA:H	1.66	0.60
1:A:2276:ALA:O	1:A:2279:SER:OG	2.20	0.60
1:D:790:ARG:HG2	1:D:1627:ALA:HB2	1.82	0.60
1:D:1128:ARG:HB2	1:D:1130:GLN:HE21	1.67	0.60
1:C:1987:SER:O	1:C:1989:ALA:N	2.34	0.60
1:B:2291:GLN:O	1:B:2293:GLN:N	2.35	0.60
1:A:219:VAL:HG12	1:A:259:LEU:HD12	1.83	0.60
1:A:3678:SER:OG	1:A:3679:LYS:N	2.34	0.60
1:C:746:CYS:SG	1:C:747:CYS:N	2.75	0.60
1:C:913:LEU:HD13	1:C:917:GLU:HB3	1.84	0.60
1:A:4719:PHE:C	1:A:4721:LYS:H	2.10	0.59
1:A:4743:MET:HE2	1:A:4746:ALA:HB2	1.84	0.59
1:D:2023:LEU:O	1:D:2028:ARG:NH2	2.35	0.59
1:B:913:LEU:HD13	1:B:917:GLU:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:919:ASN:HB2	1:A:923:GLN:HB2	1.85	0.59
1:C:219:VAL:HG12	1:C:259:LEU:HD12	1.83	0.59
1:C:4815:ASP:O	1:C:4816:ILE:C	2.45	0.59
1:B:3973:CYS:O	1:B:3976:ASN:N	2.34	0.59
1:A:975:VAL:O	1:A:1044:ARG:NH1	2.35	0.59
3:J:75:ARG:HH22	3:J:76:LYS:NZ	2.00	0.59
1:A:4235:VAL:HG13	1:A:5014:TYR:HE1	1.66	0.59
1:D:340:LYS:N	1:D:344:SER:OG	2.35	0.59
1:C:1099:GLU:O	1:C:1100:MET:HE2	2.02	0.59
3:K:75:ARG:HH22	3:K:76:LYS:NZ	2.00	0.59
1:B:919:ASN:HB2	1:B:923:GLN:HB2	1.85	0.59
1:B:1099:GLU:O	1:B:1100:MET:HE2	2.02	0.59
1:A:3826:VAL:O	1:A:3828:PHE:N	2.33	0.59
1:D:4815:ASP:O	1:D:4816:ILE:C	2.43	0.59
1:C:3826:VAL:O	1:C:3828:PHE:N	2.33	0.59
1:B:1987:SER:O	1:B:1989:ALA:N	2.35	0.59
1:A:2332:LEU:HD11	1:A:2429:LEU:HA	1.84	0.59
1:A:4815:ASP:O	1:A:4816:ILE:C	2.45	0.59
1:A:2291:GLN:O	1:A:2293:GLN:N	2.35	0.59
1:D:1987:SER:O	1:D:1989:ALA:N	2.34	0.59
1:B:760:ASN:OD1	1:B:761:GLY:N	2.36	0.59
1:B:4542:GLY:O	1:B:4546:VAL:HG12	2.02	0.59
1:A:746:CYS:SG	1:A:747:CYS:N	2.75	0.59
1:D:2276:ALA:O	1:D:2279:SER:OG	2.20	0.59
1:C:4542:GLY:O	1:C:4546:VAL:HG12	2.02	0.59
1:B:746:CYS:SG	1:B:747:CYS:N	2.75	0.59
1:B:2276:ALA:O	1:B:2279:SER:OG	2.20	0.59
1:B:4235:VAL:HG13	1:B:5014:TYR:HE1	1.66	0.59
1:A:1987:SER:O	1:A:1989:ALA:N	2.35	0.59
1:D:919:ASN:HB2	1:D:923:GLN:HB2	1.85	0.59
1:D:1099:GLU:O	1:D:1100:MET:HE2	2.02	0.59
1:C:2023:LEU:O	1:C:2028:ARG:NH2	2.35	0.59
3:K:75:ARG:HH22	3:K:76:LYS:HZ2	1.50	0.59
1:B:340:LYS:N	1:B:344:SER:OG	2.35	0.59
1:A:340:LYS:N	1:A:344:SER:OG	2.35	0.59
1:A:4543:GLU:O	1:A:4544:LEU:C	2.46	0.59
1:D:975:VAL:O	1:D:1044:ARG:NH1	2.35	0.59
3:L:75:ARG:HH22	3:L:76:LYS:NZ	2.00	0.59
1:C:760:ASN:OD1	1:C:761:GLY:N	2.36	0.59
1:D:138:GLN:HG2	1:D:139:GLU:H	1.68	0.58
1:D:760:ASN:OD1	1:D:761:GLY:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4812:HIS:CD2	1:D:4812:HIS:N	2.71	0.58
1:C:919:ASN:HB2	1:C:923:GLN:HB2	1.85	0.58
1:A:1099:GLU:O	1:A:1100:MET:HE2	2.02	0.58
1:A:4542:GLY:O	1:A:4546:VAL:HG12	2.02	0.58
1:D:2332:LEU:HD11	1:D:2429:LEU:HA	1.84	0.58
1:D:4542:GLY:O	1:D:4546:VAL:HG12	2.02	0.58
1:D:4572:ALA:O	1:D:4573:ILE:C	2.46	0.58
1:C:975:VAL:O	1:C:1044:ARG:NH1	2.35	0.58
1:B:2332:LEU:HD11	1:B:2429:LEU:HA	1.84	0.58
1:A:760:ASN:OD1	1:A:761:GLY:N	2.36	0.58
1:A:2023:LEU:O	1:A:2028:ARG:NH2	2.35	0.58
1:D:746:CYS:SG	1:D:747:CYS:N	2.75	0.58
1:D:4543:GLU:O	1:D:4544:LEU:C	2.46	0.58
1:A:1683:HIS:HB2	1:A:1797:ARG:HH22	1.69	0.58
3:I:75:ARG:HH22	3:I:76:LYS:NZ	2.00	0.58
1:C:206:CYS:SG	1:C:207:SER:N	2.76	0.58
1:C:340:LYS:N	1:C:344:SER:OG	2.35	0.58
1:C:4812:HIS:CD2	1:C:4812:HIS:N	2.71	0.58
3:K:143:VAL:O	3:K:147:THR:OG1	2.13	0.58
1:A:4812:HIS:CD2	1:A:4812:HIS:N	2.71	0.58
1:C:2276:ALA:O	1:C:2279:SER:OG	2.20	0.58
1:C:4572:ALA:O	1:C:4573:ILE:C	2.46	0.58
1:C:2868:SER:O	1:C:2872:GLN:N	2.32	0.58
1:B:1242:LEU:HD12	1:B:1243:PRO:HD2	1.86	0.58
1:B:1683:HIS:HB2	1:B:1797:ARG:HH22	1.69	0.58
1:A:2760:GLU:HG2	1:A:2794:TYR:HB3	1.86	0.58
1:D:385:ASP:HB2	1:C:156:GLN:OE1	2.03	0.58
1:C:4543:GLU:O	1:C:4544:LEU:C	2.46	0.58
1:A:4572:ALA:O	1:A:4573:ILE:C	2.46	0.58
1:D:3973:CYS:O	1:D:3976:ASN:N	2.34	0.58
3:K:48:GLU:O	3:K:52:MET:HG3	2.04	0.58
1:D:609:CYS:SG	1:D:610:ASN:N	2.73	0.58
1:D:2025:GLU:HA	1:D:2028:ARG:HG2	1.86	0.58
1:D:4570:ALA:O	1:D:4574:ASN:ND2	2.37	0.58
1:D:4719:PHE:C	1:D:4721:LYS:H	2.10	0.58
1:C:1563:GLN:O	1:C:1563:GLN:HG2	2.04	0.58
1:C:2332:LEU:HD11	1:C:2429:LEU:HA	1.84	0.58
1:A:4138:ASP:O	1:A:4140:GLY:N	2.37	0.58
1:D:1683:HIS:HB2	1:D:1797:ARG:HH22	1.69	0.58
1:D:2760:GLU:HG2	1:D:2794:TYR:HB3	1.86	0.58
1:D:4812:HIS:C	1:D:4814:LEU:H	2.12	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:CYS:SG	1:A:207:SER:N	2.76	0.57
1:B:3835:LEU:HD21	1:B:3880:PHE:HZ	1.69	0.57
1:A:138:GLN:HG2	1:A:139:GLU:H	1.68	0.57
3:I:48:GLU:O	3:I:52:MET:HG3	2.04	0.57
3:L:48:GLU:O	3:L:52:MET:HG3	2.04	0.57
1:C:359:TYR:OH	1:C:385:ASP:OD2	2.21	0.57
1:C:3401:LEU:O	1:C:3403:ARG:N	2.37	0.57
1:A:3835:LEU:HD21	1:A:3880:PHE:HZ	1.70	0.57
1:D:972:LEU:HD13	1:D:1044:ARG:HB2	1.86	0.57
1:D:1152:MET:HB2	1:D:1161:ILE:HB	1.86	0.57
1:D:3696:ASP:OD2	1:D:3773:ARG:NE	2.37	0.57
1:D:4682:GLU:HG2	1:D:4723:LYS:NZ	2.19	0.57
1:B:1433:TYR:CD1	1:B:1433:TYR:N	2.72	0.57
1:B:4138:ASP:O	1:B:4140:GLY:N	2.37	0.57
1:A:712:TYR:HE1	1:A:1470:ARG:HD2	1.70	0.57
1:A:972:LEU:HD13	1:A:1044:ARG:HB2	1.86	0.57
1:C:2291:GLN:O	1:C:2293:GLN:N	2.35	0.57
1:B:633:LEU:HG	1:B:1641:ILE:HG22	1.86	0.57
1:B:4543:GLU:O	1:B:4544:LEU:C	2.46	0.57
1:B:4719:PHE:C	1:B:4721:LYS:H	2.10	0.57
1:B:4815:ASP:O	1:B:4816:ILE:C	2.45	0.57
1:A:4235:VAL:CG1	1:A:5014:TYR:HE1	2.18	0.57
1:A:4570:ALA:O	1:A:4574:ASN:ND2	2.37	0.57
1:C:908:VAL:HA	1:C:963:ASN:HD22	1.70	0.57
1:C:3696:ASP:OD2	1:C:3773:ARG:NE	2.37	0.57
1:C:3835:LEU:HD21	1:C:3880:PHE:HZ	1.69	0.57
1:B:1776:HIS:HB3	1:B:1798:LEU:HD21	1.86	0.57
1:A:908:VAL:HA	1:A:963:ASN:HD22	1.70	0.57
1:A:1242:LEU:HD12	1:A:1243:PRO:HD2	1.86	0.57
1:A:2806:ARG:O	1:A:2810:LYS:N	2.35	0.57
1:D:1776:HIS:HB3	1:D:1798:LEU:HD21	1.86	0.57
1:C:138:GLN:HG2	1:C:139:GLU:H	1.69	0.57
1:C:1683:HIS:HB2	1:C:1797:ARG:HH22	1.69	0.57
1:C:1776:HIS:HB3	1:C:1798:LEU:HD21	1.86	0.57
1:C:4029:SER:O	1:C:4032:GLU:HG2	2.05	0.57
1:B:4085:ARG:HE	1:B:4087:LEU:HD12	1.70	0.57
1:D:4812:HIS:O	1:D:4814:LEU:N	2.37	0.57
1:C:633:LEU:HG	1:C:1641:ILE:HG22	1.86	0.57
1:C:712:TYR:HE1	1:C:1470:ARG:HD2	1.70	0.57
1:C:2025:GLU:HA	1:C:2028:ARG:HG2	1.86	0.57
1:C:4138:ASP:O	1:C:4140:GLY:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4570:ALA:O	1:C:4574:ASN:ND2	2.37	0.57
1:C:4719:PHE:C	1:C:4721:LYS:H	2.10	0.57
1:B:908:VAL:HA	1:B:963:ASN:HD22	1.70	0.57
1:B:975:VAL:O	1:B:1044:ARG:NH1	2.35	0.57
1:B:2868:SER:O	1:B:2872:GLN:N	2.32	0.57
1:A:5007:GLU:O	1:A:5008:SER:C	2.45	0.57
1:D:3401:LEU:O	1:D:3403:ARG:N	2.37	0.57
1:D:3571:TRP:O	1:D:3575:LEU:N	2.38	0.57
1:D:4085:ARG:HE	1:D:4087:LEU:HD12	1.70	0.57
1:D:5007:GLU:O	1:D:5008:SER:C	2.45	0.57
1:C:972:LEU:HD13	1:C:1044:ARG:HB2	1.86	0.57
1:C:1242:LEU:HD12	1:C:1243:PRO:HD2	1.86	0.57
1:C:4085:ARG:HE	1:C:4087:LEU:HD12	1.70	0.57
1:C:4978:HIS:HE1	1:C:4983:HIS:CD2	2.23	0.57
1:B:206:CYS:SG	1:B:207:SER:N	2.76	0.57
1:B:972:LEU:HD13	1:B:1044:ARG:HB2	1.86	0.57
1:B:1563:GLN:O	1:B:1563:GLN:HG2	2.04	0.57
1:B:3696:ASP:OD2	1:B:3773:ARG:NE	2.37	0.57
1:B:4235:VAL:CG1	1:B:5014:TYR:HE1	2.18	0.57
1:D:206:CYS:SG	1:D:207:SER:N	2.76	0.57
1:D:4138:ASP:O	1:D:4140:GLY:N	2.37	0.57
1:D:4737:ILE:HA	1:D:4740:LEU:HG	1.87	0.57
1:C:4737:ILE:HA	1:C:4740:LEU:HG	1.87	0.57
1:B:138:GLN:HG2	1:B:139:GLU:H	1.68	0.57
1:B:2025:GLU:HA	1:B:2028:ARG:HG2	1.86	0.57
1:B:2760:GLU:HG2	1:B:2794:TYR:HB3	1.86	0.57
1:B:3669:PHE:O	1:B:3670:GLU:HG2	2.05	0.57
1:B:3678:SER:OG	1:B:3679:LYS:N	2.34	0.57
1:B:4029:SER:O	1:B:4032:GLU:HG2	2.05	0.57
1:B:4682:GLU:HG2	1:B:4723:LYS:NZ	2.19	0.57
1:A:533:ASN:ND2	1:A:536:ASN:HD22	2.03	0.57
1:A:4682:GLU:HG2	1:A:4723:LYS:NZ	2.19	0.57
1:A:4978:HIS:HE1	1:A:4983:HIS:CD2	2.23	0.57
1:D:1433:TYR:N	1:D:1433:TYR:CD1	2.72	0.57
1:C:1152:MET:HB2	1:C:1161:ILE:HB	1.86	0.57
1:C:3973:CYS:O	1:C:3976:ASN:N	2.34	0.57
1:C:4682:GLU:HG2	1:C:4723:LYS:NZ	2.19	0.57
1:B:2806:ARG:O	1:B:2810:LYS:N	2.35	0.57
1:B:4570:ALA:O	1:B:4574:ASN:ND2	2.37	0.57
1:A:1152:MET:HB2	1:A:1161:ILE:HB	1.86	0.56
1:A:3669:PHE:O	1:A:3670:GLU:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4085:ARG:HE	1:A:4087:LEU:HD12	1.70	0.56
1:D:633:LEU:HG	1:D:1641:ILE:HG22	1.86	0.56
1:C:195:PHE:HB3	1:C:196:MET:SD	2.45	0.56
1:C:2760:GLU:HG2	1:C:2794:TYR:HB3	1.86	0.56
1:D:3878:ASP:OD1	1:D:3879:GLU:N	2.38	0.56
1:C:4641:PRO:O	1:C:4644:TRP:N	2.38	0.56
1:B:4572:ALA:O	1:B:4573:ILE:C	2.46	0.56
3:J:48:GLU:O	3:J:52:MET:HG3	2.04	0.56
1:A:1776:HIS:HB3	1:A:1798:LEU:HD21	1.86	0.56
1:A:5009:TYR:CE1	1:A:5013:MET:HE1	2.40	0.56
1:D:195:PHE:HB3	1:D:196:MET:SD	2.45	0.56
1:D:1170:MET:HA	1:D:1170:MET:HE3	1.87	0.56
1:D:1242:LEU:HD12	1:D:1243:PRO:HD2	1.86	0.56
1:D:2440:MET:HG2	1:D:2442:LEU:H	1.70	0.56
1:D:4235:VAL:CG1	1:D:5014:TYR:HE1	2.18	0.56
1:D:4978:HIS:HE1	1:D:4983:HIS:CD2	2.23	0.56
1:D:4985:LEU:O	1:D:4986:ALA:C	2.48	0.56
1:C:615:ARG:NH1	1:C:1677:GLY:O	2.38	0.56
1:C:1170:MET:HA	1:C:1170:MET:HE3	1.87	0.56
1:C:1433:TYR:N	1:C:1433:TYR:CD1	2.72	0.56
1:C:2440:MET:HG2	1:C:2442:LEU:H	1.70	0.56
1:C:3678:SER:OG	1:C:3679:LYS:N	2.34	0.56
1:C:5009:TYR:CE1	1:C:5013:MET:HE1	2.41	0.56
1:B:533:ASN:ND2	1:B:536:ASN:HD22	2.03	0.56
1:B:1170:MET:HA	1:B:1170:MET:HE3	1.88	0.56
1:B:4641:PRO:O	1:B:4644:TRP:N	2.38	0.56
1:B:4737:ILE:HA	1:B:4740:LEU:HG	1.87	0.56
1:B:4812:HIS:N	1:B:4812:HIS:CD2	2.71	0.56
1:A:1170:MET:HA	1:A:1170:MET:HE3	1.88	0.56
1:A:3878:ASP:OD1	1:A:3879:GLU:N	2.38	0.56
1:A:3973:CYS:O	1:A:3976:ASN:N	2.34	0.56
1:D:712:TYR:HE1	1:D:1470:ARG:HD2	1.70	0.56
1:D:4226:GLY:O	1:D:4227:GLU:HG3	2.06	0.56
1:C:3842:LEU:O	1:C:3929:SER:OG	2.23	0.56
1:C:3878:ASP:OD1	1:C:3879:GLU:N	2.38	0.56
1:B:712:TYR:HE1	1:B:1470:ARG:HD2	1.70	0.56
1:A:2025:GLU:HA	1:A:2028:ARG:HG2	1.86	0.56
1:A:3842:LEU:O	1:A:3929:SER:OG	2.23	0.56
1:D:882:TRP:HA	1:D:886:ARG:NH1	2.20	0.56
1:D:908:VAL:HA	1:D:963:ASN:HD22	1.70	0.56
1:D:2291:GLN:O	1:D:2293:GLN:N	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3669:PHE:O	1:D:3670:GLU:HG2	2.05	0.56
1:D:4029:SER:O	1:D:4032:GLU:HG2	2.05	0.56
1:C:4235:VAL:CG1	1:C:5014:TYR:HE1	2.18	0.56
1:B:3842:LEU:O	1:B:3929:SER:OG	2.23	0.56
1:B:3878:ASP:OD1	1:B:3879:GLU:N	2.38	0.56
1:B:5009:TYR:CE1	1:B:5013:MET:HE1	2.41	0.56
1:A:195:PHE:HB3	1:A:196:MET:SD	2.45	0.56
1:A:615:ARG:NH1	1:A:1677:GLY:O	2.38	0.56
1:A:1563:GLN:HG2	1:A:1563:GLN:O	2.04	0.56
1:A:4226:GLY:O	1:A:4227:GLU:HG3	2.06	0.56
1:C:533:ASN:ND2	1:C:536:ASN:HD22	2.03	0.56
1:C:3669:PHE:O	1:C:3670:GLU:HG2	2.05	0.56
1:C:4226:GLY:O	1:C:4227:GLU:HG3	2.06	0.56
1:B:195:PHE:HB3	1:B:196:MET:SD	2.45	0.56
1:A:479:GLN:HA	1:A:484:LEU:HD23	1.88	0.56
1:A:3401:LEU:O	1:A:3403:ARG:N	2.37	0.56
1:A:4737:ILE:HA	1:A:4740:LEU:HG	1.87	0.56
1:A:4842:GLY:O	1:A:4844:LEU:N	2.39	0.56
1:D:479:GLN:HA	1:D:484:LEU:HD23	1.88	0.56
1:D:533:ASN:ND2	1:D:536:ASN:HD22	2.03	0.56
1:D:1563:GLN:HG2	1:D:1563:GLN:O	2.04	0.56
1:D:4649:LEU:O	1:D:4651:THR:N	2.39	0.56
1:C:1689:VAL:HG23	1:C:1690:ASP:H	1.70	0.56
1:B:4978:HIS:HE1	1:B:4983:HIS:CD2	2.23	0.56
1:B:4985:LEU:O	1:B:4986:ALA:C	2.49	0.56
1:A:633:LEU:HG	1:A:1641:ILE:HG22	1.86	0.56
1:A:2203:MET:HE3	1:A:2235:PHE:CZ	2.41	0.56
1:D:1689:VAL:HG23	1:D:1690:ASP:H	1.70	0.56
1:D:3842:LEU:O	1:D:3929:SER:OG	2.23	0.56
1:D:5009:TYR:CE1	1:D:5013:MET:HE1	2.40	0.56
1:B:479:GLN:HA	1:B:484:LEU:HD23	1.88	0.56
1:B:891:TRP:HE1	1:B:902:ARG:HE	1.54	0.56
1:B:3188:PRO:O	1:B:3190:LEU:N	2.39	0.56
1:A:882:TRP:HA	1:A:886:ARG:NH1	2.20	0.56
1:A:2440:MET:HG2	1:A:2442:LEU:H	1.70	0.56
1:A:2865:VAL:HG11	1:A:2931:GLN:HE22	1.71	0.56
1:A:3571:TRP:O	1:A:3575:LEU:N	2.38	0.56
1:A:4649:LEU:O	1:A:4651:THR:N	2.39	0.56
1:D:615:ARG:NH1	1:D:1677:GLY:O	2.38	0.56
1:D:3188:PRO:O	1:D:3190:LEU:N	2.39	0.56
1:C:4789:PHE:CD2	1:C:4789:PHE:O	2.59	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4812:HIS:C	1:B:4814:LEU:H	2.14	0.56
1:A:3188:PRO:O	1:A:3190:LEU:N	2.39	0.56
1:A:4641:PRO:O	1:A:4644:TRP:N	2.38	0.56
1:D:2181:SER:O	1:D:2185:ILE:HG12	2.06	0.56
1:D:4789:PHE:O	1:D:4789:PHE:CD2	2.59	0.56
1:B:4189:ARG:HG2	1:B:5031:GLN:HE22	1.71	0.56
1:D:4842:GLY:O	1:D:4844:LEU:N	2.39	0.55
1:B:882:TRP:HA	1:B:886:ARG:NH1	2.20	0.55
1:B:1152:MET:HB2	1:B:1161:ILE:HB	1.86	0.55
1:D:2865:VAL:HG11	1:D:2931:GLN:HE22	1.71	0.55
1:C:2181:SER:O	1:C:2185:ILE:HG12	2.06	0.55
1:C:4842:GLY:O	1:C:4844:LEU:N	2.39	0.55
1:B:615:ARG:NH1	1:B:1677:GLY:O	2.38	0.55
1:B:2440:MET:HG2	1:B:2442:LEU:H	1.70	0.55
1:A:4029:SER:O	1:A:4032:GLU:HG2	2.05	0.55
1:C:2203:MET:HE3	1:C:2235:PHE:CZ	2.41	0.55
1:C:2271:THR:OG1	1:C:2272:PRO:HD2	2.06	0.55
1:C:4649:LEU:O	1:C:4651:THR:N	2.39	0.55
1:B:4226:GLY:O	1:B:4227:GLU:HG3	2.06	0.55
1:A:3535:LEU:O	1:A:3537:LYS:N	2.40	0.55
1:A:4789:PHE:O	1:A:4789:PHE:CD2	2.59	0.55
1:D:2271:THR:OG1	1:D:2272:PRO:HD2	2.06	0.55
1:C:479:GLN:HA	1:C:484:LEU:HD23	1.88	0.55
1:C:882:TRP:HA	1:C:886:ARG:NH1	2.20	0.55
1:B:1074:ILE:HG22	1:B:1193:SER:HB2	1.88	0.55
1:B:1689:VAL:HG23	1:B:1690:ASP:H	1.70	0.55
1:B:2271:THR:OG1	1:B:2272:PRO:HD2	2.06	0.55
1:B:4649:LEU:O	1:B:4651:THR:N	2.39	0.55
1:A:1074:ILE:HG22	1:A:1193:SER:HB2	1.88	0.55
1:D:3835:LEU:HD21	1:D:3880:PHE:HZ	1.70	0.55
1:D:4641:PRO:O	1:D:4644:TRP:N	2.38	0.55
1:B:4842:GLY:O	1:B:4844:LEU:N	2.39	0.55
1:A:1110:ARG:HD3	1:A:1111:PRO:HD2	1.88	0.55
1:A:4189:ARG:HG2	1:A:5031:GLN:HE22	1.71	0.55
1:D:4720:VAL:HG22	1:D:4720:VAL:O	2.07	0.55
1:C:4720:VAL:O	1:C:4720:VAL:HG22	2.07	0.55
1:B:2023:LEU:O	1:B:2028:ARG:NH2	2.35	0.55
1:B:4968:PHE:CE2	1:B:4978:HIS:CD2	2.95	0.55
1:D:1074:ILE:HG22	1:D:1193:SER:HB2	1.88	0.55
1:D:4189:ARG:HG2	1:D:5031:GLN:HE22	1.71	0.55
1:C:891:TRP:HE1	1:C:902:ARG:HE	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2865:VAL:HG11	1:C:2931:GLN:HE22	1.71	0.55
1:C:4218:ILE:CG2	1:C:4954:MET:HE2	2.37	0.55
1:B:2203:MET:HE3	1:B:2235:PHE:CZ	2.41	0.55
1:B:2865:VAL:HG11	1:B:2931:GLN:HE22	1.71	0.55
1:B:4720:VAL:O	1:B:4720:VAL:HG22	2.07	0.55
1:B:4789:PHE:CD2	1:B:4789:PHE:O	2.59	0.55
1:D:4823:LEU:CD2	1:C:4839:MET:HE2	2.37	0.55
1:C:1731:LEU:HD23	1:C:1772:ARG:HH11	1.72	0.55
1:B:12:GLN:O	1:B:164:ARG:NH1	2.40	0.55
1:B:2810:LYS:O	1:B:2814:LYS:N	2.40	0.55
1:B:3571:TRP:O	1:B:3575:LEU:N	2.38	0.55
2:E:41:ASP:OD1	2:E:42:ARG:N	2.40	0.55
1:D:2806:ARG:O	1:D:2810:LYS:N	2.35	0.55
1:D:2868:SER:O	1:D:2872:GLN:N	2.32	0.55
1:B:2181:SER:O	1:B:2185:ILE:HG12	2.06	0.55
1:A:1731:LEU:HD23	1:A:1772:ARG:HH11	1.72	0.55
1:A:2181:SER:O	1:A:2185:ILE:HG12	2.06	0.55
1:D:891:TRP:HE1	1:D:902:ARG:HE	1.54	0.55
1:D:1716:ILE:HD13	1:D:1844:LEU:HD12	1.89	0.55
1:D:4968:PHE:CE2	1:D:4978:HIS:CD2	2.95	0.55
1:C:4802:GLY:HA3	1:C:4809:PHE:CE1	2.42	0.55
1:B:1110:ARG:HD3	1:B:1111:PRO:HD2	1.88	0.55
1:B:1721:GLU:HA	1:B:1724:CYS:HB2	1.89	0.55
1:A:1689:VAL:HG23	1:A:1690:ASP:H	1.70	0.54
1:A:2271:THR:OG1	1:A:2272:PRO:HD2	2.06	0.54
1:A:4720:VAL:HG22	1:A:4720:VAL:O	2.07	0.54
1:D:3535:LEU:O	1:D:3537:LYS:N	2.40	0.54
1:D:4802:GLY:HA3	1:D:4809:PHE:CE1	2.42	0.54
1:C:3188:PRO:O	1:C:3190:LEU:N	2.39	0.54
1:B:3401:LEU:O	1:B:3403:ARG:N	2.37	0.54
1:B:4802:GLY:HA3	1:B:4809:PHE:CE1	2.42	0.54
1:A:1433:TYR:N	1:A:1433:TYR:CD1	2.72	0.54
1:A:3696:ASP:OD2	1:A:3773:ARG:NE	2.37	0.54
1:A:4802:GLY:HA3	1:A:4809:PHE:CE1	2.42	0.54
1:A:4968:PHE:CE2	1:A:4978:HIS:CD2	2.95	0.54
1:D:12:GLN:O	1:D:164:ARG:NH1	2.40	0.54
1:C:3535:LEU:O	1:C:3537:LYS:N	2.40	0.54
1:B:1716:ILE:HD13	1:B:1844:LEU:HD12	1.90	0.54
1:B:1731:LEU:HD23	1:B:1772:ARG:HH11	1.72	0.54
1:A:1716:ILE:HD12	1:A:1720:LEU:HD12	1.90	0.54
1:D:1110:ARG:HD3	1:D:1111:PRO:HD2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1721:GLU:HA	1:D:1724:CYS:HB2	1.89	0.54
1:A:139:GLU:O	1:A:141:ALA:N	2.41	0.54
1:A:1716:ILE:HD13	1:A:1844:LEU:HD12	1.90	0.54
1:A:1721:GLU:HA	1:A:1724:CYS:HB2	1.89	0.54
1:A:3627:GLN:O	1:A:3628:ARG:C	2.51	0.54
1:D:567:VAL:HG23	1:D:568:LEU:HD12	1.89	0.54
1:D:4834:GLY:O	1:D:4838:VAL:HG22	2.08	0.54
1:C:139:GLU:O	1:C:141:ALA:N	2.41	0.54
1:C:1716:ILE:HD12	1:C:1720:LEU:HD12	1.90	0.54
1:C:4189:ARG:HG2	1:C:5031:GLN:HE22	1.72	0.54
1:C:4812:HIS:C	1:C:4814:LEU:H	2.15	0.54
1:B:941:MET:HE2	1:B:941:MET:HA	1.90	0.54
1:A:1252:HIS:O	1:A:1253:PRO:C	2.51	0.54
1:A:4834:GLY:O	1:A:4838:VAL:HG22	2.08	0.54
1:D:1716:ILE:HD12	1:D:1720:LEU:HD12	1.90	0.54
2:H:41:ASP:OD1	2:H:42:ARG:N	2.40	0.54
1:C:1252:HIS:O	1:C:1253:PRO:C	2.51	0.54
1:C:4968:PHE:CE2	1:C:4978:HIS:CD2	2.95	0.54
1:A:891:TRP:HE1	1:A:902:ARG:HE	1.54	0.54
1:A:977:LEU:HB3	1:A:1044:ARG:HH12	1.73	0.54
1:D:977:LEU:HB3	1:D:1044:ARG:HH12	1.73	0.54
1:C:1074:ILE:HG22	1:C:1193:SER:HB2	1.88	0.54
1:C:2810:LYS:O	1:C:2814:LYS:N	2.40	0.54
1:B:1716:ILE:HD12	1:B:1720:LEU:HD12	1.90	0.54
1:A:181:HIS:N	1:A:192:ASP:O	2.40	0.54
1:A:2810:LYS:O	1:A:2814:LYS:N	2.40	0.54
1:A:4960:ILE:HD11	1:A:4985:LEU:HD23	1.89	0.54
1:D:1731:LEU:HD23	1:D:1772:ARG:HH11	1.72	0.54
1:D:2810:LYS:O	1:D:2814:LYS:N	2.40	0.54
1:D:3921:ASP:OD1	1:D:3922:TYR:N	2.41	0.54
1:C:4820:VAL:O	1:C:4821:LYS:C	2.51	0.54
1:C:4985:LEU:O	1:C:4986:ALA:C	2.49	0.54
1:A:12:GLN:O	1:A:164:ARG:NH1	2.40	0.54
1:A:4985:LEU:O	1:A:4986:ALA:C	2.49	0.54
1:C:12:GLN:O	1:C:164:ARG:NH1	2.40	0.54
1:C:110:ARG:HH22	1:C:115:ARG:HH21	1.56	0.54
1:B:567:VAL:HG23	1:B:568:LEU:HD12	1.89	0.54
1:A:3921:ASP:OD1	1:A:3922:TYR:N	2.41	0.54
1:A:4914:VAL:HG23	1:B:4888:TYR:HD2	1.73	0.54
1:D:4218:ILE:CG2	1:D:4954:MET:HE2	2.37	0.54
1:C:941:MET:HA	1:C:941:MET:HE2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1110:ARG:HD3	1:C:1111:PRO:HD2	1.88	0.54
1:B:3921:ASP:OD1	1:B:3922:TYR:N	2.41	0.54
1:A:914:PRO:HD2	1:A:917:GLU:HG3	1.89	0.54
1:D:1252:HIS:O	1:D:1253:PRO:C	2.51	0.54
1:D:3627:GLN:O	1:D:3628:ARG:C	2.51	0.54
1:C:1716:ILE:HD13	1:C:1844:LEU:HD12	1.90	0.54
1:C:1721:GLU:HA	1:C:1724:CYS:HB2	1.89	0.54
1:C:3921:ASP:OD1	1:C:3922:TYR:N	2.41	0.54
2:G:41:ASP:OD1	2:G:42:ARG:N	2.40	0.54
1:B:139:GLU:O	1:B:141:ALA:N	2.41	0.54
1:B:1252:HIS:O	1:B:1253:PRO:C	2.51	0.54
1:A:4218:ILE:CG2	1:A:4954:MET:HE2	2.37	0.53
1:D:3901:ASN:OD1	1:D:3904:ARG:NH1	2.29	0.53
1:C:567:VAL:HG23	1:C:568:LEU:HD12	1.89	0.53
1:C:914:PRO:HD2	1:C:917:GLU:HG3	1.89	0.53
1:C:3758:MET:HB3	1:C:3762:ARG:HH22	1.73	0.53
1:C:4175:ARG:HH21	1:C:4175:ARG:HG3	1.74	0.53
1:C:4834:GLY:O	1:C:4838:VAL:HG22	2.08	0.53
1:B:110:ARG:HH22	1:B:115:ARG:HH21	1.56	0.53
1:B:4834:GLY:O	1:B:4838:VAL:HG22	2.08	0.53
2:F:41:ASP:OD1	2:F:42:ARG:N	2.40	0.53
1:A:567:VAL:HG23	1:A:568:LEU:HD12	1.89	0.53
1:A:941:MET:HE2	1:A:941:MET:HA	1.90	0.53
1:C:977:LEU:HB3	1:C:1044:ARG:HH12	1.73	0.53
1:C:2760:GLU:O	1:C:2764:GLU:N	2.38	0.53
1:C:2806:ARG:O	1:C:2810:LYS:N	2.35	0.53
1:C:3627:GLN:O	1:C:3628:ARG:C	2.51	0.53
1:B:694:PRO:HG3	1:B:826:ILE:HG23	1.91	0.53
1:B:805:PRO:HB2	1:B:808:TYR:HE2	1.73	0.53
1:B:914:PRO:HD2	1:B:917:GLU:HG3	1.89	0.53
1:A:2368:LEU:HA	1:A:2374:SER:HA	1.91	0.53
1:A:3528:THR:CA	1:D:1220:GLN:HG2	2.37	0.53
1:D:1802:ILE:HD12	1:D:1803:PRO:HD2	1.90	0.53
1:D:2355:ARG:NH2	1:D:2355:ARG:HB2	2.24	0.53
1:D:2368:LEU:HA	1:D:2374:SER:HA	1.90	0.53
1:D:2760:GLU:O	1:D:2764:GLU:N	2.38	0.53
1:D:4960:ILE:HD11	1:D:4985:LEU:HD23	1.90	0.53
1:C:3571:TRP:O	1:C:3575:LEU:N	2.38	0.53
1:B:3535:LEU:O	1:B:3537:LYS:N	2.40	0.53
1:B:3758:MET:HB3	1:B:3762:ARG:HH22	1.73	0.53
1:B:5007:GLU:O	1:B:5008:SER:C	2.45	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ARG:HH22	1:A:115:ARG:HH21	1.56	0.53
1:D:694:PRO:HG3	1:D:826:ILE:HG23	1.91	0.53
1:D:4773:VAL:O	1:D:4777:ILE:HG13	2.09	0.53
1:C:229:GLU:OE2	1:C:247:TYR:HB3	2.09	0.53
1:C:5011:TRP:CG	1:C:5011:TRP:O	2.60	0.53
1:B:2355:ARG:HB2	1:B:2355:ARG:NH2	2.24	0.53
1:B:4960:ILE:HD11	1:B:4985:LEU:HD23	1.90	0.53
1:D:229:GLU:OE2	1:D:247:TYR:HB3	2.09	0.53
1:D:914:PRO:HD2	1:D:917:GLU:HG3	1.90	0.53
1:C:694:PRO:HG3	1:C:826:ILE:HG23	1.91	0.53
1:C:4960:ILE:HD11	1:C:4985:LEU:HD23	1.89	0.53
1:A:1947:CYS:SG	1:A:1948:ASP:N	2.82	0.53
1:A:2868:SER:O	1:A:2872:GLN:N	2.32	0.53
1:A:5011:TRP:O	1:A:5011:TRP:CG	2.60	0.53
1:D:4820:VAL:O	1:D:4821:LYS:C	2.51	0.53
1:C:805:PRO:HB2	1:C:808:TYR:HE2	1.73	0.53
1:C:1802:ILE:HD12	1:C:1803:PRO:HD2	1.90	0.53
1:B:345:LEU:HD22	1:B:387:ALA:HB1	1.91	0.53
1:B:4218:ILE:CG2	1:B:4954:MET:HE2	2.37	0.53
1:A:345:LEU:HD22	1:A:387:ALA:HB1	1.91	0.53
1:A:5009:TYR:CZ	1:A:5013:MET:HE1	2.44	0.53
1:D:110:ARG:HH22	1:D:115:ARG:HH21	1.56	0.53
1:D:181:HIS:N	1:D:192:ASP:O	2.40	0.53
1:D:5009:TYR:CZ	1:D:5013:MET:HE1	2.44	0.53
1:C:345:LEU:HD22	1:C:387:ALA:HB1	1.91	0.53
1:B:168:ASP:OD1	1:B:168:ASP:N	2.42	0.53
1:B:3627:GLN:O	1:B:3628:ARG:C	2.51	0.53
1:B:5009:TYR:CZ	1:B:5013:MET:HE1	2.44	0.53
2:F:73:LYS:HE2	2:F:73:LYS:HA	1.91	0.53
1:A:76:ARG:HG3	1:B:3932:ASP:OD1	2.08	0.53
1:A:805:PRO:HB2	1:A:808:TYR:HE2	1.73	0.53
1:D:3758:MET:HB3	1:D:3762:ARG:HH22	1.73	0.53
1:C:4897:ILE:HG22	1:C:4897:ILE:O	2.09	0.53
1:A:872:GLU:HA	1:A:875:ALA:HB3	1.91	0.53
1:D:139:GLU:O	1:D:141:ALA:N	2.41	0.53
1:D:1724:CYS:HB3	1:D:1728:ARG:HH12	1.74	0.53
1:C:609:CYS:SG	1:C:610:ASN:N	2.74	0.53
1:C:2355:ARG:HB2	1:C:2355:ARG:NH2	2.24	0.53
1:C:5009:TYR:CZ	1:C:5013:MET:HE1	2.44	0.53
1:B:977:LEU:HB3	1:B:1044:ARG:HH12	1.73	0.53
1:B:1948:ASP:OD1	1:B:1948:ASP:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:GLU:OE2	1:A:247:TYR:HB3	2.09	0.53
1:A:1676:LEU:HB3	1:A:2167:ILE:HD12	1.91	0.53
1:C:4773:VAL:O	1:C:4777:ILE:HG13	2.08	0.53
1:C:5007:GLU:O	1:C:5008:SER:C	2.45	0.53
1:B:1947:CYS:SG	1:B:1948:ASP:N	2.82	0.53
1:B:4175:ARG:HH21	1:B:4175:ARG:HG3	1.74	0.53
1:D:941:MET:HE2	1:D:941:MET:HA	1.90	0.52
1:D:3293:PRO:O	1:D:3295:ALA:N	2.42	0.52
1:C:219:VAL:HG22	1:C:261:ARG:HG3	1.91	0.52
1:C:1733:GLU:OE1	1:C:1733:GLU:N	2.42	0.52
1:B:872:GLU:HA	1:B:875:ALA:HB3	1.91	0.52
1:A:694:PRO:HG3	1:A:826:ILE:HG23	1.91	0.52
1:A:1733:GLU:OE1	1:A:1733:GLU:N	2.42	0.52
1:A:3293:PRO:O	1:A:3295:ALA:N	2.42	0.52
1:A:3592:ILE:O	1:A:3594:ARG:N	2.43	0.52
1:A:4066:LEU:HD22	1:A:4169:SER:HB3	1.91	0.52
1:A:4773:VAL:O	1:A:4777:ILE:HG13	2.09	0.52
1:A:4820:VAL:O	1:A:4821:LYS:C	2.51	0.52
1:A:4950:VAL:HG22	1:A:4951:LYS:N	2.24	0.52
1:D:345:LEU:HD22	1:D:387:ALA:HB1	1.91	0.52
1:D:872:GLU:HA	1:D:875:ALA:HB3	1.91	0.52
1:D:4175:ARG:HH21	1:D:4175:ARG:HG3	1.74	0.52
1:C:5034:ASP:C	1:C:5036:LEU:N	2.65	0.52
1:B:4066:LEU:HD22	1:B:4169:SER:HB3	1.91	0.52
1:B:4812:HIS:O	1:B:4814:LEU:N	2.42	0.52
1:A:2355:ARG:HB2	1:A:2355:ARG:NH2	2.24	0.52
1:D:805:PRO:HB2	1:D:808:TYR:HE2	1.73	0.52
3:L:33:LEU:HA	3:L:36:VAL:HG22	1.92	0.52
1:C:872:GLU:HA	1:C:875:ALA:HB3	1.91	0.52
1:C:4066:LEU:HD22	1:C:4169:SER:HB3	1.91	0.52
1:C:4951:LYS:O	1:C:4951:LYS:HG2	2.09	0.52
1:D:4066:LEU:HD22	1:D:4169:SER:HB3	1.91	0.52
1:C:1724:CYS:HB3	1:C:1728:ARG:HH12	1.74	0.52
3:K:33:LEU:HA	3:K:36:VAL:HG22	1.92	0.52
1:B:3293:PRO:O	1:B:3295:ALA:N	2.42	0.52
1:A:359:TYR:OH	1:A:385:ASP:OD2	2.21	0.52
1:A:1802:ILE:HD12	1:A:1803:PRO:HD2	1.90	0.52
1:A:4175:ARG:HH21	1:A:4175:ARG:HG3	1.74	0.52
2:E:73:LYS:HA	2:E:73:LYS:HE2	1.91	0.52
1:D:1947:CYS:SG	1:D:1948:ASP:N	2.82	0.52
1:D:2203:MET:HE3	1:D:2235:PHE:CZ	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4823:LEU:HD21	1:C:4839:MET:HE2	1.91	0.52
1:D:4897:ILE:O	1:D:4897:ILE:HG22	2.09	0.52
1:C:4812:HIS:O	1:C:4814:LEU:N	2.43	0.52
1:C:4966:ASP:O	1:C:4968:PHE:N	2.43	0.52
1:B:1724:CYS:HB3	1:B:1728:ARG:HH12	1.74	0.52
1:A:3756:LYS:HG3	1:A:3757:GLU:OE2	2.10	0.52
1:A:3758:MET:HB3	1:A:3762:ARG:HH22	1.73	0.52
1:D:3570:ARG:O	1:D:3572:GLN:N	2.42	0.52
1:D:3592:ILE:O	1:D:3594:ARG:N	2.43	0.52
1:D:3756:LYS:HG3	1:D:3757:GLU:OE2	2.10	0.52
1:C:1947:CYS:SG	1:C:1948:ASP:N	2.82	0.52
1:C:2889:LYS:O	1:C:2893:GLU:N	2.43	0.52
1:C:3293:PRO:O	1:C:3295:ALA:N	2.42	0.52
1:B:219:VAL:HG22	1:B:261:ARG:HG3	1.91	0.52
1:B:2889:LYS:O	1:B:2893:GLU:N	2.43	0.52
1:B:3592:ILE:O	1:B:3594:ARG:N	2.43	0.52
1:B:4773:VAL:O	1:B:4777:ILE:HG13	2.09	0.52
1:D:219:VAL:HG22	1:D:261:ARG:HG3	1.91	0.52
1:D:1676:LEU:HB3	1:D:2167:ILE:HD12	1.91	0.52
1:D:4951:LYS:HG2	1:D:4951:LYS:O	2.09	0.52
1:D:4991:PHE:C	1:D:4993:MET:H	2.18	0.52
1:C:3756:LYS:HG3	1:C:3757:GLU:OE2	2.10	0.52
1:B:229:GLU:OE2	1:B:247:TYR:HB3	2.09	0.52
1:B:3756:LYS:HG3	1:B:3757:GLU:OE2	2.10	0.52
1:A:123:THR:OG1	1:A:134:ASP:OD1	2.28	0.52
1:A:1724:CYS:HB3	1:A:1728:ARG:HH12	1.74	0.52
1:D:470:SER:O	1:D:474:ARG:NH2	2.43	0.52
1:D:4950:VAL:HG22	1:D:4951:LYS:N	2.24	0.52
2:H:73:LYS:HE2	2:H:73:LYS:HA	1.91	0.52
1:C:952:LYS:HG2	1:C:970:LEU:HG	1.92	0.52
1:C:2296:GLU:HG2	1:C:2356:LEU:HD21	1.92	0.52
1:C:4950:VAL:HG22	1:C:4951:LYS:N	2.24	0.52
1:B:1100:MET:HB2	1:B:1143:TRP:CH2	2.45	0.52
1:B:1802:ILE:HD12	1:B:1803:PRO:HD2	1.90	0.52
1:B:4897:ILE:O	1:B:4897:ILE:HG22	2.08	0.52
1:A:1100:MET:HB2	1:A:1143:TRP:CH2	2.45	0.52
1:A:2296:GLU:HG2	1:A:2356:LEU:HD21	1.92	0.52
1:D:3817:LEU:HB2	1:D:3899:PHE:CE1	2.45	0.52
1:C:3592:ILE:O	1:C:3594:ARG:N	2.43	0.52
1:C:3817:LEU:HB2	1:C:3899:PHE:CE1	2.45	0.52
3:J:33:LEU:HA	3:J:36:VAL:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2953:LYS:O	1:A:2957:PHE:N	2.43	0.52
1:A:4549:VAL:O	1:A:4550:LYS:C	2.53	0.52
1:A:4897:ILE:O	1:A:4897:ILE:HG22	2.09	0.52
1:D:952:LYS:HG2	1:D:970:LEU:HG	1.92	0.52
1:D:4549:VAL:O	1:D:4550:LYS:C	2.53	0.52
1:C:907:LEU:O	1:C:963:ASN:ND2	2.44	0.52
1:C:1100:MET:HB2	1:C:1143:TRP:CH2	2.45	0.52
1:B:4950:VAL:HG22	1:B:4951:LYS:N	2.24	0.52
1:A:315:CYS:SG	1:A:316:PHE:N	2.84	0.51
1:A:4547:GLN:O	1:A:4548:ARG:C	2.53	0.51
1:A:4966:ASP:O	1:A:4968:PHE:N	2.43	0.51
1:D:4899:ASP:O	1:D:4900:GLU:CB	2.59	0.51
1:C:315:CYS:SG	1:C:316:PHE:N	2.84	0.51
1:C:961:MET:HB2	1:C:963:ASN:OD1	2.10	0.51
1:C:1676:LEU:HB3	1:C:2167:ILE:HD12	1.91	0.51
1:C:2368:LEU:HA	1:C:2374:SER:HA	1.91	0.51
1:B:40:GLU:OE2	1:B:44:ASN:N	2.44	0.51
1:B:315:CYS:SG	1:B:316:PHE:N	2.84	0.51
1:B:1733:GLU:OE1	1:B:1733:GLU:N	2.42	0.51
1:B:4966:ASP:O	1:B:4968:PHE:N	2.43	0.51
1:A:219:VAL:HG22	1:A:261:ARG:HG3	1.91	0.51
1:A:2889:LYS:O	1:A:2893:GLU:N	2.43	0.51
1:A:3725:TYR:HA	1:A:3728:ILE:HG12	1.93	0.51
1:A:5034:ASP:C	1:A:5036:LEU:N	2.65	0.51
3:I:33:LEU:HA	3:I:36:VAL:HG22	1.92	0.51
1:D:775:GLY:C	1:D:776:LEU:HD12	2.35	0.51
1:C:4991:PHE:C	1:C:4993:MET:H	2.18	0.51
1:B:1969:LEU:HD21	1:B:2009:LEU:HD13	1.92	0.51
1:B:2368:LEU:HA	1:B:2374:SER:HA	1.91	0.51
1:B:4820:VAL:O	1:B:4821:LYS:C	2.51	0.51
1:B:4951:LYS:O	1:B:4951:LYS:HG2	2.09	0.51
1:A:775:GLY:C	1:A:776:LEU:HD12	2.35	0.51
1:A:961:MET:HB2	1:A:963:ASN:OD1	2.10	0.51
1:D:315:CYS:SG	1:D:316:PHE:N	2.84	0.51
1:D:2889:LYS:O	1:D:2893:GLU:N	2.43	0.51
1:D:4966:ASP:O	1:D:4968:PHE:N	2.43	0.51
1:C:775:GLY:C	1:C:776:LEU:HD12	2.35	0.51
1:B:787:VAL:HG13	1:B:789:VAL:HG23	1.93	0.51
1:B:1730:MET:HA	1:B:1730:MET:HE3	1.93	0.51
1:B:2296:GLU:HG2	1:B:2356:LEU:HD21	1.92	0.51
1:B:4966:ASP:O	1:B:4969:ASP:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:SER:O	1:A:474:ARG:NH2	2.43	0.51
1:A:4812:HIS:C	1:A:4814:LEU:H	2.18	0.51
1:A:4899:ASP:O	1:A:4900:GLU:CB	2.59	0.51
1:A:4951:LYS:HG2	1:A:4951:LYS:O	2.09	0.51
1:A:4991:PHE:C	1:A:4993:MET:H	2.18	0.51
1:D:4764:LEU:O	1:D:4766:THR:N	2.44	0.51
1:C:1101:ARG:HB3	1:C:1123:VAL:HG21	1.93	0.51
1:C:1948:ASP:N	1:C:1948:ASP:OD1	2.42	0.51
1:C:4966:ASP:O	1:C:4969:ASP:N	2.43	0.51
1:B:340:LYS:H	1:B:344:SER:HG	1.56	0.51
1:B:1580:PHE:CE2	1:B:1592:PRO:HG2	2.45	0.51
1:B:3039:ILE:O	1:B:3041:SER:N	2.43	0.51
1:B:5034:ASP:C	1:B:5036:LEU:N	2.65	0.51
1:A:787:VAL:HG13	1:A:789:VAL:HG23	1.93	0.51
1:A:1948:ASP:N	1:A:1948:ASP:OD1	2.42	0.51
1:A:3817:LEU:HB2	1:A:3899:PHE:CE1	2.45	0.51
1:D:5011:TRP:CG	1:D:5011:TRP:O	2.60	0.51
1:C:1730:MET:HE3	1:C:1730:MET:HA	1.93	0.51
1:B:2953:LYS:O	1:B:2957:PHE:N	2.43	0.51
1:B:4242:ILE:HD11	1:B:4993:MET:HG2	1.92	0.51
1:B:4649:LEU:O	1:B:4650:HIS:C	2.53	0.51
1:A:907:LEU:O	1:A:963:ASN:ND2	2.44	0.51
1:A:1730:MET:HA	1:A:1730:MET:HE3	1.93	0.51
1:A:3901:ASN:OD1	1:A:3904:ARG:NH1	2.29	0.51
1:D:787:VAL:HG13	1:D:789:VAL:HG23	1.93	0.51
1:C:1948:ASP:HA	1:C:1951:LEU:HB2	1.93	0.51
2:G:73:LYS:HE2	2:G:73:LYS:HA	1.91	0.51
1:B:683:ARG:NH2	1:B:707:VAL:O	2.44	0.51
1:B:775:GLY:C	1:B:776:LEU:HD12	2.35	0.51
1:B:1948:ASP:HA	1:B:1951:LEU:HB2	1.93	0.51
1:B:4991:PHE:C	1:B:4993:MET:H	2.18	0.51
1:D:40:GLU:OE2	1:D:44:ASN:N	2.44	0.51
1:D:1733:GLU:N	1:D:1733:GLU:OE1	2.42	0.51
1:D:2296:GLU:HG2	1:D:2356:LEU:HD21	1.92	0.51
1:D:3039:ILE:O	1:D:3041:SER:N	2.44	0.51
1:D:4686:LEU:HD11	1:D:4692:PRO:HA	1.92	0.51
1:C:645:ARG:HG3	1:C:778:PHE:CD1	2.46	0.51
1:C:683:ARG:NH2	1:C:707:VAL:O	2.44	0.51
1:C:1675:ALA:O	1:C:1677:GLY:N	2.42	0.51
1:B:181:HIS:N	1:B:192:ASP:O	2.40	0.51
1:B:470:SER:O	1:B:474:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1976:ARG:NH1	1:B:2022:PRO:O	2.44	0.51
1:B:4949:GLN:O	1:B:4950:VAL:C	2.54	0.51
1:A:1969:LEU:HD21	1:A:2009:LEU:HD13	1.92	0.51
1:A:1976:ARG:NH1	1:A:2022:PRO:O	2.44	0.51
1:A:3039:ILE:O	1:A:3041:SER:N	2.43	0.51
1:D:961:MET:HB2	1:D:963:ASN:OD1	2.10	0.51
1:D:1101:ARG:HB3	1:D:1123:VAL:HG21	1.93	0.51
1:D:3725:TYR:HA	1:D:3728:ILE:HG12	1.93	0.51
1:C:40:GLU:OE2	1:C:44:ASN:N	2.44	0.51
1:C:123:THR:OG1	1:C:134:ASP:OD1	2.28	0.51
1:B:1676:LEU:HB3	1:B:2167:ILE:HD12	1.91	0.51
1:A:1580:PHE:CE2	1:A:1592:PRO:HG2	2.46	0.51
1:A:2321:ILE:HG13	1:A:2322:GLY:N	2.26	0.51
1:D:1240:LYS:O	1:D:1241:SER:OG	2.29	0.51
1:D:1976:ARG:NH1	1:D:2022:PRO:O	2.44	0.51
1:D:3648:ARG:HG3	1:D:3648:ARG:HH21	1.76	0.51
1:D:4823:LEU:HD21	1:C:4839:MET:HB3	1.92	0.51
1:C:470:SER:O	1:C:474:ARG:NH2	2.43	0.51
1:C:2321:ILE:HG13	1:C:2322:GLY:N	2.26	0.51
1:C:3648:ARG:HG3	1:C:3648:ARG:HH21	1.76	0.51
1:C:4242:ILE:HD11	1:C:4993:MET:HG2	1.92	0.51
1:B:907:LEU:O	1:B:963:ASN:ND2	2.44	0.51
1:B:961:MET:HB2	1:B:963:ASN:OD1	2.10	0.51
1:B:3725:TYR:HA	1:B:3728:ILE:HG12	1.93	0.51
1:B:4567:LEU:HD11	1:B:4816:ILE:HD13	1.93	0.51
1:A:689:THR:HG22	1:A:778:PHE:CE2	2.46	0.51
1:A:1196:PRO:O	1:A:1198:GLN:NE2	2.44	0.51
1:D:1580:PHE:CE2	1:D:1592:PRO:HG2	2.46	0.51
1:C:600:LEU:HD21	1:C:1666:THR:HA	1.93	0.51
1:C:787:VAL:HG13	1:C:789:VAL:HG23	1.93	0.51
1:C:1580:PHE:CE2	1:C:1592:PRO:HG2	2.46	0.51
1:B:3817:LEU:HB2	1:B:3899:PHE:CE1	2.45	0.51
1:B:3850:GLN:CD	1:B:3873:LYS:HD2	2.36	0.51
1:A:4242:ILE:HD11	1:A:4993:MET:HG2	1.92	0.50
1:A:4567:LEU:HD11	1:A:4816:ILE:HD13	1.93	0.50
1:D:1969:LEU:HD21	1:D:2009:LEU:HD13	1.92	0.50
1:D:2956:ALA:O	1:D:2960:LEU:N	2.44	0.50
1:D:3850:GLN:CD	1:D:3873:LYS:HD2	2.37	0.50
1:C:168:ASP:OD1	1:C:168:ASP:N	2.42	0.50
1:C:1969:LEU:HD21	1:C:2009:LEU:HD13	1.92	0.50
1:C:2927:LEU:HD23	1:C:2930:LEU:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4899:ASP:O	1:C:4900:GLU:CB	2.59	0.50
1:B:123:THR:OG1	1:B:134:ASP:OD1	2.28	0.50
1:B:243:ARG:HB3	1:B:300:VAL:HG13	1.93	0.50
1:B:2695:LEU:O	1:B:2951:ILE:N	2.39	0.50
1:B:2956:ALA:O	1:B:2960:LEU:N	2.44	0.50
1:B:4899:ASP:O	1:B:4900:GLU:CB	2.59	0.50
1:B:5011:TRP:CG	1:B:5011:TRP:O	2.60	0.50
1:A:110:ARG:HH22	1:A:115:ARG:NH2	2.09	0.50
1:A:648:ILE:HD11	1:A:779:PRO:HG2	1.93	0.50
1:A:3648:ARG:HH21	1:A:3648:ARG:HG3	1.76	0.50
1:A:3850:GLN:CD	1:A:3873:LYS:HD2	2.37	0.50
1:D:4966:ASP:O	1:D:4969:ASP:N	2.44	0.50
3:L:73:MET:SD	3:L:77:MET:HE3	2.52	0.50
1:B:1762:LEU:HD12	1:B:1863:LEU:HD13	1.94	0.50
1:A:1675:ALA:O	1:A:1677:GLY:N	2.42	0.50
1:A:2695:LEU:O	1:A:2951:ILE:N	2.39	0.50
1:A:5035:GLN:O	1:A:5036:LEU:CB	2.60	0.50
1:C:1976:ARG:NH1	1:C:2022:PRO:O	2.44	0.50
1:C:3039:ILE:O	1:C:3041:SER:N	2.43	0.50
1:C:3850:GLN:CD	1:C:3873:LYS:HD2	2.37	0.50
1:A:168:ASP:OD1	1:A:168:ASP:N	2.42	0.50
1:A:243:ARG:HB3	1:A:300:VAL:HG13	1.93	0.50
1:A:1243:PRO:HG2	1:A:1458:HIS:HB3	1.93	0.50
1:D:110:ARG:HH22	1:D:115:ARG:NH2	2.09	0.50
1:D:123:THR:OG1	1:D:134:ASP:OD1	2.28	0.50
1:D:600:LEU:HD21	1:D:1666:THR:HA	1.93	0.50
1:D:1730:MET:HA	1:D:1730:MET:HE3	1.93	0.50
1:D:2470:ILE:O	1:D:2470:ILE:HG13	2.11	0.50
1:D:2927:LEU:HD23	1:D:2930:LEU:HD12	1.94	0.50
1:D:5035:GLN:O	1:D:5036:LEU:CB	2.60	0.50
1:C:181:HIS:N	1:C:192:ASP:O	2.40	0.50
1:C:292:ALA:HB1	1:C:311:ALA:HB1	1.93	0.50
1:C:2470:ILE:HG13	1:C:2470:ILE:O	2.11	0.50
1:C:2763:HIS:O	1:C:2767:ALA:N	2.38	0.50
1:C:3932:ASP:OD1	1:B:76:ARG:HG3	2.12	0.50
1:B:110:ARG:HH22	1:B:115:ARG:NH2	2.09	0.50
1:B:952:LYS:HG2	1:B:970:LEU:HG	1.92	0.50
1:B:4547:GLN:O	1:B:4548:ARG:C	2.53	0.50
1:B:4686:LEU:HD11	1:B:4692:PRO:HA	1.92	0.50
1:A:683:ARG:NH2	1:A:707:VAL:O	2.44	0.50
1:A:952:LYS:HG2	1:A:970:LEU:HG	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1101:ARG:HB3	1:A:1123:VAL:HG21	1.93	0.50
1:A:1689:VAL:HG23	1:A:1690:ASP:N	2.27	0.50
1:D:689:THR:HG22	1:D:778:PHE:CE2	2.46	0.50
1:C:1762:LEU:HD12	1:C:1863:LEU:HD13	1.94	0.50
1:B:645:ARG:HG3	1:B:778:PHE:CD1	2.46	0.50
1:B:1689:VAL:HG23	1:B:1690:ASP:N	2.26	0.50
1:B:2321:ILE:HG13	1:B:2322:GLY:N	2.26	0.50
1:B:3648:ARG:HH21	1:B:3648:ARG:HG3	1.76	0.50
1:A:2760:GLU:O	1:A:2764:GLU:N	2.38	0.50
1:D:1649:ASP:OD1	1:D:1650:ILE:N	2.45	0.50
1:D:1707:LEU:O	1:D:1709:ALA:N	2.45	0.50
1:D:2618:MET:O	1:D:2622:LEU:N	2.43	0.50
1:C:110:ARG:HH22	1:C:115:ARG:NH2	2.09	0.50
1:C:3725:TYR:HA	1:C:3728:ILE:HG12	1.93	0.50
1:B:533:ASN:OD1	1:B:534:ARG:N	2.45	0.50
1:B:1649:ASP:OD1	1:B:1650:ILE:N	2.45	0.50
1:A:40:GLU:OE2	1:A:44:ASN:N	2.44	0.50
1:A:1477:GLY:HA2	1:A:1484:HIS:HB2	1.94	0.50
1:D:907:LEU:O	1:D:963:ASN:ND2	2.44	0.50
1:D:1100:MET:HB2	1:D:1143:TRP:CH2	2.45	0.50
1:D:1948:ASP:N	1:D:1948:ASP:OD1	2.42	0.50
1:D:4242:ILE:HD11	1:D:4993:MET:HG2	1.92	0.50
1:C:648:ILE:HD11	1:C:779:PRO:HG2	1.93	0.50
1:C:1707:LEU:O	1:C:1709:ALA:N	2.45	0.50
1:C:4562:LEU:HD12	1:C:4657:MET:HG3	1.94	0.50
3:K:73:MET:SD	3:K:77:MET:HE3	2.52	0.50
1:B:1101:ARG:HB3	1:B:1123:VAL:HG21	1.93	0.50
1:A:1762:LEU:HD12	1:A:1863:LEU:HD13	1.94	0.50
1:A:2470:ILE:HG13	1:A:2470:ILE:O	2.11	0.50
1:A:4678:ALA:HB2	1:A:4720:VAL:HG21	1.94	0.50
1:A:4686:LEU:HD11	1:A:4692:PRO:HA	1.92	0.50
1:A:4764:LEU:O	1:A:4766:THR:N	2.44	0.50
2:E:25:HIS:NE2	2:E:40:ARG:HG2	2.27	0.50
1:D:648:ILE:HD11	1:D:779:PRO:HG2	1.93	0.50
1:D:683:ARG:NH2	1:D:707:VAL:O	2.44	0.50
1:D:1152:MET:HE3	1:D:1223:PHE:CE2	2.47	0.50
1:D:1243:PRO:HG2	1:D:1458:HIS:HB3	1.93	0.50
1:D:4705:VAL:O	1:D:4708:THR:HG22	2.12	0.50
3:L:125:MET:HE3	3:L:145:MET:HG2	1.94	0.50
1:C:822:ARG:HG2	1:C:822:ARG:HH21	1.77	0.50
1:C:4649:LEU:O	1:C:4650:HIS:C	2.53	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4686:LEU:HD11	1:C:4692:PRO:HA	1.92	0.50
2:G:25:HIS:NE2	2:G:40:ARG:HG2	2.27	0.50
1:B:822:ARG:HH21	1:B:822:ARG:HG2	1.77	0.50
2:F:25:HIS:NE2	2:F:40:ARG:HG2	2.27	0.50
1:A:533:ASN:OD1	1:A:534:ARG:N	2.45	0.50
1:A:2956:ALA:O	1:A:2960:LEU:N	2.44	0.50
1:A:4812:HIS:O	1:A:4814:LEU:N	2.44	0.50
1:A:4820:VAL:O	1:A:4822:THR:N	2.45	0.50
1:D:645:ARG:HG3	1:D:778:PHE:CD1	2.46	0.50
1:D:1689:VAL:HG23	1:D:1690:ASP:N	2.27	0.50
1:D:1948:ASP:HA	1:D:1951:LEU:HB2	1.93	0.50
1:C:243:ARG:HB3	1:C:300:VAL:HG13	1.93	0.50
1:C:1496:TRP:CD1	1:C:1498:GLY:H	2.30	0.50
1:B:233:ILE:HG22	1:B:234:SER:H	1.77	0.50
1:B:4820:VAL:O	1:B:4822:THR:N	2.45	0.50
1:B:5017:ARG:NH1	1:B:5019:TRP:HH2	2.10	0.50
1:A:600:LEU:HD21	1:A:1666:THR:HA	1.93	0.49
1:A:1451:GLY:HA3	1:A:1494:MET:HA	1.94	0.49
1:A:3327:LEU:O	1:A:3331:GLU:N	2.44	0.49
1:D:243:ARG:HB3	1:D:300:VAL:HG13	1.93	0.49
1:D:292:ALA:HB1	1:D:311:ALA:HB1	1.93	0.49
1:D:1451:GLY:HA3	1:D:1494:MET:HA	1.94	0.49
1:D:1477:GLY:HA2	1:D:1484:HIS:HB2	1.94	0.49
1:D:4678:ALA:HB2	1:D:4720:VAL:HG21	1.94	0.49
1:C:883:ALA:O	1:C:887:ILE:N	2.45	0.49
1:C:2956:ALA:O	1:C:2960:LEU:N	2.44	0.49
1:C:4547:GLN:O	1:C:4548:ARG:C	2.53	0.49
1:C:4567:LEU:HD11	1:C:4816:ILE:HD13	1.93	0.49
1:B:1707:LEU:O	1:B:1709:ALA:N	2.45	0.49
1:B:4549:VAL:O	1:B:4550:LYS:C	2.53	0.49
1:B:4562:LEU:HD12	1:B:4657:MET:HG3	1.94	0.49
1:B:4678:ALA:HB2	1:B:4720:VAL:HG21	1.94	0.49
1:A:1649:ASP:OD1	1:A:1650:ILE:N	2.45	0.49
1:A:1948:ASP:HA	1:A:1951:LEU:HB2	1.93	0.49
1:A:5017:ARG:NH1	1:A:5019:TRP:HH2	2.10	0.49
3:I:73:MET:SD	3:I:77:MET:HE3	2.52	0.49
1:D:359:TYR:OH	1:D:385:ASP:OD2	2.21	0.49
1:D:501:ALA:HB1	1:D:512:ALA:HB1	1.94	0.49
1:D:4571:PHE:HE2	1:D:4816:ILE:CG1	2.25	0.49
1:C:1243:PRO:HG2	1:C:1458:HIS:HB3	1.93	0.49
1:C:4820:VAL:O	1:C:4822:THR:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:125:MET:HE3	3:K:145:MET:HG2	1.94	0.49
1:B:1243:PRO:HG2	1:B:1458:HIS:HB3	1.93	0.49
1:A:4075:GLU:HA	1:A:4078:GLN:HG2	1.94	0.49
2:E:8:SER:HB2	2:E:71:ARG:HG2	1.95	0.49
1:D:4982:GLU:O	1:D:4983:HIS:C	2.55	0.49
2:H:25:HIS:NE2	2:H:40:ARG:HG2	2.27	0.49
1:C:4549:VAL:O	1:C:4550:LYS:C	2.53	0.49
1:C:4551:PHE:C	1:C:4553:ASN:N	2.69	0.49
1:B:4945:ASP:C	1:B:4947:GLN:N	2.71	0.49
1:A:1707:LEU:O	1:A:1709:ALA:N	2.45	0.49
1:A:4649:LEU:O	1:A:4650:HIS:C	2.53	0.49
1:A:4743:MET:HG3	1:A:4743:MET:O	2.13	0.49
1:D:4567:LEU:HD11	1:D:4816:ILE:HD13	1.93	0.49
1:D:4743:MET:O	1:D:4743:MET:HG3	2.13	0.49
1:D:5034:ASP:C	1:D:5036:LEU:N	2.65	0.49
1:C:1689:VAL:HG23	1:C:1690:ASP:N	2.27	0.49
1:B:292:ALA:HB1	1:B:311:ALA:HB1	1.93	0.49
1:B:600:LEU:HD21	1:B:1666:THR:HA	1.93	0.49
1:B:2760:GLU:O	1:B:2764:GLU:N	2.38	0.49
1:B:5035:GLN:O	1:B:5036:LEU:CB	2.60	0.49
1:A:2777:TYR:HB2	1:A:2791:LEU:HD22	1.95	0.49
1:A:4705:VAL:O	1:A:4708:THR:HG22	2.12	0.49
1:A:4966:ASP:O	1:A:4969:ASP:N	2.43	0.49
1:D:223:PHE:CE2	1:D:391:THR:HG21	2.48	0.49
1:D:233:ILE:HG22	1:D:234:SER:H	1.77	0.49
1:D:1762:LEU:HD12	1:D:1863:LEU:HD13	1.94	0.49
1:D:4547:GLN:O	1:D:4548:ARG:C	2.53	0.49
1:D:4820:VAL:O	1:D:4822:THR:N	2.45	0.49
1:C:533:ASN:OD1	1:C:534:ARG:N	2.45	0.49
1:C:689:THR:HG22	1:C:778:PHE:CE2	2.46	0.49
1:C:1649:ASP:OD1	1:C:1650:ILE:N	2.45	0.49
1:C:2777:TYR:HB2	1:C:2791:LEU:HD22	1.95	0.49
1:C:2953:LYS:O	1:C:2957:PHE:N	2.43	0.49
1:B:1451:GLY:HA3	1:B:1494:MET:HA	1.94	0.49
2:F:8:SER:HB2	2:F:71:ARG:HG2	1.95	0.49
1:A:292:ALA:HB1	1:A:311:ALA:HB1	1.93	0.49
1:A:645:ARG:HG3	1:A:778:PHE:CD1	2.46	0.49
1:A:822:ARG:HG2	1:A:822:ARG:HH21	1.77	0.49
1:A:4562:LEU:HD12	1:A:4657:MET:HG3	1.94	0.49
1:A:4682:GLU:HG2	1:A:4723:LYS:HZ3	1.77	0.49
1:A:4982:GLU:O	1:A:4983:HIS:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:125:MET:HE3	3:I:145:MET:HG2	1.94	0.49
1:D:625:LEU:O	1:D:626:LEU:HB2	2.13	0.49
1:D:4949:GLN:O	1:D:4950:VAL:C	2.54	0.49
2:H:8:SER:HB2	2:H:71:ARG:HG2	1.95	0.49
3:L:143:VAL:O	3:L:147:THR:OG1	2.13	0.49
1:C:233:ILE:HG22	1:C:234:SER:H	1.77	0.49
1:C:1977:TYR:HA	1:C:1997:GLU:OE2	2.13	0.49
1:B:648:ILE:HD11	1:B:779:PRO:HG2	1.93	0.49
2:F:77:THR:OG1	2:F:78:PRO:HD2	2.13	0.49
3:J:73:MET:SD	3:J:77:MET:HE3	2.52	0.49
1:A:2862:LEU:HB3	1:A:2928:LYS:HB3	1.95	0.49
1:D:533:ASN:OD1	1:D:534:ARG:N	2.45	0.49
1:D:1977:TYR:HA	1:D:1997:GLU:OE2	2.13	0.49
1:C:4678:ALA:HB2	1:C:4720:VAL:HG21	1.94	0.49
1:C:4794:TRP:CG	1:C:4794:TRP:O	2.65	0.49
1:B:4794:TRP:CG	1:B:4794:TRP:O	2.65	0.49
3:J:90:PHE:HE2	3:J:99:GLY:HA2	1.78	0.49
3:J:125:MET:HE3	3:J:145:MET:HG2	1.94	0.49
1:A:223:PHE:CE2	1:A:391:THR:HG21	2.48	0.49
1:A:2763:HIS:O	1:A:2767:ALA:N	2.38	0.49
1:D:883:ALA:O	1:D:887:ILE:N	2.45	0.49
1:D:1703:LEU:HA	1:D:1708:ARG:HH22	1.78	0.49
1:D:4649:LEU:O	1:D:4650:HIS:C	2.53	0.49
1:D:5017:ARG:NH1	1:D:5019:TRP:HH2	2.10	0.49
1:C:501:ALA:HB1	1:C:512:ALA:HB1	1.94	0.49
3:K:90:PHE:HE2	3:K:99:GLY:HA2	1.78	0.49
1:B:689:THR:HG22	1:B:778:PHE:CE2	2.46	0.49
1:B:1477:GLY:HA2	1:B:1484:HIS:HB2	1.94	0.49
1:B:4075:GLU:HA	1:B:4078:GLN:HG2	1.94	0.49
1:D:2777:TYR:HB2	1:D:2791:LEU:HD22	1.95	0.49
1:D:3327:LEU:O	1:D:3331:GLU:N	2.45	0.49
1:D:4794:TRP:CG	1:D:4794:TRP:O	2.65	0.49
1:D:4842:GLY:O	1:D:4843:LEU:C	2.56	0.49
1:D:4844:LEU:O	1:D:4847:VAL:N	2.46	0.49
1:C:625:LEU:O	1:C:626:LEU:HB2	2.13	0.49
1:C:2618:MET:O	1:C:2622:LEU:N	2.43	0.49
1:C:4743:MET:HG3	1:C:4743:MET:O	2.13	0.49
1:C:5013:MET:HE2	1:C:5013:MET:HB2	1.64	0.49
2:G:8:SER:HB2	2:G:71:ARG:HG2	1.95	0.49
2:G:77:THR:OG1	2:G:78:PRO:HD2	2.13	0.49
1:B:164:ARG:HH11	1:B:165:VAL:HB	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1716:ILE:HD11	1:B:1847:THR:HG21	1.95	0.49
1:B:1977:TYR:HA	1:B:1997:GLU:OE2	2.13	0.49
1:B:2862:LEU:HB3	1:B:2928:LYS:HB3	1.95	0.49
1:B:2927:LEU:HD23	1:B:2930:LEU:HD12	1.93	0.49
1:B:4728:HIS:O	1:B:4731:ILE:HG22	2.13	0.49
1:A:1549:PHE:N	1:A:1549:PHE:CD1	2.81	0.49
1:A:2927:LEU:HD23	1:A:2930:LEU:HD12	1.94	0.49
1:A:4551:PHE:C	1:A:4553:ASN:N	2.69	0.49
1:A:4945:ASP:C	1:A:4947:GLN:N	2.71	0.49
2:E:77:THR:OG1	2:E:78:PRO:HD2	2.13	0.49
1:D:1099:GLU:HG2	1:D:1195:GLY:HA3	1.95	0.49
1:D:2196:ASN:OD1	1:D:2199:ARG:NH1	2.46	0.49
1:C:1716:ILE:HD11	1:C:1847:THR:HG21	1.95	0.49
1:C:4705:VAL:O	1:C:4708:THR:HG22	2.12	0.49
1:B:4705:VAL:O	1:B:4708:THR:HG22	2.12	0.49
1:A:952:LYS:HA	1:A:970:LEU:HA	1.95	0.48
1:A:1496:TRP:CD1	1:A:1498:GLY:H	2.30	0.48
1:D:164:ARG:HH11	1:D:165:VAL:HB	1.78	0.48
1:C:164:ARG:HH11	1:C:165:VAL:HB	1.78	0.48
1:C:1451:GLY:HA3	1:C:1494:MET:HA	1.94	0.48
1:C:1703:LEU:HA	1:C:1708:ARG:HH22	1.78	0.48
1:C:4982:GLU:O	1:C:4983:HIS:C	2.55	0.48
1:B:220:LEU:HB2	1:B:391:THR:O	2.13	0.48
1:B:2470:ILE:O	1:B:2470:ILE:HG13	2.11	0.48
1:A:501:ALA:HB1	1:A:512:ALA:HB1	1.94	0.48
1:A:1152:MET:HE3	1:A:1223:PHE:CE2	2.48	0.48
1:A:4794:TRP:O	1:A:4794:TRP:CG	2.65	0.48
1:D:233:ILE:HG22	1:D:234:SER:N	2.28	0.48
1:D:1496:TRP:CD1	1:D:1498:GLY:H	2.30	0.48
1:D:4562:LEU:HD12	1:D:4657:MET:HG3	1.94	0.48
1:C:5017:ARG:NH1	1:C:5019:TRP:HH2	2.10	0.48
1:B:223:PHE:CE2	1:B:391:THR:HG21	2.48	0.48
1:B:501:ALA:HB1	1:B:512:ALA:HB1	1.94	0.48
1:B:2618:MET:O	1:B:2622:LEU:N	2.43	0.48
1:A:233:ILE:HG22	1:A:234:SER:N	2.28	0.48
1:A:516:LYS:HG3	1:A:555:GLU:HG3	1.95	0.48
1:A:883:ALA:O	1:A:887:ILE:N	2.45	0.48
1:A:1099:GLU:HG2	1:A:1195:GLY:HA3	1.95	0.48
1:A:1977:TYR:HA	1:A:1997:GLU:OE2	2.13	0.48
1:A:4571:PHE:HE2	1:A:4816:ILE:CG1	2.26	0.48
3:I:90:PHE:HE2	3:I:99:GLY:HA2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:516:LYS:HG3	1:D:555:GLU:HG3	1.95	0.48
1:D:1196:PRO:O	1:D:1198:GLN:NE2	2.44	0.48
1:C:1152:MET:HE3	1:C:1223:PHE:CE2	2.48	0.48
1:C:2196:ASN:OD1	1:C:2199:ARG:NH1	2.46	0.48
1:C:4728:HIS:O	1:C:4731:ILE:HG22	2.13	0.48
1:B:2777:TYR:HB2	1:B:2791:LEU:HD22	1.95	0.48
1:B:4950:VAL:C	1:B:4952:GLU:N	2.71	0.48
1:B:4982:GLU:O	1:B:4983:HIS:C	2.55	0.48
1:A:164:ARG:HH11	1:A:165:VAL:HB	1.78	0.48
1:A:220:LEU:HB2	1:A:391:THR:O	2.13	0.48
1:A:625:LEU:O	1:A:626:LEU:HB2	2.13	0.48
1:A:1952:GLN:O	1:A:1956:GLU:HG2	2.14	0.48
1:A:4728:HIS:O	1:A:4731:ILE:HG22	2.13	0.48
1:D:822:ARG:HG2	1:D:822:ARG:HH21	1.77	0.48
1:D:4075:GLU:HA	1:D:4078:GLN:HG2	1.95	0.48
3:L:90:PHE:HE2	3:L:99:GLY:HA2	1.78	0.48
1:C:2777:TYR:C	1:C:2787:THR:HB	2.39	0.48
1:C:4075:GLU:HA	1:C:4078:GLN:HG2	1.94	0.48
1:C:4888:TYR:HD2	1:B:4914:VAL:HG23	1.78	0.48
1:B:1496:TRP:CD1	1:B:1498:GLY:H	2.31	0.48
1:A:2777:TYR:C	1:A:2787:THR:HB	2.38	0.48
1:A:4827:LEU:HD12	1:A:4827:LEU:HA	1.66	0.48
1:A:4991:PHE:C	1:A:4993:MET:N	2.71	0.48
1:C:223:PHE:CE2	1:C:391:THR:HG21	2.48	0.48
1:C:1079:LYS:HE3	1:C:1107:PRO:HB2	1.96	0.48
1:C:3901:ASN:OD1	1:C:3904:ARG:NH1	2.29	0.48
1:C:4003:LEU:HD21	1:C:4012:LEU:HD22	1.95	0.48
1:C:4571:PHE:HE2	1:C:4816:ILE:CG1	2.26	0.48
3:K:123:ASP:O	3:K:127:ARG:HB2	2.14	0.48
1:B:555:GLU:O	1:B:555:GLU:HG2	2.14	0.48
1:B:1152:MET:HE3	1:B:1223:PHE:CE2	2.48	0.48
1:B:1703:LEU:HA	1:B:1708:ARG:HH22	1.78	0.48
1:B:4764:LEU:O	1:B:4766:THR:N	2.44	0.48
1:B:4835:LYS:HE3	1:B:4835:LYS:HB3	1.58	0.48
1:D:883:ALA:O	1:D:887:ILE:HG12	2.14	0.48
1:D:4551:PHE:C	1:D:4553:ASN:N	2.69	0.48
1:C:2770:LYS:HD2	1:C:2788:HIS:CG	2.49	0.48
1:B:1952:GLN:O	1:B:1956:GLU:HG2	2.14	0.48
1:B:3652:MET:O	1:B:3656:SER:OG	2.24	0.48
1:B:4551:PHE:C	1:B:4553:ASN:N	2.69	0.48
1:A:555:GLU:HG2	1:A:555:GLU:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1079:LYS:HE3	1:A:1107:PRO:HB2	1.96	0.48
1:A:4216:GLN:NE2	1:A:4220:ASP:OD2	2.47	0.48
2:E:77:THR:O	2:E:80:VAL:HG12	2.14	0.48
1:D:1698:LEU:HD13	1:D:1712:TYR:CZ	2.49	0.48
1:D:2695:LEU:O	1:D:2951:ILE:N	2.39	0.48
1:D:2777:TYR:C	1:D:2787:THR:HB	2.38	0.48
1:D:4897:ILE:HD13	1:D:4897:ILE:HA	1.69	0.48
1:C:12:GLN:HG3	1:C:13:PHE:CD2	2.49	0.48
1:C:686:TRP:HD1	1:C:755:ILE:HD13	1.79	0.48
1:C:883:ALA:O	1:C:887:ILE:HG12	2.14	0.48
1:C:1549:PHE:N	1:C:1549:PHE:CD1	2.81	0.48
1:C:4682:GLU:HG2	1:C:4723:LYS:HZ2	1.78	0.48
1:B:863:LEU:HD11	1:B:867:LEU:HD22	1.96	0.48
1:B:952:LYS:HA	1:B:970:LEU:HA	1.95	0.48
1:B:1079:LYS:HE3	1:B:1107:PRO:HB2	1.96	0.48
1:B:4743:MET:HG3	1:B:4743:MET:O	2.13	0.48
3:J:123:ASP:O	3:J:127:ARG:HB2	2.14	0.48
1:A:1087:ARG:HH11	1:A:1222:GLY:HA3	1.78	0.48
1:A:1253:PRO:HB2	1:A:1254:HIS:H	1.48	0.48
1:A:1703:LEU:HA	1:A:1708:ARG:HH22	1.78	0.48
1:A:4794:TRP:O	1:A:4794:TRP:CD2	2.67	0.48
1:D:667:MET:O	1:D:789:VAL:HG13	2.14	0.48
1:D:1079:LYS:HE3	1:D:1107:PRO:HB2	1.96	0.48
1:D:1716:ILE:HD11	1:D:1847:THR:HG21	1.95	0.48
1:D:1952:GLN:O	1:D:1956:GLU:HG2	2.14	0.48
1:D:2871:LEU:HD22	1:D:2927:LEU:HD22	1.96	0.48
2:H:77:THR:O	2:H:80:VAL:HG12	2.14	0.48
3:L:90:PHE:CE2	3:L:99:GLY:HA2	2.49	0.48
1:C:233:ILE:HG22	1:C:234:SER:N	2.28	0.48
1:C:555:GLU:HG2	1:C:555:GLU:O	2.14	0.48
1:C:1087:ARG:HH11	1:C:1222:GLY:HA3	1.78	0.48
1:C:1698:LEU:HD13	1:C:1712:TYR:CZ	2.49	0.48
1:C:2862:LEU:HB3	1:C:2928:LYS:HB3	1.94	0.48
1:C:4949:GLN:O	1:C:4950:VAL:C	2.54	0.48
1:C:4991:PHE:C	1:C:4993:MET:N	2.72	0.48
1:B:12:GLN:HG3	1:B:13:PHE:CD2	2.49	0.48
1:B:1099:GLU:HG2	1:B:1195:GLY:HA3	1.95	0.48
1:B:2196:ASN:OD1	1:B:2199:ARG:NH1	2.46	0.48
1:B:4216:GLN:NE2	1:B:4220:ASP:OD2	2.47	0.48
1:A:5026:ASP:OD1	1:A:5027:CYS:N	2.47	0.48
1:D:2110:TYR:HD1	1:D:3700:GLN:HE21	1.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:77:THR:OG1	2:H:78:PRO:HD2	2.13	0.48
1:C:1477:GLY:HA2	1:C:1484:HIS:HB2	1.94	0.48
1:C:4216:GLN:NE2	1:C:4220:ASP:OD2	2.47	0.48
1:B:233:ILE:HG22	1:B:234:SER:N	2.28	0.48
1:B:759:ILE:HG13	1:B:760:ASN:H	1.79	0.48
1:B:1196:PRO:O	1:B:1198:GLN:NE2	2.44	0.48
1:B:4842:GLY:O	1:B:4843:LEU:C	2.56	0.48
1:A:759:ILE:HG13	1:A:760:ASN:H	1.79	0.48
1:A:894:GLY:N	1:A:904:HIS:O	2.47	0.48
1:A:1977:TYR:O	1:A:1981:MET:N	2.47	0.48
1:A:2770:LYS:HD2	1:A:2788:HIS:CG	2.49	0.48
1:D:220:LEU:HB2	1:D:391:THR:O	2.14	0.48
1:D:470:SER:O	1:D:474:ARG:HG3	2.14	0.48
1:D:863:LEU:HD11	1:D:867:LEU:HD22	1.96	0.48
1:D:932:LEU:HA	1:D:935:LEU:HD13	1.96	0.48
1:D:2862:LEU:HB3	1:D:2928:LYS:HB3	1.95	0.48
1:D:5013:MET:HE2	1:D:5013:MET:HB2	1.64	0.48
1:D:5026:ASP:OD1	1:D:5027:CYS:N	2.47	0.48
1:C:516:LYS:HG3	1:C:555:GLU:HG3	1.95	0.48
1:C:958:THR:HG23	1:C:959:TYR:N	2.29	0.48
1:C:1158:ASN:HB3	1:C:1182:ILE:H	1.79	0.48
1:C:4794:TRP:O	1:C:4794:TRP:CD2	2.67	0.48
1:C:4842:GLY:O	1:C:4843:LEU:C	2.56	0.48
1:C:5026:ASP:OD1	1:C:5027:CYS:N	2.47	0.48
3:K:90:PHE:CE2	3:K:99:GLY:HA2	2.49	0.48
1:B:1158:ASN:HB3	1:B:1182:ILE:H	1.79	0.48
1:B:1675:ALA:O	1:B:1677:GLY:N	2.42	0.48
1:B:4571:PHE:HE2	1:B:4816:ILE:CG1	2.25	0.48
1:B:4794:TRP:O	1:B:4794:TRP:CD2	2.67	0.48
1:A:233:ILE:HG22	1:A:234:SER:H	1.77	0.47
1:A:795:GLY:H	1:A:812:HIS:HD2	1.62	0.47
1:A:932:LEU:HA	1:A:935:LEU:HD13	1.96	0.47
1:A:4842:GLY:O	1:A:4843:LEU:C	2.56	0.47
1:A:4949:GLN:O	1:A:4950:VAL:C	2.54	0.47
1:D:1087:ARG:HH11	1:D:1222:GLY:HA3	1.78	0.47
1:D:4216:GLN:NE2	1:D:4220:ASP:OD2	2.47	0.47
1:C:667:MET:O	1:C:789:VAL:HG13	2.14	0.47
1:C:1099:GLU:HG2	1:C:1195:GLY:HA3	1.95	0.47
1:A:108:LEU:HD12	1:A:147:TRP:CZ2	2.49	0.47
1:A:2760:GLU:OE2	1:A:2794:TYR:N	2.48	0.47
1:A:3292:PRO:O	1:A:3294:PRO:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4003:LEU:HD21	1:A:4012:LEU:HD22	1.95	0.47
1:D:108:LEU:HD12	1:D:147:TRP:CZ2	2.49	0.47
1:D:894:GLY:N	1:D:904:HIS:O	2.47	0.47
1:D:958:THR:HG23	1:D:959:TYR:N	2.29	0.47
1:D:1835:GLU:O	1:D:1839:VAL:HG12	2.15	0.47
1:D:1977:TYR:O	1:D:1981:MET:N	2.47	0.47
1:D:4678:ALA:CB	1:D:4720:VAL:HG21	2.44	0.47
1:D:4950:VAL:C	1:D:4952:GLU:N	2.71	0.47
1:C:1452:TRP:N	1:C:1493:TYR:O	2.42	0.47
1:C:4764:LEU:O	1:C:4766:THR:N	2.44	0.47
2:G:77:THR:O	2:G:80:VAL:HG12	2.14	0.47
1:B:883:ALA:O	1:B:887:ILE:HG12	2.14	0.47
1:B:1698:LEU:HD13	1:B:1712:TYR:CZ	2.49	0.47
1:B:2271:THR:HG22	1:B:2274:ASP:OD2	2.14	0.47
1:A:667:MET:O	1:A:789:VAL:HG13	2.14	0.47
1:A:686:TRP:HD1	1:A:755:ILE:HD13	1.79	0.47
1:A:863:LEU:HD11	1:A:867:LEU:HD22	1.96	0.47
1:A:883:ALA:O	1:A:887:ILE:HG12	2.14	0.47
1:A:1716:ILE:HD11	1:A:1847:THR:HG21	1.95	0.47
1:A:2110:TYR:HD1	1:A:3700:GLN:HE21	1.62	0.47
3:I:90:PHE:CE2	3:I:99:GLY:HA2	2.49	0.47
1:D:2953:LYS:O	1:D:2957:PHE:N	2.43	0.47
1:D:4003:LEU:HD21	1:D:4012:LEU:HD22	1.95	0.47
1:C:220:LEU:HB2	1:C:391:THR:O	2.14	0.47
1:C:863:LEU:HD11	1:C:867:LEU:HD22	1.96	0.47
1:C:1240:LYS:O	1:C:1241:SER:OG	2.29	0.47
1:C:2909:ASP:O	1:C:2916:LYS:NZ	2.38	0.47
1:B:625:LEU:O	1:B:626:LEU:HB2	2.13	0.47
1:B:3636:PHE:CB	3:J:89:ALA:HB1	2.43	0.47
1:B:5026:ASP:OD1	1:B:5027:CYS:N	2.47	0.47
1:A:4983:HIS:ND1	1:A:4983:HIS:N	2.63	0.47
3:I:123:ASP:O	3:I:127:ARG:HB2	2.14	0.47
1:D:686:TRP:HD1	1:D:755:ILE:HD13	1.79	0.47
1:D:759:ILE:HG13	1:D:760:ASN:H	1.79	0.47
1:D:2760:GLU:OE2	1:D:2794:TYR:N	2.48	0.47
2:H:59:PHE:HE1	2:H:101:VAL:HG21	1.80	0.47
1:C:108:LEU:HD12	1:C:147:TRP:CZ2	2.49	0.47
1:B:516:LYS:HG3	1:B:555:GLU:HG3	1.95	0.47
1:B:686:TRP:HD1	1:B:755:ILE:HD13	1.79	0.47
1:B:795:GLY:H	1:B:812:HIS:HD2	1.62	0.47
1:B:2770:LYS:HD2	1:B:2788:HIS:CG	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3528:THR:HA	1:D:1220:GLN:CG	2.42	0.47
2:E:59:PHE:HE1	2:E:101:VAL:HG21	1.80	0.47
1:D:4794:TRP:O	1:D:4794:TRP:CD2	2.67	0.47
3:L:123:ASP:O	3:L:127:ARG:HB2	2.14	0.47
1:C:1443:GLN:OE1	1:C:1557:THR:N	2.47	0.47
1:C:4945:ASP:O	1:C:4946:GLN:C	2.58	0.47
1:C:4945:ASP:C	1:C:4947:GLN:N	2.71	0.47
1:B:908:VAL:HG12	1:B:963:ASN:HB3	1.96	0.47
1:B:1835:GLU:O	1:B:1839:VAL:HG12	2.14	0.47
1:B:3327:LEU:O	1:B:3331:GLU:N	2.45	0.47
1:B:4003:LEU:HD21	1:B:4012:LEU:HD22	1.95	0.47
3:J:90:PHE:CE2	3:J:99:GLY:HA2	2.49	0.47
1:A:1698:LEU:HD13	1:A:1712:TYR:CZ	2.48	0.47
1:A:2871:LEU:HD22	1:A:2927:LEU:HD22	1.96	0.47
1:D:2770:LYS:HD2	1:D:2788:HIS:CG	2.49	0.47
1:C:759:ILE:HG13	1:C:760:ASN:H	1.79	0.47
1:C:894:GLY:N	1:C:904:HIS:O	2.47	0.47
1:C:952:LYS:HA	1:C:970:LEU:HA	1.95	0.47
1:C:2271:THR:HG22	1:C:2274:ASP:OD2	2.14	0.47
1:C:2760:GLU:OE2	1:C:2794:TYR:N	2.48	0.47
1:C:4678:ALA:CB	1:C:4720:VAL:HG21	2.44	0.47
1:B:894:GLY:N	1:B:904:HIS:O	2.47	0.47
1:B:932:LEU:HA	1:B:935:LEU:HD13	1.96	0.47
1:B:1087:ARG:HH11	1:B:1222:GLY:HA3	1.78	0.47
1:B:2777:TYR:C	1:B:2787:THR:HB	2.38	0.47
1:B:4682:GLU:HG2	1:B:4723:LYS:HZ3	1.77	0.47
2:F:77:THR:O	2:F:80:VAL:HG12	2.14	0.47
1:A:426:ARG:HD2	1:A:431:PRO:HA	1.97	0.47
1:A:470:SER:O	1:A:474:ARG:HG3	2.14	0.47
1:A:1855:GLY:O	1:A:1857:GLU:N	2.47	0.47
1:A:2271:THR:HG22	1:A:2274:ASP:OD2	2.14	0.47
1:A:3836:MET:HE1	1:A:3919:THR:HG22	1.97	0.47
1:A:4844:LEU:O	1:A:4847:VAL:N	2.46	0.47
1:D:821:LEU:HD23	1:D:821:LEU:H	1.80	0.47
1:D:1158:ASN:HB3	1:D:1182:ILE:H	1.79	0.47
1:D:1855:GLY:O	1:D:1857:GLU:N	2.47	0.47
1:D:2271:THR:HG22	1:D:2274:ASP:OD2	2.14	0.47
1:D:3292:PRO:O	1:D:3294:PRO:N	2.48	0.47
1:D:4659:ILE:HD12	1:D:4659:ILE:HA	1.75	0.47
1:C:350:HIS:HE1	1:C:352:ALA:HB3	1.80	0.47
1:C:821:LEU:HD23	1:C:821:LEU:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1549:PHE:N	1:C:1549:PHE:HD1	2.13	0.47
1:C:1952:GLN:O	1:C:1956:GLU:HG2	2.14	0.47
1:C:1977:TYR:O	1:C:1981:MET:N	2.47	0.47
1:C:3696:ASP:OD1	1:C:3699:HIS:HB2	2.14	0.47
1:C:3836:MET:HE1	1:C:3919:THR:HG22	1.97	0.47
1:C:4835:LYS:HE3	1:C:4835:LYS:HB3	1.58	0.47
1:B:3292:PRO:O	1:B:3294:PRO:N	2.48	0.47
1:A:12:GLN:HG3	1:A:13:PHE:CD2	2.49	0.47
1:A:350:HIS:HE1	1:A:352:ALA:HB3	1.80	0.47
1:A:908:VAL:HG12	1:A:963:ASN:HB3	1.96	0.47
1:A:958:THR:HG23	1:A:959:TYR:N	2.29	0.47
1:D:225:GLY:HA2	1:C:156:GLN:NE2	2.30	0.47
1:D:350:HIS:HE1	1:D:352:ALA:HB3	1.80	0.47
1:D:555:GLU:HG2	1:D:555:GLU:O	2.14	0.47
1:D:1075:PHE:HE2	1:D:1194:LEU:HD12	1.80	0.47
1:D:1549:PHE:N	1:D:1549:PHE:HD1	2.13	0.47
1:D:4991:PHE:C	1:D:4993:MET:N	2.71	0.47
1:C:932:LEU:HA	1:C:935:LEU:HD13	1.96	0.47
1:C:2871:LEU:HD22	1:C:2927:LEU:HD22	1.96	0.47
1:C:3327:LEU:O	1:C:3331:GLU:N	2.44	0.47
1:C:4844:LEU:O	1:C:4847:VAL:N	2.46	0.47
1:C:5035:GLN:O	1:C:5036:LEU:CB	2.60	0.47
1:B:426:ARG:HD2	1:B:431:PRO:HA	1.97	0.47
1:B:667:MET:O	1:B:789:VAL:HG13	2.14	0.47
1:B:2257:LEU:HD11	1:B:2275:VAL:HG13	1.96	0.47
1:B:2760:GLU:OE2	1:B:2794:TYR:N	2.48	0.47
1:B:3696:ASP:OD1	1:B:3699:HIS:HB2	2.14	0.47
1:A:1443:GLN:OE1	1:A:1557:THR:N	2.47	0.47
3:I:37:MET:HE2	3:I:73:MET:HE1	1.97	0.47
1:D:3632:VAL:O	1:D:3633:VAL:C	2.58	0.47
1:C:1075:PHE:HE2	1:C:1194:LEU:HD12	1.80	0.47
1:C:3292:PRO:O	1:C:3294:PRO:N	2.48	0.47
3:K:45:THR:OG1	3:K:46:GLU:N	2.48	0.47
1:B:350:HIS:HE1	1:B:352:ALA:HB3	1.80	0.47
1:B:359:TYR:OH	1:B:385:ASP:OD2	2.21	0.47
1:B:470:SER:O	1:B:474:ARG:HG3	2.14	0.47
1:A:1158:ASN:HB3	1:A:1182:ILE:H	1.79	0.47
1:D:795:GLY:H	1:D:812:HIS:HD2	1.62	0.47
1:D:952:LYS:HA	1:D:970:LEU:HA	1.95	0.47
1:D:1253:PRO:HB2	1:D:1254:HIS:H	1.48	0.47
1:D:5002:GLU:O	1:D:5003:HIS:C	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2110:TYR:HD1	1:C:3700:GLN:HE21	1.62	0.47
1:B:958:THR:HG23	1:B:959:TYR:N	2.29	0.47
1:B:1075:PHE:HE2	1:B:1194:LEU:HD12	1.80	0.47
1:B:4978:HIS:CE1	1:B:4983:HIS:CG	3.03	0.47
1:A:3696:ASP:OD1	1:A:3699:HIS:HB2	2.14	0.46
1:A:4678:ALA:CB	1:A:4720:VAL:HG21	2.44	0.46
1:D:546:TRP:O	1:D:550:LYS:NZ	2.47	0.46
1:D:1549:PHE:N	1:D:1549:PHE:CD1	2.81	0.46
1:D:1863:LEU:HD21	1:D:1946:PHE:HE2	1.80	0.46
1:D:3836:MET:HE1	1:D:3919:THR:HG22	1.97	0.46
1:D:4728:HIS:O	1:D:4731:ILE:HG22	2.13	0.46
1:C:876:GLU:O	1:C:880:GLU:HG2	2.15	0.46
1:C:1835:GLU:O	1:C:1839:VAL:HG12	2.15	0.46
1:C:4823:LEU:HD21	1:B:4839:MET:HE2	1.97	0.46
1:C:4983:HIS:O	1:C:4984:ASN:HB2	2.15	0.46
1:A:649:PHE:HB3	1:A:776:LEU:HD23	1.98	0.46
1:D:101:LEU:HB2	1:D:163:VAL:HG11	1.98	0.46
1:D:830:ARG:HD3	1:D:1612:PHE:CE2	2.51	0.46
1:D:4842:GLY:C	1:D:4844:LEU:N	2.74	0.46
1:D:4945:ASP:C	1:D:4947:GLN:N	2.71	0.46
1:C:1484:HIS:ND1	1:C:1484:HIS:C	2.72	0.46
1:C:2695:LEU:O	1:C:2951:ILE:N	2.39	0.46
1:C:4551:PHE:CE1	1:C:4555:LEU:HD13	2.50	0.46
1:B:108:LEU:HD12	1:B:147:TRP:CZ2	2.49	0.46
1:B:1193:SER:OG	1:B:1194:LEU:N	2.49	0.46
1:B:1863:LEU:HD21	1:B:1946:PHE:HE2	1.80	0.46
1:B:1977:TYR:O	1:B:1981:MET:N	2.47	0.46
1:B:4983:HIS:O	1:B:4984:ASN:HB2	2.15	0.46
1:B:4991:PHE:C	1:B:4993:MET:N	2.71	0.46
1:A:2196:ASN:OD1	1:A:2199:ARG:NH1	2.46	0.46
1:A:4551:PHE:CE1	1:A:4555:LEU:HD13	2.50	0.46
1:D:12:GLN:HG3	1:D:13:PHE:CD2	2.49	0.46
1:D:3648:ARG:HG3	1:D:3648:ARG:NH2	2.31	0.46
1:D:4551:PHE:CE1	1:D:4555:LEU:HD13	2.50	0.46
1:D:4704:LEU:O	1:D:4774:LYS:HE2	2.16	0.46
1:C:3636:PHE:CB	3:K:89:ALA:HB1	2.43	0.46
1:C:4704:LEU:O	1:C:4774:LYS:HE2	2.16	0.46
1:C:4719:PHE:C	1:C:4721:LYS:N	2.73	0.46
1:C:4978:HIS:CE1	1:C:4983:HIS:CG	3.03	0.46
1:B:887:ILE:HG13	1:B:959:TYR:CE1	2.51	0.46
1:B:1443:GLN:OE1	1:B:1557:THR:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1549:PHE:N	1:B:1549:PHE:CD1	2.81	0.46
1:B:4551:PHE:CE1	1:B:4555:LEU:HD13	2.50	0.46
1:B:4897:ILE:HD13	1:B:4897:ILE:HA	1.69	0.46
1:A:977:LEU:HB3	1:A:1044:ARG:HH22	1.80	0.46
1:A:4978:HIS:CE1	1:A:4983:HIS:CG	3.03	0.46
1:D:426:ARG:HD2	1:D:431:PRO:HA	1.97	0.46
1:D:908:VAL:HG12	1:D:963:ASN:HB3	1.96	0.46
1:D:4889:VAL:O	1:D:4889:VAL:HG12	2.15	0.46
1:C:470:SER:O	1:C:474:ARG:HG3	2.14	0.46
1:C:1855:GLY:O	1:C:1857:GLU:N	2.47	0.46
1:C:3671:ASP:OD1	1:C:3672:ARG:N	2.49	0.46
1:C:4978:HIS:HE1	1:C:4983:HIS:CG	2.33	0.46
1:C:4995:LEU:HD11	1:C:5007:GLU:HB3	1.97	0.46
1:B:1549:PHE:N	1:B:1549:PHE:HD1	2.13	0.46
1:B:1855:GLY:O	1:B:1857:GLU:N	2.47	0.46
1:B:3628:ARG:O	1:B:3629:ARG:C	2.58	0.46
1:B:3836:MET:HE1	1:B:3919:THR:HG22	1.97	0.46
1:A:876:GLU:O	1:A:880:GLU:HG2	2.15	0.46
1:A:3135:ALA:O	1:A:3137:LEU:N	2.48	0.46
1:A:3648:ARG:HG3	1:A:3648:ARG:NH2	2.31	0.46
1:D:2257:LEU:HD11	1:D:2275:VAL:HG13	1.96	0.46
1:D:3264:THR:O	1:D:3266:MET:N	2.48	0.46
1:D:3628:ARG:O	1:D:3629:ARG:C	2.58	0.46
1:D:4995:LEU:HD11	1:D:5007:GLU:HB3	1.97	0.46
1:C:1196:PRO:O	1:C:1198:GLN:NE2	2.44	0.46
1:C:2152:THR:HG22	1:C:2190:VAL:HG11	1.97	0.46
1:B:418:LEU:HD12	1:B:421:PHE:CZ	2.51	0.46
1:B:4071:ILE:HG21	1:B:4097:MET:HE1	1.97	0.46
1:B:4562:LEU:O	1:B:4563:LYS:C	2.57	0.46
1:A:1835:GLU:O	1:A:1839:VAL:HG12	2.15	0.46
1:A:2257:LEU:HD11	1:A:2275:VAL:HG13	1.96	0.46
1:A:3264:THR:O	1:A:3266:MET:N	2.48	0.46
1:A:4945:ASP:O	1:A:4946:GLN:C	2.58	0.46
1:A:4952:GLU:O	1:A:4952:GLU:HG2	2.15	0.46
1:A:4983:HIS:O	1:A:4984:ASN:HB2	2.15	0.46
1:D:887:ILE:HG13	1:D:959:TYR:CE1	2.51	0.46
1:D:1452:TRP:N	1:D:1493:TYR:O	2.42	0.46
1:D:1675:ALA:O	1:D:1677:GLY:N	2.42	0.46
1:D:2807:TRP:HA	1:D:2810:LYS:HB2	1.98	0.46
1:D:3135:ALA:O	1:D:3137:LEU:N	2.48	0.46
1:D:3696:ASP:OD1	1:D:3699:HIS:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3768:SER:HA	1:D:3771:HIS:CD2	2.51	0.46
1:D:4952:GLU:O	1:D:4952:GLU:HG2	2.15	0.46
1:D:4983:HIS:ND1	1:D:4983:HIS:N	2.63	0.46
1:C:649:PHE:HB3	1:C:776:LEU:HD23	1.98	0.46
1:C:908:VAL:HG12	1:C:963:ASN:HB3	1.96	0.46
1:C:2257:LEU:HD11	1:C:2275:VAL:HG13	1.96	0.46
1:B:883:ALA:O	1:B:887:ILE:N	2.45	0.46
1:B:4842:GLY:C	1:B:4844:LEU:N	2.74	0.46
1:B:5002:GLU:O	1:B:5003:HIS:C	2.55	0.46
3:J:45:THR:OG1	3:J:46:GLU:N	2.48	0.46
1:A:1549:PHE:N	1:A:1549:PHE:HD1	2.13	0.46
1:A:3628:ARG:O	1:A:3629:ARG:C	2.58	0.46
1:A:4995:LEU:HD11	1:A:5007:GLU:HB3	1.97	0.46
1:D:768:PHE:C	1:D:769:GLU:HG3	2.41	0.46
1:D:977:LEU:HB3	1:D:1044:ARG:HH22	1.80	0.46
1:D:2909:ASP:O	1:D:2916:LYS:NZ	2.38	0.46
1:D:4920:PHE:O	1:D:4924:VAL:HG22	2.16	0.46
1:D:4978:HIS:HE1	1:D:4983:HIS:CG	2.33	0.46
1:C:4071:ILE:HG21	1:C:4097:MET:HE1	1.97	0.46
3:K:37:MET:HE2	3:K:73:MET:HE1	1.97	0.46
1:B:834:PRO:HB2	1:B:835:ARG:NH1	2.31	0.46
1:B:876:GLU:O	1:B:880:GLU:HG2	2.15	0.46
1:B:3768:SER:HA	1:B:3771:HIS:CD2	2.51	0.46
1:B:4719:PHE:C	1:B:4721:LYS:N	2.73	0.46
1:B:4983:HIS:ND1	1:B:4983:HIS:N	2.63	0.46
1:A:418:LEU:HD12	1:A:421:PHE:CZ	2.51	0.46
1:A:875:ALA:O	1:A:879:HIS:N	2.47	0.46
1:A:3632:VAL:O	1:A:3633:VAL:C	2.58	0.46
1:A:3768:SER:HA	1:A:3771:HIS:CD2	2.51	0.46
1:A:4704:LEU:O	1:A:4774:LYS:HE2	2.16	0.46
3:I:45:THR:OG1	3:I:46:GLU:N	2.48	0.46
1:D:649:PHE:HB3	1:D:776:LEU:HD23	1.98	0.46
1:D:1193:SER:OG	1:D:1194:LEU:N	2.49	0.46
1:D:2321:ILE:HG13	1:D:2322:GLY:N	2.26	0.46
1:C:101:LEU:HB2	1:C:163:VAL:HG11	1.98	0.46
1:C:1863:LEU:HD21	1:C:1946:PHE:HE2	1.80	0.46
1:C:4813:LEU:HD23	1:C:4813:LEU:HA	1.70	0.46
1:B:131:LEU:HD12	1:B:178:ARG:CZ	2.46	0.46
1:B:821:LEU:HD23	1:B:821:LEU:H	1.80	0.46
1:B:977:LEU:HB3	1:B:1044:ARG:HH22	1.80	0.46
1:B:2871:LEU:HD22	1:B:2927:LEU:HD22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3632:VAL:O	1:B:3633:VAL:C	2.58	0.46
1:B:4561:THR:OG1	1:B:4562:LEU:N	2.49	0.46
1:B:4678:ALA:CB	1:B:4720:VAL:HG21	2.45	0.46
1:A:834:PRO:HB2	1:A:835:ARG:NH1	2.31	0.46
1:A:4920:PHE:O	1:A:4924:VAL:HG22	2.16	0.46
1:D:4552:LEU:HA	1:D:4555:LEU:CD2	2.45	0.46
1:D:4945:ASP:O	1:D:4946:GLN:C	2.58	0.46
1:D:4978:HIS:CE1	1:D:4983:HIS:CG	3.03	0.46
1:D:4983:HIS:O	1:D:4984:ASN:HB2	2.15	0.46
1:C:830:ARG:HD3	1:C:1612:PHE:CE2	2.51	0.46
1:C:834:PRO:HB2	1:C:835:ARG:NH1	2.31	0.46
1:C:4920:PHE:O	1:C:4924:VAL:HG22	2.16	0.46
1:C:4952:GLU:HG2	1:C:4952:GLU:O	2.15	0.46
1:C:4977:THR:O	1:C:4978:HIS:C	2.59	0.46
2:G:59:PHE:HE1	2:G:101:VAL:HG21	1.79	0.46
1:B:101:LEU:HB2	1:B:163:VAL:HG11	1.98	0.46
1:B:649:PHE:HB3	1:B:776:LEU:HD23	1.98	0.46
1:B:2110:TYR:HD1	1:B:3700:GLN:HE21	1.62	0.46
1:B:3901:ASN:OD1	1:B:3904:ARG:NH1	2.29	0.46
1:B:4561:THR:O	1:B:4562:LEU:C	2.58	0.46
1:B:4819:GLU:HB3	1:B:4820:VAL:H	1.59	0.46
1:B:4889:VAL:O	1:B:4889:VAL:HG12	2.15	0.46
3:J:37:MET:HE2	3:J:73:MET:HE1	1.97	0.46
1:A:717:ASP:OD1	1:A:720:HIS:N	2.44	0.46
1:A:4901:ILE:O	1:A:4902:GLU:O	2.34	0.46
1:D:131:LEU:HD12	1:D:178:ARG:CZ	2.46	0.46
1:D:418:LEU:HD12	1:D:421:PHE:CZ	2.51	0.46
1:C:426:ARG:HD2	1:C:431:PRO:HA	1.97	0.46
1:C:2811:GLU:HA	1:C:2814:LYS:HB2	1.98	0.46
1:C:4903:ASP:HA	1:C:4904:PRO:HD3	1.76	0.46
1:B:3363:GLY:O	1:B:3367:LYS:N	2.49	0.46
1:B:3909:ASN:HB3	1:B:3910:THR:H	1.63	0.46
1:B:4952:GLU:HG2	1:B:4952:GLU:O	2.15	0.46
1:A:768:PHE:C	1:A:769:GLU:HG3	2.41	0.45
1:A:887:ILE:HG13	1:A:959:TYR:CE1	2.51	0.45
1:A:1075:PHE:HE2	1:A:1194:LEU:HD12	1.80	0.45
1:A:2811:GLU:HA	1:A:2814:LYS:HB2	1.98	0.45
1:A:3671:ASP:OD1	1:A:3672:ARG:N	2.49	0.45
1:A:3829:PHE:HB3	1:A:3913:ILE:HG13	1.98	0.45
1:D:2152:THR:HG22	1:D:2190:VAL:HG11	1.97	0.45
1:D:3829:PHE:HB3	1:D:3913:ILE:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:37:MET:HE2	3:L:73:MET:HE1	1.97	0.45
1:C:131:LEU:HD12	1:C:178:ARG:CZ	2.46	0.45
1:C:418:LEU:HD12	1:C:421:PHE:CZ	2.51	0.45
1:C:1193:SER:OG	1:C:1194:LEU:N	2.49	0.45
1:C:2775:TRP:CZ3	1:C:2786:LYS:HA	2.51	0.45
1:C:3363:GLY:O	1:C:3367:LYS:N	2.48	0.45
1:B:138:GLN:HG2	1:B:139:GLU:N	2.32	0.45
1:B:3829:PHE:HB3	1:B:3913:ILE:HG13	1.98	0.45
1:B:4977:THR:O	1:B:4978:HIS:C	2.59	0.45
1:A:2775:TRP:CZ3	1:A:2786:LYS:HA	2.51	0.45
1:A:3826:VAL:C	1:A:3828:PHE:H	2.25	0.45
1:D:3636:PHE:CB	3:L:89:ALA:HB1	2.43	0.45
1:D:3671:ASP:OD1	1:D:3672:ARG:N	2.49	0.45
1:D:4977:THR:O	1:D:4978:HIS:C	2.59	0.45
1:C:138:GLN:HG2	1:C:139:GLU:N	2.32	0.45
1:C:977:LEU:HB3	1:C:1044:ARG:HH22	1.80	0.45
1:C:3514:LEU:O	1:C:3516:LYS:N	2.50	0.45
1:B:745:SER:O	1:B:758:ARG:N	2.48	0.45
1:B:2152:THR:HG22	1:B:2190:VAL:HG11	1.97	0.45
1:B:4978:HIS:HE1	1:B:4983:HIS:CG	2.33	0.45
1:A:101:LEU:HB2	1:A:163:VAL:HG11	1.98	0.45
1:A:483:MET:HA	1:A:486:LEU:HB2	1.98	0.45
1:A:821:LEU:H	1:A:821:LEU:HD23	1.80	0.45
1:A:830:ARG:HD3	1:A:1612:PHE:CE2	2.51	0.45
1:A:1863:LEU:HD21	1:A:1946:PHE:HE2	1.80	0.45
1:A:4071:ILE:HG21	1:A:4097:MET:HE1	1.97	0.45
1:A:4889:VAL:O	1:A:4889:VAL:HG12	2.15	0.45
1:A:5004:THR:OG1	1:A:5005:GLY:N	2.46	0.45
1:C:768:PHE:C	1:C:769:GLU:HG3	2.41	0.45
1:C:910:PHE:O	1:C:913:LEU:HB2	2.16	0.45
1:C:3135:ALA:O	1:C:3137:LEU:N	2.48	0.45
1:C:3628:ARG:O	1:C:3629:ARG:C	2.58	0.45
1:C:3768:SER:HA	1:C:3771:HIS:CD2	2.51	0.45
1:B:483:MET:HA	1:B:486:LEU:HB2	1.98	0.45
1:B:1240:LYS:O	1:B:1241:SER:OG	2.29	0.45
1:B:2775:TRP:CZ3	1:B:2786:LYS:HA	2.52	0.45
1:B:3135:ALA:O	1:B:3137:LEU:N	2.48	0.45
1:B:4204:GLN:HA	1:B:4207:MET:HE2	1.98	0.45
1:B:4704:LEU:O	1:B:4774:LYS:HE2	2.16	0.45
1:B:4706:LEU:H	1:B:4706:LEU:HD12	1.82	0.45
1:A:131:LEU:HD12	1:A:178:ARG:CZ	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3514:LEU:O	1:A:3516:LYS:N	2.50	0.45
1:A:4903:ASP:HA	1:A:4904:PRO:HD3	1.76	0.45
1:D:876:GLU:O	1:D:880:GLU:HG2	2.16	0.45
1:D:910:PHE:O	1:D:913:LEU:HB2	2.16	0.45
1:D:2811:GLU:HA	1:D:2814:LYS:HB2	1.99	0.45
1:D:4071:ILE:HG21	1:D:4097:MET:HE1	1.97	0.45
1:D:4562:LEU:O	1:D:4563:LYS:C	2.57	0.45
1:D:5004:THR:OG1	1:D:5005:GLY:N	2.46	0.45
1:C:483:MET:HE3	1:C:483:MET:HB3	1.88	0.45
1:C:875:ALA:O	1:C:879:HIS:N	2.47	0.45
1:C:4552:LEU:HA	1:C:4555:LEU:CD2	2.45	0.45
1:C:4561:THR:OG1	1:C:4562:LEU:N	2.49	0.45
1:C:4706:LEU:H	1:C:4706:LEU:HD12	1.82	0.45
1:C:4844:LEU:HD12	1:C:4844:LEU:HA	1.61	0.45
1:B:768:PHE:C	1:B:769:GLU:HG3	2.41	0.45
1:B:910:PHE:O	1:B:913:LEU:HB2	2.16	0.45
1:B:2920:ARG:O	1:B:2924:GLN:N	2.38	0.45
1:B:3514:LEU:O	1:B:3516:LYS:N	2.50	0.45
1:B:3671:ASP:OD1	1:B:3672:ARG:N	2.49	0.45
1:B:4945:ASP:O	1:B:4946:GLN:C	2.58	0.45
1:A:910:PHE:O	1:A:913:LEU:HB2	2.16	0.45
1:A:1040:CYS:O	1:A:1044:ARG:N	2.49	0.45
1:A:2807:TRP:HA	1:A:2810:LYS:HB2	1.98	0.45
1:A:4097:MET:HB3	1:A:4108:ILE:HD12	1.99	0.45
1:A:4839:MET:HE2	1:B:4823:LEU:HD21	1.98	0.45
1:D:2191:PHE:CG	1:D:2191:PHE:O	2.69	0.45
1:D:4204:GLN:HA	1:D:4207:MET:HE2	1.98	0.45
1:D:4901:ILE:O	1:D:4902:GLU:O	2.34	0.45
1:B:2811:GLU:HA	1:B:2814:LYS:HB2	1.98	0.45
1:B:3648:ARG:HG3	1:B:3648:ARG:NH2	2.31	0.45
1:B:4901:ILE:O	1:B:4902:GLU:O	2.34	0.45
1:A:138:GLN:HG2	1:A:139:GLU:N	2.32	0.45
1:A:1440:PHE:HD1	1:A:1561:VAL:O	2.00	0.45
1:A:3630:ARG:O	1:A:3631:ALA:C	2.60	0.45
1:A:4561:THR:OG1	1:A:4562:LEU:N	2.49	0.45
1:A:4842:GLY:C	1:A:4844:LEU:N	2.74	0.45
1:D:138:GLN:HG2	1:D:139:GLU:N	2.32	0.45
1:D:560:ILE:HA	1:D:563:VAL:HG12	1.99	0.45
1:D:4020:GLN:HB2	1:D:4139:ILE:HD12	1.99	0.45
1:C:745:SER:O	1:C:758:ARG:N	2.48	0.45
1:C:1253:PRO:HB2	1:C:1254:HIS:H	1.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3648:ARG:HG3	1:C:3648:ARG:NH2	2.31	0.45
1:C:4553:ASN:O	1:C:4557:ARG:HG3	2.17	0.45
1:C:4889:VAL:O	1:C:4889:VAL:HG12	2.15	0.45
1:B:1440:PHE:HD1	1:B:1561:VAL:O	2.00	0.45
1:A:415:ILE:HD11	1:A:490:CYS:SG	2.57	0.45
1:A:4978:HIS:HE1	1:A:4983:HIS:CG	2.33	0.45
1:D:1040:CYS:O	1:D:1044:ARG:N	2.49	0.45
1:D:1100:MET:H	1:D:1143:TRP:HH2	1.65	0.45
1:C:546:TRP:O	1:C:550:LYS:NZ	2.47	0.45
1:C:4983:HIS:ND1	1:C:4983:HIS:N	2.63	0.45
1:B:830:ARG:HD3	1:B:1612:PHE:CE2	2.51	0.45
1:B:1040:CYS:O	1:B:1044:ARG:N	2.49	0.45
1:B:1130:GLN:OE1	1:B:1136:SER:OG	2.24	0.45
1:B:4903:ASP:HA	1:B:4904:PRO:HD3	1.75	0.45
1:B:4920:PHE:O	1:B:4924:VAL:HG22	2.16	0.45
2:F:59:PHE:HE1	2:F:101:VAL:HG21	1.79	0.45
1:A:1240:LYS:O	1:A:1241:SER:OG	2.29	0.45
1:A:2959:PHE:O	1:A:2963:LEU:N	2.48	0.45
1:A:3202:PRO:O	1:A:3206:LEU:N	2.38	0.45
3:I:20:PHE:CE2	3:I:32:ALA:HB1	2.52	0.45
1:D:168:ASP:N	1:D:168:ASP:OD1	2.42	0.45
1:D:445:LEU:O	1:D:449:ILE:HG13	2.17	0.45
1:D:717:ASP:OD1	1:D:720:HIS:N	2.44	0.45
1:D:4553:ASN:O	1:D:4557:ARG:HG3	2.17	0.45
1:D:4733:GLY:H	1:D:4736:ARG:NH2	2.15	0.45
1:C:445:LEU:O	1:C:449:ILE:HG13	2.17	0.45
1:C:483:MET:HA	1:C:486:LEU:HB2	1.98	0.45
1:C:887:ILE:HG13	1:C:959:TYR:CE1	2.51	0.45
1:C:1440:PHE:HD1	1:C:1561:VAL:O	2.00	0.45
1:C:2247:GLN:HE21	1:C:2280:VAL:HA	1.82	0.45
1:C:3829:PHE:HB3	1:C:3913:ILE:HG13	1.98	0.45
1:C:4562:LEU:O	1:C:4563:LYS:C	2.57	0.45
1:B:1237:TRP:CZ2	1:B:1655:GLU:HG3	2.52	0.45
1:B:2165:LEU:HD11	1:B:2170:MET:HE1	1.99	0.45
1:B:4995:LEU:HD11	1:B:5007:GLU:HB3	1.97	0.45
1:A:1193:SER:OG	1:A:1194:LEU:N	2.49	0.45
1:A:2191:PHE:O	1:A:2191:PHE:CG	2.69	0.45
1:A:4687:TYR:CE1	1:A:4692:PRO:HG3	2.49	0.45
1:A:4706:LEU:H	1:A:4706:LEU:HD12	1.82	0.45
1:D:1484:HIS:ND1	1:D:1484:HIS:C	2.72	0.45
1:D:3216:CYS:O	1:D:3218:VAL:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:63:ALA:HA	2:H:66:MET:HE3	1.98	0.45
1:C:2959:PHE:O	1:C:2963:LEU:N	2.48	0.45
1:C:3826:VAL:C	1:C:3828:PHE:H	2.25	0.45
1:B:3826:VAL:C	1:B:3828:PHE:H	2.25	0.45
1:A:955:LEU:N	1:A:956:PRO:HD3	2.32	0.45
1:A:3216:CYS:O	1:A:3218:VAL:N	2.50	0.45
1:D:415:ILE:HD11	1:D:490:CYS:SG	2.57	0.45
1:D:483:MET:HA	1:D:486:LEU:HB2	1.98	0.45
1:D:955:LEU:N	1:D:956:PRO:HD3	2.32	0.45
1:D:3889:GLN:HG3	1:D:3967:GLU:HG3	1.99	0.45
3:L:20:PHE:CE2	3:L:32:ALA:HB1	2.52	0.45
1:C:2191:PHE:CG	1:C:2191:PHE:O	2.69	0.45
1:C:4659:ILE:HD12	1:C:4659:ILE:HA	1.75	0.45
1:C:4766:THR:O	1:C:4769:MET:HG3	2.17	0.45
1:B:415:ILE:HD11	1:B:490:CYS:SG	2.57	0.45
1:B:560:ILE:HA	1:B:563:VAL:HG12	1.99	0.45
1:B:717:ASP:OD1	1:B:720:HIS:N	2.44	0.45
1:B:1079:LYS:HG2	1:B:1655:GLU:OE1	2.18	0.45
1:B:2807:TRP:HA	1:B:2810:LYS:HB2	1.98	0.45
1:B:3889:GLN:HG3	1:B:3967:GLU:HG3	1.99	0.45
1:A:745:SER:O	1:A:758:ARG:N	2.48	0.44
1:A:3856:LEU:H	1:A:3856:LEU:HG	1.52	0.44
1:A:4733:GLY:H	1:A:4736:ARG:NH2	2.15	0.44
1:D:705:ASN:OD1	1:D:709:ASP:HB2	2.17	0.44
1:C:415:ILE:HD11	1:C:490:CYS:SG	2.57	0.44
1:C:705:ASN:OD1	1:C:709:ASP:HB2	2.17	0.44
1:C:955:LEU:N	1:C:956:PRO:HD3	2.32	0.44
1:C:1079:LYS:HG2	1:C:1655:GLU:OE1	2.17	0.44
1:C:1243:PRO:HB2	1:C:1600:LEU:HG	2.00	0.44
1:C:3632:VAL:O	1:C:3633:VAL:C	2.58	0.44
1:C:4020:GLN:HB2	1:C:4139:ILE:HD12	1.99	0.44
1:B:4572:ALA:O	1:B:4575:PHE:N	2.48	0.44
1:B:4844:LEU:O	1:B:4847:VAL:N	2.46	0.44
1:A:1100:MET:H	1:A:1143:TRP:HH2	1.65	0.44
1:A:2447:LYS:HG2	1:A:2449:GLU:H	1.83	0.44
1:A:2618:MET:O	1:A:2622:LEU:N	2.43	0.44
1:A:3951:PHE:HE1	1:A:3955:MET:HE3	1.83	0.44
1:D:3514:LEU:O	1:D:3516:LYS:N	2.50	0.44
1:D:3897:ASN:OD1	1:D:3901:ASN:ND2	2.51	0.44
1:D:3951:PHE:HE1	1:D:3955:MET:HE3	1.83	0.44
1:C:1484:HIS:C	1:C:1484:HIS:HD1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3456:GLN:O	1:C:3460:VAL:N	2.51	0.44
1:C:4204:GLN:HA	1:C:4207:MET:HE2	1.98	0.44
1:C:4901:ILE:O	1:C:4902:GLU:O	2.34	0.44
2:G:63:ALA:HA	2:G:66:MET:HE3	1.98	0.44
1:B:1552:VAL:HG11	1:B:1562:ILE:HD13	2.00	0.44
1:B:3264:THR:O	1:B:3266:MET:N	2.48	0.44
1:A:1079:LYS:HG2	1:A:1655:GLU:OE1	2.18	0.44
1:A:1237:TRP:CZ2	1:A:1655:GLU:HG3	2.52	0.44
1:A:1552:VAL:HG11	1:A:1562:ILE:HD13	2.00	0.44
1:A:2152:THR:HG22	1:A:2190:VAL:HG11	1.97	0.44
1:A:3873:LYS:HG3	1:A:3874:VAL:H	1.82	0.44
1:A:3889:GLN:HG3	1:A:3967:GLU:HG3	1.99	0.44
2:E:63:ALA:HA	2:E:66:MET:HE3	1.98	0.44
3:I:44:PRO:HG2	3:I:48:GLU:OE2	2.18	0.44
1:D:1440:PHE:HD1	1:D:1561:VAL:O	2.00	0.44
1:D:2880:GLU:HG2	1:D:2884:ASN:OD1	2.18	0.44
1:C:1829:PRO:HG2	1:C:1834:VAL:H	1.82	0.44
1:C:2165:LEU:HD11	1:C:2170:MET:HE1	1.99	0.44
1:C:2447:LYS:HG2	1:C:2449:GLU:H	1.83	0.44
1:C:2807:TRP:HA	1:C:2810:LYS:HB2	1.98	0.44
1:C:4733:GLY:H	1:C:4736:ARG:NH2	2.15	0.44
1:B:445:LEU:O	1:B:449:ILE:HG13	2.17	0.44
1:B:540:PHE:HD2	1:B:567:VAL:HG11	1.83	0.44
1:B:1731:LEU:HA	1:B:1772:ARG:HH11	1.82	0.44
1:B:2191:PHE:CG	1:B:2191:PHE:O	2.69	0.44
1:B:2447:LYS:HG2	1:B:2449:GLU:H	1.83	0.44
1:B:3216:CYS:O	1:B:3218:VAL:N	2.50	0.44
1:B:4575:PHE:CD1	1:B:4575:PHE:C	2.96	0.44
1:A:3456:GLN:O	1:A:3460:VAL:N	2.51	0.44
1:A:3897:ASN:OD1	1:A:3901:ASN:ND2	2.51	0.44
1:D:1079:LYS:HG2	1:D:1655:GLU:OE1	2.17	0.44
1:D:2378:ALA:O	1:D:2382:GLU:N	2.40	0.44
1:D:2382:GLU:O	1:D:2386:ILE:HG12	2.18	0.44
1:D:2775:TRP:CZ3	1:D:2786:LYS:HA	2.52	0.44
1:C:2259:GLU:HA	1:C:2297:LYS:HZ2	1.82	0.44
1:C:3889:GLN:HG3	1:C:3967:GLU:HG3	1.99	0.44
1:C:4097:MET:HB3	1:C:4108:ILE:HD12	1.99	0.44
1:C:4842:GLY:C	1:C:4844:LEU:N	2.74	0.44
1:C:4897:ILE:HD13	1:C:4897:ILE:HA	1.69	0.44
1:B:705:ASN:OD1	1:B:709:ASP:HB2	2.17	0.44
1:B:1829:PRO:HG2	1:B:1834:VAL:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2880:GLU:HG2	1:B:2884:ASN:OD1	2.18	0.44
1:B:4097:MET:HB3	1:B:4108:ILE:HD12	1.99	0.44
3:J:44:PRO:HG2	3:J:48:GLU:OE2	2.18	0.44
1:A:705:ASN:OD1	1:A:709:ASP:HB2	2.17	0.44
1:A:2382:GLU:O	1:A:2386:ILE:HG12	2.18	0.44
1:A:3363:GLY:O	1:A:3367:LYS:N	2.49	0.44
1:A:4115:SER:OG	1:A:4116:GLU:N	2.50	0.44
1:A:4575:PHE:CD1	1:A:4575:PHE:C	2.96	0.44
1:D:540:PHE:HD2	1:D:567:VAL:HG11	1.83	0.44
1:D:834:PRO:HB2	1:D:835:ARG:NH1	2.31	0.44
1:D:1237:TRP:CZ2	1:D:1655:GLU:HG3	2.52	0.44
1:D:1243:PRO:HB2	1:D:1600:LEU:HG	1.99	0.44
1:D:3630:ARG:O	1:D:3631:ALA:C	2.60	0.44
1:D:3718:GLU:O	1:D:3793:MET:HE1	2.18	0.44
1:C:1100:MET:H	1:C:1143:TRP:HH2	1.65	0.44
1:C:2880:GLU:HG2	1:C:2884:ASN:OD1	2.18	0.44
1:C:3873:LYS:HG3	1:C:3874:VAL:H	1.82	0.44
1:C:3951:PHE:HE1	1:C:3955:MET:HE3	1.82	0.44
1:C:4575:PHE:CD1	1:C:4575:PHE:C	2.96	0.44
1:B:419:ASP:O	1:B:422:SER:OG	2.30	0.44
1:B:2187:ASN:OD1	3:J:14:LYS:NZ	2.44	0.44
1:B:3873:LYS:HG3	1:B:3874:VAL:H	1.82	0.44
1:B:4844:LEU:HD12	1:B:4844:LEU:HA	1.61	0.44
1:A:560:ILE:HA	1:A:563:VAL:HG12	1.99	0.44
1:A:2816:MET:SD	1:A:2878:LEU:HD21	2.58	0.44
1:A:2880:GLU:HG2	1:A:2884:ASN:OD1	2.18	0.44
1:A:4020:GLN:HB2	1:A:4139:ILE:HD12	1.99	0.44
1:A:4552:LEU:HA	1:A:4555:LEU:CD2	2.45	0.44
1:A:4553:ASN:O	1:A:4557:ARG:HG3	2.17	0.44
1:D:1552:VAL:HG11	1:D:1562:ILE:HD13	2.00	0.44
1:D:2247:GLN:HE21	1:D:2280:VAL:HA	1.82	0.44
1:D:4097:MET:HB3	1:D:4108:ILE:HD12	1.99	0.44
1:D:4575:PHE:CD1	1:D:4575:PHE:C	2.96	0.44
1:D:4766:THR:O	1:D:4769:MET:HG3	2.17	0.44
1:D:4911:LEU:HA	1:D:4914:VAL:HG12	2.00	0.44
3:L:44:PRO:HG2	3:L:48:GLU:OE2	2.18	0.44
1:C:540:PHE:HD2	1:C:567:VAL:HG11	1.83	0.44
1:C:1237:TRP:CZ2	1:C:1655:GLU:HG3	2.52	0.44
1:C:1731:LEU:HA	1:C:1772:ARG:HH11	1.82	0.44
1:C:3216:CYS:O	1:C:3218:VAL:N	2.50	0.44
1:C:4569:LEU:O	1:C:4573:ILE:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4572:ALA:O	1:C:4575:PHE:N	2.48	0.44
1:C:4914:VAL:O	1:C:4918:ILE:HG12	2.18	0.44
3:K:20:PHE:CE2	3:K:32:ALA:HB1	2.52	0.44
1:B:2959:PHE:O	1:B:2963:LEU:N	2.48	0.44
1:B:3631:ALA:O	1:B:3632:VAL:C	2.60	0.44
1:B:4115:SER:OG	1:B:4116:GLU:N	2.50	0.44
1:B:4766:THR:O	1:B:4769:MET:HG3	2.17	0.44
1:B:4914:VAL:O	1:B:4918:ILE:HG12	2.18	0.44
1:A:1731:LEU:HA	1:A:1772:ARG:HH11	1.82	0.44
1:A:2247:GLN:HE21	1:A:2280:VAL:HA	1.82	0.44
1:A:4911:LEU:HA	1:A:4914:VAL:HG12	2.00	0.44
3:I:106:LEU:HA	3:I:109:VAL:HG22	2.00	0.44
1:D:875:ALA:O	1:D:879:HIS:N	2.47	0.44
1:D:2447:LYS:HG2	1:D:2449:GLU:H	1.83	0.44
1:D:3670:GLU:OE1	1:D:3731:LYS:HB2	2.18	0.44
1:D:4682:GLU:HG2	1:D:4723:LYS:HZ3	1.83	0.44
1:D:4706:LEU:HD12	1:D:4706:LEU:H	1.82	0.44
1:C:1552:VAL:HG11	1:C:1562:ILE:HD13	2.00	0.44
1:C:3010:PHE:O	1:C:3014:CYS:N	2.51	0.44
1:C:4650:HIS:CE1	1:C:4812:HIS:CE1	3.06	0.44
1:B:3718:GLU:O	1:B:3793:MET:HE1	2.18	0.44
1:B:4733:GLY:H	1:B:4736:ARG:NH2	2.15	0.44
2:F:63:ALA:HA	2:F:66:MET:HE3	1.98	0.44
3:J:20:PHE:CE2	3:J:32:ALA:HB1	2.52	0.44
1:A:4680:LYS:HE3	1:A:4686:LEU:HD22	2.00	0.44
1:A:4766:THR:O	1:A:4769:MET:HG3	2.17	0.44
1:A:4897:ILE:HA	1:A:4897:ILE:HD13	1.69	0.44
1:A:4977:THR:O	1:A:4978:HIS:C	2.59	0.44
1:D:645:ARG:HD2	1:D:826:ILE:HB	2.00	0.44
1:D:745:SER:O	1:D:758:ARG:N	2.48	0.44
3:L:106:LEU:HA	3:L:109:VAL:HG22	2.00	0.44
1:C:316:PHE:CE1	1:C:348:VAL:HG12	2.53	0.44
1:C:645:ARG:HD2	1:C:826:ILE:HB	2.00	0.44
1:C:3668:SER:HB2	1:C:3672:ARG:HH22	1.83	0.44
1:C:3670:GLU:OE1	1:C:3731:LYS:HB2	2.18	0.44
1:C:3718:GLU:O	1:C:3793:MET:HE1	2.18	0.44
1:C:4115:SER:OG	1:C:4116:GLU:N	2.50	0.44
1:C:4680:LYS:HE3	1:C:4686:LEU:HD22	2.00	0.44
3:K:44:PRO:HG2	3:K:48:GLU:OE2	2.18	0.44
1:B:1452:TRP:N	1:B:1493:TYR:O	2.42	0.44
1:B:2247:GLN:HE21	1:B:2280:VAL:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3456:GLN:O	1:B:3460:VAL:N	2.51	0.44
1:B:4226:GLY:C	1:B:4227:GLU:HG3	2.43	0.44
1:A:331:VAL:HG12	1:A:333:GLY:H	1.83	0.44
1:A:4204:GLN:HA	1:A:4207:MET:HE2	1.98	0.44
1:A:5002:GLU:O	1:A:5003:HIS:C	2.55	0.44
1:D:316:PHE:CE1	1:D:348:VAL:HG12	2.53	0.44
1:D:1093:GLU:HB3	1:D:1201:HIS:HB3	2.00	0.44
1:D:4572:ALA:O	1:D:4575:PHE:N	2.48	0.44
1:D:4680:LYS:HE3	1:D:4686:LEU:HD22	2.00	0.44
1:D:4914:VAL:O	1:D:4918:ILE:HG12	2.18	0.44
1:C:1093:GLU:HB3	1:C:1201:HIS:HB3	2.00	0.44
1:C:2755:ILE:HG13	1:C:2813:LEU:HD12	2.00	0.44
1:C:4817:ALA:O	1:C:4818:MET:HG2	2.18	0.44
1:C:4911:LEU:HA	1:C:4914:VAL:HG12	2.00	0.44
1:B:945:LYS:C	1:B:947:GLU:H	2.26	0.44
1:B:3951:PHE:HE1	1:B:3955:MET:HE3	1.83	0.44
1:A:445:LEU:O	1:A:449:ILE:HG13	2.17	0.43
1:A:3668:SER:HB2	1:A:3672:ARG:HH22	1.83	0.43
1:A:4650:HIS:CE1	1:A:4812:HIS:CE1	3.06	0.43
1:D:2763:HIS:O	1:D:2767:ALA:N	2.38	0.43
1:D:3363:GLY:O	1:D:3367:LYS:N	2.49	0.43
1:D:3396:ASP:O	1:D:3400:VAL:N	2.48	0.43
1:D:3456:GLN:O	1:D:3460:VAL:N	2.51	0.43
1:D:4115:SER:OG	1:D:4116:GLU:N	2.50	0.43
1:D:4975:PHE:O	1:D:4979:THR:HG22	2.18	0.43
1:B:4553:ASN:O	1:B:4557:ARG:HG3	2.17	0.43
1:B:4680:LYS:HE3	1:B:4686:LEU:HD22	2.00	0.43
1:B:4715:TYR:O	1:B:4715:TYR:CG	2.71	0.43
1:A:750:LEU:HA	1:A:753:PRO:HB3	2.00	0.43
1:A:4797:VAL:O	1:A:4797:VAL:HG13	2.18	0.43
1:A:4975:PHE:O	1:A:4979:THR:HG22	2.18	0.43
1:D:1829:PRO:HG2	1:D:1834:VAL:H	1.82	0.43
1:D:4715:TYR:O	1:D:4715:TYR:CG	2.71	0.43
1:C:3630:ARG:O	1:C:3631:ALA:C	2.60	0.43
1:B:168:ASP:HB2	1:B:199:LEU:HD12	2.00	0.43
1:B:483:MET:HE3	1:B:483:MET:HB3	1.88	0.43
1:B:686:TRP:HZ3	1:B:779:PRO:HG3	1.83	0.43
1:B:1100:MET:H	1:B:1143:TRP:HH2	1.65	0.43
1:B:2755:ILE:HG13	1:B:2813:LEU:HD12	2.00	0.43
1:B:2763:HIS:O	1:B:2767:ALA:N	2.38	0.43
1:B:3668:SER:HB2	1:B:3672:ARG:HH22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3897:ASN:OD1	1:B:3901:ASN:ND2	2.51	0.43
1:B:4817:ALA:O	1:B:4818:MET:HG2	2.18	0.43
1:A:1243:PRO:HB2	1:A:1600:LEU:HG	2.00	0.43
1:A:4743:MET:HE2	1:A:4746:ALA:CB	2.48	0.43
3:I:5:LEU:HD11	3:I:74:ALA:HA	2.01	0.43
1:D:331:VAL:HG12	1:D:333:GLY:H	1.83	0.43
1:D:1731:LEU:HA	1:D:1772:ARG:HH11	1.82	0.43
1:D:2959:PHE:O	1:D:2963:LEU:N	2.48	0.43
1:D:3668:SER:HB2	1:D:3672:ARG:HH22	1.83	0.43
1:D:4817:ALA:O	1:D:4818:MET:HG2	2.18	0.43
2:H:25:HIS:O	2:H:40:ARG:NH2	2.52	0.43
3:L:45:THR:OG1	3:L:46:GLU:N	2.48	0.43
1:C:168:ASP:HB2	1:C:199:LEU:HD12	2.00	0.43
1:C:1040:CYS:O	1:C:1044:ARG:N	2.49	0.43
1:C:1431:THR:O	1:C:1431:THR:OG1	2.36	0.43
1:C:3897:ASN:OD1	1:C:3901:ASN:ND2	2.51	0.43
1:C:4975:PHE:O	1:C:4979:THR:HG22	2.18	0.43
1:C:5007:GLU:O	1:C:5009:TYR:N	2.51	0.43
1:B:2189:LYS:HG2	1:B:2189:LYS:O	2.19	0.43
1:B:3372:VAL:O	1:B:3376:GLU:N	2.46	0.43
1:B:4552:LEU:HA	1:B:4555:LEU:CD2	2.45	0.43
1:B:4650:HIS:CE1	1:B:4812:HIS:CE1	3.06	0.43
1:A:168:ASP:HB2	1:A:199:LEU:HD12	2.00	0.43
1:A:830:ARG:HD3	1:A:1612:PHE:CZ	2.53	0.43
1:A:945:LYS:C	1:A:947:GLU:H	2.26	0.43
1:A:1001:VAL:HA	1:A:1005:TRP:HA	2.00	0.43
1:A:2165:LEU:HD11	1:A:2170:MET:HE1	1.99	0.43
1:A:2920:ARG:O	1:A:2924:GLN:N	2.38	0.43
2:E:25:HIS:O	2:E:40:ARG:NH2	2.52	0.43
1:D:2755:ILE:HG13	1:D:2813:LEU:HD12	2.00	0.43
1:D:2782:ASP:OD1	1:D:2783:GLU:N	2.51	0.43
1:D:2816:MET:SD	1:D:2878:LEU:HD21	2.58	0.43
1:D:2920:ARG:O	1:D:2924:GLN:N	2.38	0.43
1:D:3757:GLU:HA	1:D:3760:LYS:HG2	2.01	0.43
1:D:4650:HIS:CE1	1:D:4812:HIS:CE1	3.06	0.43
1:C:556:ALA:HB1	1:C:560:ILE:HG12	2.01	0.43
1:C:3372:VAL:O	1:C:3376:GLU:N	2.46	0.43
1:C:4823:LEU:HD21	1:B:4839:MET:HB3	2.00	0.43
1:B:620:LEU:HA	1:B:623:GLU:HG3	2.01	0.43
1:B:649:PHE:HB3	1:B:776:LEU:CD2	2.48	0.43
1:B:955:LEU:N	1:B:956:PRO:HD3	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3202:PRO:O	1:B:3206:LEU:N	2.38	0.43
1:A:453:GLU:HA	1:A:454:PRO:HD3	1.91	0.43
1:A:1130:GLN:OE1	1:A:1136:SER:OG	2.24	0.43
1:A:1565:GLU:O	1:A:1566:LEU:HD12	2.19	0.43
1:A:2755:ILE:HG13	1:A:2813:LEU:HD12	2.00	0.43
1:A:2782:ASP:OD1	1:A:2783:GLU:N	2.51	0.43
1:A:2873:ALA:O	1:A:2876:GLU:HB3	2.19	0.43
1:A:4226:GLY:C	1:A:4227:GLU:HG3	2.43	0.43
1:A:4562:LEU:O	1:A:4563:LYS:C	2.57	0.43
1:D:168:ASP:HB2	1:D:199:LEU:HD12	2.00	0.43
1:D:620:LEU:HA	1:D:623:GLU:HG3	2.01	0.43
1:D:697:GLY:O	1:D:704:GLY:N	2.50	0.43
1:D:2189:LYS:O	1:D:2189:LYS:HG2	2.19	0.43
1:D:4743:MET:HE2	1:D:4746:ALA:CB	2.48	0.43
1:C:548:VAL:O	1:C:551:LEU:HD23	2.19	0.43
1:C:560:ILE:HA	1:C:563:VAL:HG12	1.99	0.43
1:C:4797:VAL:O	1:C:4797:VAL:HG13	2.18	0.43
1:B:316:PHE:CE1	1:B:348:VAL:HG12	2.53	0.43
1:B:331:VAL:HG12	1:B:333:GLY:H	1.83	0.43
1:B:619:ASP:O	1:B:622:THR:OG1	2.25	0.43
1:B:1834:VAL:HG13	1:B:1835:GLU:N	2.33	0.43
1:B:3630:ARG:O	1:B:3631:ALA:C	2.60	0.43
1:B:3856:LEU:H	1:B:3856:LEU:HG	1.50	0.43
3:J:106:LEU:HA	3:J:109:VAL:HG22	2.00	0.43
1:A:3631:ALA:O	1:A:3632:VAL:C	2.60	0.43
1:A:4175:ARG:HG3	1:A:4175:ARG:NH2	2.34	0.43
1:A:4569:LEU:O	1:A:4573:ILE:HG22	2.18	0.43
1:A:4572:ALA:O	1:A:4575:PHE:N	2.48	0.43
1:D:1431:THR:O	1:D:1431:THR:OG1	2.36	0.43
1:D:1443:GLN:OE1	1:D:1557:THR:N	2.47	0.43
1:D:2284:ASN:H	1:D:2341:VAL:HG21	1.84	0.43
1:D:3849:ARG:H	1:D:3849:ARG:HG2	1.66	0.43
1:D:4569:LEU:O	1:D:4573:ILE:HG22	2.18	0.43
1:D:4816:ILE:O	1:D:4818:MET:N	2.50	0.43
1:C:1569:GLN:HB2	1:C:1572:ILE:HD11	2.00	0.43
1:C:2189:LYS:O	1:C:2189:LYS:HG2	2.19	0.43
1:C:2816:MET:SD	1:C:2878:LEU:HD21	2.58	0.43
1:B:1569:GLN:HB2	1:B:1572:ILE:HD11	2.00	0.43
1:B:2284:ASN:H	1:B:2341:VAL:HG21	1.84	0.43
1:B:2816:MET:SD	1:B:2878:LEU:HD21	2.58	0.43
1:B:4839:MET:HE2	1:B:4839:MET:HB3	1.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5004:THR:OG1	1:B:5005:GLY:N	2.46	0.43
1:A:316:PHE:CE1	1:A:348:VAL:HG12	2.53	0.43
1:A:548:VAL:O	1:A:551:LEU:HD23	2.19	0.43
1:A:649:PHE:HB3	1:A:776:LEU:CD2	2.48	0.43
1:A:686:TRP:HZ3	1:A:779:PRO:HG3	1.84	0.43
1:A:1561:VAL:HG12	1:A:1562:ILE:HG23	2.01	0.43
1:A:1834:VAL:HG13	1:A:1835:GLU:N	2.33	0.43
1:A:2032:GLN:OE1	1:A:2032:GLN:N	2.52	0.43
1:A:3718:GLU:O	1:A:3793:MET:HE1	2.18	0.43
1:A:4561:THR:O	1:A:4562:LEU:C	2.58	0.43
1:A:4715:TYR:CG	1:A:4715:TYR:O	2.71	0.43
1:D:359:TYR:HD2	1:D:361:ALA:HB2	1.84	0.43
1:D:830:ARG:HD3	1:D:1612:PHE:CZ	2.53	0.43
1:D:2032:GLN:N	1:D:2032:GLN:OE1	2.52	0.43
1:D:2165:LEU:HD11	1:D:2170:MET:HE1	1.99	0.43
1:D:4561:THR:OG1	1:D:4562:LEU:N	2.49	0.43
1:D:4649:LEU:C	1:D:4651:THR:N	2.77	0.43
1:D:4797:VAL:O	1:D:4797:VAL:HG13	2.18	0.43
1:C:144:GLU:O	1:C:175:SER:HB3	2.19	0.43
1:C:548:VAL:HG11	1:C:582:HIS:ND1	2.34	0.43
1:C:945:LYS:C	1:C:947:GLU:H	2.26	0.43
1:C:4175:ARG:HG3	1:C:4175:ARG:NH2	2.34	0.43
2:G:25:HIS:O	2:G:40:ARG:NH2	2.52	0.43
1:B:144:GLU:O	1:B:175:SER:HB3	2.19	0.43
1:B:556:ALA:HB1	1:B:560:ILE:HG12	2.00	0.43
1:B:750:LEU:HA	1:B:753:PRO:HB3	2.00	0.43
1:B:875:ALA:O	1:B:879:HIS:N	2.47	0.43
1:B:1565:GLU:O	1:B:1566:LEU:HD12	2.19	0.43
1:B:5007:GLU:O	1:B:5009:TYR:N	2.51	0.43
1:A:540:PHE:HD2	1:A:567:VAL:HG11	1.83	0.43
1:A:2189:LYS:O	1:A:2189:LYS:HG2	2.19	0.43
1:A:2284:ASN:H	1:A:2341:VAL:HG21	1.84	0.43
1:A:4184:MET:HB2	1:A:4190:ILE:HD13	2.01	0.43
1:A:4817:ALA:O	1:A:4818:MET:HG2	2.18	0.43
1:A:4978:HIS:HA	1:A:4982:GLU:HG3	2.01	0.43
1:D:548:VAL:HG11	1:D:582:HIS:ND1	2.34	0.43
1:D:3873:LYS:HG3	1:D:3874:VAL:H	1.82	0.43
1:D:4226:GLY:C	1:D:4227:GLU:HG3	2.43	0.43
3:L:107:ARG:HA	3:L:107:ARG:HD2	1.82	0.43
1:C:1561:VAL:HG12	1:C:1562:ILE:HG23	2.01	0.43
1:C:1565:GLU:O	1:C:1566:LEU:HD12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3757:GLU:HA	1:C:3760:LYS:HG2	2.01	0.43
1:C:4226:GLY:C	1:C:4227:GLU:HG3	2.43	0.43
1:B:546:TRP:O	1:B:550:LYS:NZ	2.47	0.43
1:B:894:GLY:HA2	1:B:903:LEU:HD13	2.01	0.43
1:B:2382:GLU:O	1:B:2386:ILE:HG12	2.18	0.43
1:B:4175:ARG:HG3	1:B:4175:ARG:NH2	2.34	0.43
1:A:359:TYR:HD2	1:A:361:ALA:HB2	1.84	0.43
1:A:620:LEU:HA	1:A:623:GLU:HG3	2.01	0.43
1:A:1452:TRP:N	1:A:1493:TYR:O	2.42	0.43
1:A:1569:GLN:HB2	1:A:1572:ILE:HD11	2.00	0.43
1:A:2414:ASN:N	1:A:2417:HIS:O	2.52	0.43
1:A:2760:GLU:OE2	1:A:2795:LYS:N	2.52	0.43
1:A:3670:GLU:OE1	1:A:3731:LYS:HB2	2.18	0.43
1:A:4914:VAL:O	1:A:4918:ILE:HG12	2.18	0.43
1:D:548:VAL:O	1:D:551:LEU:HD23	2.19	0.43
1:D:750:LEU:HA	1:D:753:PRO:HB3	2.00	0.43
1:D:1001:VAL:HA	1:D:1005:TRP:HA	2.00	0.43
1:D:1452:TRP:HB3	1:D:1548:LEU:HD22	2.01	0.43
1:C:459:LEU:HD23	1:C:459:LEU:HA	1.92	0.43
1:C:1119:GLU:H	1:C:1119:GLU:CD	2.27	0.43
1:C:2382:GLU:O	1:C:2386:ILE:HG12	2.18	0.43
1:C:2751:LEU:HD22	1:C:2813:LEU:HB3	2.01	0.43
1:C:3631:ALA:O	1:C:3632:VAL:C	2.60	0.43
1:C:4715:TYR:CG	1:C:4715:TYR:O	2.71	0.43
1:C:4978:HIS:HA	1:C:4982:GLU:HG3	2.01	0.43
1:C:5002:GLU:O	1:C:5003:HIS:C	2.55	0.43
1:B:830:ARG:HD3	1:B:1612:PHE:CZ	2.53	0.43
1:B:956:PRO:HG2	1:B:959:TYR:CG	2.54	0.43
1:B:1001:VAL:HA	1:B:1005:TRP:HA	2.00	0.43
1:B:1561:VAL:HG12	1:B:1562:ILE:HG23	2.01	0.43
1:B:1863:LEU:HD21	1:B:1946:PHE:CE2	2.54	0.43
1:B:4020:GLN:HB2	1:B:4139:ILE:HD12	1.99	0.43
2:F:25:HIS:O	2:F:40:ARG:NH2	2.52	0.43
1:A:548:VAL:HG11	1:A:582:HIS:ND1	2.34	0.43
1:A:645:ARG:HD2	1:A:826:ILE:HB	2.00	0.43
1:A:1829:PRO:HG2	1:A:1834:VAL:H	1.82	0.43
1:A:4545:GLU:O	1:A:4546:VAL:C	2.62	0.43
1:D:144:GLU:O	1:D:175:SER:HB3	2.18	0.43
1:D:649:PHE:HB3	1:D:776:LEU:CD2	2.48	0.43
1:D:1119:GLU:H	1:D:1119:GLU:CD	2.27	0.43
1:D:1569:GLN:HB2	1:D:1572:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1834:VAL:HG13	1:D:1835:GLU:N	2.33	0.43
1:D:3010:PHE:O	1:D:3014:CYS:N	2.51	0.43
1:D:4730:ASP:OD1	1:D:4731:ILE:N	2.52	0.43
1:D:5007:GLU:O	1:D:5009:TYR:N	2.51	0.43
1:C:649:PHE:HB3	1:C:776:LEU:CD2	2.48	0.43
1:C:1001:VAL:HA	1:C:1005:TRP:HA	2.00	0.43
1:C:1863:LEU:HD21	1:C:1946:PHE:CE2	2.54	0.43
1:C:3202:PRO:O	1:C:3206:LEU:N	2.38	0.43
1:C:3699:HIS:O	1:C:3703:LEU:HD23	2.19	0.43
3:K:5:LEU:HD11	3:K:74:ALA:HA	2.01	0.43
1:B:645:ARG:HD2	1:B:826:ILE:HB	2.00	0.43
1:B:4184:MET:HB2	1:B:4190:ILE:HD13	2.01	0.43
1:B:4569:LEU:O	1:B:4573:ILE:HG22	2.18	0.43
1:B:4975:PHE:O	1:B:4979:THR:HG22	2.18	0.43
3:J:5:LEU:HD11	3:J:74:ALA:HA	2.01	0.43
1:A:144:GLU:O	1:A:175:SER:HB3	2.19	0.42
1:A:662:TRP:CD1	1:A:748:LEU:HD22	2.51	0.42
1:A:2568:LEU:O	1:A:2572:THR:N	2.52	0.42
1:A:2883:HIS:O	1:A:2887:GLY:HA3	2.19	0.42
1:A:4012:LEU:HA	1:A:4015:GLU:OE2	2.19	0.42
1:A:4649:LEU:C	1:A:4651:THR:N	2.77	0.42
1:D:945:LYS:C	1:D:947:GLU:H	2.26	0.42
1:D:1565:GLU:O	1:D:1566:LEU:HD12	2.19	0.42
1:D:2873:ALA:O	1:D:2876:GLU:HB3	2.19	0.42
1:D:3631:ALA:O	1:D:3632:VAL:C	2.60	0.42
1:D:4184:MET:HB2	1:D:4190:ILE:HD13	2.01	0.42
1:D:5012:LYS:HE3	1:D:5012:LYS:HB3	1.18	0.42
1:C:686:TRP:HZ3	1:C:779:PRO:HG3	1.83	0.42
1:C:3696:ASP:OD1	1:C:3696:ASP:N	2.52	0.42
1:B:1119:GLU:H	1:B:1119:GLU:CD	2.27	0.42
1:B:1641:ILE:HA	1:B:1642:PRO:HD3	1.80	0.42
1:B:3670:GLU:OE1	1:B:3731:LYS:HB2	2.18	0.42
1:B:4038:GLY:O	1:B:4042:ARG:HG3	2.19	0.42
1:B:4827:LEU:HD12	1:B:4827:LEU:HA	1.66	0.42
2:F:23:VAL:HG12	2:F:47:LYS:HB3	2.01	0.42
1:A:1607:ARG:HD3	1:A:1652:GLU:HB3	2.02	0.42
1:A:1863:LEU:HD21	1:A:1946:PHE:CE2	2.54	0.42
1:A:2187:ASN:OD1	3:I:14:LYS:NZ	2.44	0.42
1:A:2447:LYS:HG2	1:A:2448:GLY:H	1.84	0.42
1:A:3010:PHE:O	1:A:3014:CYS:N	2.51	0.42
1:A:5007:GLU:O	1:A:5009:TYR:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1561:VAL:HG12	1:D:1562:ILE:HG23	2.01	0.42
1:D:2414:ASN:N	1:D:2417:HIS:O	2.52	0.42
1:D:2754:PHE:HA	1:D:2757:LYS:HE2	2.02	0.42
1:D:3629:ARG:O	1:D:3630:ARG:C	2.62	0.42
1:D:4545:GLU:O	1:D:4546:VAL:C	2.62	0.42
1:D:4835:LYS:HE3	1:D:4835:LYS:HB3	1.58	0.42
2:H:23:VAL:HG12	2:H:47:LYS:HB3	2.01	0.42
1:C:289:ARG:HG2	1:C:303:ASP:HA	2.01	0.42
1:C:359:TYR:HD2	1:C:361:ALA:HB2	1.84	0.42
1:C:1452:TRP:HB3	1:C:1548:LEU:HD22	2.01	0.42
1:C:2414:ASN:N	1:C:2417:HIS:O	2.52	0.42
1:C:2873:ALA:O	1:C:2876:GLU:HB3	2.19	0.42
1:C:2951:ILE:O	1:C:2955:PHE:N	2.46	0.42
1:C:4038:GLY:O	1:C:4042:ARG:HG3	2.19	0.42
1:C:4802:GLY:C	1:C:4804:TYR:N	2.77	0.42
1:B:548:VAL:HG11	1:B:582:HIS:ND1	2.34	0.42
1:B:1703:LEU:HD12	1:B:1704:PRO:HD2	2.00	0.42
1:B:3010:PHE:O	1:B:3014:CYS:N	2.51	0.42
1:B:4168:GLU:OE1	1:B:4168:GLU:HA	2.20	0.42
1:B:4743:MET:HE2	1:B:4746:ALA:CB	2.48	0.42
1:B:4911:LEU:HA	1:B:4914:VAL:HG12	2.00	0.42
1:B:4980:LEU:HD23	1:B:4980:LEU:HA	1.80	0.42
1:A:2378:ALA:O	1:A:2382:GLU:N	2.40	0.42
1:A:2875:ALA:HA	1:A:2878:LEU:HB2	2.02	0.42
1:A:3757:GLU:HA	1:A:3760:LYS:HG2	2.01	0.42
1:D:347:PHE:HB3	1:D:356:TRP:HZ3	1.84	0.42
1:D:2883:HIS:O	1:D:2887:GLY:HA3	2.19	0.42
1:D:3699:HIS:O	1:D:3703:LEU:HD23	2.20	0.42
1:D:4561:THR:O	1:D:4562:LEU:C	2.58	0.42
3:L:30:THR:O	3:L:33:LEU:HG	2.20	0.42
1:C:620:LEU:HA	1:C:623:GLU:HG3	2.01	0.42
1:C:1703:LEU:HD12	1:C:1704:PRO:HD2	2.01	0.42
1:C:2032:GLN:OE1	1:C:2032:GLN:N	2.52	0.42
1:C:4649:LEU:C	1:C:4651:THR:N	2.77	0.42
1:B:548:VAL:O	1:B:551:LEU:HD23	2.19	0.42
1:B:618:GLN:HG3	1:B:618:GLN:O	2.19	0.42
1:B:1253:PRO:HB2	1:B:1254:HIS:H	1.48	0.42
1:B:2414:ASN:N	1:B:2417:HIS:O	2.52	0.42
1:B:3757:GLU:HA	1:B:3760:LYS:HG2	2.01	0.42
1:B:4977:THR:HG22	1:B:4978:HIS:N	2.35	0.42
1:A:320:LYS:NZ	1:A:383:HIS:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:TRP:O	1:A:550:LYS:NZ	2.47	0.42
1:A:894:GLY:HA2	1:A:903:LEU:HD13	2.01	0.42
1:A:1093:GLU:HB3	1:A:1201:HIS:HB3	2.00	0.42
1:A:1703:LEU:HD12	1:A:1704:PRO:HD2	2.00	0.42
1:A:2456:ILE:O	1:A:2459:SER:OG	2.35	0.42
1:A:4730:ASP:OD1	1:A:4731:ILE:N	2.52	0.42
2:E:23:VAL:HG12	2:E:47:LYS:HB3	2.01	0.42
1:D:618:GLN:HG3	1:D:618:GLN:O	2.19	0.42
1:D:1779:PRO:HA	1:D:1780:PRO:HD3	1.91	0.42
1:D:1863:LEU:HD21	1:D:1946:PHE:CE2	2.54	0.42
1:D:2777:TYR:CG	1:D:2778:GLY:N	2.87	0.42
1:D:4682:GLU:HG2	1:D:4723:LYS:HZ2	1.85	0.42
1:C:331:VAL:HG12	1:C:333:GLY:H	1.83	0.42
1:C:750:LEU:HA	1:C:753:PRO:HB3	2.00	0.42
1:C:795:GLY:H	1:C:812:HIS:HD2	1.62	0.42
1:C:2782:ASP:OD1	1:C:2783:GLU:N	2.51	0.42
1:C:3909:ASN:HB3	1:C:3910:THR:H	1.63	0.42
1:C:4977:THR:HG22	1:C:4978:HIS:N	2.34	0.42
1:B:453:GLU:HA	1:B:454:PRO:HD3	1.91	0.42
1:B:1093:GLU:HB3	1:B:1201:HIS:HB3	2.00	0.42
1:B:2032:GLN:OE1	1:B:2032:GLN:N	2.52	0.42
1:A:316:PHE:HE1	1:A:348:VAL:HG12	1.85	0.42
1:A:556:ALA:HB1	1:A:560:ILE:HG12	2.01	0.42
1:A:1119:GLU:H	1:A:1119:GLU:CD	2.27	0.42
1:A:2751:LEU:HD22	1:A:2813:LEU:HB3	2.01	0.42
1:A:2816:MET:HG2	1:A:2819:TRP:CZ2	2.55	0.42
1:D:289:ARG:HG2	1:D:303:ASP:HA	2.01	0.42
1:D:340:LYS:H	1:D:344:SER:HG	1.66	0.42
1:D:686:TRP:HZ3	1:D:779:PRO:HG3	1.83	0.42
1:D:2284:ASN:N	1:D:2341:VAL:HG21	2.35	0.42
1:D:2751:LEU:HD22	1:D:2813:LEU:HB3	2.01	0.42
1:D:4012:LEU:HA	1:D:4015:GLU:OE2	2.19	0.42
1:D:4813:LEU:HD22	1:D:4813:LEU:HA	1.80	0.42
3:L:5:LEU:HD11	3:L:74:ALA:HA	2.01	0.42
1:C:830:ARG:HD3	1:C:1612:PHE:CZ	2.53	0.42
1:C:2875:ALA:HA	1:C:2878:LEU:HB2	2.01	0.42
1:C:3361:THR:O	1:C:3363:GLY:N	2.53	0.42
1:C:3629:ARG:O	1:C:3630:ARG:C	2.62	0.42
1:C:4687:TYR:OH	1:C:4702:ASP:OD1	2.36	0.42
3:K:106:LEU:HA	3:K:109:VAL:HG22	2.00	0.42
1:B:1243:PRO:HB2	1:B:1600:LEU:HG	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2260:ASN:OD1	1:B:2260:ASN:N	2.52	0.42
1:B:2284:ASN:N	1:B:2341:VAL:HG21	2.35	0.42
1:B:2751:LEU:HD22	1:B:2813:LEU:HB3	2.01	0.42
1:B:2873:ALA:O	1:B:2876:GLU:HB3	2.19	0.42
1:A:688:LEU:HD12	1:A:690:GLU:H	1.85	0.42
1:A:2284:ASN:N	1:A:2341:VAL:HG21	2.35	0.42
1:A:3629:ARG:O	1:A:3630:ARG:C	2.62	0.42
1:A:3636:PHE:CB	3:I:89:ALA:HB1	2.43	0.42
1:A:3667:HIS:HB3	1:A:3668:SER:H	1.67	0.42
3:I:122:VAL:O	3:I:126:ILE:HG12	2.20	0.42
1:D:894:GLY:HA2	1:D:903:LEU:HD13	2.01	0.42
1:D:956:PRO:HG2	1:D:959:TYR:CG	2.54	0.42
1:D:3372:VAL:O	1:D:3376:GLU:N	2.46	0.42
1:D:3804:ILE:O	1:D:3809:ASN:ND2	2.53	0.42
3:L:82:SER:O	3:L:85:GLU:HG2	2.19	0.42
3:L:122:VAL:O	3:L:126:ILE:HG12	2.20	0.42
1:C:759:ILE:HG22	1:C:762:CYS:O	2.20	0.42
1:C:1937:LEU:HB2	1:C:2116:LEU:HD13	2.02	0.42
1:C:2883:HIS:O	1:C:2887:GLY:HA3	2.19	0.42
1:C:3652:MET:O	1:C:3656:SER:OG	2.24	0.42
1:C:3804:ILE:O	1:C:3809:ASN:ND2	2.53	0.42
1:C:4730:ASP:OD1	1:C:4731:ILE:N	2.52	0.42
1:C:4819:GLU:HB3	1:C:4820:VAL:H	1.59	0.42
3:K:30:THR:O	3:K:33:LEU:HG	2.20	0.42
3:K:122:VAL:O	3:K:126:ILE:HG12	2.20	0.42
1:B:285:VAL:HG23	1:B:286:THR:N	2.35	0.42
1:B:1607:ARG:HD3	1:B:1652:GLU:HB3	2.02	0.42
1:A:2260:ASN:OD1	1:A:2260:ASN:N	2.52	0.42
1:A:3923:LEU:HD22	1:A:3961:VAL:HG12	2.02	0.42
1:D:1720:LEU:C	1:D:1722:SER:H	2.28	0.42
1:D:2875:ALA:HA	1:D:2878:LEU:HB2	2.02	0.42
1:C:1641:ILE:HG13	1:C:1641:ILE:O	2.20	0.42
1:C:2754:PHE:HA	1:C:2757:LYS:HE2	2.01	0.42
1:B:1703:LEU:HD13	1:B:1708:ARG:HB3	2.02	0.42
1:B:1859:VAL:HA	1:B:1862:ILE:HG22	2.02	0.42
1:B:2447:LYS:HG2	1:B:2448:GLY:H	1.84	0.42
1:B:3629:ARG:O	1:B:3630:ARG:C	2.62	0.42
1:B:4967:TYR:C	1:B:4967:TYR:CD1	2.97	0.42
1:A:224:HIS:O	1:A:229:GLU:HB3	2.20	0.42
1:A:1703:LEU:HD13	1:A:1708:ARG:HB3	2.02	0.42
1:A:1720:LEU:C	1:A:1722:SER:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3804:ILE:O	1:A:3809:ASN:ND2	2.53	0.42
1:D:224:HIS:O	1:D:229:GLU:HB3	2.20	0.42
1:D:247:TYR:HE1	1:D:376:ALA:HB2	1.85	0.42
1:D:316:PHE:HE1	1:D:348:VAL:HG12	1.85	0.42
1:D:320:LYS:NZ	1:D:383:HIS:O	2.52	0.42
1:D:688:LEU:HD12	1:D:690:GLU:H	1.85	0.42
1:D:4038:GLY:O	1:D:4042:ARG:HG3	2.19	0.42
1:D:4251:ILE:HD12	1:D:4557:ARG:HG2	2.02	0.42
1:C:224:HIS:O	1:C:229:GLU:HB3	2.20	0.42
1:C:285:VAL:HG23	1:C:286:THR:N	2.35	0.42
1:C:320:LYS:NZ	1:C:383:HIS:O	2.52	0.42
1:C:956:PRO:HG2	1:C:959:TYR:CG	2.54	0.42
1:C:2816:MET:HG2	1:C:2819:TRP:CZ2	2.55	0.42
1:C:3669:PHE:O	1:C:3669:PHE:CG	2.73	0.42
1:C:4168:GLU:OE1	1:C:4168:GLU:HA	2.20	0.42
1:B:224:HIS:O	1:B:229:GLU:HB3	2.20	0.42
1:B:759:ILE:HD12	1:B:759:ILE:HA	1.94	0.42
1:B:1119:GLU:HA	1:B:1133:HIS:CE1	2.55	0.42
1:B:1641:ILE:O	1:B:1641:ILE:HG13	2.20	0.42
1:B:2023:LEU:H	1:B:2028:ARG:HH12	1.68	0.42
1:B:2284:ASN:HA	1:B:2341:VAL:HG11	2.02	0.42
1:B:2883:HIS:O	1:B:2887:GLY:HA3	2.19	0.42
1:B:4545:GLU:O	1:B:4546:VAL:C	2.62	0.42
1:B:4813:LEU:HD23	1:B:4813:LEU:HA	1.70	0.42
1:B:4976:GLU:HA	1:B:4976:GLU:OE1	2.20	0.42
1:A:247:TYR:HE1	1:A:376:ALA:HB2	1.85	0.42
1:A:1455:PRO:HG3	1:A:1549:PHE:CZ	2.55	0.42
1:A:2951:ILE:O	1:A:2955:PHE:N	2.46	0.42
1:A:3669:PHE:O	1:A:3669:PHE:CG	2.73	0.42
1:A:4251:ILE:HD12	1:A:4557:ARG:HG2	2.02	0.42
1:A:4816:ILE:O	1:A:4818:MET:N	2.50	0.42
1:A:4976:GLU:HA	1:A:4976:GLU:OE1	2.20	0.42
1:D:285:VAL:HG23	1:D:286:THR:N	2.35	0.42
1:D:759:ILE:HG22	1:D:762:CYS:O	2.20	0.42
1:D:1703:LEU:HD12	1:D:1704:PRO:HD2	2.01	0.42
1:D:3669:PHE:O	1:D:3669:PHE:CG	2.73	0.42
1:D:4175:ARG:HG3	1:D:4175:ARG:NH2	2.34	0.42
1:D:4687:TYR:CE1	1:D:4692:PRO:HG3	2.49	0.42
1:D:4972:PRO:O	1:D:4973:HIS:C	2.63	0.42
1:D:4977:THR:HG22	1:D:4978:HIS:N	2.34	0.42
1:D:4978:HIS:HA	1:D:4982:GLU:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:PHE:HE1	1:C:348:VAL:HG12	1.85	0.42
1:C:697:GLY:O	1:C:704:GLY:N	2.50	0.42
1:C:1720:LEU:C	1:C:1722:SER:H	2.28	0.42
1:C:2284:ASN:N	1:C:2341:VAL:HG21	2.35	0.42
1:C:4743:MET:HE2	1:C:4746:ALA:CB	2.48	0.42
1:C:4980:LEU:HD23	1:C:4980:LEU:HA	1.80	0.42
1:B:316:PHE:HE1	1:B:348:VAL:HG12	1.85	0.42
1:B:320:LYS:NZ	1:B:383:HIS:O	2.52	0.42
1:B:347:PHE:HB3	1:B:356:TRP:HZ3	1.84	0.42
1:B:759:ILE:HG22	1:B:762:CYS:O	2.20	0.42
1:B:2754:PHE:HA	1:B:2757:LYS:HE2	2.01	0.42
1:B:2777:TYR:CG	1:B:2778:GLY:N	2.87	0.42
1:B:4012:LEU:HA	1:B:4015:GLU:OE2	2.19	0.42
3:J:82:SER:O	3:J:85:GLU:HG2	2.19	0.42
3:J:122:VAL:O	3:J:126:ILE:HG12	2.20	0.42
1:A:956:PRO:HG2	1:A:959:TYR:CG	2.54	0.42
1:A:1452:TRP:HB3	1:A:1548:LEU:HD22	2.01	0.42
1:A:1859:VAL:HA	1:A:1862:ILE:HG22	2.02	0.42
1:A:2259:GLU:HA	1:A:2297:LYS:HZ2	1.85	0.42
1:A:3434:LEU:O	1:A:3436:ARG:N	2.44	0.42
1:A:4802:GLY:C	1:A:4804:TYR:N	2.77	0.42
1:D:3718:GLU:HA	1:D:3718:GLU:OE1	2.20	0.42
1:D:4705:VAL:HG22	1:D:4711:PHE:HD1	1.85	0.42
1:C:669:ASP:OD1	1:C:669:ASP:N	2.53	0.42
1:C:670:GLU:CD	1:C:788:LYS:H	2.28	0.42
1:C:894:GLY:HA2	1:C:903:LEU:HD13	2.01	0.42
1:C:1653:LEU:HD23	1:C:1653:LEU:HA	1.86	0.42
1:C:1703:LEU:HD13	1:C:1708:ARG:HB3	2.02	0.42
1:C:1859:VAL:HA	1:C:1862:ILE:HG22	2.02	0.42
1:C:1969:LEU:HD21	1:C:2009:LEU:CD1	2.50	0.42
1:C:3718:GLU:OE1	1:C:3718:GLU:HA	2.20	0.42
1:C:4984:ASN:HA	6:C:5103:ATP:HN61	1.85	0.42
1:B:485:SER:O	1:B:489:ASN:N	2.48	0.42
1:B:1580:PHE:HE2	1:B:1592:PRO:HG2	1.85	0.42
1:B:1937:LEU:HB2	1:B:2116:LEU:HD13	2.02	0.42
1:B:2782:ASP:OD1	1:B:2783:GLU:N	2.51	0.42
1:B:3361:THR:O	1:B:3363:GLY:N	2.53	0.42
1:B:3804:ILE:O	1:B:3809:ASN:ND2	2.53	0.42
1:B:4730:ASP:OD1	1:B:4731:ILE:N	2.52	0.42
1:B:5013:MET:HE2	1:B:5013:MET:HB2	1.64	0.42
1:A:618:GLN:O	1:A:618:GLN:HG3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:GLN:OE1	1:A:1673:VAL:HA	2.20	0.41
1:A:759:ILE:HG22	1:A:762:CYS:O	2.20	0.41
1:A:1580:PHE:HE2	1:A:1592:PRO:HG2	1.85	0.41
1:A:1928:GLN:OE1	1:A:1928:GLN:HA	2.20	0.41
1:A:4844:LEU:HA	1:A:4844:LEU:HD12	1.61	0.41
1:A:4984:ASN:HA	6:A:5103:ATP:HN61	1.85	0.41
1:D:117:TYR:HB3	1:D:146:CYS:SG	2.60	0.41
1:D:1639:LEU:O	1:D:1647:CYS:HA	2.20	0.41
1:D:1767:VAL:HG13	1:D:1767:VAL:O	2.20	0.41
1:D:2163:ARG:H	1:D:2163:ARG:HG2	1.69	0.41
1:D:3202:PRO:O	1:D:3206:LEU:N	2.38	0.41
1:D:3696:ASP:OD1	1:D:3696:ASP:N	2.52	0.41
1:D:4168:GLU:OE1	1:D:4168:GLU:HA	2.20	0.41
1:D:4546:VAL:HG13	1:D:4547:GLN:H	1.85	0.41
1:D:4802:GLY:C	1:D:4804:TYR:N	2.77	0.41
1:C:717:ASP:OD1	1:C:720:HIS:N	2.44	0.41
1:C:3922:TYR:C	1:C:3924:LEU:H	2.28	0.41
1:C:4184:MET:HB2	1:C:4190:ILE:HD13	2.01	0.41
1:C:4976:GLU:HA	1:C:4976:GLU:OE1	2.20	0.41
2:G:23:VAL:HG12	2:G:47:LYS:HB3	2.01	0.41
1:B:118:LEU:HA	1:B:137:LEU:HB3	2.02	0.41
1:B:359:TYR:HD2	1:B:361:ALA:HB2	1.84	0.41
1:B:670:GLU:CD	1:B:788:LYS:H	2.28	0.41
1:B:2033:ASP:O	1:B:2037:ASP:N	2.47	0.41
1:A:118:LEU:HA	1:A:137:LEU:HB3	2.02	0.41
1:A:347:PHE:HB3	1:A:356:TRP:HZ3	1.84	0.41
1:A:1119:GLU:HA	1:A:1133:HIS:CE1	2.55	0.41
1:A:1767:VAL:O	1:A:1767:VAL:HG13	2.20	0.41
1:A:2023:LEU:H	1:A:2028:ARG:HH12	1.68	0.41
1:A:3361:THR:O	1:A:3363:GLY:N	2.53	0.41
1:A:3696:ASP:OD1	1:A:3696:ASP:N	2.52	0.41
1:A:4038:GLY:O	1:A:4042:ARG:HG3	2.19	0.41
1:A:4546:VAL:HG13	1:A:4547:GLN:H	1.85	0.41
1:A:4719:PHE:C	1:A:4721:LYS:N	2.73	0.41
1:D:319:SER:OG	1:D:320:LYS:N	2.53	0.41
1:D:662:TRP:CD1	1:D:748:LEU:HD22	2.51	0.41
1:D:1607:ARG:HD3	1:D:1652:GLU:HB3	2.02	0.41
1:D:2568:LEU:O	1:D:2572:THR:N	2.52	0.41
1:D:3361:THR:O	1:D:3363:GLY:N	2.53	0.41
1:D:3923:LEU:HD22	1:D:3961:VAL:HG12	2.02	0.41
1:C:1607:ARG:HD3	1:C:1652:GLU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1834:VAL:HG13	1:C:1835:GLU:N	2.33	0.41
1:C:4546:VAL:HG13	1:C:4547:GLN:H	1.85	0.41
1:B:247:TYR:HE1	1:B:376:ALA:HB2	1.85	0.41
1:B:688:LEU:HD12	1:B:690:GLU:H	1.85	0.41
1:B:1731:LEU:HA	1:B:1772:ARG:NH1	2.35	0.41
1:B:3699:HIS:O	1:B:3703:LEU:HD23	2.19	0.41
1:B:4649:LEU:C	1:B:4651:THR:N	2.77	0.41
1:B:4978:HIS:HA	1:B:4982:GLU:HG3	2.01	0.41
1:B:4984:ASN:HA	6:B:5103:ATP:HN61	1.85	0.41
3:J:107:ARG:HD2	3:J:107:ARG:HA	1.82	0.41
1:A:805:PRO:HB2	1:A:808:TYR:CE2	2.55	0.41
1:A:877:ASN:HD21	1:A:970:LEU:HB2	1.85	0.41
1:A:1519:LEU:HD23	1:A:1519:LEU:HA	1.91	0.41
1:A:1641:ILE:HG13	1:A:1641:ILE:O	2.20	0.41
1:A:1731:LEU:HA	1:A:1772:ARG:NH1	2.35	0.41
1:A:4977:THR:HG22	1:A:4978:HIS:N	2.34	0.41
1:D:618:GLN:OE1	1:D:1673:VAL:HA	2.20	0.41
1:D:1097:THR:HG23	1:D:1143:TRP:HB2	2.03	0.41
1:D:1731:LEU:HA	1:D:1772:ARG:NH1	2.35	0.41
1:D:2284:ASN:HA	1:D:2341:VAL:HG11	2.02	0.41
1:C:1097:THR:HG23	1:C:1143:TRP:HB2	2.03	0.41
1:C:1767:VAL:O	1:C:1767:VAL:HG13	2.20	0.41
1:C:1808:ARG:HD2	1:C:1858:ASP:OD2	2.21	0.41
1:C:4972:PRO:O	1:C:4973:HIS:C	2.63	0.41
2:G:37:ASP:OD1	2:G:38:SER:N	2.54	0.41
1:B:805:PRO:HB2	1:B:808:TYR:CE2	2.55	0.41
1:B:1455:PRO:HG3	1:B:1549:PHE:CZ	2.55	0.41
1:B:1720:LEU:C	1:B:1722:SER:H	2.28	0.41
1:B:2568:LEU:O	1:B:2572:THR:N	2.52	0.41
1:B:3669:PHE:O	1:B:3669:PHE:CG	2.73	0.41
1:B:3923:LEU:HD22	1:B:3961:VAL:HG12	2.02	0.41
1:A:224:HIS:NE2	1:A:385:ASP:O	2.54	0.41
1:A:1033:ARG:HE	1:A:1036:ARG:HH11	1.68	0.41
1:A:1639:LEU:O	1:A:1647:CYS:HA	2.21	0.41
1:A:2777:TYR:CG	1:A:2778:GLY:N	2.87	0.41
1:A:3941:ASP:OD1	1:A:3942:VAL:N	2.54	0.41
1:A:4705:VAL:HG22	1:A:4711:PHE:HD1	1.85	0.41
1:A:4818:MET:HE3	1:A:4818:MET:HB3	1.74	0.41
1:A:4967:TYR:C	1:A:4967:TYR:CD1	2.97	0.41
1:A:4980:LEU:HD23	1:A:4980:LEU:HA	1.80	0.41
2:E:54:GLU:HG2	2:E:55:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:66:PHE:CE2	3:I:70:LEU:HD12	2.55	0.41
1:D:1119:GLU:HA	1:D:1133:HIS:CE1	2.55	0.41
1:D:2447:LYS:HG2	1:D:2448:GLY:H	1.84	0.41
1:D:3941:ASP:OD1	1:D:3942:VAL:N	2.54	0.41
1:D:4567:LEU:HD11	1:D:4816:ILE:CD1	2.51	0.41
1:C:224:HIS:NE2	1:C:385:ASP:O	2.54	0.41
1:C:2284:ASN:H	1:C:2341:VAL:HG21	1.84	0.41
1:C:3941:ASP:OD1	1:C:3942:VAL:N	2.54	0.41
1:C:4687:TYR:CE1	1:C:4692:PRO:HG3	2.50	0.41
1:C:5010:VAL:HG12	1:C:5010:VAL:O	2.21	0.41
1:B:2816:MET:HG2	1:B:2819:TRP:CZ2	2.55	0.41
1:B:3718:GLU:HA	1:B:3718:GLU:OE1	2.20	0.41
1:B:4034:ASN:OD1	1:B:4035:VAL:O	2.39	0.41
1:B:4797:VAL:O	1:B:4797:VAL:HG13	2.18	0.41
1:A:669:ASP:N	1:A:669:ASP:OD1	2.53	0.41
1:A:1937:LEU:HB2	1:A:2116:LEU:HD13	2.02	0.41
1:A:2280:VAL:HG13	1:A:2280:VAL:O	2.21	0.41
1:A:3909:ASN:HB3	1:A:3910:THR:H	1.63	0.41
1:A:4554:TYR:CE2	1:A:4558:ASN:ND2	2.89	0.41
1:A:4986:ALA:O	1:A:4987:ASN:C	2.63	0.41
1:D:669:ASP:N	1:D:669:ASP:OD1	2.53	0.41
1:D:670:GLU:CD	1:D:788:LYS:H	2.28	0.41
1:D:1130:GLN:OE1	1:D:1136:SER:OG	2.24	0.41
1:D:4647:SER:OG	1:D:4803:HIS:HE1	2.04	0.41
3:L:66:PHE:CE2	3:L:70:LEU:HD12	2.55	0.41
3:L:94:ASP:OD1	3:L:94:ASP:N	2.54	0.41
1:C:117:TYR:HB3	1:C:146:CYS:SG	2.60	0.41
1:C:618:GLN:HG3	1:C:618:GLN:O	2.19	0.41
1:C:1236:THR:OG1	1:C:1608:MET:SD	2.76	0.41
1:C:4687:TYR:HD2	1:C:4706:LEU:HD21	1.85	0.41
1:C:4952:GLU:O	1:C:4952:GLU:CG	2.69	0.41
1:B:319:SER:OG	1:B:320:LYS:N	2.53	0.41
1:B:618:GLN:OE1	1:B:1673:VAL:HA	2.20	0.41
1:B:2311:PRO:HA	1:B:2314:LEU:HB3	2.03	0.41
1:A:689:THR:HA	1:A:778:PHE:HE2	1.86	0.41
1:A:697:GLY:O	1:A:704:GLY:N	2.50	0.41
1:A:2814:LYS:O	1:A:2817:ILE:HG22	2.21	0.41
1:A:3699:HIS:O	1:A:3703:LEU:HD23	2.19	0.41
1:A:3775:ALA:O	1:A:3778:MET:N	2.53	0.41
1:A:4168:GLU:OE1	1:A:4168:GLU:HA	2.20	0.41
3:I:40:LEU:HD23	3:I:40:LEU:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:82:SER:O	3:I:85:GLU:HG2	2.19	0.41
1:D:443:LEU:HD23	1:D:443:LEU:HA	1.87	0.41
1:D:891:TRP:HE3	1:D:904:HIS:HB2	1.85	0.41
1:D:1033:ARG:HE	1:D:1036:ARG:HH11	1.68	0.41
1:D:1099:GLU:N	1:D:1099:GLU:OE1	2.54	0.41
1:D:1782:PHE:CE2	2:H:90:VAL:HG11	2.55	0.41
1:D:1928:GLN:OE1	1:D:1928:GLN:HA	2.20	0.41
1:D:2763:HIS:NE2	1:D:2767:ALA:HB2	2.36	0.41
1:D:4967:TYR:C	1:D:4967:TYR:CD1	2.97	0.41
1:D:4977:THR:O	1:D:4979:THR:N	2.54	0.41
1:C:347:PHE:HB3	1:C:356:TRP:HZ3	1.84	0.41
1:C:1119:GLU:HA	1:C:1133:HIS:CE1	2.55	0.41
1:C:2023:LEU:H	1:C:2028:ARG:HH12	1.68	0.41
1:C:2763:HIS:NE2	1:C:2767:ALA:HB2	2.36	0.41
1:C:2777:TYR:CG	1:C:2778:GLY:N	2.87	0.41
1:C:3598:GLU:HA	1:C:3601:ALA:HB3	2.03	0.41
1:C:4001:MET:HE2	1:C:4001:MET:HB2	1.94	0.41
1:C:5004:THR:OG1	1:C:5005:GLY:N	2.46	0.41
3:K:82:SER:O	3:K:85:GLU:HG2	2.19	0.41
1:B:1452:TRP:HB3	1:B:1548:LEU:HD22	2.01	0.41
1:B:1782:PHE:CE2	2:F:90:VAL:HG11	2.55	0.41
1:B:2875:ALA:HA	1:B:2878:LEU:HB2	2.01	0.41
1:B:2951:ILE:O	1:B:2955:PHE:N	2.46	0.41
1:B:3696:ASP:OD1	1:B:3696:ASP:N	2.52	0.41
1:B:3775:ALA:O	1:B:3778:MET:N	2.53	0.41
1:B:4546:VAL:HG13	1:B:4547:GLN:H	1.85	0.41
1:B:4972:PRO:O	1:B:4973:HIS:C	2.63	0.41
2:F:37:ASP:OD1	2:F:38:SER:N	2.54	0.41
1:A:285:VAL:HG23	1:A:286:THR:N	2.35	0.41
1:A:289:ARG:HG2	1:A:303:ASP:HA	2.01	0.41
1:A:2437:ALA:HB1	1:A:2438:PRO:HD2	2.03	0.41
1:D:1641:ILE:HG13	1:D:1641:ILE:O	2.20	0.41
1:D:1937:LEU:HB2	1:D:2116:LEU:HD13	2.02	0.41
1:D:1969:LEU:HD21	1:D:2009:LEU:CD1	2.50	0.41
1:D:2816:MET:HG2	1:D:2819:TRP:CZ2	2.55	0.41
1:C:118:LEU:HA	1:C:137:LEU:HB3	2.02	0.41
1:C:618:GLN:OE1	1:C:1673:VAL:HA	2.20	0.41
1:C:877:ASN:HD21	1:C:970:LEU:HB2	1.85	0.41
1:C:3775:ALA:O	1:C:3778:MET:N	2.53	0.41
1:C:4151:SER:HA	1:C:4160:LEU:HD21	2.02	0.41
1:C:4567:LEU:HD11	1:C:4816:ILE:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1256:GLU:HB2	1:B:1273:ALA:HB3	2.02	0.41
1:B:2280:VAL:O	1:B:2280:VAL:HG13	2.21	0.41
1:B:4151:SER:HA	1:B:4160:LEU:HD21	2.03	0.41
1:B:4554:TYR:CE2	1:B:4558:ASN:ND2	2.89	0.41
3:J:30:THR:O	3:J:33:LEU:HG	2.20	0.41
1:A:117:TYR:HB3	1:A:146:CYS:SG	2.60	0.41
1:A:1808:ARG:HD2	1:A:1858:ASP:OD2	2.21	0.41
1:A:3372:VAL:O	1:A:3376:GLU:N	2.46	0.41
1:A:4034:ASN:OD1	1:A:4035:VAL:O	2.39	0.41
1:A:4813:LEU:HD23	1:A:4813:LEU:HA	1.74	0.41
3:I:30:THR:O	3:I:33:LEU:HG	2.20	0.41
1:D:556:ALA:HB1	1:D:560:ILE:HG12	2.01	0.41
1:D:1859:VAL:HA	1:D:1862:ILE:HG22	2.02	0.41
1:D:2280:VAL:O	1:D:2280:VAL:HG13	2.21	0.41
1:D:2814:LYS:O	1:D:2817:ILE:HG22	2.21	0.41
1:D:4034:ASN:OD1	1:D:4035:VAL:O	2.39	0.41
1:D:4181:ILE:HG23	1:D:4988:TYR:CE1	2.56	0.41
1:D:4687:TYR:HD2	1:D:4706:LEU:HD21	1.85	0.41
1:D:5010:VAL:O	1:D:5010:VAL:HG12	2.21	0.41
2:H:54:GLU:HG2	2:H:55:VAL:HG23	2.02	0.41
1:C:247:TYR:HE1	1:C:376:ALA:HB2	1.85	0.41
1:C:2280:VAL:HG13	1:C:2280:VAL:O	2.21	0.41
1:C:2284:ASN:HA	1:C:2341:VAL:HG11	2.02	0.41
1:C:3849:ARG:H	1:C:3849:ARG:HG2	1.66	0.41
1:C:3856:LEU:H	1:C:3856:LEU:HG	1.50	0.41
1:C:4181:ILE:HG23	1:C:4988:TYR:CE1	2.56	0.41
1:C:4226:GLY:C	1:C:4228:ALA:H	2.28	0.41
3:K:107:ARG:HD2	3:K:107:ARG:HA	1.82	0.41
1:B:443:LEU:HD23	1:B:443:LEU:HA	1.87	0.41
1:B:689:THR:HA	1:B:778:PHE:HE2	1.86	0.41
1:B:886:ARG:HA	1:B:889:GLN:HB2	2.03	0.41
1:B:891:TRP:HE3	1:B:904:HIS:HB2	1.85	0.41
1:B:1808:ARG:HD2	1:B:1858:ASP:OD2	2.21	0.41
1:B:2763:HIS:NE2	1:B:2767:ALA:HB2	2.36	0.41
1:B:3713:LYS:HD3	1:B:3713:LYS:HA	1.85	0.41
1:B:4802:GLY:C	1:B:4804:TYR:N	2.77	0.41
1:A:297:GLN:HG3	1:A:300:VAL:HG21	2.03	0.41
1:A:2794:TYR:HA	1:A:2797:PHE:HB2	2.03	0.41
1:A:2882:TYR:OH	1:A:2922:LYS:O	2.38	0.41
1:A:4151:SER:HA	1:A:4160:LEU:HD21	2.02	0.41
1:A:4544:LEU:O	1:A:4545:GLU:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4551:PHE:C	1:A:4553:ASN:H	2.29	0.41
1:A:4687:TYR:OH	1:A:4702:ASP:OD1	2.36	0.41
1:A:4693:GLY:C	1:A:4695:ASP:H	2.29	0.41
1:A:4839:MET:HB3	1:B:4823:LEU:HD21	2.02	0.41
3:I:107:ARG:HD2	3:I:107:ARG:HA	1.82	0.41
1:D:118:LEU:HA	1:D:137:LEU:HB3	2.02	0.41
1:D:224:HIS:NE2	1:D:385:ASP:O	2.54	0.41
1:D:619:ASP:O	1:D:622:THR:OG1	2.25	0.41
1:D:1703:LEU:HD13	1:D:1708:ARG:HB3	2.02	0.41
1:D:2927:LEU:HA	1:D:2930:LEU:HD12	2.03	0.41
1:D:3909:ASN:HB3	1:D:3910:THR:H	1.63	0.41
1:D:4137:ARG:HH21	1:D:4137:ARG:HG3	1.86	0.41
1:D:4226:GLY:C	1:D:4228:ALA:H	2.28	0.41
1:D:4693:GLY:C	1:D:4695:ASP:H	2.29	0.41
1:D:4976:GLU:OE1	1:D:4976:GLU:HA	2.20	0.41
3:L:27:THR:HG23	3:L:63:THR:HG23	2.02	0.41
1:C:688:LEU:HD12	1:C:690:GLU:H	1.85	0.41
1:C:689:THR:HA	1:C:778:PHE:HE2	1.86	0.41
1:C:805:PRO:HB2	1:C:808:TYR:CE2	2.55	0.41
1:C:891:TRP:HE3	1:C:904:HIS:HB2	1.85	0.41
1:C:1033:ARG:HE	1:C:1036:ARG:NH1	2.19	0.41
1:C:1252:HIS:HA	1:C:1253:PRO:HD2	1.94	0.41
1:C:1639:LEU:O	1:C:1647:CYS:HA	2.20	0.41
1:C:1782:PHE:CE2	2:G:90:VAL:HG11	2.55	0.41
1:C:4034:ASN:OD1	1:C:4035:VAL:O	2.39	0.41
1:C:4251:ILE:HD12	1:C:4557:ARG:HG2	2.02	0.41
1:C:4561:THR:O	1:C:4562:LEU:C	2.58	0.41
1:C:5015:GLN:C	1:C:5016:GLU:O	2.59	0.41
3:K:27:THR:HG23	3:K:63:THR:HG23	2.02	0.41
1:B:117:TYR:HB3	1:B:146:CYS:SG	2.60	0.41
1:B:289:ARG:HG2	1:B:303:ASP:HA	2.01	0.41
1:B:707:VAL:HG23	1:B:713:SER:HB2	2.03	0.41
1:B:877:ASN:HD21	1:B:970:LEU:HB2	1.85	0.41
1:B:1099:GLU:N	1:B:1099:GLU:OE1	2.54	0.41
1:B:1928:GLN:HA	1:B:1928:GLN:OE1	2.20	0.41
1:B:2378:ALA:O	1:B:2382:GLU:N	2.40	0.41
1:B:2437:ALA:HB1	1:B:2438:PRO:HD2	2.03	0.41
1:B:2970:SER:O	1:B:2974:ILE:N	2.44	0.41
1:B:4567:LEU:HD11	1:B:4816:ILE:CD1	2.51	0.41
1:B:4977:THR:O	1:B:4979:THR:N	2.54	0.41
3:J:66:PHE:CE2	3:J:70:LEU:HD12	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:891:TRP:HE3	1:A:904:HIS:HB2	1.85	0.41
1:A:1252:HIS:HA	1:A:1253:PRO:HD2	1.94	0.41
1:D:561:LEU:HD21	1:D:589:LEU:HD21	2.02	0.41
1:D:622:THR:HA	1:D:626:LEU:HD13	2.03	0.41
1:D:1653:LEU:HD23	1:D:1653:LEU:HA	1.86	0.41
1:D:1808:ARG:HD2	1:D:1858:ASP:OD2	2.21	0.41
1:D:4134:GLU:HB3	1:D:4135:PRO:HD3	2.03	0.41
1:D:4554:TYR:CE2	1:D:4558:ASN:ND2	2.89	0.41
1:D:4577:LEU:C	1:D:4579:PHE:H	2.29	0.41
1:D:4984:ASN:HA	6:D:5103:ATP:HN61	1.85	0.41
3:L:52:MET:HA	3:L:55:GLU:OE1	2.21	0.41
1:C:319:SER:OG	1:C:320:LYS:N	2.53	0.41
1:C:1126:GLY:O	1:C:1142:PRO:HA	2.21	0.41
1:C:3264:THR:O	1:C:3266:MET:N	2.48	0.41
1:C:3974:THR:O	1:C:3978:GLN:HG2	2.21	0.41
1:B:1126:GLY:O	1:B:1142:PRO:HA	2.21	0.41
1:B:1767:VAL:HG13	1:B:1767:VAL:O	2.20	0.41
1:B:2456:ILE:O	1:B:2459:SER:OG	2.35	0.41
1:B:2794:TYR:HA	1:B:2797:PHE:HB2	2.03	0.41
1:B:3598:GLU:HA	1:B:3601:ALA:HB3	2.03	0.41
1:B:3974:THR:O	1:B:3978:GLN:HG2	2.21	0.41
1:B:4137:ARG:HH21	1:B:4137:ARG:HG3	1.86	0.41
1:B:4181:ILE:HG23	1:B:4988:TYR:CE1	2.56	0.41
1:B:4951:LYS:O	1:B:4951:LYS:CG	2.69	0.41
1:B:5010:VAL:O	1:B:5010:VAL:HG12	2.21	0.41
1:A:622:THR:HA	1:A:626:LEU:HD13	2.03	0.40
1:A:864:PRO:HA	1:A:865:PRO:HD3	2.00	0.40
1:A:886:ARG:HA	1:A:889:GLN:HB2	2.03	0.40
1:A:1969:LEU:HD21	1:A:2009:LEU:CD1	2.50	0.40
1:A:2311:PRO:HA	1:A:2314:LEU:HB3	2.03	0.40
1:A:4181:ILE:HG23	1:A:4988:TYR:CE1	2.56	0.40
1:A:4567:LEU:HD11	1:A:4816:ILE:CD1	2.51	0.40
1:D:805:PRO:HB2	1:D:808:TYR:CE2	2.55	0.40
1:D:1455:PRO:HG3	1:D:1549:PHE:CZ	2.55	0.40
1:C:111:HIS:CE1	1:C:114:SER:H	2.39	0.40
1:C:297:GLN:HG3	1:C:300:VAL:HG21	2.03	0.40
1:C:608:VAL:HG23	1:C:613:ALA:HB2	2.03	0.40
1:C:2447:LYS:HG2	1:C:2448:GLY:H	1.84	0.40
1:C:2927:LEU:HA	1:C:2930:LEU:HD12	2.03	0.40
1:C:4012:LEU:HA	1:C:4015:GLU:OE2	2.19	0.40
1:C:4554:TYR:CE2	1:C:4558:ASN:ND2	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4977:THR:O	1:C:4979:THR:N	2.54	0.40
1:B:102:LEU:HB2	1:B:105:HIS:CE1	2.57	0.40
1:B:561:LEU:HD21	1:B:589:LEU:HD21	2.02	0.40
1:B:1969:LEU:HD21	1:B:2009:LEU:CD1	2.50	0.40
1:B:2259:GLU:HA	1:B:2297:LYS:HZ2	1.87	0.40
1:B:3922:TYR:C	1:B:3924:LEU:H	2.28	0.40
1:B:4693:GLY:C	1:B:4695:ASP:H	2.29	0.40
1:B:4705:VAL:HG22	1:B:4711:PHE:HD1	1.85	0.40
3:J:27:THR:HG23	3:J:63:THR:HG23	2.02	0.40
1:A:196:MET:HB3	1:A:197:GLN:H	1.73	0.40
1:A:670:GLU:CD	1:A:788:LYS:H	2.28	0.40
1:A:2573:GLU:O	1:A:2577:ILE:N	2.54	0.40
1:A:3718:GLU:HA	1:A:3718:GLU:OE1	2.20	0.40
1:A:4134:GLU:HB3	1:A:4135:PRO:HD3	2.03	0.40
1:A:4647:SER:OG	1:A:4803:HIS:HE1	2.04	0.40
1:A:4991:PHE:HD1	1:A:4991:PHE:HA	1.78	0.40
3:I:52:MET:HA	3:I:55:GLU:OE1	2.21	0.40
1:D:102:LEU:HB2	1:D:105:HIS:CE1	2.57	0.40
1:D:111:HIS:CE1	1:D:114:SER:H	2.39	0.40
1:D:297:GLN:HG3	1:D:300:VAL:HG21	2.03	0.40
1:D:622:THR:O	1:D:627:PRO:HD3	2.21	0.40
1:D:877:ASN:HD21	1:D:970:LEU:HB2	1.86	0.40
1:D:950:LEU:HD23	1:D:971:ASP:HB3	2.03	0.40
1:D:1033:ARG:HE	1:D:1036:ARG:NH1	2.19	0.40
1:D:3598:GLU:HA	1:D:3601:ALA:HB3	2.03	0.40
1:D:3775:ALA:O	1:D:3778:MET:N	2.53	0.40
1:D:4945:ASP:C	1:D:4947:GLN:H	2.29	0.40
1:C:950:LEU:HD23	1:C:971:ASP:HB3	2.03	0.40
1:C:1033:ARG:HE	1:C:1036:ARG:HH11	1.68	0.40
1:C:1641:ILE:HA	1:C:1642:PRO:HD3	1.80	0.40
1:C:2311:PRO:HA	1:C:2314:LEU:HB3	2.03	0.40
1:C:3713:LYS:HD3	1:C:3713:LYS:HA	1.85	0.40
1:C:4647:SER:OG	1:C:4803:HIS:HE1	2.04	0.40
2:G:54:GLU:HG2	2:G:55:VAL:HG23	2.02	0.40
3:K:14:LYS:HA	3:K:14:LYS:HD2	1.89	0.40
3:K:66:PHE:CE2	3:K:70:LEU:HD12	2.55	0.40
1:B:924:MET:O	1:B:928:THR:OG1	2.38	0.40
1:B:1033:ARG:HE	1:B:1036:ARG:NH1	2.19	0.40
1:B:2167:ILE:HG13	1:B:2168:VAL:N	2.37	0.40
1:B:4226:GLY:C	1:B:4228:ALA:H	2.28	0.40
1:A:308:HIS:C	1:A:310:LYS:H	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:622:THR:O	1:A:627:PRO:HD3	2.21	0.40
1:A:707:VAL:HG23	1:A:713:SER:HB2	2.03	0.40
1:A:1099:GLU:OE1	1:A:1099:GLU:N	2.54	0.40
1:A:1213:PHE:O	1:A:1214:PHE:C	2.65	0.40
1:A:1782:PHE:CE2	2:E:90:VAL:HG11	2.55	0.40
1:A:2030:ASP:N	1:A:2030:ASP:OD1	2.54	0.40
1:A:2763:HIS:NE2	1:A:2767:ALA:HB2	2.36	0.40
1:A:4820:VAL:O	1:A:4823:LEU:N	2.55	0.40
1:D:308:HIS:C	1:D:310:LYS:H	2.30	0.40
1:D:1641:ILE:HA	1:D:1642:PRO:HD3	1.80	0.40
1:D:2437:ALA:HB1	1:D:2438:PRO:HD2	2.03	0.40
1:D:2794:TYR:HA	1:D:2797:PHE:HB2	2.03	0.40
1:D:4062:PHE:HB2	1:D:4170:ILE:HD11	2.04	0.40
1:D:4154:VAL:HG13	1:D:4154:VAL:O	2.21	0.40
1:D:5015:GLN:C	1:D:5016:GLU:O	2.59	0.40
2:H:37:ASP:OD1	2:H:38:SER:N	2.54	0.40
1:C:622:THR:HA	1:C:626:LEU:HD13	2.03	0.40
1:C:622:THR:O	1:C:627:PRO:HD3	2.21	0.40
1:C:662:TRP:HB3	1:C:811:CYS:SG	2.62	0.40
1:C:707:VAL:HG23	1:C:713:SER:HB2	2.03	0.40
1:C:1256:GLU:HB2	1:C:1273:ALA:HB3	2.02	0.40
1:C:1455:PRO:HG3	1:C:1549:PHE:CZ	2.55	0.40
1:C:1752:ARG:O	1:C:1754:GLY:N	2.54	0.40
1:C:1928:GLN:HA	1:C:1928:GLN:OE1	2.20	0.40
1:C:2167:ILE:HG13	1:C:2168:VAL:N	2.37	0.40
1:C:2920:ARG:O	1:C:2924:GLN:N	2.38	0.40
1:C:3434:LEU:O	1:C:3436:ARG:N	2.44	0.40
1:C:3923:LEU:HD22	1:C:3961:VAL:HG12	2.02	0.40
1:C:4154:VAL:O	1:C:4154:VAL:HG13	2.21	0.40
1:B:669:ASP:N	1:B:669:ASP:OD1	2.53	0.40
1:B:1033:ARG:HE	1:B:1036:ARG:HH11	1.68	0.40
1:B:1164:LEU:HD12	1:B:1164:LEU:HA	1.94	0.40
1:B:1278:GLY:O	1:B:1280:GLN:N	2.55	0.40
1:B:2805:TYR:O	1:B:2808:PRO:HD2	2.22	0.40
1:B:2927:LEU:HA	1:B:2930:LEU:HD12	2.03	0.40
1:B:3941:ASP:OD1	1:B:3942:VAL:N	2.54	0.40
1:B:4687:TYR:HD2	1:B:4706:LEU:HD21	1.85	0.40
2:F:54:GLU:HG2	2:F:55:VAL:HG23	2.02	0.40
3:J:32:ALA:O	3:J:35:THR:OG1	2.35	0.40
1:A:257:ARG:O	1:A:284:HIS:NE2	2.55	0.40
1:A:1256:GLU:HB2	1:A:1273:ALA:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2284:ASN:HA	1:A:2341:VAL:HG11	2.02	0.40
1:A:2754:PHE:HA	1:A:2757:LYS:HE2	2.01	0.40
1:A:3396:ASP:O	1:A:3400:VAL:N	2.48	0.40
1:A:4137:ARG:HG3	1:A:4137:ARG:HH21	1.86	0.40
1:A:4154:VAL:O	1:A:4154:VAL:HG13	2.21	0.40
1:A:4226:GLY:C	1:A:4228:ALA:H	2.28	0.40
1:A:4687:TYR:HD2	1:A:4706:LEU:HD21	1.85	0.40
1:D:207:SER:OG	1:D:208:CYS:N	2.54	0.40
1:D:662:TRP:HB3	1:D:811:CYS:SG	2.62	0.40
1:D:689:THR:HA	1:D:778:PHE:HE2	1.86	0.40
1:D:2167:ILE:HG13	1:D:2168:VAL:N	2.37	0.40
1:D:2751:LEU:N	1:D:2755:ILE:HD12	2.37	0.40
1:D:2790:MET:HE2	1:D:2801:ASP:OD2	2.22	0.40
1:D:4951:LYS:O	1:D:4951:LYS:CG	2.69	0.40
3:L:40:LEU:H	3:L:40:LEU:HD23	1.85	0.40
1:C:561:LEU:HD21	1:C:589:LEU:HD21	2.02	0.40
1:C:1731:LEU:HA	1:C:1772:ARG:NH1	2.35	0.40
1:C:2751:LEU:N	1:C:2755:ILE:HD12	2.37	0.40
1:C:2757:LYS:O	1:C:2760:GLU:HB2	2.22	0.40
1:C:2794:TYR:HA	1:C:2797:PHE:HB2	2.03	0.40
1:C:4705:VAL:HG22	1:C:4711:PHE:HD1	1.85	0.40
1:C:4802:GLY:C	1:C:4804:TYR:H	2.30	0.40
1:B:224:HIS:NE2	1:B:385:ASP:O	2.54	0.40
1:B:257:ARG:O	1:B:284:HIS:NE2	2.55	0.40
1:B:297:GLN:HG3	1:B:300:VAL:HG21	2.03	0.40
1:B:950:LEU:HD23	1:B:971:ASP:HB3	2.03	0.40
1:B:1639:LEU:O	1:B:1647:CYS:HA	2.20	0.40
1:B:4154:VAL:O	1:B:4154:VAL:HG13	2.21	0.40
1:B:4251:ILE:HD12	1:B:4557:ARG:HG2	2.02	0.40
1:B:4702:ASP:O	1:B:4705:VAL:HG12	2.21	0.40
1:A:561:LEU:HD21	1:A:589:LEU:HD21	2.02	0.40
1:A:2347:GLU:OE1	1:A:2347:GLU:N	2.53	0.40
1:A:4839:MET:HE2	1:A:4839:MET:HB3	1.49	0.40
1:A:4972:PRO:O	1:A:4973:HIS:C	2.63	0.40
1:A:4977:THR:O	1:A:4979:THR:N	2.54	0.40
1:A:5010:VAL:O	1:A:5010:VAL:HG12	2.21	0.40
1:D:608:VAL:HG23	1:D:613:ALA:HB2	2.03	0.40
1:D:1752:ARG:O	1:D:1754:GLY:N	2.54	0.40
1:D:2023:LEU:H	1:D:2028:ARG:HH12	1.68	0.40
1:D:2805:TYR:O	1:D:2808:PRO:HD2	2.22	0.40
1:D:4687:TYR:OH	1:D:4702:ASP:OD1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:HIS:C	1:C:310:LYS:H	2.30	0.40
1:C:485:SER:O	1:C:489:ASN:N	2.48	0.40
1:C:886:ARG:HA	1:C:889:GLN:HB2	2.03	0.40
1:C:1166:GLY:HA3	1:C:1216:ILE:HD11	2.04	0.40
1:C:2136:ARG:O	1:C:2140:ARG:NH1	2.55	0.40
1:C:2790:MET:HE2	1:C:2801:ASP:OD2	2.22	0.40
1:C:3183:VAL:O	1:C:3187:ARG:N	2.55	0.40
1:B:1097:THR:HG23	1:B:1143:TRP:HB2	2.03	0.40
1:B:2030:ASP:OD1	1:B:2030:ASP:N	2.54	0.40
1:B:4820:VAL:O	1:B:4823:LEU:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4081/5037 (81%)	3348 (82%)	598 (15%)	135 (3%)	3	21
1	B	4081/5037 (81%)	3348 (82%)	598 (15%)	135 (3%)	3	21
1	C	4081/5037 (81%)	3351 (82%)	596 (15%)	134 (3%)	3	21
1	D	4081/5037 (81%)	3348 (82%)	598 (15%)	135 (3%)	3	21
2	E	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
2	F	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
2	G	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
2	H	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
3	I	133/149 (89%)	129 (97%)	4 (3%)	0	100	100
3	J	133/149 (89%)	129 (97%)	4 (3%)	0	100	100
3	K	133/149 (89%)	129 (97%)	4 (3%)	0	100	100
3	L	133/149 (89%)	129 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	17276/21172 (82%)	14307 (83%)	2430 (14%)	539 (3%)	5	22

All (539) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	626	LEU
1	A	1215	ALA
1	A	1241	SER
1	A	1291	LEU
1	A	1708	ARG
1	A	1767	VAL
1	A	1834	VAL
1	A	1856	ASP
1	A	2393	ASP
1	A	2496	PRO
1	A	2701	PRO
1	A	3020	THR
1	A	3021	PRO
1	A	3039	ILE
1	A	3138	PRO
1	A	3232	LEU
1	A	3233	PRO
1	A	3267	PRO
1	A	3289	PRO
1	A	3293	PRO
1	A	3294	PRO
1	A	3343	GLN
1	A	3351	PRO
1	A	3533	ILE
1	A	3567	PRO
1	A	3580	PRO
1	A	3592	ILE
1	A	4806	ASN
1	A	4820	VAL
1	A	4843	LEU
1	A	4845	ALA
1	A	4900	GLU
1	A	4901	ILE
1	A	4902	GLU
1	A	4904	PRO
1	A	4946	GLN
1	A	4951	LYS

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Mol	Chain	Res	Type
1	A	4966	ASP
1	A	4985	LEU
1	A	5004	THR
1	D	626	LEU
1	D	1215	ALA
1	D	1241	SER
1	D	1291	LEU
1	D	1708	ARG
1	D	1767	VAL
1	D	1834	VAL
1	D	1856	ASP
1	D	2393	ASP
1	D	2496	PRO
1	D	2701	PRO
1	D	3020	THR
1	D	3021	PRO
1	D	3039	ILE
1	D	3138	PRO
1	D	3232	LEU
1	D	3233	PRO
1	D	3267	PRO
1	D	3289	PRO
1	D	3293	PRO
1	D	3294	PRO
1	D	3343	GLN
1	D	3351	PRO
1	D	3533	ILE
1	D	3567	PRO
1	D	3580	PRO
1	D	3592	ILE
1	D	4806	ASN
1	D	4820	VAL
1	D	4843	LEU
1	D	4845	ALA
1	D	4900	GLU
1	D	4901	ILE
1	D	4902	GLU
1	D	4904	PRO
1	D	4946	GLN
1	D	4951	LYS
1	D	4966	ASP
1	D	4985	LEU

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Mol	Chain	Res	Type
1	D	5004	THR
1	C	626	LEU
1	C	1215	ALA
1	C	1241	SER
1	C	1291	LEU
1	C	1708	ARG
1	C	1767	VAL
1	C	1834	VAL
1	C	1856	ASP
1	C	2393	ASP
1	C	2496	PRO
1	C	2701	PRO
1	C	3020	THR
1	C	3021	PRO
1	C	3039	ILE
1	C	3138	PRO
1	C	3232	LEU
1	C	3233	PRO
1	C	3267	PRO
1	C	3289	PRO
1	C	3293	PRO
1	C	3294	PRO
1	C	3343	GLN
1	C	3351	PRO
1	C	3533	ILE
1	C	3567	PRO
1	C	3580	PRO
1	C	3592	ILE
1	C	4806	ASN
1	C	4820	VAL
1	C	4843	LEU
1	C	4845	ALA
1	C	4900	GLU
1	C	4901	ILE
1	C	4902	GLU
1	C	4904	PRO
1	C	4946	GLN
1	C	4951	LYS
1	C	4966	ASP
1	C	4985	LEU
1	C	5004	THR
1	B	626	LEU

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Mol	Chain	Res	Type
1	B	1215	ALA
1	B	1241	SER
1	B	1291	LEU
1	B	1708	ARG
1	B	1767	VAL
1	B	1834	VAL
1	B	1856	ASP
1	B	2393	ASP
1	B	2496	PRO
1	B	2701	PRO
1	B	3020	THR
1	B	3021	PRO
1	B	3039	ILE
1	B	3138	PRO
1	B	3232	LEU
1	B	3233	PRO
1	B	3267	PRO
1	B	3289	PRO
1	B	3293	PRO
1	B	3294	PRO
1	B	3343	GLN
1	B	3351	PRO
1	B	3533	ILE
1	B	3567	PRO
1	B	3580	PRO
1	B	3592	ILE
1	B	4806	ASN
1	B	4820	VAL
1	B	4843	LEU
1	B	4845	ALA
1	B	4900	GLU
1	B	4901	ILE
1	B	4902	GLU
1	B	4904	PRO
1	B	4946	GLN
1	B	4951	LYS
1	B	4966	ASP
1	B	4985	LEU
1	B	5004	THR
1	A	1279	SER
1	A	1295	VAL
1	A	2346	VAL

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Mol	Chain	Res	Type
1	A	2509	VAL
1	A	2514	ASN
1	A	2692	ASP
1	A	2965	ARG
1	A	3003	LEU
1	A	3040	THR
1	A	3062	PRO
1	A	3136	LEU
1	A	3188	PRO
1	A	3189	ALA
1	A	3217	SER
1	A	3243	ILE
1	A	3336	LYS
1	A	3350	ARG
1	A	3362	ILE
1	A	3515	LYS
1	A	3571	TRP
1	A	3593	VAL
1	A	3670	GLU
1	A	3873	LYS
1	A	4650	HIS
1	A	4818	MET
1	A	4955	GLU
1	A	4961	CYS
1	A	4967	TYR
1	A	4984	ASN
1	A	4992	LEU
1	A	5036	LEU
1	D	1279	SER
1	D	1295	VAL
1	D	2346	VAL
1	D	2509	VAL
1	D	2514	ASN
1	D	2692	ASP
1	D	2965	ARG
1	D	3003	LEU
1	D	3040	THR
1	D	3062	PRO
1	D	3136	LEU
1	D	3188	PRO
1	D	3189	ALA
1	D	3217	SER

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Mol	Chain	Res	Type
1	D	3243	ILE
1	D	3336	LYS
1	D	3350	ARG
1	D	3362	ILE
1	D	3432	GLU
1	D	3515	LYS
1	D	3571	TRP
1	D	3593	VAL
1	D	3670	GLU
1	D	3873	LYS
1	D	4650	HIS
1	D	4818	MET
1	D	4955	GLU
1	D	4961	CYS
1	D	4967	TYR
1	D	4984	ASN
1	D	4992	LEU
1	D	5036	LEU
1	C	1279	SER
1	C	1295	VAL
1	C	2346	VAL
1	C	2509	VAL
1	C	2514	ASN
1	C	2692	ASP
1	C	2965	ARG
1	C	3003	LEU
1	C	3040	THR
1	C	3062	PRO
1	C	3136	LEU
1	C	3188	PRO
1	C	3189	ALA
1	C	3217	SER
1	C	3243	ILE
1	C	3336	LYS
1	C	3350	ARG
1	C	3362	ILE
1	C	3432	GLU
1	C	3515	LYS
1	C	3571	TRP
1	C	3593	VAL
1	C	3670	GLU
1	C	3873	LYS

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Mol	Chain	Res	Type
1	C	4650	HIS
1	C	4818	MET
1	C	4955	GLU
1	C	4967	TYR
1	C	4984	ASN
1	C	4992	LEU
1	C	5036	LEU
1	B	1279	SER
1	B	1295	VAL
1	B	2346	VAL
1	B	2509	VAL
1	B	2514	ASN
1	B	2692	ASP
1	B	2965	ARG
1	B	3003	LEU
1	B	3040	THR
1	B	3062	PRO
1	B	3136	LEU
1	B	3188	PRO
1	B	3189	ALA
1	B	3217	SER
1	B	3243	ILE
1	B	3336	LYS
1	B	3350	ARG
1	B	3362	ILE
1	B	3515	LYS
1	B	3571	TRP
1	B	3593	VAL
1	B	3670	GLU
1	B	3873	LYS
1	B	4650	HIS
1	B	4818	MET
1	B	4955	GLU
1	B	4961	CYS
1	B	4967	TYR
1	B	4984	ASN
1	B	4992	LEU
1	B	5036	LEU
1	A	1253	PRO
1	A	1753	LYS
1	A	1985	THR
1	A	2540	THR

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Mol	Chain	Res	Type
1	A	2587	TYR
1	A	2616	PRO
1	A	2966	TRP
1	A	3190	LEU
1	A	3193	CYS
1	A	3333	THR
1	A	3427	PRO
1	A	3432	GLU
1	A	3434	LEU
1	A	3462	ASN
1	A	3530	GLN
1	A	3610	GLU
1	A	4102	GLN
1	A	4907	ASP
1	A	4908	GLU
1	A	4962	GLY
1	D	771	PHE
1	D	1214	PHE
1	D	1253	PRO
1	D	1753	LYS
1	D	1985	THR
1	D	2540	THR
1	D	2587	TYR
1	D	2616	PRO
1	D	2966	TRP
1	D	3190	LEU
1	D	3193	CYS
1	D	3333	THR
1	D	3427	PRO
1	D	3434	LEU
1	D	3462	ASN
1	D	3530	GLN
1	D	3610	GLU
1	D	4102	GLN
1	D	4718	LYS
1	D	4907	ASP
1	D	4908	GLU
1	D	4962	GLY
1	C	1253	PRO
1	C	1753	LYS
1	C	1985	THR
1	C	2540	THR

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Mol	Chain	Res	Type
1	C	2587	TYR
1	C	2616	PRO
1	C	2966	TRP
1	C	3190	LEU
1	C	3193	CYS
1	C	3333	THR
1	C	3427	PRO
1	C	3434	LEU
1	C	3462	ASN
1	C	3530	GLN
1	C	3610	GLU
1	C	4102	GLN
1	C	4907	ASP
1	C	4908	GLU
1	C	4961	CYS
1	C	4962	GLY
1	B	1253	PRO
1	B	1753	LYS
1	B	1985	THR
1	B	2540	THR
1	B	2587	TYR
1	B	2616	PRO
1	B	2966	TRP
1	B	3190	LEU
1	B	3193	CYS
1	B	3333	THR
1	B	3427	PRO
1	B	3432	GLU
1	B	3434	LEU
1	B	3462	ASN
1	B	3530	GLN
1	B	3610	GLU
1	B	4102	GLN
1	B	4907	ASP
1	B	4908	GLU
1	B	4962	GLY
1	A	771	PHE
1	A	1988	ALA
1	A	2539	ALA
1	A	2604	GLU
1	A	2645	THR
1	A	2666	VAL

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Mol	Chain	Res	Type
1	A	2699	ALA
1	A	2950	SER
1	A	3262	ARG
1	A	3265	GLU
1	A	3299	GLY
1	A	3360	PRO
1	A	3402	CYS
1	A	3536	ALA
1	A	3568	SER
1	A	3827	GLY
1	A	4715	TYR
1	A	4821	LYS
1	A	4898	GLY
1	D	1988	ALA
1	D	2539	ALA
1	D	2604	GLU
1	D	2645	THR
1	D	2666	VAL
1	D	2699	ALA
1	D	2950	SER
1	D	3262	ARG
1	D	3299	GLY
1	D	3360	PRO
1	D	3402	CYS
1	D	3536	ALA
1	D	3568	SER
1	D	3827	GLY
1	D	4715	TYR
1	D	4821	LYS
1	D	4898	GLY
1	C	771	PHE
1	C	1214	PHE
1	C	1988	ALA
1	C	2539	ALA
1	C	2604	GLU
1	C	2645	THR
1	C	2666	VAL
1	C	2699	ALA
1	C	2950	SER
1	C	3262	ARG
1	C	3265	GLU
1	C	3299	GLY

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Mol	Chain	Res	Type
1	C	3360	PRO
1	C	3402	CYS
1	C	3536	ALA
1	C	3568	SER
1	C	3827	GLY
1	C	4641	PRO
1	C	4715	TYR
1	C	4821	LYS
1	C	4898	GLY
1	B	771	PHE
1	B	1988	ALA
1	B	2539	ALA
1	B	2604	GLU
1	B	2645	THR
1	B	2666	VAL
1	B	2699	ALA
1	B	2950	SER
1	B	3262	ARG
1	B	3265	GLU
1	B	3299	GLY
1	B	3360	PRO
1	B	3402	CYS
1	B	3536	ALA
1	B	3568	SER
1	B	3827	GLY
1	B	4641	PRO
1	B	4715	TYR
1	B	4821	LYS
1	B	4898	GLY
1	A	1214	PHE
1	A	2495	VAL
1	A	2531	ARG
1	A	2562	ILE
1	A	2566	ALA
1	A	2630	VAL
1	A	3015	LEU
1	A	3356	SER
1	A	3426	GLU
1	A	3579	LEU
1	A	4118	ASP
1	A	4641	PRO
1	A	4844	LEU

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Mol	Chain	Res	Type
1	A	4886	HIS
1	D	2495	VAL
1	D	2531	ARG
1	D	2562	ILE
1	D	2566	ALA
1	D	2630	VAL
1	D	3015	LEU
1	D	3265	GLU
1	D	3356	SER
1	D	3426	GLU
1	D	3579	LEU
1	D	4118	ASP
1	D	4641	PRO
1	D	4844	LEU
1	C	2495	VAL
1	C	2531	ARG
1	C	2562	ILE
1	C	2566	ALA
1	C	2630	VAL
1	C	3015	LEU
1	C	3356	SER
1	C	3426	GLU
1	C	3579	LEU
1	C	4118	ASP
1	C	4844	LEU
1	B	1214	PHE
1	B	2495	VAL
1	B	2531	ARG
1	B	2562	ILE
1	B	2566	ALA
1	B	2630	VAL
1	B	3015	LEU
1	B	3356	SER
1	B	3426	GLU
1	B	3579	LEU
1	B	4118	ASP
1	B	4844	LEU
1	A	677	ALA
1	A	2559	LEU
1	A	3775	ALA
1	A	4897	ILE
1	D	677	ALA

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Mol	Chain	Res	Type
1	D	2559	LEU
1	D	3775	ALA
1	D	4897	ILE
1	D	4968	PHE
1	C	677	ALA
1	C	2559	LEU
1	C	3775	ALA
1	C	4897	ILE
1	B	677	ALA
1	B	2559	LEU
1	B	3775	ALA
1	B	4897	ILE
1	A	4637	GLY
1	B	4637	GLY
1	A	3588	ASP
1	D	3588	ASP
1	D	4720	VAL
1	C	3588	ASP
1	C	4720	VAL
1	B	3588	ASP
1	A	4720	VAL
1	A	4950	VAL
1	D	4950	VAL
1	C	4637	GLY
1	C	4692	PRO
1	C	4950	VAL
1	B	4720	VAL
1	B	4950	VAL
1	A	753	PRO
1	A	3300	ALA
1	A	4692	PRO
1	D	753	PRO
1	D	3300	ALA
1	D	4692	PRO
1	C	753	PRO
1	C	3300	ALA
1	B	753	PRO
1	B	3300	ALA
1	B	4692	PRO
1	B	3633	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2516/4277 (59%)	2456 (98%)	60 (2%)	43	60
1	B	2516/4277 (59%)	2456 (98%)	60 (2%)	43	60
1	C	2516/4277 (59%)	2455 (98%)	61 (2%)	43	60
1	D	2516/4277 (59%)	2455 (98%)	61 (2%)	43	60
2	E	84/88 (96%)	84 (100%)	0	100	100
2	F	84/88 (96%)	84 (100%)	0	100	100
2	G	84/88 (96%)	84 (100%)	0	100	100
2	H	84/88 (96%)	84 (100%)	0	100	100
3	I	102/123 (83%)	102 (100%)	0	100	100
3	J	102/123 (83%)	102 (100%)	0	100	100
3	K	102/123 (83%)	102 (100%)	0	100	100
3	L	102/123 (83%)	102 (100%)	0	100	100
All	All	10808/17952 (60%)	10566 (98%)	242 (2%)	45	62

All (242) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1253	PRO
1	A	1433	TYR
1	A	1549	PHE
1	A	3632	VAL
1	A	3636	PHE
1	A	3639	THR
1	A	3856	LEU
1	A	4546	VAL
1	A	4552	LEU
1	A	4554	TYR
1	A	4555	LEU
1	A	4562	LEU
1	A	4563	LYS
1	A	4569	LEU

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Mol	Chain	Res	Type
1	A	4573	ILE
1	A	4575	PHE
1	A	4645	CYS
1	A	4648	LEU
1	A	4649	LEU
1	A	4651	THR
1	A	4659	ILE
1	A	4662	ASN
1	A	4668	LEU
1	A	4669	VAL
1	A	4716	TRP
1	A	4718	LYS
1	A	4792	SER
1	A	4797	VAL
1	A	4798	MET
1	A	4800	LEU
1	A	4806	ASN
1	A	4818	MET
1	A	4819	GLU
1	A	4820	VAL
1	A	4825	THR
1	A	4827	LEU
1	A	4828	SER
1	A	4838	VAL
1	A	4839	MET
1	A	4843	LEU
1	A	4846	VAL
1	A	4884	LEU
1	A	4897	ILE
1	A	4911	LEU
1	A	4945	ASP
1	A	4949	GLN
1	A	4950	VAL
1	A	4952	GLU
1	A	4957	LYS
1	A	4960	ILE
1	A	4963	ILE
1	A	4965	SER
1	A	4977	THR
1	A	4983	HIS
1	A	4985	LEU
1	A	5008	SER

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Mol	Chain	Res	Type
1	A	5012	LYS
1	A	5013	MET
1	A	5014	TYR
1	A	5037	SER
1	D	1253	PRO
1	D	1433	TYR
1	D	1549	PHE
1	D	3632	VAL
1	D	3636	PHE
1	D	3639	THR
1	D	3856	LEU
1	D	4546	VAL
1	D	4552	LEU
1	D	4554	TYR
1	D	4555	LEU
1	D	4562	LEU
1	D	4563	LYS
1	D	4569	LEU
1	D	4573	ILE
1	D	4575	PHE
1	D	4645	CYS
1	D	4648	LEU
1	D	4649	LEU
1	D	4651	THR
1	D	4659	ILE
1	D	4668	LEU
1	D	4716	TRP
1	D	4718	LYS
1	D	4792	SER
1	D	4797	VAL
1	D	4798	MET
1	D	4800	LEU
1	D	4806	ASN
1	D	4813	LEU
1	D	4814	LEU
1	D	4818	MET
1	D	4819	GLU
1	D	4820	VAL
1	D	4825	THR
1	D	4826	ILE
1	D	4827	LEU
1	D	4828	SER

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Mol	Chain	Res	Type
1	D	4838	VAL
1	D	4839	MET
1	D	4843	LEU
1	D	4846	VAL
1	D	4884	LEU
1	D	4897	ILE
1	D	4911	LEU
1	D	4945	ASP
1	D	4949	GLN
1	D	4950	VAL
1	D	4952	GLU
1	D	4957	LYS
1	D	4960	ILE
1	D	4963	ILE
1	D	4965	SER
1	D	4977	THR
1	D	4983	HIS
1	D	4985	LEU
1	D	5008	SER
1	D	5012	LYS
1	D	5013	MET
1	D	5014	TYR
1	D	5037	SER
1	C	1253	PRO
1	C	1433	TYR
1	C	1549	PHE
1	C	3632	VAL
1	C	3636	PHE
1	C	3639	THR
1	C	3856	LEU
1	C	4546	VAL
1	C	4552	LEU
1	C	4554	TYR
1	C	4555	LEU
1	C	4562	LEU
1	C	4563	LYS
1	C	4569	LEU
1	C	4573	ILE
1	C	4575	PHE
1	C	4645	CYS
1	C	4648	LEU
1	C	4649	LEU

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Mol	Chain	Res	Type
1	C	4651	THR
1	C	4659	ILE
1	C	4662	ASN
1	C	4668	LEU
1	C	4669	VAL
1	C	4716	TRP
1	C	4718	LYS
1	C	4792	SER
1	C	4797	VAL
1	C	4798	MET
1	C	4800	LEU
1	C	4806	ASN
1	C	4818	MET
1	C	4819	GLU
1	C	4820	VAL
1	C	4825	THR
1	C	4827	LEU
1	C	4828	SER
1	C	4838	VAL
1	C	4839	MET
1	C	4843	LEU
1	C	4846	VAL
1	C	4884	LEU
1	C	4897	ILE
1	C	4911	LEU
1	C	4933	GLN
1	C	4945	ASP
1	C	4949	GLN
1	C	4950	VAL
1	C	4952	GLU
1	C	4957	LYS
1	C	4960	ILE
1	C	4963	ILE
1	C	4965	SER
1	C	4977	THR
1	C	4983	HIS
1	C	4985	LEU
1	C	5008	SER
1	C	5012	LYS
1	C	5013	MET
1	C	5014	TYR
1	C	5037	SER

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Mol	Chain	Res	Type
1	B	1253	PRO
1	B	1433	TYR
1	B	1549	PHE
1	B	3632	VAL
1	B	3636	PHE
1	B	3639	THR
1	B	3856	LEU
1	B	4546	VAL
1	B	4552	LEU
1	B	4554	TYR
1	B	4555	LEU
1	B	4562	LEU
1	B	4563	LYS
1	B	4569	LEU
1	B	4573	ILE
1	B	4575	PHE
1	B	4645	CYS
1	B	4648	LEU
1	B	4649	LEU
1	B	4651	THR
1	B	4659	ILE
1	B	4662	ASN
1	B	4669	VAL
1	B	4716	TRP
1	B	4718	LYS
1	B	4792	SER
1	B	4797	VAL
1	B	4798	MET
1	B	4800	LEU
1	B	4806	ASN
1	B	4814	LEU
1	B	4818	MET
1	B	4819	GLU
1	B	4820	VAL
1	B	4825	THR
1	B	4827	LEU
1	B	4828	SER
1	B	4838	VAL
1	B	4839	MET
1	B	4843	LEU
1	B	4846	VAL
1	B	4884	LEU

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Mol	Chain	Res	Type
1	B	4897	ILE
1	B	4911	LEU
1	B	4945	ASP
1	B	4949	GLN
1	B	4950	VAL
1	B	4952	GLU
1	B	4957	LYS
1	B	4960	ILE
1	B	4963	ILE
1	B	4965	SER
1	B	4977	THR
1	B	4983	HIS
1	B	4985	LEU
1	B	5008	SER
1	B	5012	LYS
1	B	5013	MET
1	B	5014	TYR
1	B	5037	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (123) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	79	GLN
1	A	151	HIS
1	A	218	HIS
1	A	465	GLN
1	A	536	ASN
1	A	618	GLN
1	A	812	HIS
1	A	1041	GLN
1	A	1429	ASN
1	A	1560	ASN
1	A	1563	GLN
1	A	1598	GLN
1	A	1660	GLN
1	A	1719	HIS
1	A	2213	ASN
1	A	2772	GLN
1	A	2884	ASN
1	A	2931	GLN
1	A	3814	GLN

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Mol	Chain	Res	Type
1	A	3889	GLN
1	A	3895	HIS
1	A	3909	ASN
1	A	4078	GLN
1	A	4133	GLN
1	A	4803	HIS
1	A	4836	GLN
1	A	4886	HIS
1	A	4946	GLN
1	A	4949	GLN
1	A	4978	HIS
1	A	5003	HIS
2	E	70	GLN
1	D	57	ASN
1	D	151	HIS
1	D	218	HIS
1	D	465	GLN
1	D	536	ASN
1	D	618	GLN
1	D	681	HIS
1	D	812	HIS
1	D	1041	GLN
1	D	1429	ASN
1	D	1560	ASN
1	D	1563	GLN
1	D	1837	GLN
1	D	2213	ASN
1	D	2772	GLN
1	D	2884	ASN
1	D	2931	GLN
1	D	3814	GLN
1	D	3889	GLN
1	D	3895	HIS
1	D	3909	ASN
1	D	4078	GLN
1	D	4133	GLN
1	D	4803	HIS
1	D	4836	GLN
1	D	4946	GLN
1	D	4949	GLN
1	D	4978	HIS
1	D	5003	HIS

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Mol	Chain	Res	Type
1	C	57	ASN
1	C	151	HIS
1	C	218	HIS
1	C	536	ASN
1	C	618	GLN
1	C	681	HIS
1	C	812	HIS
1	C	1041	GLN
1	C	1429	ASN
1	C	1560	ASN
1	C	1563	GLN
1	C	1719	HIS
1	C	1837	GLN
1	C	2213	ASN
1	C	2772	GLN
1	C	2884	ASN
1	C	2931	GLN
1	C	3814	GLN
1	C	3889	GLN
1	C	3895	HIS
1	C	3909	ASN
1	C	4078	GLN
1	C	4133	GLN
1	C	4803	HIS
1	C	4886	HIS
1	C	4946	GLN
1	C	4949	GLN
1	C	4978	HIS
1	C	5003	HIS
2	G	70	GLN
2	G	87	HIS
1	B	57	ASN
1	B	218	HIS
1	B	536	ASN
1	B	681	HIS
1	B	812	HIS
1	B	1041	GLN
1	B	1429	ASN
1	B	1560	ASN
1	B	1563	GLN
1	B	1719	HIS
1	B	1837	GLN

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Mol	Chain	Res	Type
1	B	2213	ASN
1	B	2772	GLN
1	B	2884	ASN
1	B	2931	GLN
1	B	3699	HIS
1	B	3814	GLN
1	B	3889	GLN
1	B	3895	HIS
1	B	3909	ASN
1	B	4078	GLN
1	B	4133	GLN
1	B	4803	HIS
1	B	4836	GLN
1	B	4886	HIS
1	B	4946	GLN
1	B	4949	GLN
1	B	4978	HIS
1	B	5003	HIS
2	F	70	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 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	$\# Z > 2$
6	ATP	B	5103	-	32,33,33	1.30	4 (12%)	48,52,52	1.77	12 (25%)
6	ATP	A	5103	-	32,33,33	1.31	4 (12%)	48,52,52	1.76	12 (25%)
7	CFF	D	5104	-	15,15,15	0.71	0	23,23,23	0.90	0
7	CFF	A	5104	-	15,15,15	0.73	0	23,23,23	0.92	0
6	ATP	C	5103	-	32,33,33	1.31	4 (12%)	48,52,52	1.76	12 (25%)
7	CFF	B	5104	-	15,15,15	0.73	0	23,23,23	0.91	0
7	CFF	C	5104	-	15,15,15	0.73	0	23,23,23	0.93	0
6	ATP	D	5103	-	32,33,33	1.30	4 (12%)	48,52,52	1.76	13 (27%)

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
6	ATP	B	5103	-	-	3/22/38/38	0/3/3/3
6	ATP	A	5103	-	-	3/22/38/38	0/3/3/3
7	CFF	D	5104	-	-	-	0/2/2/2
7	CFF	A	5104	-	-	-	0/2/2/2
6	ATP	C	5103	-	-	3/22/38/38	0/3/3/3
7	CFF	B	5104	-	-	-	0/2/2/2
7	CFF	C	5104	-	-	-	0/2/2/2
6	ATP	D	5103	-	-	3/22/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	5103	ATP	C5-C4	3.77	1.45	1.39
6	A	5103	ATP	C5-C4	3.74	1.45	1.39
6	B	5103	ATP	C5-C4	3.74	1.45	1.39
6	D	5103	ATP	C5-C4	3.72	1.45	1.39
6	A	5103	ATP	C4-N9	-2.90	1.31	1.37
6	C	5103	ATP	C4-N9	-2.90	1.31	1.37
6	B	5103	ATP	C4-N9	-2.90	1.31	1.37
6	D	5103	ATP	C4-N9	-2.89	1.31	1.37
6	D	5103	ATP	C5-N7	-2.70	1.34	1.39
6	A	5103	ATP	C5-N7	-2.68	1.34	1.39
6	C	5103	ATP	C5-N7	-2.68	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	5103	ATP	C5-N7	-2.67	1.34	1.39
6	D	5103	ATP	C8-N7	2.24	1.36	1.31
6	A	5103	ATP	C8-N7	2.24	1.36	1.31
6	C	5103	ATP	C8-N7	2.23	1.36	1.31
6	B	5103	ATP	C8-N7	2.20	1.35	1.31

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	5103	ATP	C5-C4-N3	-4.45	120.59	126.72
6	A	5103	ATP	C5-C4-N3	-4.45	120.59	126.72
6	B	5103	ATP	C5-C4-N3	-4.45	120.59	126.72
6	D	5103	ATP	C5-C4-N3	-4.43	120.62	126.72
6	B	5103	ATP	N3-C2-N1	-3.73	122.94	128.58
6	A	5103	ATP	C4-N9-C8	3.73	109.65	105.74
6	C	5103	ATP	C4-N9-C8	3.73	109.65	105.74
6	B	5103	ATP	C4-N9-C8	3.73	109.65	105.74
6	D	5103	ATP	N3-C2-N1	-3.71	122.96	128.58
6	D	5103	ATP	C4-N9-C8	3.71	109.63	105.74
6	A	5103	ATP	N3-C2-N1	-3.71	122.97	128.58
6	C	5103	ATP	N3-C4-N9	3.70	133.45	127.17
6	C	5103	ATP	N3-C2-N1	-3.68	123.01	128.58
6	A	5103	ATP	N3-C4-N9	3.68	133.42	127.17
6	B	5103	ATP	N3-C4-N9	3.68	133.42	127.17
6	D	5103	ATP	N3-C4-N9	3.66	133.39	127.17
6	A	5103	ATP	C2-N3-C4	3.30	119.88	111.83
6	C	5103	ATP	C2-N3-C4	3.30	119.88	111.83
6	B	5103	ATP	C2-N3-C4	3.30	119.88	111.83
6	D	5103	ATP	C2-N3-C4	3.29	119.86	111.83
6	B	5103	ATP	C4-C5-N7	-3.00	107.15	110.58
6	A	5103	ATP	C4-C5-N7	-2.97	107.18	110.58
6	D	5103	ATP	C4-C5-N7	-2.95	107.20	110.58
6	C	5103	ATP	C2'-C1'-N9	-2.95	105.97	113.30
6	D	5103	ATP	C2'-C1'-N9	-2.95	105.97	113.30
6	C	5103	ATP	C4-C5-N7	-2.94	107.22	110.58
6	A	5103	ATP	C2'-C1'-N9	-2.94	106.00	113.30
6	B	5103	ATP	C2'-C1'-N9	-2.94	106.00	113.30
6	A	5103	ATP	N9-C8-N7	-2.83	109.92	113.94
6	B	5103	ATP	N9-C8-N7	-2.83	109.92	113.94
6	D	5103	ATP	N9-C8-N7	-2.82	109.93	113.94
6	C	5103	ATP	N9-C8-N7	-2.80	109.96	113.94
6	B	5103	ATP	C5-N7-C8	2.44	107.28	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	5103	ATP	C5-N7-C8	2.42	107.25	103.45
6	D	5103	ATP	C5-N7-C8	2.41	107.24	103.45
6	B	5103	ATP	C6-C5-N7	2.40	136.72	132.09
6	A	5103	ATP	C6-C5-N7	2.40	136.72	132.09
6	C	5103	ATP	C6-C5-N7	2.40	136.72	132.09
6	C	5103	ATP	C5-N7-C8	2.39	107.21	103.45
6	D	5103	ATP	C6-C5-N7	2.38	136.68	132.09
6	D	5103	ATP	C2-N1-C6	2.27	122.47	118.73
6	B	5103	ATP	C2-N1-C6	2.27	122.45	118.73
6	A	5103	ATP	C2-N1-C6	2.26	122.44	118.73
6	C	5103	ATP	C2-N1-C6	2.24	122.41	118.73
6	A	5103	ATP	C4-N9-C1'	-2.17	121.57	126.63
6	C	5103	ATP	C4-N9-C1'	-2.17	121.57	126.63
6	B	5103	ATP	C4-N9-C1'	-2.17	121.57	126.63
6	D	5103	ATP	C4-N9-C1'	-2.16	121.59	126.63
6	D	5103	ATP	O4'-C1'-N9	2.01	111.95	108.09

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	5103	ATP	C4'-C5'-O5'-PA
6	D	5103	ATP	C4'-C5'-O5'-PA
6	C	5103	ATP	C4'-C5'-O5'-PA
6	B	5103	ATP	C4'-C5'-O5'-PA
6	A	5103	ATP	PG-O3B-PB-O1B
6	D	5103	ATP	PG-O3B-PB-O1B
6	C	5103	ATP	PG-O3B-PB-O1B
6	B	5103	ATP	PG-O3B-PB-O1B
6	A	5103	ATP	PG-O3B-PB-O2B
6	D	5103	ATP	PG-O3B-PB-O2B
6	C	5103	ATP	PG-O3B-PB-O2B
6	B	5103	ATP	PG-O3B-PB-O2B

There are no ring outliers.

4 monomers are involved in 4 short contacts:

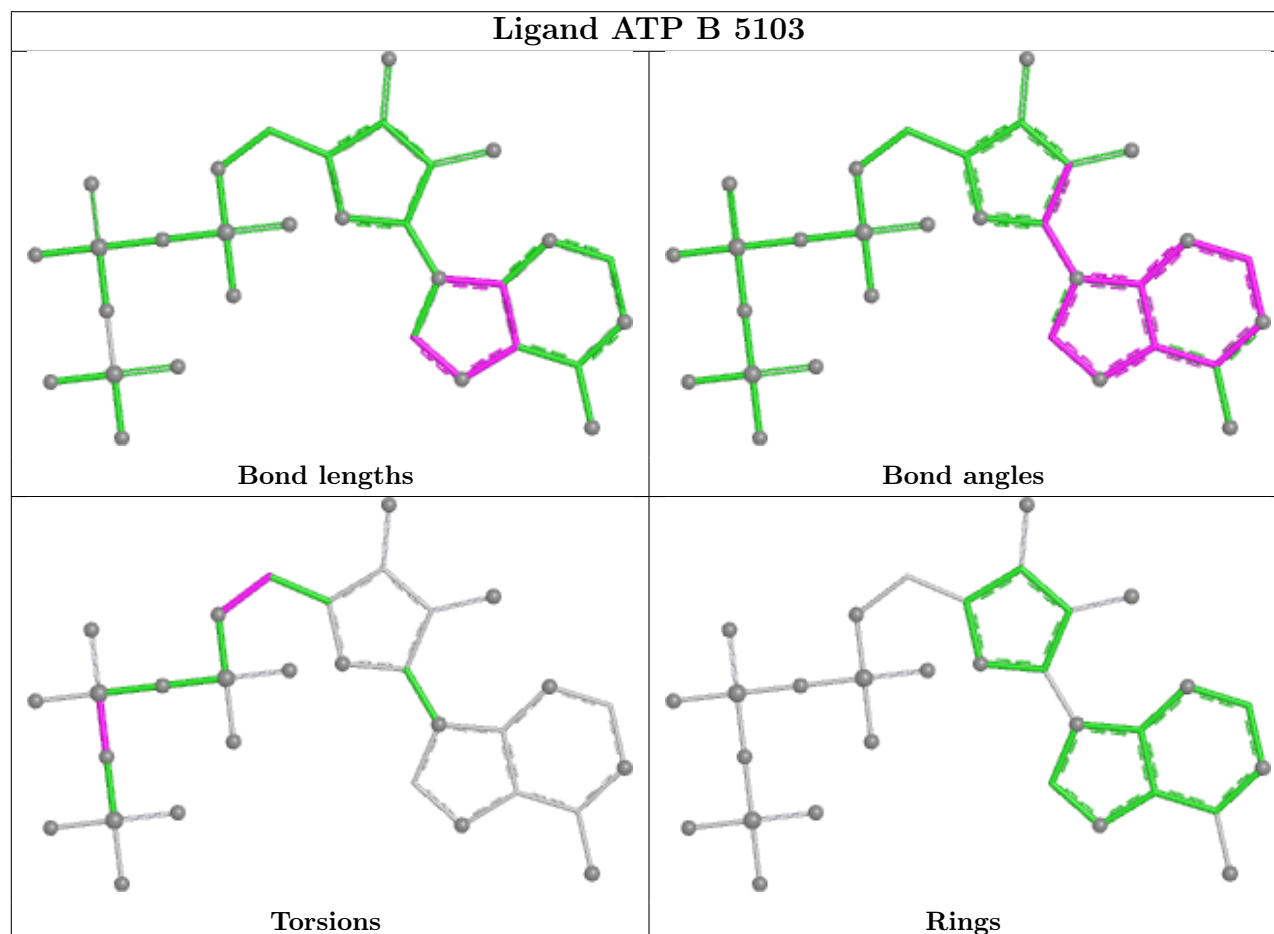
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	5103	ATP	1	0
6	A	5103	ATP	1	0
6	C	5103	ATP	1	0

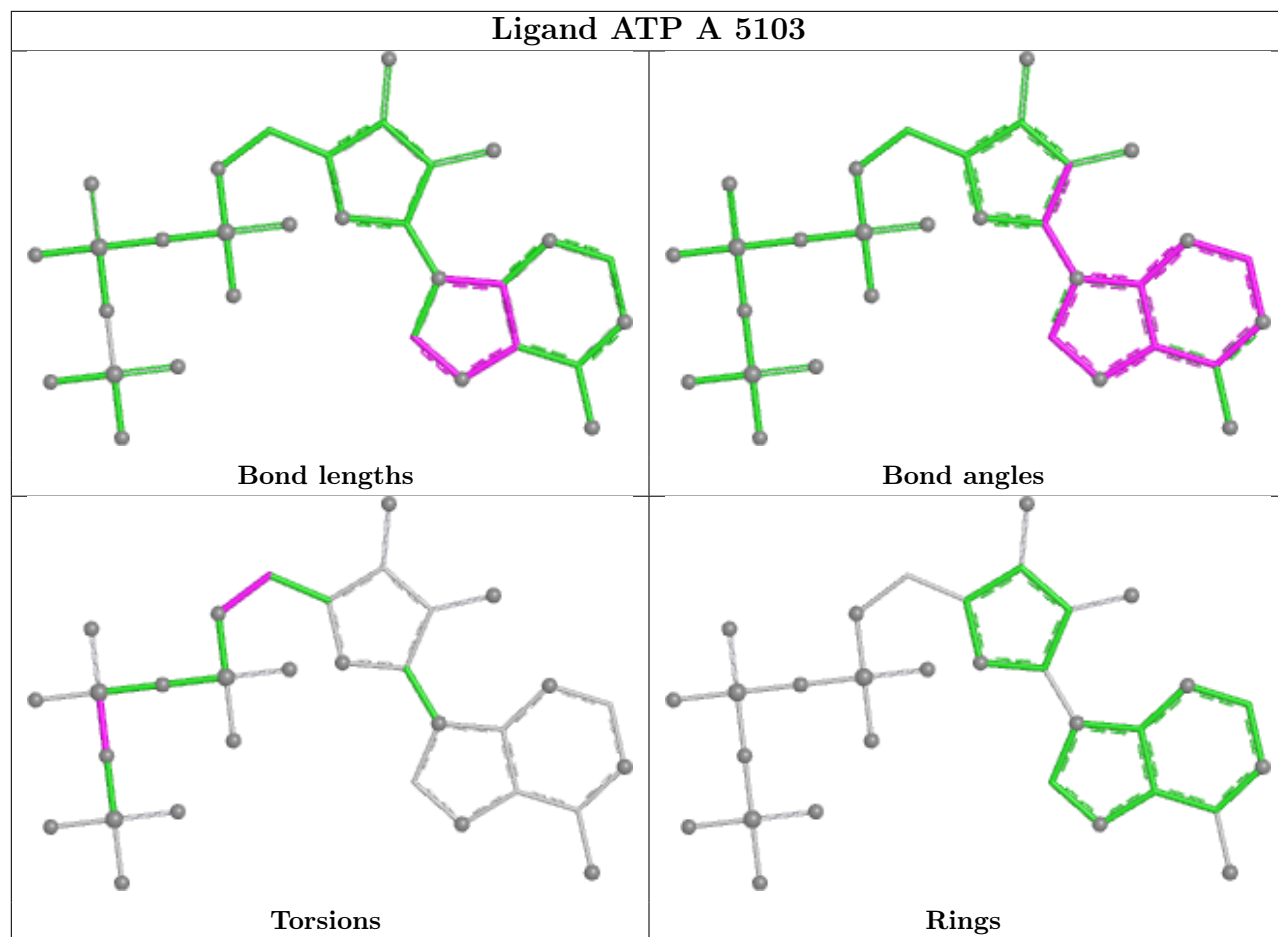
Continued on next page...

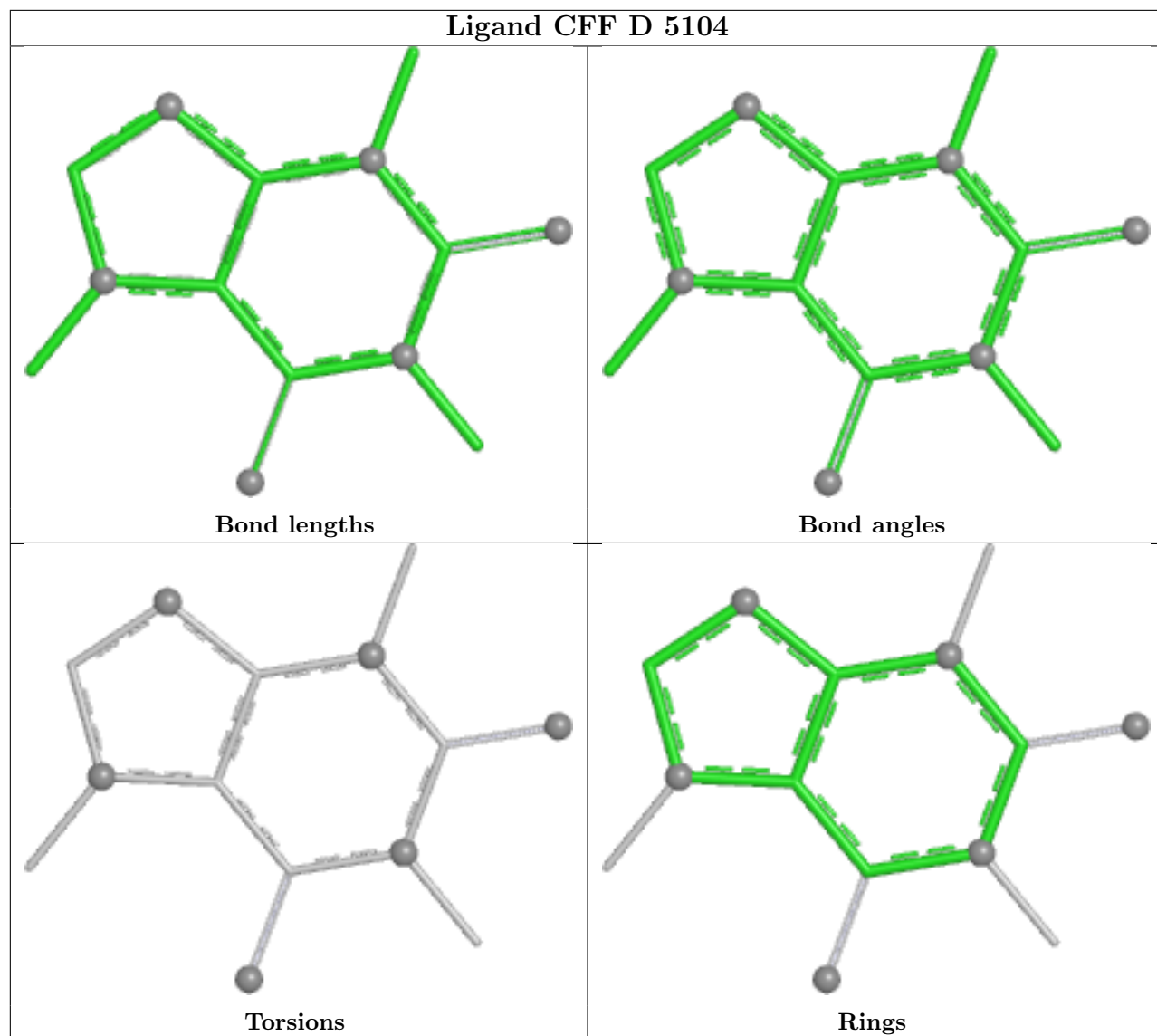
Continued from previous page...

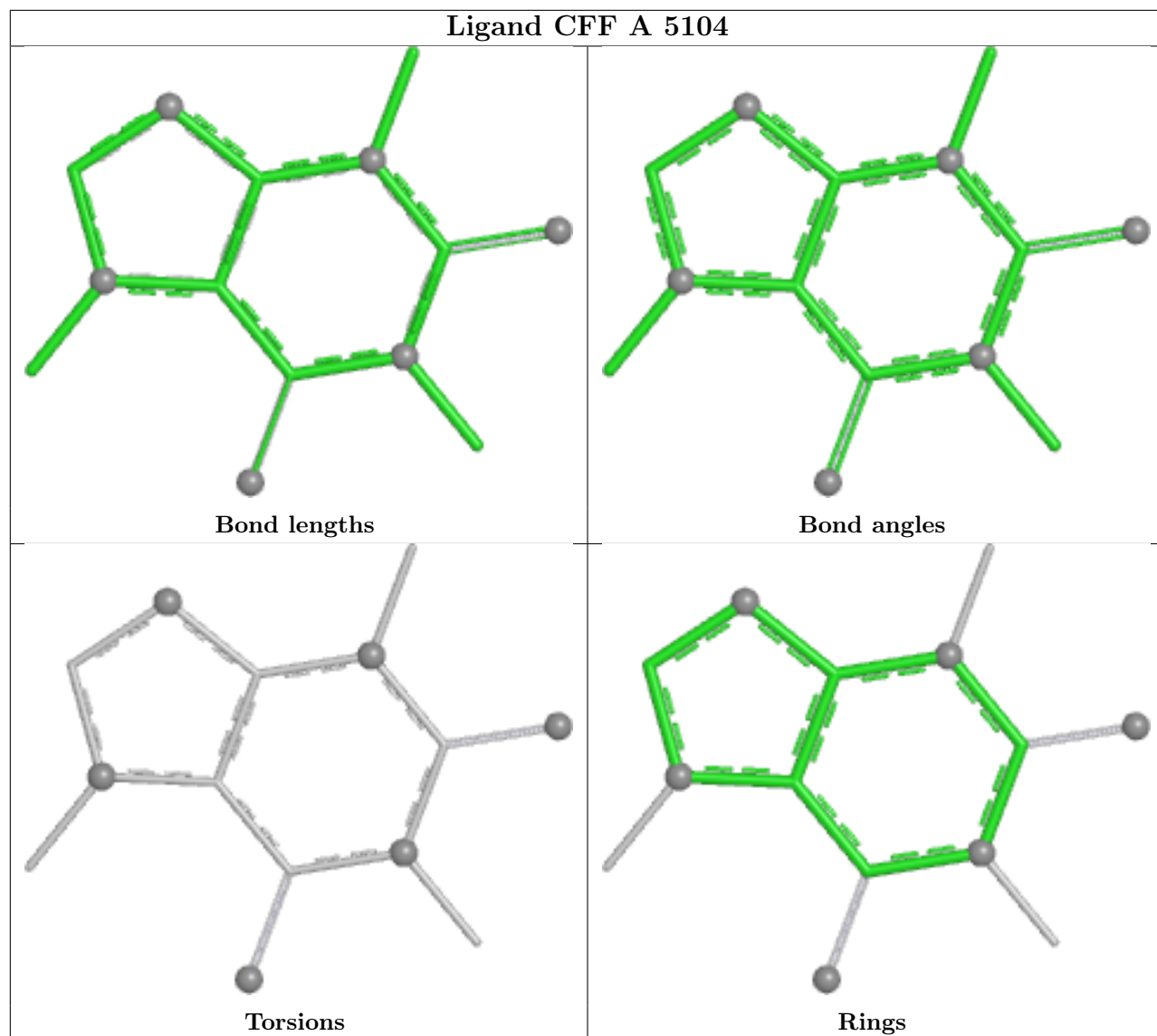
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	5103	ATP	1	0

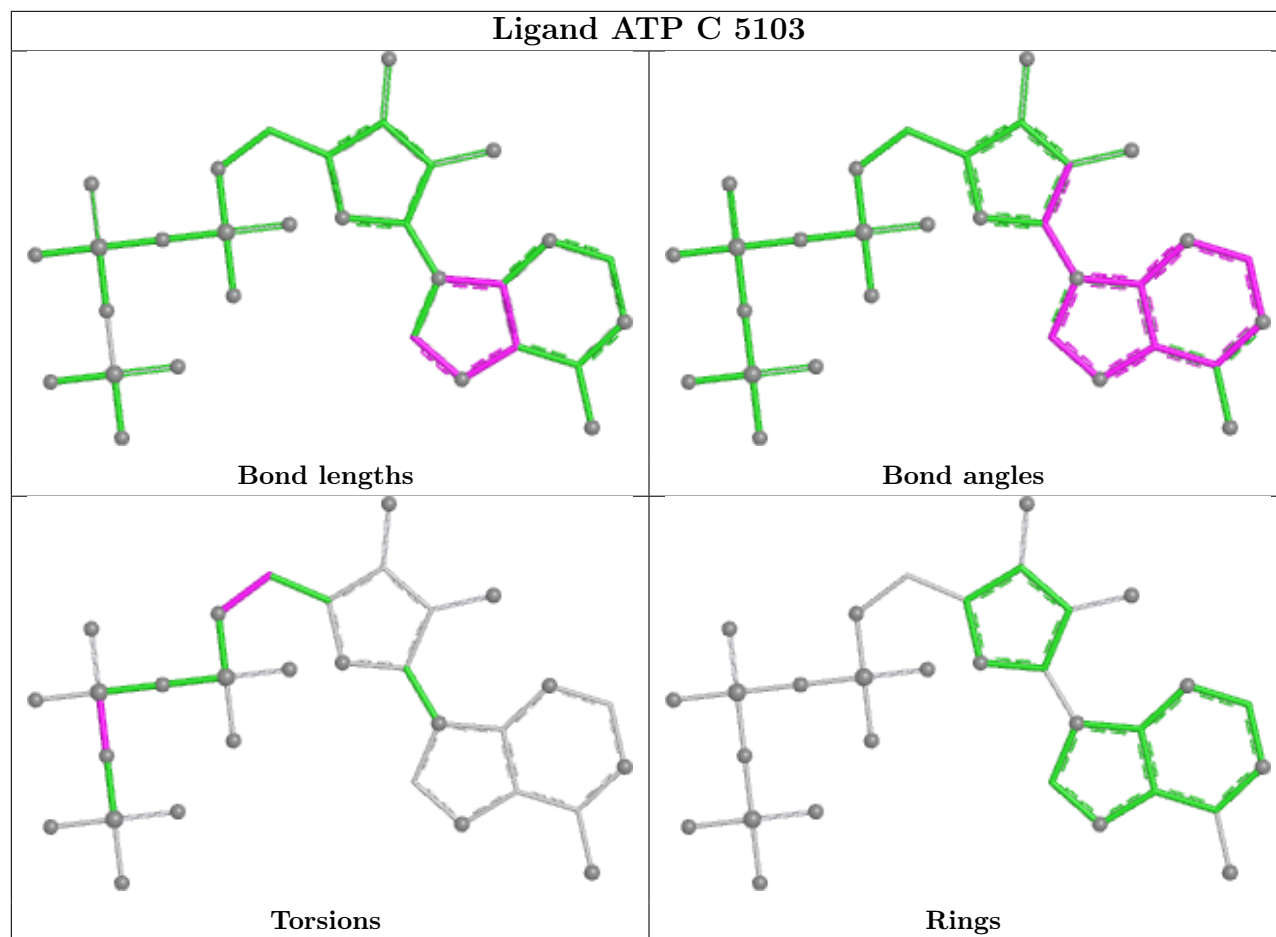
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

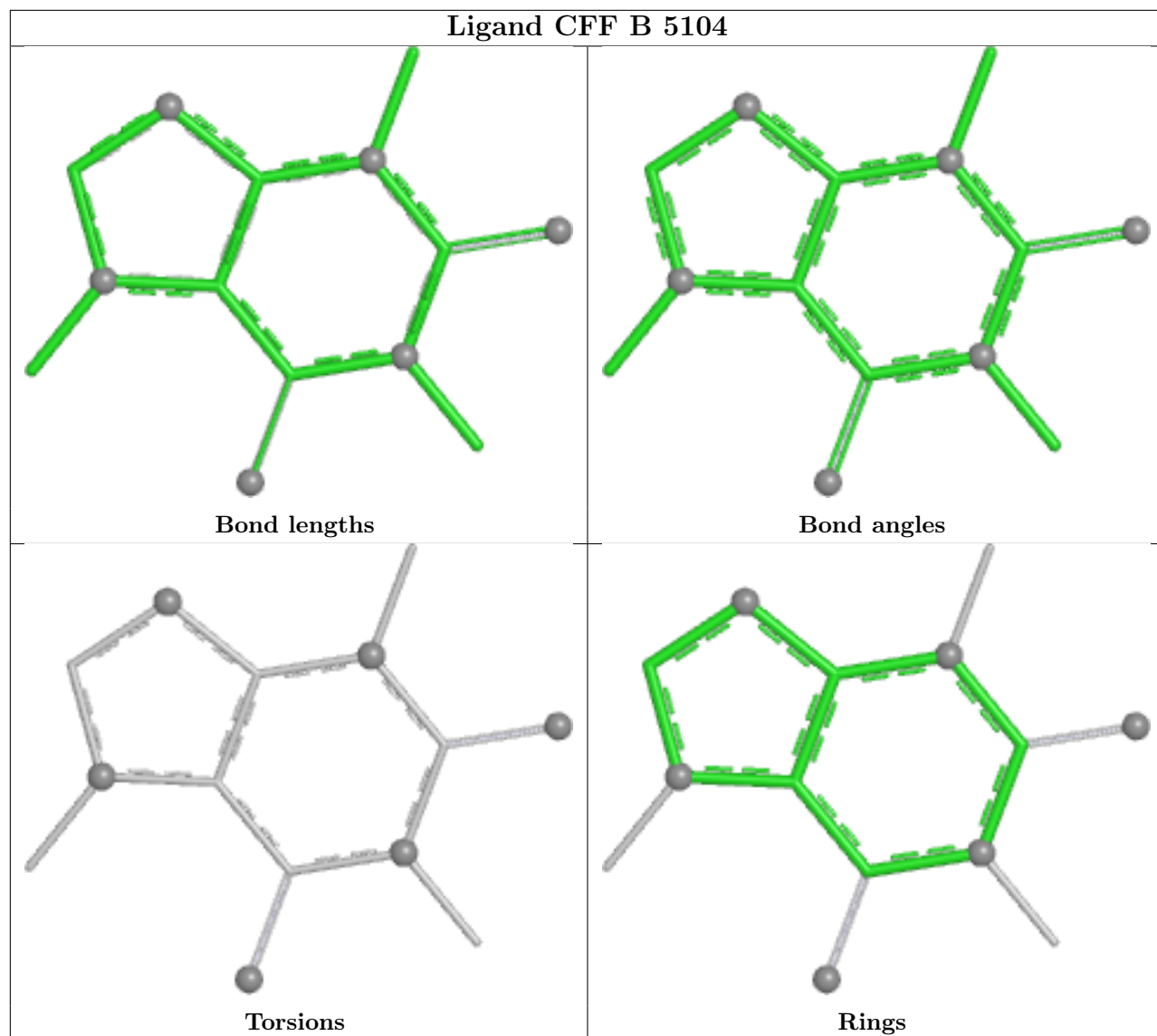


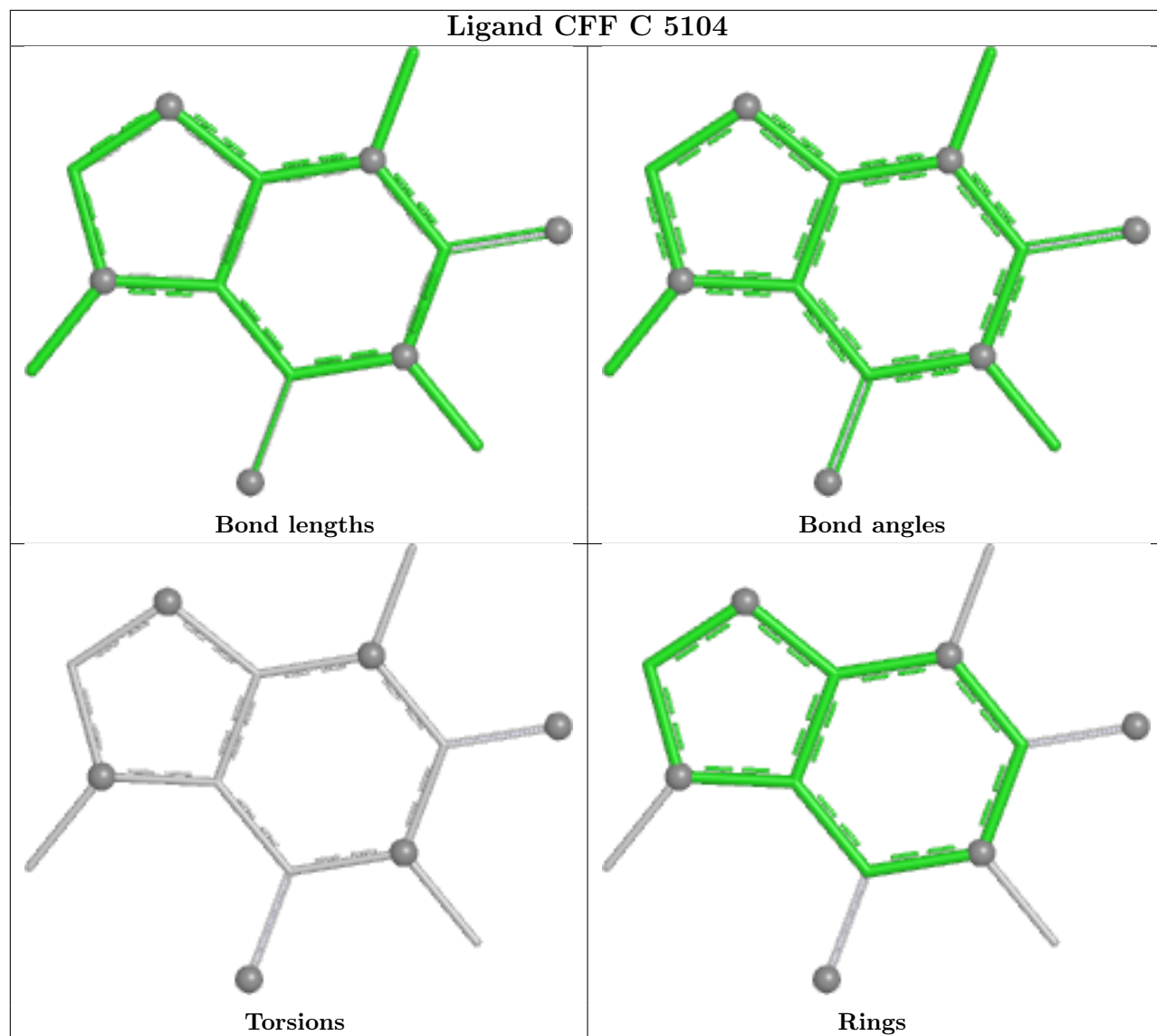


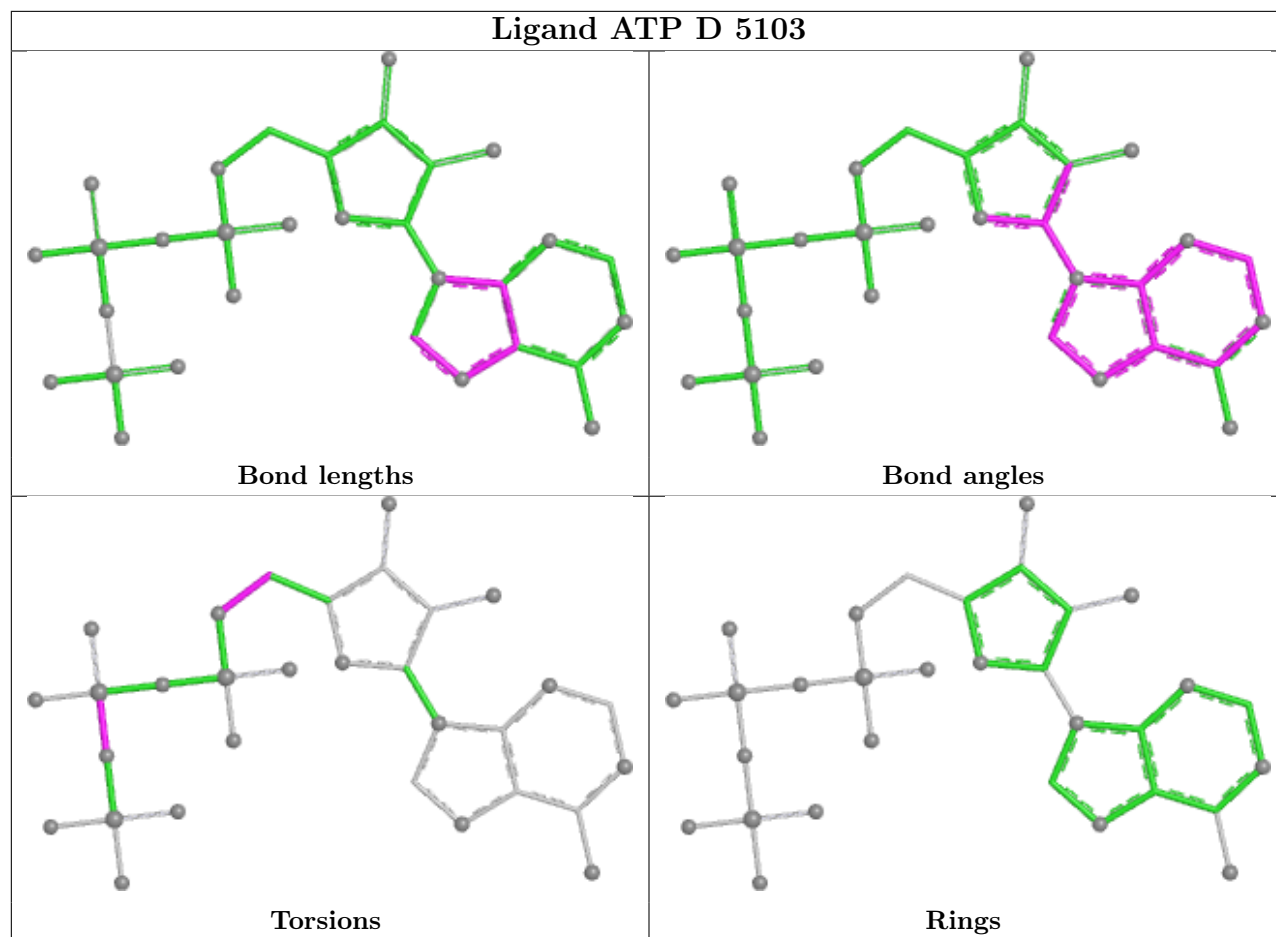












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

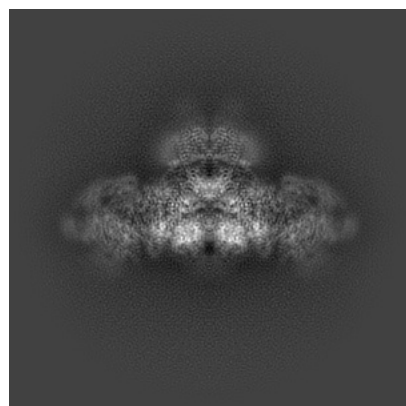
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38448. These allow visual inspection of the internal detail of the map and identification of artifacts.

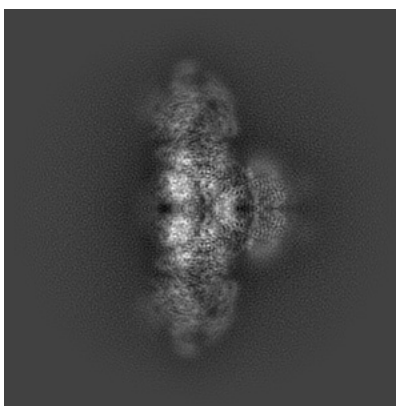
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

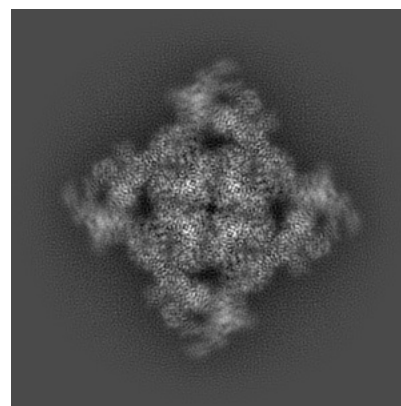
6.1.1 Primary map



X

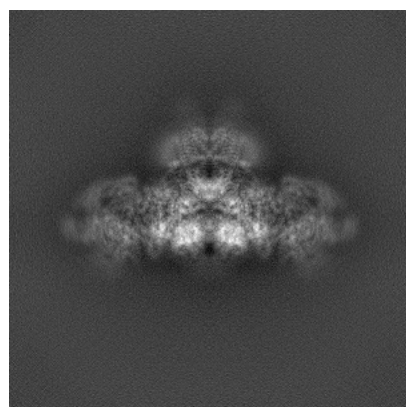


Y

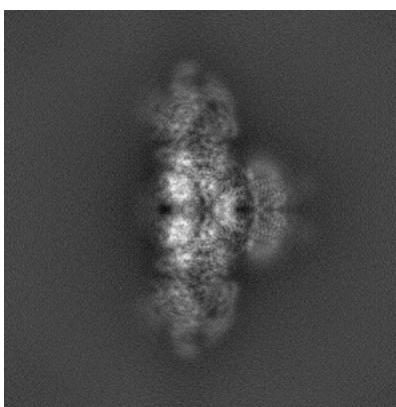


Z

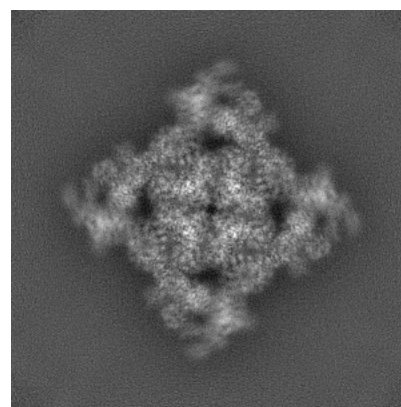
6.1.2 Raw map



X



Y

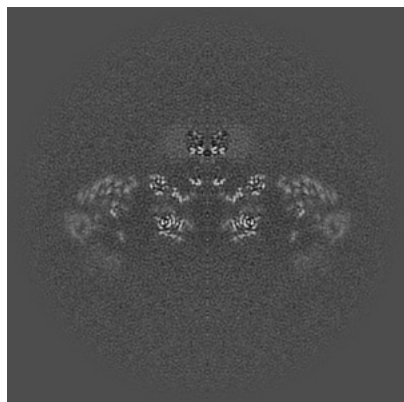


Z

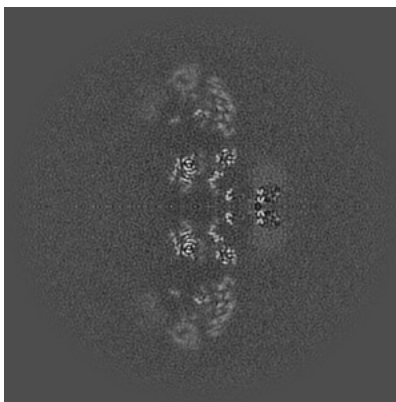
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

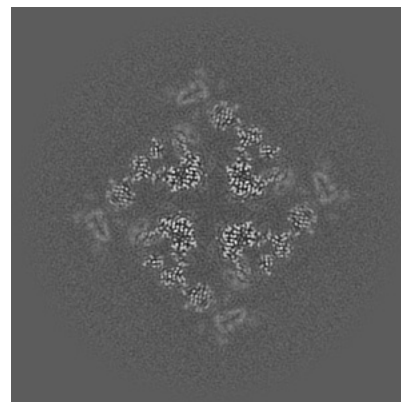
6.2.1 Primary map



X Index: 240

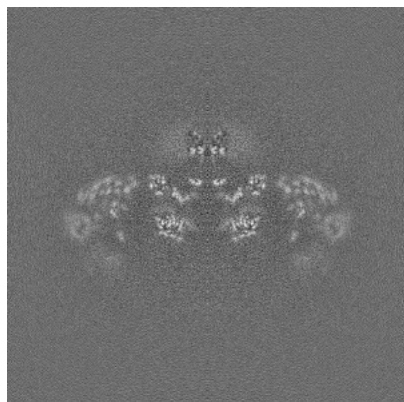


Y Index: 240

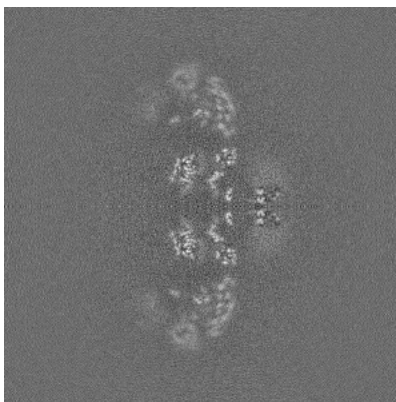


Z Index: 240

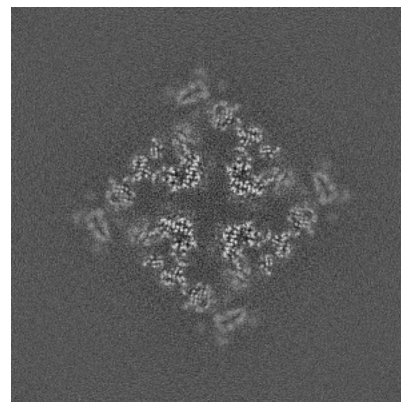
6.2.2 Raw map



X Index: 240



Y Index: 240

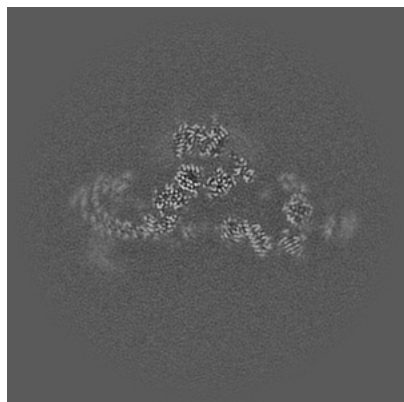


Z Index: 240

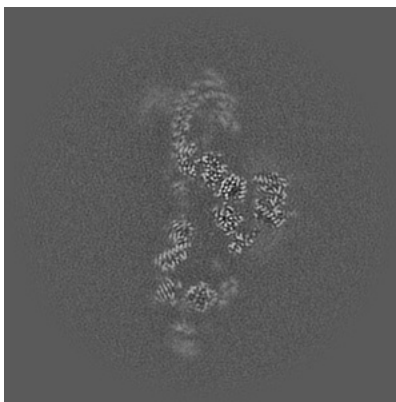
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

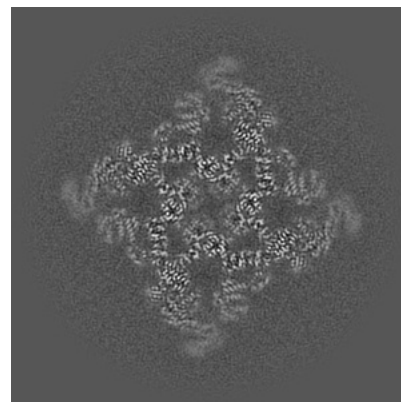
6.3.1 Primary map



X Index: 256

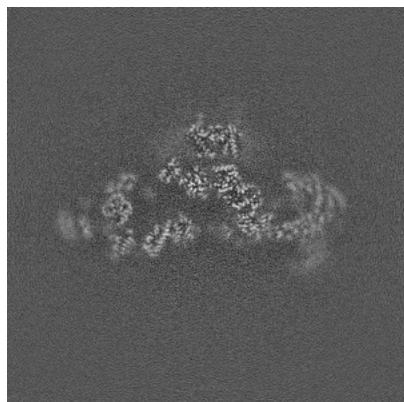


Y Index: 256

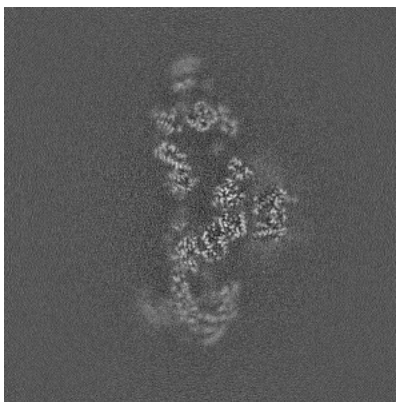


Z Index: 218

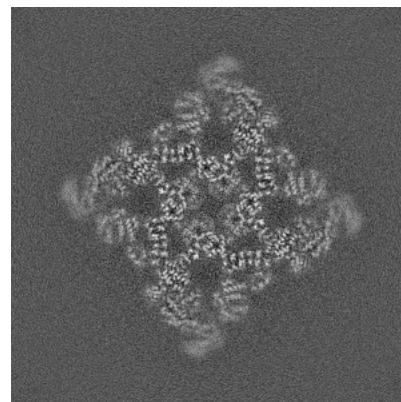
6.3.2 Raw map



X Index: 225



Y Index: 225

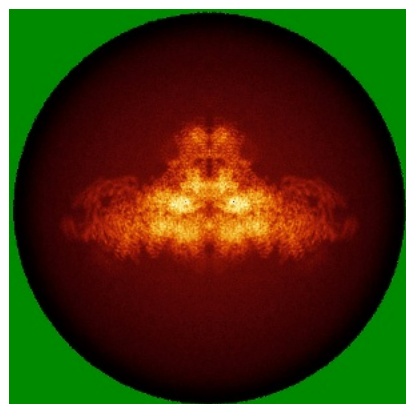


Z Index: 218

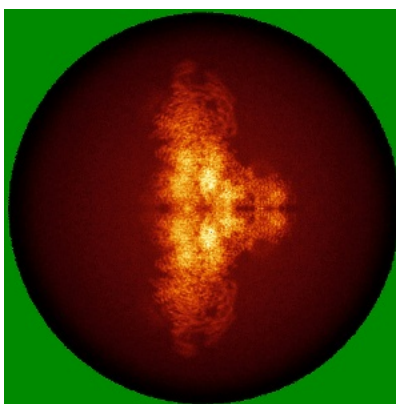
The images above show the largest variance slices of the map in three orthogonal directions.

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

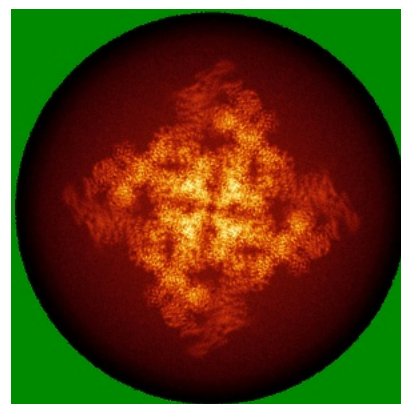
6.4.1 Primary map



X

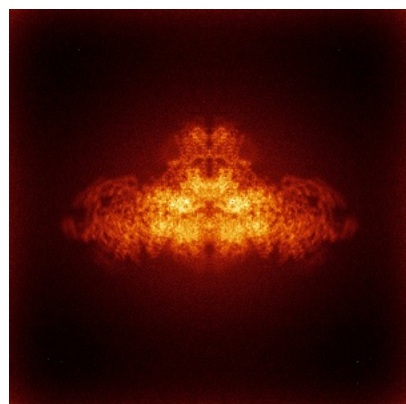


Y

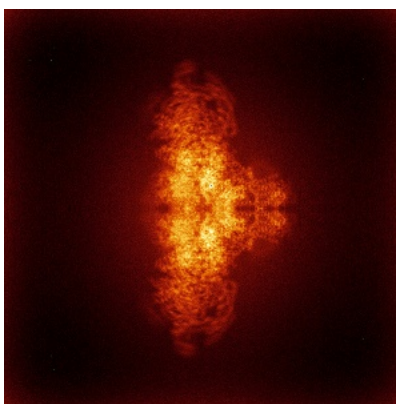


Z

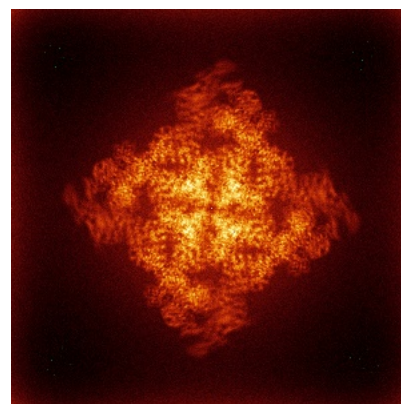
6.4.2 Raw map



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](#)

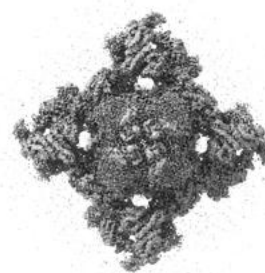
6.5.1 Primary map



X



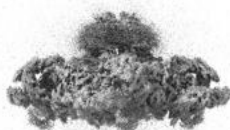
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.135. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

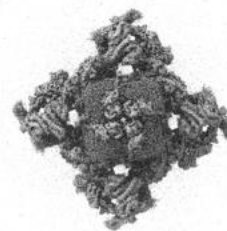
6.5.2 Raw map



X



Y



Z

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

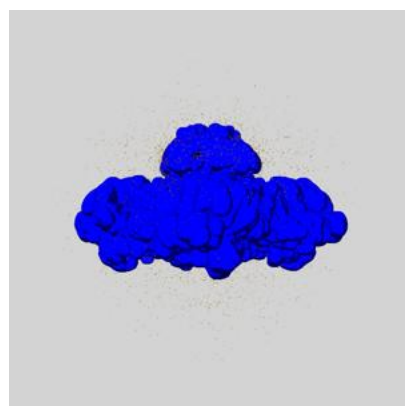
6.6 Mask visualisation [i](#)

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

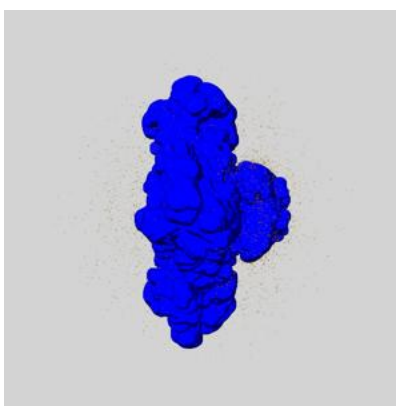
A mask typically either:

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

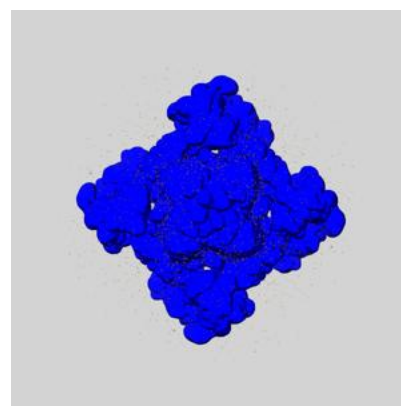
6.6.1 emd_38448_msk_1.map [i](#)



X



Y

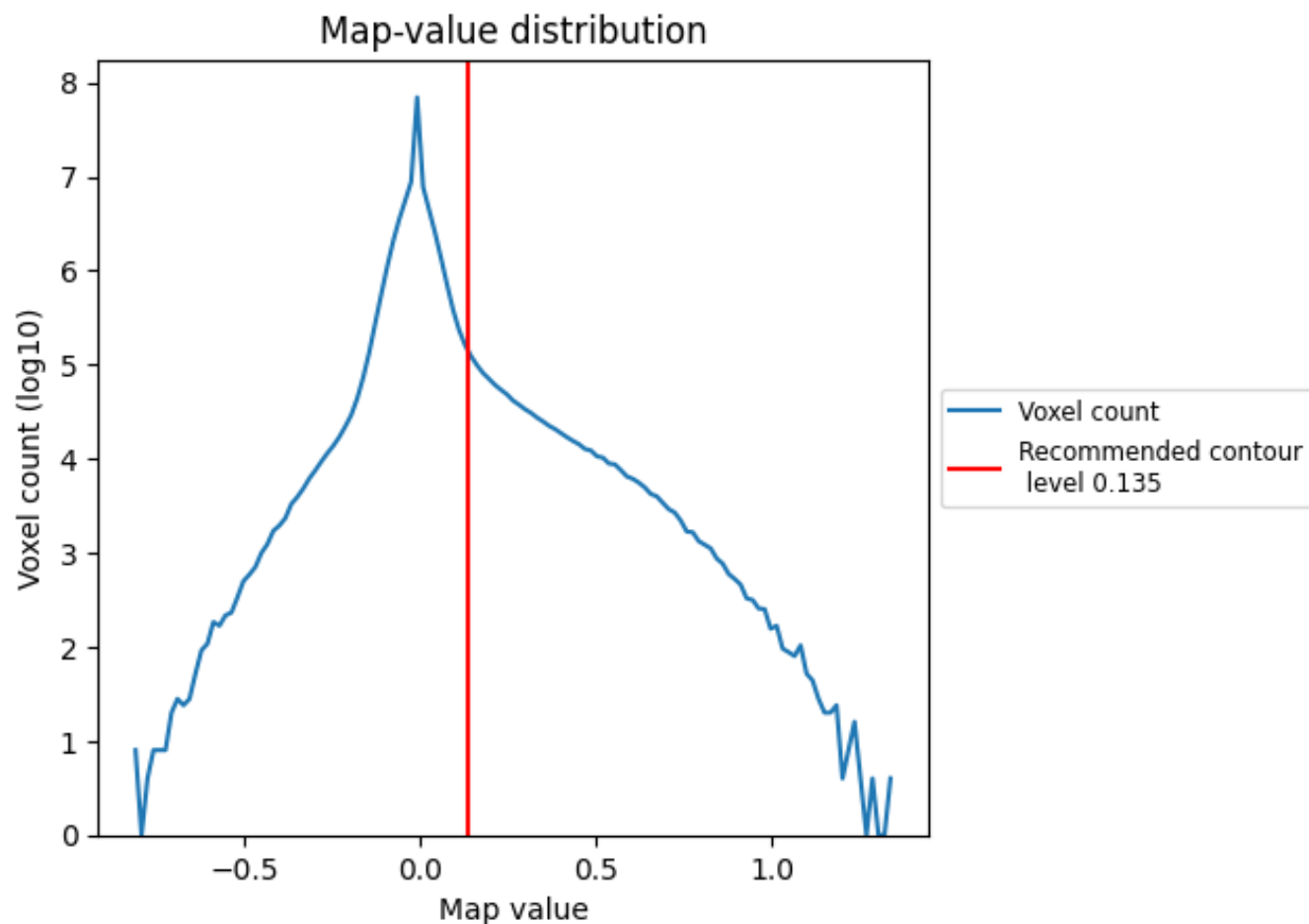


Z

7 Map analysis [i](#)

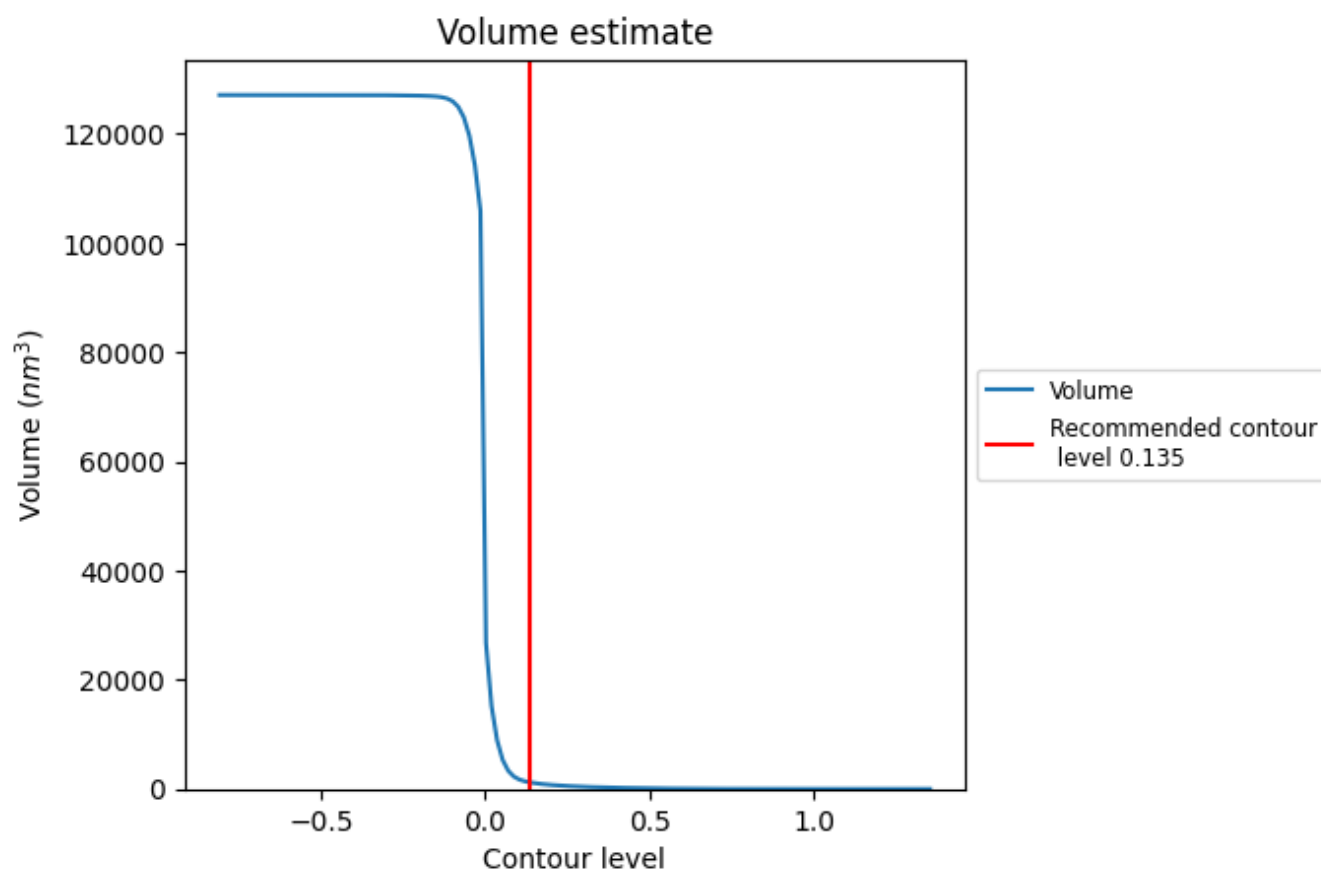
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

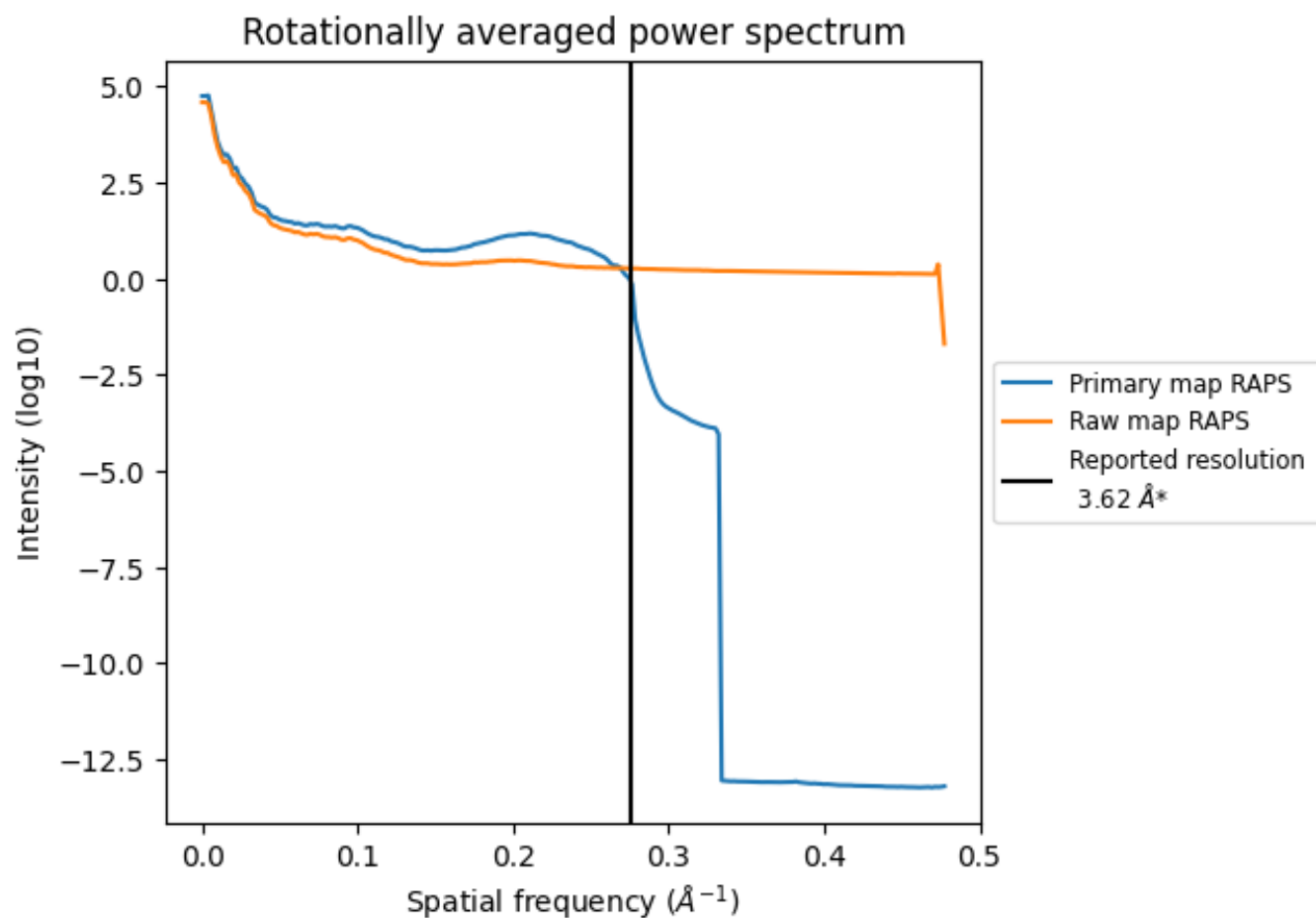
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1226 nm^3 ; this corresponds to an approximate mass of 1107 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 ⓘ

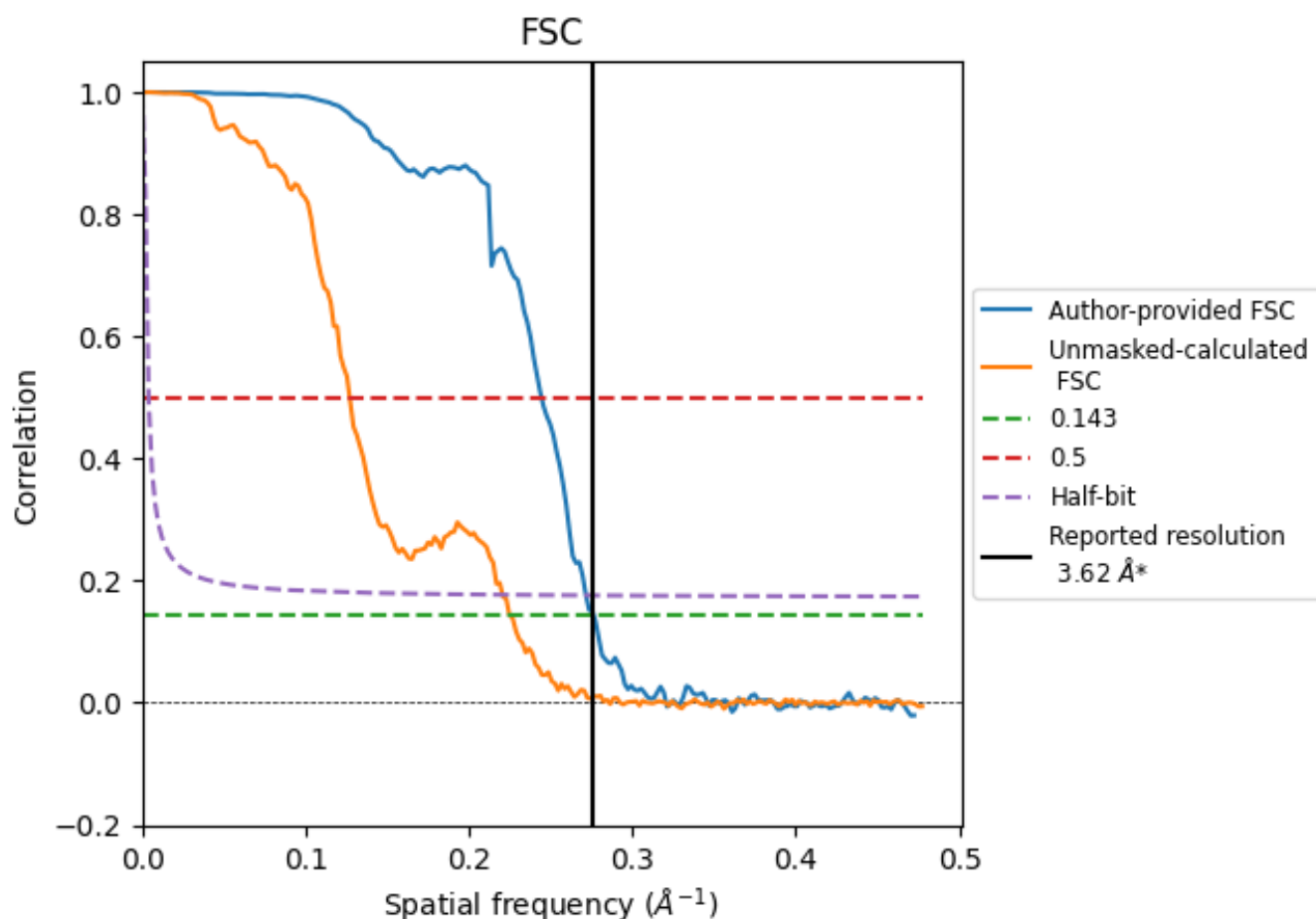


*Reported resolution corresponds to spatial frequency of $0.276 \text{ \AA}^{-1}$

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 0.276 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.62	-	-
Author-provided FSC curve	3.62	4.09	3.68
Unmasked-calculated*	4.44	7.88	4.54

*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 4.44 differs from the reported value 3.62 by more than 10 %

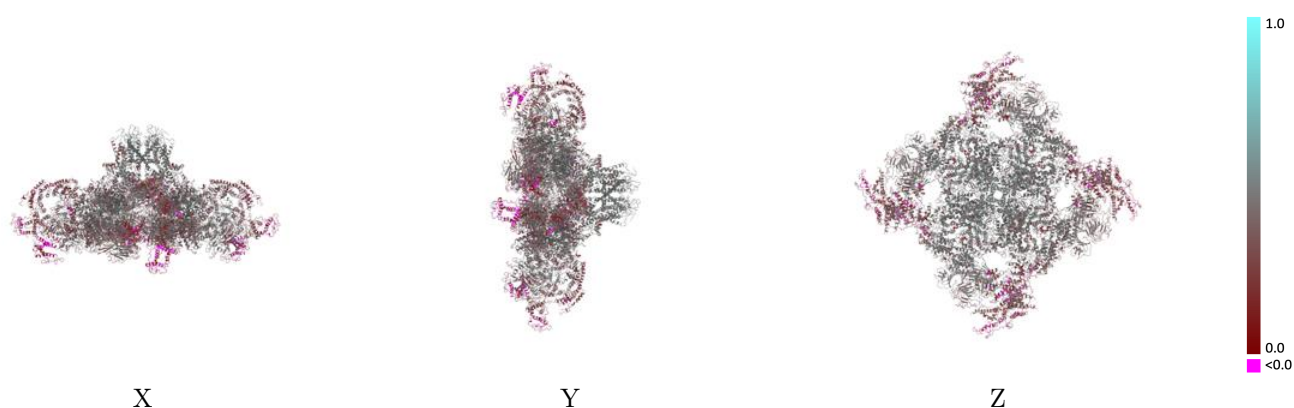
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38448 and PDB model 8XLH. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

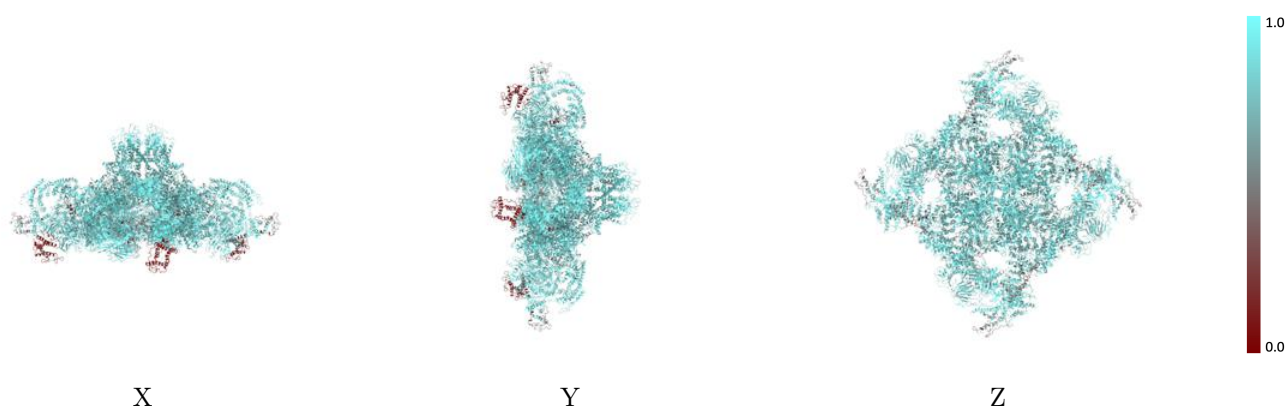
This section was not generated.

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



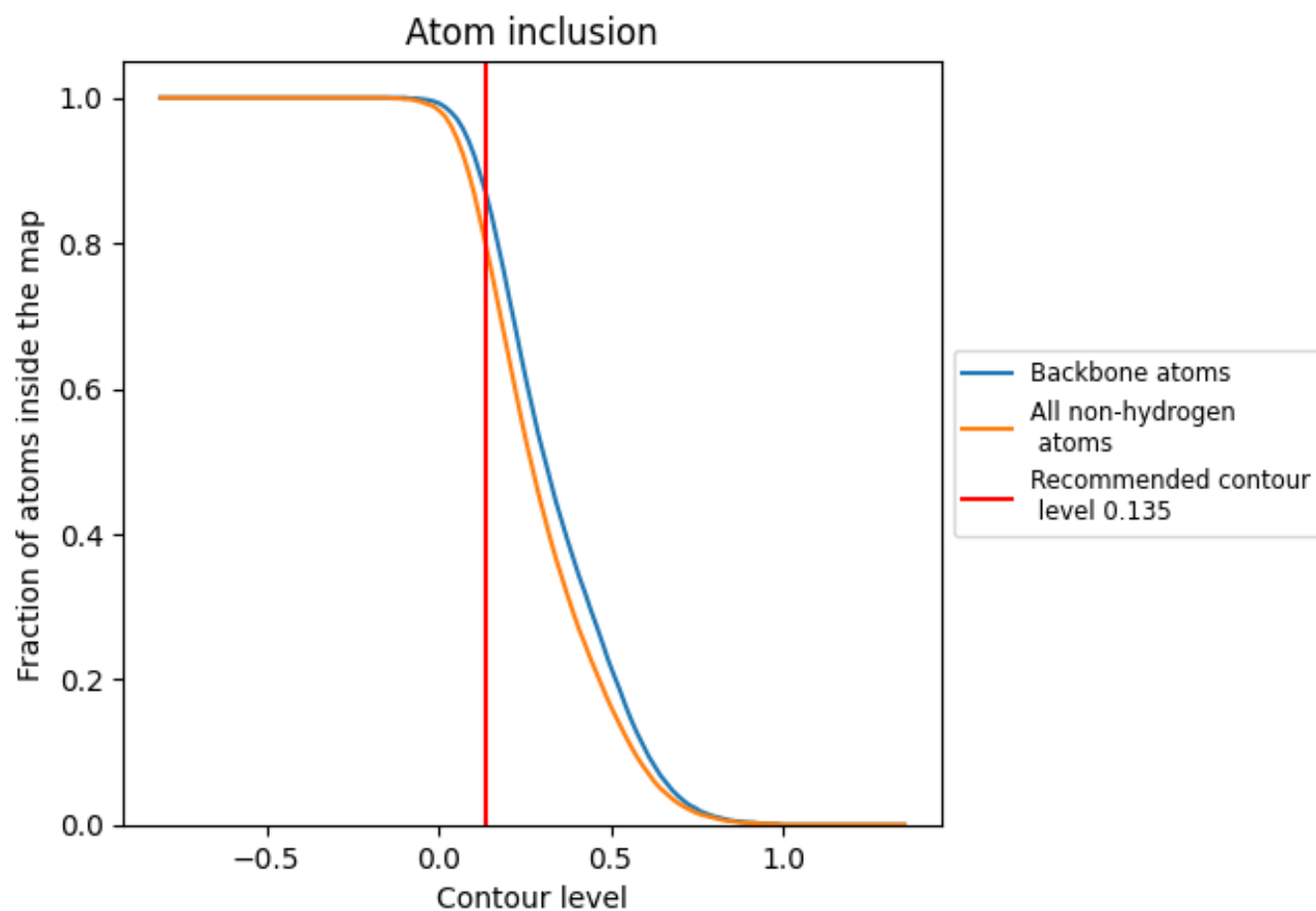
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.135).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 80% 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 (0.135) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8030	0.3860
A	0.8120	0.3950
B	0.8110	0.3950
C	0.8110	0.3960
D	0.7960	0.3770
E	0.8380	0.4100
F	0.8380	0.4150
G	0.8360	0.4110
H	0.8190	0.3940
I	0.6560	0.2530
J	0.6550	0.2540
K	0.6580	0.2500
L	0.6400	0.2360

