



## Full wwPDB EM Validation Report ⓘ

Oct 14, 2024 – 10:14 AM EDT

PDB ID : 8SEP  
EMDB ID : EMD-40424  
Title : Cryo-EM Structure of RyR1 + ADP  
Authors : Cholak, S.; Saville, J.W.; Zhu, X.; Berezuk, A.M.; Tuttle, K.S.; Haji-Ghassemi, O.; Van Petegem, F.; Subramaniam, S.  
Deposited on : 2023-04-10  
Resolution : 3.57 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

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

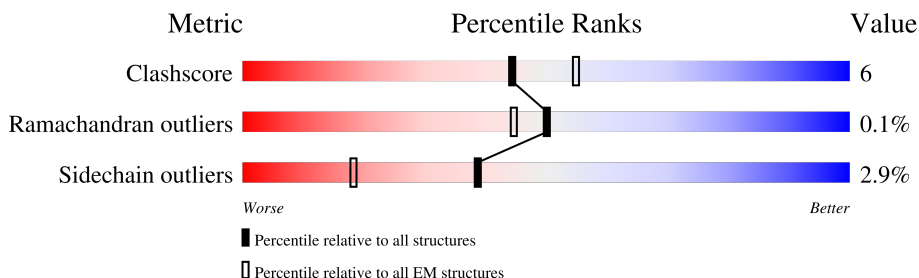
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.57 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	5037	<div> <div>13%</div> <div>71%</div> <div>16%</div> <div>•</div> <div>13%</div> </div>
1	B	5037	<div> <div>13%</div> <div>71%</div> <div>16%</div> <div>•</div> <div>13%</div> </div>
1	C	5037	<div> <div>13%</div> <div>70%</div> <div>16%</div> <div>•</div> <div>13%</div> </div>
1	D	5037	<div> <div>13%</div> <div>70%</div> <div>16%</div> <div>•</div> <div>13%</div> </div>
2	E	350	<div> <div>23%</div> <div>7%</div> <div>69%</div> </div>
2	F	350	<div> <div>23%</div> <div>8%</div> <div>69%</div> </div>
2	G	350	<div> <div>23%</div> <div>7%</div> <div>69%</div> </div>
2	H	350	<div> <div>23%</div> <div>7%</div> <div>69%</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 143100 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	4379	Total	C	N	O	S	9	0
			34929	22223	6026	6444	236		
1	B	4379	Total	C	N	O	S	9	0
			34929	22223	6026	6444	236		
1	C	4379	Total	C	N	O	S	9	0
			34929	22223	6026	6444	236		
1	D	4379	Total	C	N	O	S	9	0
			34929	22223	6026	6444	236		

- Molecule 2 is a protein called Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	G	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-242	MET	-	expression tag	UNP P08515
E	-241	LYS	-	expression tag	UNP P08515
E	-240	SER	-	expression tag	UNP P08515
E	-239	SER	-	expression tag	UNP P08515
E	-238	HIS	-	expression tag	UNP P08515
E	-237	HIS	-	expression tag	UNP P08515
E	-236	HIS	-	expression tag	UNP P08515
E	-235	HIS	-	expression tag	UNP P08515

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-234	HIS	-	expression tag	UNP P08515
E	-233	HIS	-	expression tag	UNP P08515
E	-232	GLY	-	expression tag	UNP P08515
E	-231	SER	-	expression tag	UNP P08515
E	-230	SER	-	expression tag	UNP P08515
E	-11	GLY	-	linker	UNP P08515
E	-10	ILE	-	linker	UNP P08515
E	-9	GLU	-	linker	UNP P08515
E	-8	GLU	-	linker	UNP P08515
E	-7	ASN	-	linker	UNP P08515
E	-6	LEU	-	linker	UNP P08515
E	-5	TYR	-	linker	UNP P08515
E	-4	PHE	-	linker	UNP P08515
E	-3	GLN	-	linker	UNP P08515
E	-2	SER	-	linker	UNP P08515
E	-1	ASN	-	linker	UNP P08515
E	0	ALA	-	linker	UNP P08515
F	-242	MET	-	expression tag	UNP P08515
F	-241	LYS	-	expression tag	UNP P08515
F	-240	SER	-	expression tag	UNP P08515
F	-239	SER	-	expression tag	UNP P08515
F	-238	HIS	-	expression tag	UNP P08515
F	-237	HIS	-	expression tag	UNP P08515
F	-236	HIS	-	expression tag	UNP P08515
F	-235	HIS	-	expression tag	UNP P08515
F	-234	HIS	-	expression tag	UNP P08515
F	-233	HIS	-	expression tag	UNP P08515
F	-232	GLY	-	expression tag	UNP P08515
F	-231	SER	-	expression tag	UNP P08515
F	-230	SER	-	expression tag	UNP P08515
F	-11	GLY	-	linker	UNP P08515
F	-10	ILE	-	linker	UNP P08515
F	-9	GLU	-	linker	UNP P08515
F	-8	GLU	-	linker	UNP P08515
F	-7	ASN	-	linker	UNP P08515
F	-6	LEU	-	linker	UNP P08515
F	-5	TYR	-	linker	UNP P08515
F	-4	PHE	-	linker	UNP P08515
F	-3	GLN	-	linker	UNP P08515
F	-2	SER	-	linker	UNP P08515
F	-1	ASN	-	linker	UNP P08515
F	0	ALA	-	linker	UNP P08515

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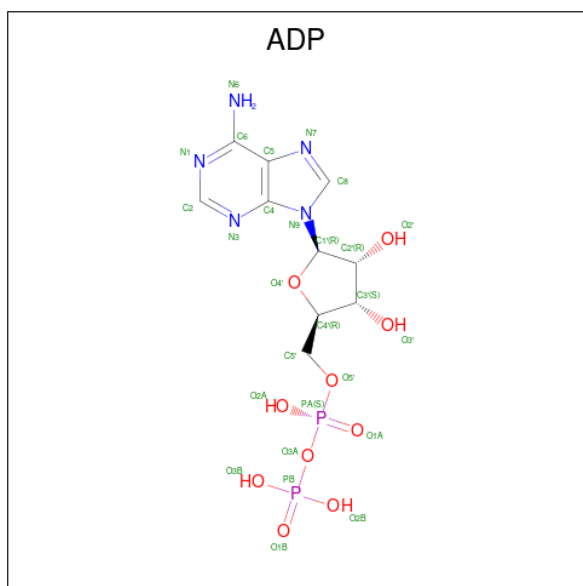
Chain	Residue	Modelled	Actual	Comment	Reference
G	-242	MET	-	expression tag	UNP P08515
G	-241	LYS	-	expression tag	UNP P08515
G	-240	SER	-	expression tag	UNP P08515
G	-239	SER	-	expression tag	UNP P08515
G	-238	HIS	-	expression tag	UNP P08515
G	-237	HIS	-	expression tag	UNP P08515
G	-236	HIS	-	expression tag	UNP P08515
G	-235	HIS	-	expression tag	UNP P08515
G	-234	HIS	-	expression tag	UNP P08515
G	-233	HIS	-	expression tag	UNP P08515
G	-232	GLY	-	expression tag	UNP P08515
G	-231	SER	-	expression tag	UNP P08515
G	-230	SER	-	expression tag	UNP P08515
G	-11	GLY	-	linker	UNP P08515
G	-10	ILE	-	linker	UNP P08515
G	-9	GLU	-	linker	UNP P08515
G	-8	GLU	-	linker	UNP P08515
G	-7	ASN	-	linker	UNP P08515
G	-6	LEU	-	linker	UNP P08515
G	-5	TYR	-	linker	UNP P08515
G	-4	PHE	-	linker	UNP P08515
G	-3	GLN	-	linker	UNP P08515
G	-2	SER	-	linker	UNP P08515
G	-1	ASN	-	linker	UNP P08515
G	0	ALA	-	linker	UNP P08515
H	-242	MET	-	expression tag	UNP P08515
H	-241	LYS	-	expression tag	UNP P08515
H	-240	SER	-	expression tag	UNP P08515
H	-239	SER	-	expression tag	UNP P08515
H	-238	HIS	-	expression tag	UNP P08515
H	-237	HIS	-	expression tag	UNP P08515
H	-236	HIS	-	expression tag	UNP P08515
H	-235	HIS	-	expression tag	UNP P08515
H	-234	HIS	-	expression tag	UNP P08515
H	-233	HIS	-	expression tag	UNP P08515
H	-232	GLY	-	expression tag	UNP P08515
H	-231	SER	-	expression tag	UNP P08515
H	-230	SER	-	expression tag	UNP P08515
H	-11	GLY	-	linker	UNP P08515
H	-10	ILE	-	linker	UNP P08515
H	-9	GLU	-	linker	UNP P08515
H	-8	GLU	-	linker	UNP P08515

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-7	ASN	-	linker	UNP P08515
H	-6	LEU	-	linker	UNP P08515
H	-5	TYR	-	linker	UNP P08515
H	-4	PHE	-	linker	UNP P08515
H	-3	GLN	-	linker	UNP P08515
H	-2	SER	-	linker	UNP P08515
H	-1	ASN	-	linker	UNP P08515
H	0	ALA	-	linker	UNP P08515

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).



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

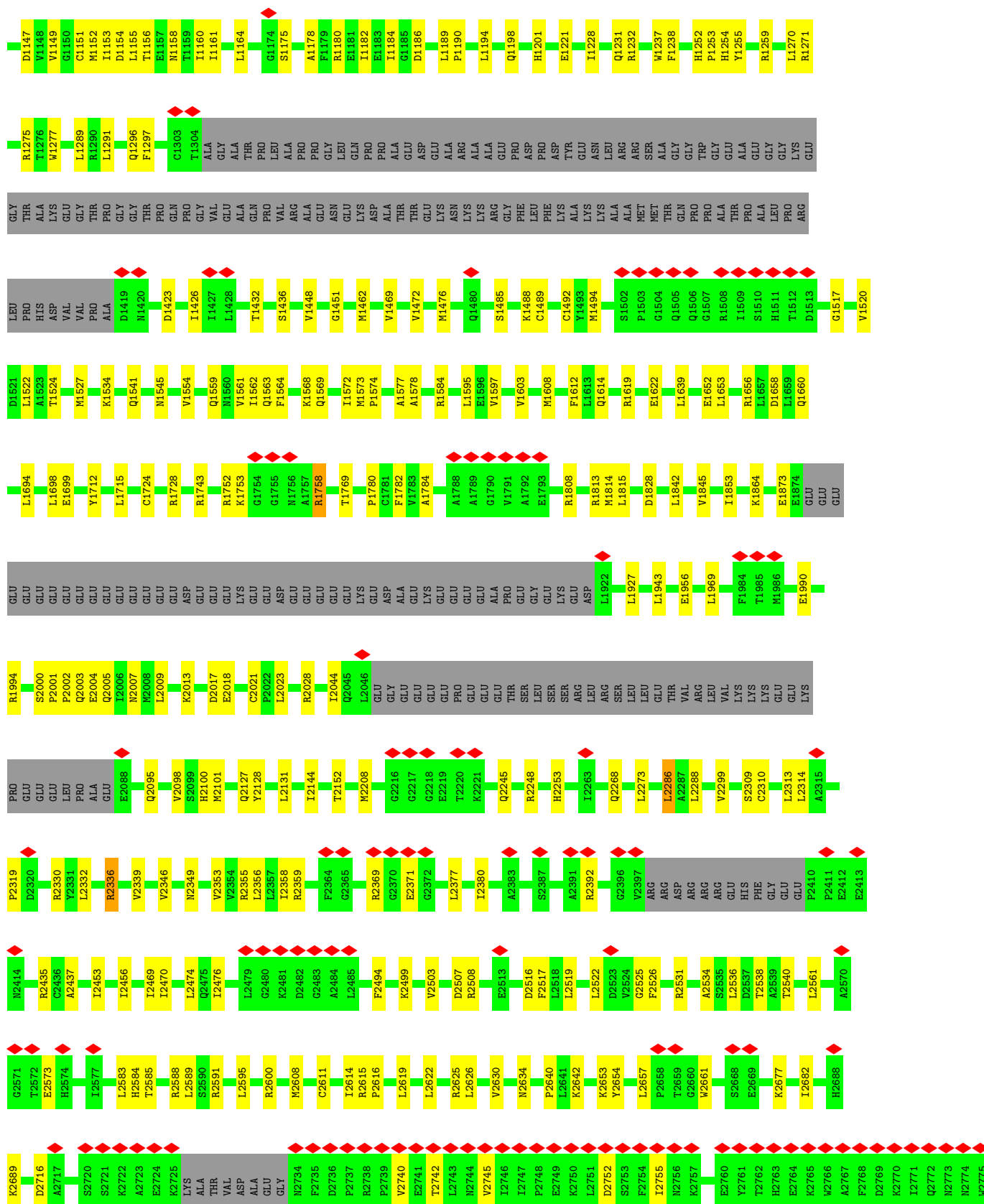
### 3 Residue-property plots

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







M4057	T3864	K3614	D5531	L3434	I3322	V3065	L2963	A2896	LYS	S2776
I4058	V3865	S3615	D5532	F3435	I3323	V3066	L2964	K2897	LYS	V2777
D4063	I3866	K3616	I3532	R3436	V3324	L3068	R2965	G2898	LYS	G2778
M4064	N3867	K3617	M5534	R3453	N3325	H3069	M2966	G2899	ARG	E2779
L4068	Q3868	A3618	K3537	E3454	N3326	L3075	S2970	G2900	LYS	M2780
K4069	R3869	V3619	K3538	N3457	L3327	D3076	Q2971	H2901	ILE	V2781
D4070	N3870	W3620	T3538	F3458	L3328	D3077	Q2972	H2902	SER	D2782
E3871	H3871	H3621	Y3540	V3459	I3329	R3078	L2974	H2903	THR	E2783
E3872	K3622	K3622	A3541	V3460	V3218	E2978	E2978	P2903	ALA	L2785
K3873	L3623	L3623	L3542	Q3461	Y3219	A2979	A2979	L2904	GLN	E2786
M3875	L3624	L3624	K3543	E3463	T3220	V2980	V2980	L2905	THR	L2785
D3878	S3625	S3625	K3544	I3464	K3222	V2981	V2981	V2906	TTR	K2786
Q3889	K3626	K3626	E3548	N3465	S3223	S2982	S2982	P2907	ASP	T2787
L3890	Q3627	Q3627	V3549	N3466	F3224	S2983	S2983	D2908	ARG	H2788
L3891	R3628	R3628	R3550	M3467	R3225	K3114	K3114	D2909	PRO	P2789
F3899	R3629	R3629	E3551	S3468	R3225	G3113	G3113	D2910	GLY	H2790
L3924	R3630	R3630	N3555	F3469	R3348	V3115	V2985	L2911	GLY	M2791
S3929	A3631	A3631	N3556	F3470	R3350	S3116	V2986	T2912	Y2855	L2791
W3935	V3632	V3632	L3557	T3471	P3351	ALA	E2987	T2912	P2857	R2792
K4095	A3634	A3634	H3558	A3472	L3354	ARG	K2988	K2914	Q2858	P2793
A4096	C3635	C3635	Q3560	S3473	F3358	THR	P2989	E2915	P2859	L2794
M4097	F3636	F3636	G3561	D3474	I3362	GLN	P2990	K2916	P2860	K2795
D4098	R3637	R3637	K3562	S3475	I3362	VAL	H2991	A2917	D2861	L2796
Q4099	M3638	M3638	V3563	K3476	E3377	K3123	E2992	R2918	L2862	F2797
E3967	L3641	L3641	G3564	K3477	E3377	Y3131	Q2993	D2919	S2863	S2798
L3980	M3652	M3652	E3564	A3479	V3245	H3146	F2997	R2920	G2864	E2799
R3984	E3655	E3655	S3568	L3479	R3248	Q3149	I3001	E2921	V2865	K2800
L3985	E3656	E3656	W3571	ALA	E3382	H3150	T3020	K2922	T2867	D2801
V3990	A3659	A3659	L3579	GLY	A3383	Q3151	A3021	A2923	S2868	K2802
F3995	R3660	R3660	L3579	ASP	K3384	V3156	A3022	E2925	R2869	E2803
A3997	W3661	W3661	R3582	ALA	A3385	I3157	L2926	L2927	E2870	I2804
H3998	I3662	I3662	E3583	GLN	K3386	L3158	K3023	L2927	L2871	Y2805
M3999	L3663	L3663	E3584	SER	E3387	V3161	V3024	K2928	Q2872	R2806
K4002	D3676	D3676	E3585	GLY	E3388	Q3162	L3025	F2929	A2873	W2807
E4011	A3680	A3680	A3586	ASP	E3389	L3261	G3026	L2930	M2874	P2808
L3842	G3681	G3681	D3587	GLN	R3395	N3180	G3028	L2931	A2875	K2810
A3846	E3682	E3682	I3592	THR	R3403	V3183	N3033	W2811	E2876	E2811
V4035	Q3683	Q3683	R3595	LYS	D3404	E3184	E3037	Q2877	Q2877	S2812
M4039	E3684	E3684	V3596	LYS	L3405	K3185	L3046	L2878	A2879	L2813
Q4043	E3685	E3685	L3603	R3498	L3408	L3190	K3045	G2934	L2879	K2814
E4121	E3686	E3686	V3604	R3499	Y3409	L3194	E3037	Y2935	E2880	A2815
S4051	E3687	E3687	H3605	R3499	L3413	L3194	L3049	V2937	F2881	K2816
M4054	E3688	E3688	L3606	D3501	R3414	L3197	V3050	T2938	Y2882	A2818
D4138	V3690	V3690	Q3607	R3502	D3417	A3204	R2939	K2939	H2883	W2819
N4142	E3691	E3691	T3609	R3502	N3418	F3205	LEU	GLY	N2884	E2820
E4152	E3692	E3692	H3610	Q3506	K3418	E3207	LYS	ASP	T2885	W2821
P4155	D3696	D3696	H3611	K3515	L3424	E3207	ASP	ASP	W2886	T2822
	C3733	C3733	P3612	N3523	E3433	E3207	GLU	GLU	R2887	T2823
	E3735	E3735	Y3613	M3524	E3433	E3207	L2948	L2946	R2888	E2824
							S2949	D2947	K2889	K2825
							E2952	K2890	K2891	A2826
							E2952	Q2892	Q2892	R2827
							E2952	E2893	E2893	G2828
							E2952	L2894	L2894	E2830
							E2952	E2895	E2895	GLU
							E2952	E2895	E2895	GLU
							E2952	E2895	E2895	THR
							E2952	E2895	E2895	THR
							E2952	E2895	E2895	GLU



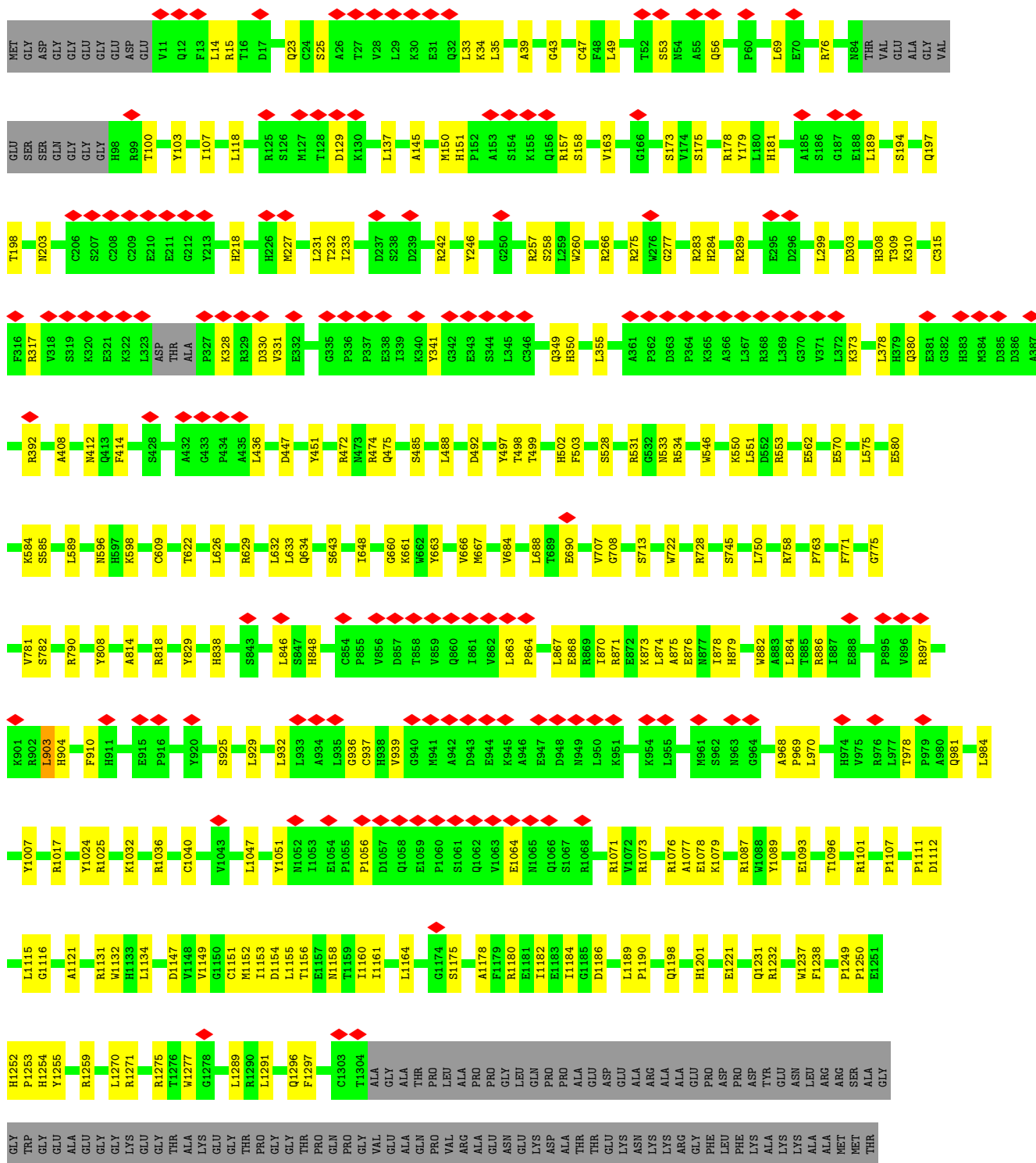




M4857	K4721	T4636	M4574	GLU	GLY	VAL	THR	VAL	GLY	THR	VAL	ARG	GLY	A4117	I4010	Q3846	E3689	L3603	R3499
R4860	R4722	G4637	M4577	PRO	VAL	THR	THR	VAL	GLY	THR	VAL	ARG	GLY	D4118	E4011	A3846	V3690	Y3604	Q3500
K4861	R4734	M4639	L4577	PRO	ALA	LEU	LEU	ARG	PRO	LEU	ARG	ARG	PRO	E4119	K4014	Q3850	E3691	L3606	D3501
M4864	R4736	L4643	Y4580	LYS	ALA	GLY	GLY	ARG	ALA	ALA	ARG	ARG	ALA	W4120	V4035	H3858	E3692	Q3608	R3502
D4870	L4741	L4646	K4581	ASP	ASP	GLY	MET	LEU	ASP	GLY	ARG	LEU	ASP	E4125	M4039	V3859	D3696	T3609	Q3506
M4874	G4742	S4647	V4582	GLU	GLY	PRO	ASP	THR	GLY	THR	ARG	THR	GLY	D4138	Q4043	Q3860	C3733	E3610	K3615
D4878	M4744	T4651	D4584	ASN	PHE	PRO	ASP	THR	GLY	THR	ARG	THR	MET	N4142	S4051	D3862	E3736	P3612	K3623
L4745	L4745	L4658	P4587	GLY	GLY	PRO	ASP	SER	GLY	SER	GLY	GLY	GLY	N4142	Q4051	G3863	GLY	Y3613	N3523
L4748	L4748	M4662	GLY	GLY	GLY	GLY	ASP	ALA	GLY	ASP	ALA	ALA	GLY	E4152	M4054	T3864	GLY	K3614	K3614
M4879	E4749	GLY	ASP	GLY	GLY	GLY	GLY	THR	ALA	GLY	THR	THR	ALA	E4152	M4057	V3865	GLY	S3616	D3531
M4880	I4750	VAL	ASP	GLY	ALA	VAL	VAL	ALA	ALA	VAL	ALA	ALA	ALA	E4165	I4058	T3866	ASN	K3616	L3532
T4881	THR	GLY	MET	VAL	GLY	HIS	GLY	GLY	GLY	HIS	GLY	GLY	GLY	E4165	I4058	T3866	GLY	K3617	I3533
L4884	ALA	GLY	GLY	PRO	GLY	GLY	GLY	ALA	GLY	GLY	ALA	ALA	GLY	E4168	D4063	N3867	GLY	A3618	M3534
V4889	HIS	LEU	GLY	GLY	LEU	GLY	GLY	ALA	GLY	GLY	ALA	ALA	GLY	E4172	M4064	R3868	ALA	W3619	K3537
P4904	ASN	ASP	ALA	ALA	GLY	PRO	PRO	LEU	GLY	PRO	LEU	LEU	GLY	R4175	K4068	Q3869	GLY	V3620	T3538
L4911	ARG	E4675	GLY	PRO	ASP	GLY	GLY	THR	GLY	GLY	GLY	THR	GLY	R4175	L4068	G3871	GLY	H3621	R3539
Y4912	LYS	E4676	GLY	PRO	GLY	GLY	GLY	THR	ALA	GLY	VAL	VAL	ALA	L4178	K4069	E3872	V3749	K3622	Y3540
R4913	PRO	L4677	LEU	PRO	THR	GLY	GLY	THR	ALA	GLY	VAL	VAL	ALA	G4179	D4070	Q3873	E3750	L3623	A3541
I4927	ASP	R4678	ALA	LYS	THR	GLY	GLY	THR	ALA	GLY	ALA	ALA	ALA	E4181	I4071	V3874	V3751	L3624	L3542
L4932	PRO	L4681	GLY	LYS	PRO	GLY	ASP	PRO	ALA	ASP	ARG	ARG	ALA	E4182	S4074	N3875	S3752	S3625	K3543
Q4933	GLY	E4682	GLY	PRO	ALA	ALA	ASP	GLY	GLY	GLY	GLY	GLY	GLY	E4182	E4075	D3878	F3753	K3626	E3548
D4945	LEU	F4683	GLY	PRO	PRO	ALA	PRO	PRO	ALA	ALA	ALA	ALA	ALA	E4184	D4079	L3888	E3755	Q3627	V3549
E4948	THR	D4684	GLY	SER	THR	GLY	ALA	THR	GLY	GLY	GLY	GLY	GLY	R4188	K4079	L3890	K3756	R3628	R3550
D4966	LEU	G4685	GLY	PRO	THR	GLY	GLY	THR	GLY	GLY	GLY	GLY	GLY	R4188	E4075	L3891	E3757	R3629	E3551
T4971	TRP	L4686	GLY	PRO	PRO	GLY	GLY	PRO	ALA	GLY	VAL	VAL	THR	R4189	T4082	L3891	K3760	R3630	N3555
P4972	MET	Y4687	GLY	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VAL	R4190	D4083	L3891	Q3766	A3631	N3556
D4966	SER	T4688	TRP	LYS	SER	GLY	GLY	GLY	ALA	GLY	ALA	ALA	ALA	E4191	K4090	F3899	Q3767	R3632	L3557
T4977	ILE	E4690	GLY	GLY	GLY	GLY	GLY	GLY	ALA	GLY	GLY	GLY	ALA	R4192	K4090	L3924	S3768	V3633	R3558
H4978	GLY	Q4691	SER	GLY	ILE	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	T4200	K4091	L3924	R3769	A3634	Q3560
E4982	GLY	P4692	ALA	ALA	LEU	ASP	ASP	ASP	LEU	ASP	ALA	LEU	ALA	E4206	D4092	S3929	L3770	C3636	F3636
H4983	GLY	Q4693	GLY	GLY	ARG	ALA	ALA	ARG	ARG	ALA	ARG	ARG	ARG	E4206	F4093	W3935	H3771	R3637	G3561
M4989	ALA	D4694	GLY	ALA	LYS	GLY	GLY	LEU	LEU	GLY	LEU	LEU	ALA	Q4209	Q4094	W3935	T3772	N3638	K3562
L4992	GLY	D4695	GLY	MET	GLY	ASP	GLY	THR	ALA	GLY	THR	THR	ALA	V4210	K4095	K3940	R3773	H3638	V3563
M4993	ASP	V4696	GLY	GLY	VAL	GLY	GLY	GLY	ALA	GLY	GLY	GLY	ALA	K4211	A4096	E3967	G3788	L3641	E3564
Y4994	GLY	L4703	ASP	W4541	ASP	ASP	ASP	SER	ALA	SER	SER	SER	ALA	E4212	M4097	E3967	G3801	L3641	G3565
L4995	GLY	V4705	GLY	G4542	GLY	GLY	GLY	GLY	ALA	GLY	GLY	GLY	ALA	V4221	D4098	L3980	G3801	M3652	S3568
I4996	ASP	L4706	ASP	E4543	GLY	VAL	VAL	PHE	ARG	ARG	GLY	ARG	GLY	E4224	Q4100	R3984	L3905	E3655	K3571
K4997	PRO	Y4715	GLY	L4544	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ARG	ARG	E4227	K4101	L3985	L3905	E3655	K3571
K4998	GLY	P4717	GLY	L4555	GLY	HIS	HIS	LEU	GLY	LEU	LEU	GLY	GLY	E4227	Q4102	V3990	N3909	A3659	L3579
E5002	GLY	Y4719	GLY	S4556	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4103	V3990	N3909	A3659	L3579
H5003	GLY	F4719	GLY	S4556	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	T4104	V3990	N3909	A3659	L3579
		V4720	GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561	GLY	VAL	VAL	VAL	LEU	LEU	VAL	LEU	LEU	E4227	Q4105	V3990	N3909	A3659	L3579
			GLY	T4561</															



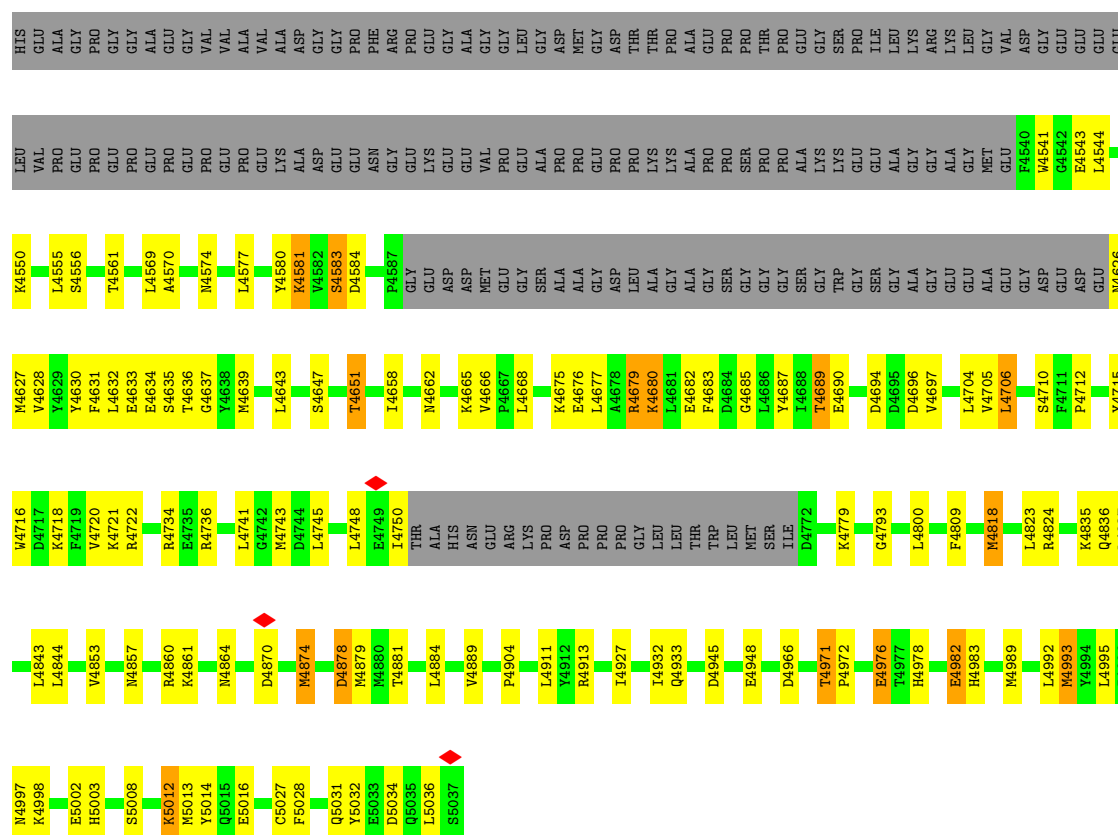
• Molecule 1: Ryanodine receptor 1



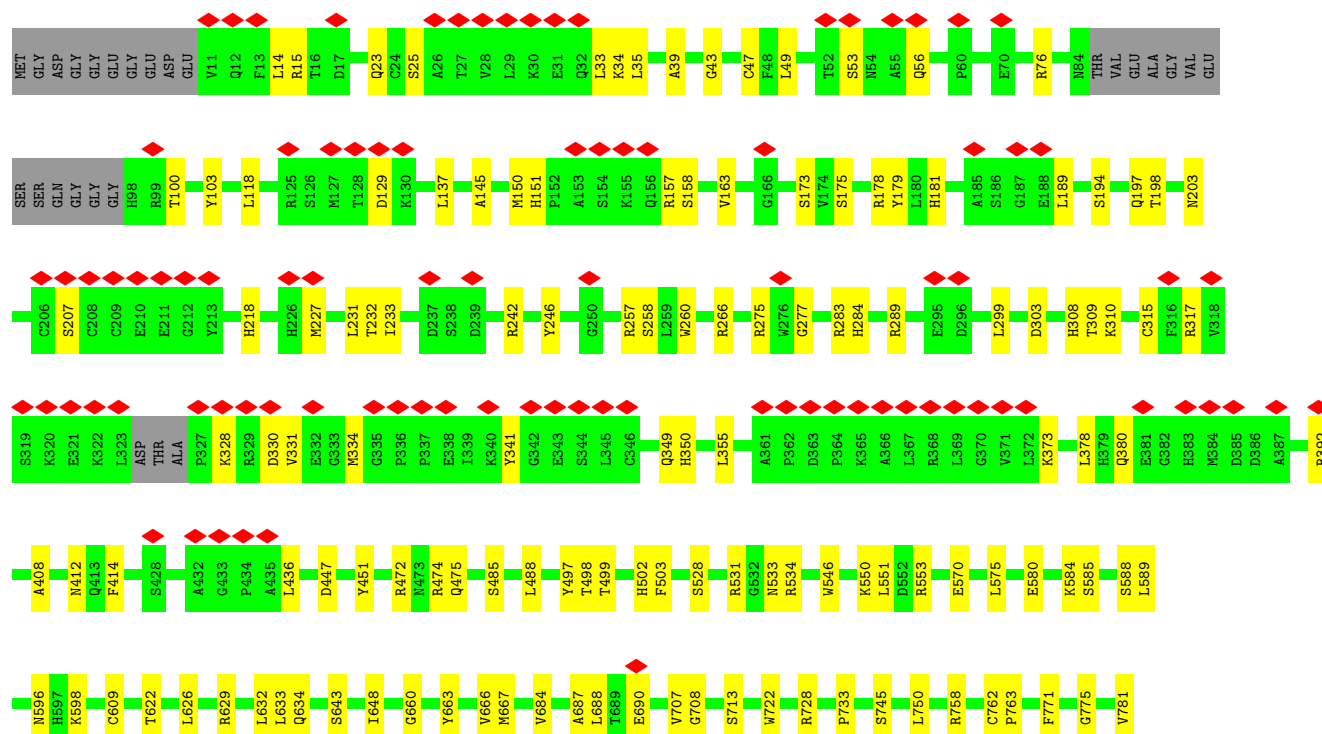


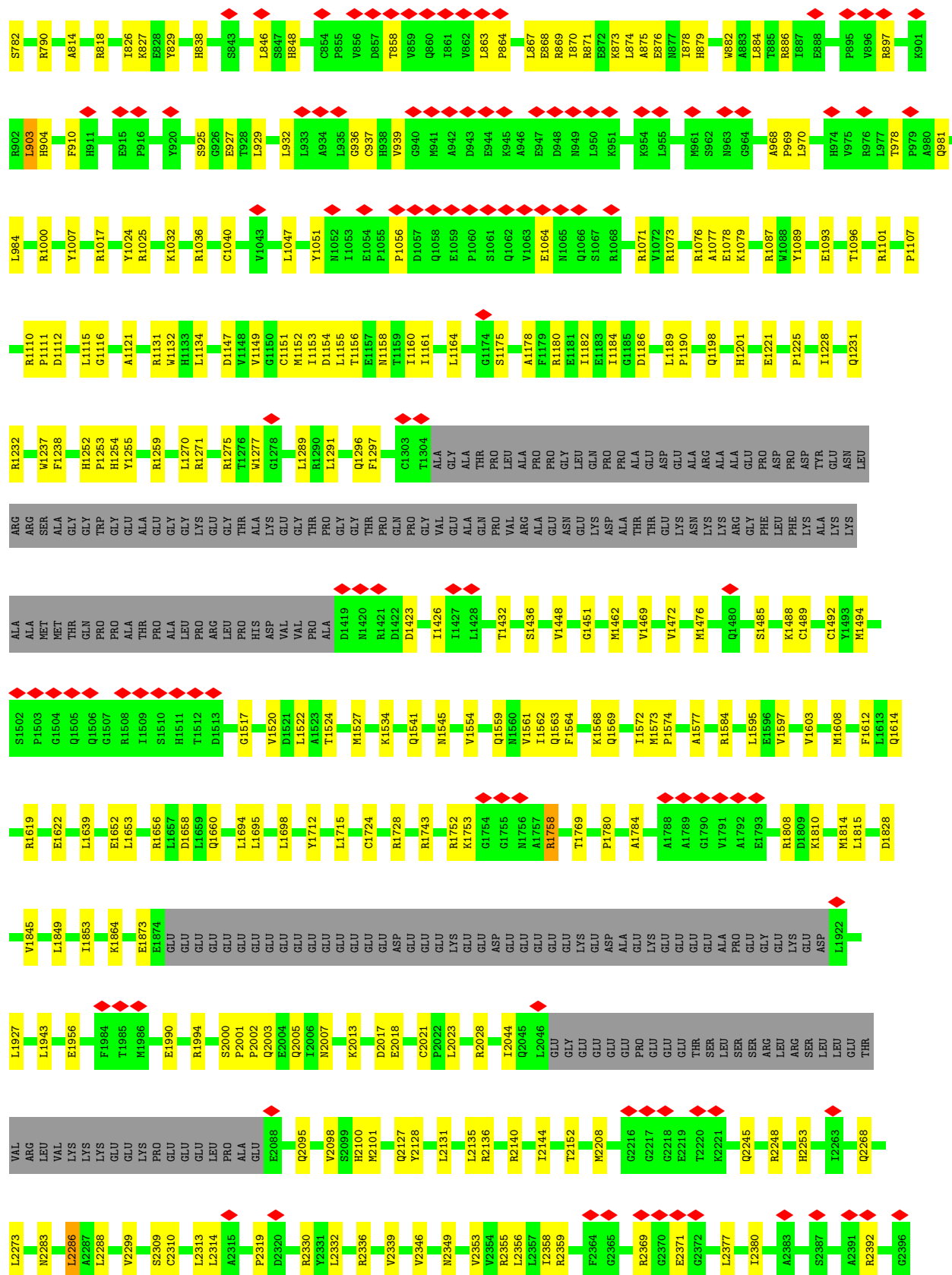




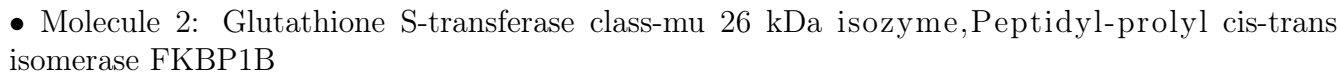


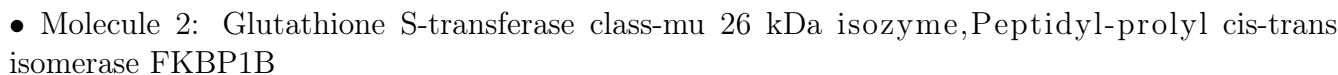
# • Molecule 1: Ryanodine receptor 1





K3571	A3385	G3026	G2934	M2874	K2814	S2753	L2841	G3525	V2397
L3579	E3386	S3027	Y2935	A2875	A2815	F2754	K2642	F2526	ARG
R3582	A3387	G3028	A2936	E2876	M2816	I2755	K2653	R2531	ARG
E3583	E3388	L3281	V2937	Q2877	L2817	N2756	Y2654	A2534	ARG
E3584	E3389	R3033	T2938	L2878	A2818	K2757	L2657	S2535	ARG
R3595	R3395	E3037	GLY	A2879	W2819	E2760	P2658	L2536	ARG
R3403	R3403	K3045	LEU	E2880	E2820	Y2761	T2659	G2537	GLU
D3404	D3404	L3046	LYS	W2881	W2821	T2762	G2659	T2538	HIS
L3405	L3405	V3183	ASP	Y2882	T2822	H2763	G2660	A2539	PHE
L3408	L3408	L3049	GLU	W2884	L2823	E2764	W2661	T2540	GLY
Y3409	Y3409	V3050	L2946	T2885	E2824	K2765	S2668	Y2553	GLU
L3413	L3413	R3051	D2947	W2886	K2825	K2766	E2669	L2561	P2410
R3414	R3414	R3052	T2948	G2887	A2826	A2767	K2677	E2412	P2411
D3417	D3417	L3056	S2949	R2888	E2828	F2768	I2682	E2413	W2414
N3418	N3418	T3059	E2952	K2889	Q2829	D2769	I2682	T2572	A2437
R3419	R3419	P3062	L2960	K2890	E2830	K2770	H2688	H2574	I2453
R3420	R3420	V3065	Q2961	Q2892	GLU	I2771	K2689	I2577	I2456
L3424	L3424	F3205	Q2962	E2893	ARG	Q2772	E2694	I2577	I2469
E3433	E3433	L3206	L2963	L2894	THR	N2773	D2716	I2583	I2469
F3435	F3435	E3207	L2964	E2895	GLU	N2774	A2717	H2584	I2479
R3436	R3436	L3210	R2965	A2896	LYS	S2776	S2720	T2588	I2474
R3437	R3437	Y3213	W2966	K2897	LYS	Y2777	S2721	R2588	I2475
R3453	R3453	N3214	M2967	G2898	THR	Q2778	S2722	S2589	I2476
E3454	E3454	A3215	S2970	G2899	LYS	E2779	A2723	S2590	L2479
N3457	N3457	R3078	I2974	G2900	ILE	N2780	E2724	R2591	G2480
F3458	F3458	L3075	Q2971	T2901	SER	D2781	K2725	L2595	K2481
V3459	V3459	S3083	E2978	H2902	THR	V2782	LYS	R2600	D2482
V3460	V3460	E3086	A2979	P2903	ALA	E2783	ALA	G2608	G2483
Q3461	Q3461	S3087	V2980	L2904	GLN	E2784	THR	C2611	A2484
N3462	N3462	V3107	S2982	V2906	ASP	K2786	ASP	I2614	F2494
R3463	R3463	G3113	S2983	P2907	PRO	T2787	ALA	R2615	K2499
I3464	I3464	K3114	G2984	Y2908	ARG	H2788	GLY	P2616	A2500
N3465	N3465	V3115	R2985	D2909	GLY	P2789	N2734	L2619	V2503
N3466	N3466	S3116	V2986	T2910	Y2855	M2790	F2735	L2622	D2507
N3467	N3467	GLN	E2987	L2911	N2856	L2791	D2736	R2625	R2508
F3468	F3468	ALA	K2988	T2912	P2857	R2792	P2737	L2626	E2513
F3469	F3469	ARG	S2989	A2913	Q2858	P2793	R2738	V2630	D2516
L3470	L3470	THR	P2990	K2914	P2859	Y2794	P2739	N2634	F2517
T3471	T3471	GLN	H2991	E2915	P2860	K2795	V2740	K2638	L2518
A3472	A3472	VAL	E2992	K2916	L2862	T2796	E2741	H2639	L2519
D3473	D3473	K3123	Q2993	A2917	L2862	F2797	T2742	P2640	L2522
S3474	S3474	Y3131	F2997	R2918	S2863	S2798	L2743	L2523	V2524
K3475	K3475	H3146	I3001	D2919	G2864	E2799	N2744		
K3476	K3476	H3149	T3020	R2920	V2865	K2800	V2745		
K3477	K3477	Q3149	P3021	E2921	T2866	D2801	I2746		
N3478	N3478	H3150	A3022	K2922	L2867	K2802	I2747		
L3479	L3479	Q3151	K3023	A2923	S2868	E2803	P2748		
LYS	LYS		V3024	Q2924	R2869	I2804	E2749		
ALA	ALA		L3025	E2925	E2870	K2750	K2751		
GLY	GLY			L2926	L2871	R2806	D2752		
ASP	ASP			L2927	Q2872	W2807			
				K2928	A2873	P2808			
				F2929		I2809			
				L2930		K2810			
				Q2931		E2811			
				N2932		S2812			
				N2933		L2813			





- Chain H:  23% 7% 69%

[illegible]

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	171805	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.602	Depositor
Minimum map value	-0.818	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.062	Depositor
Recommended contour level	0.263	Depositor
Map size (Å)	515.2, 515.2, 515.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.288, 1.288, 1.288	Depositor



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.33	0/35746	0.66	14/48409 (0.0%)
1	B	0.33	0/35746	0.66	14/48409 (0.0%)
1	C	0.33	0/35746	0.66	14/48409 (0.0%)
1	D	0.33	0/35746	0.66	14/48409 (0.0%)
2	E	0.33	0/834	0.62	0/1123
2	F	0.33	0/834	0.62	0/1123
2	G	0.33	0/834	0.62	0/1123
2	H	0.33	0/834	0.62	0/1123
All	All	0.33	0/146320	0.66	56/198128 (0.0%)

There are no bond length outliers.

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	4945	ASP	CB-CG-OD1	7.59	125.13	118.30
1	A	4945	ASP	CB-CG-OD1	7.57	125.11	118.30
1	B	4945	ASP	CB-CG-OD1	7.53	125.07	118.30
1	D	4945	ASP	CB-CG-OD1	7.51	125.06	118.30
1	D	903	LEU	CA-CB-CG	6.81	130.97	115.30
1	B	903	LEU	CA-CB-CG	6.81	130.97	115.30
1	C	903	LEU	CA-CB-CG	6.81	130.97	115.30
1	A	903	LEU	CA-CB-CG	6.78	130.89	115.30
1	C	4581	LYS	CA-CB-CG	6.52	127.75	113.40
1	A	4581	LYS	CA-CB-CG	6.52	127.75	113.40
1	B	4581	LYS	CA-CB-CG	6.52	127.75	113.40
1	D	4581	LYS	CA-CB-CG	6.51	127.72	113.40
1	C	1186	ASP	CB-CG-OD1	6.50	124.15	118.30
1	A	1186	ASP	CB-CG-OD1	6.48	124.13	118.30
1	B	1186	ASP	CB-CG-OD1	6.47	124.13	118.30
1	D	1186	ASP	CB-CG-OD1	6.43	124.09	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	227	MET	CA-CB-CG	5.97	123.45	113.30
1	B	227	MET	CA-CB-CG	5.97	123.45	113.30
1	C	227	MET	CA-CB-CG	5.96	123.43	113.30
1	A	227	MET	CA-CB-CG	5.95	123.42	113.30
1	B	2286	LEU	CA-CB-CG	5.74	128.49	115.30
1	A	2286	LEU	CA-CB-CG	5.72	128.45	115.30
1	C	2286	LEU	CA-CB-CG	5.71	128.42	115.30
1	D	2286	LEU	CA-CB-CG	5.70	128.41	115.30
1	D	3197	LEU	CA-CB-CG	5.63	128.24	115.30
1	B	3999	MET	CA-CB-CG	5.62	122.86	113.30
1	C	3999	MET	CA-CB-CG	5.62	122.86	113.30
1	A	3999	MET	CA-CB-CG	5.60	122.83	113.30
1	D	3999	MET	CA-CB-CG	5.60	122.82	113.30
1	C	3197	LEU	CA-CB-CG	5.60	128.18	115.30
1	A	3197	LEU	CA-CB-CG	5.60	128.17	115.30
1	B	3197	LEU	CA-CB-CG	5.59	128.16	115.30
1	B	4878	ASP	CB-CG-OD1	5.45	123.20	118.30
1	A	4878	ASP	CB-CG-OD1	5.45	123.20	118.30
1	D	4878	ASP	CB-CG-OD1	5.44	123.20	118.30
1	C	4878	ASP	CB-CG-OD1	5.41	123.17	118.30
1	C	3835	LEU	CA-CB-CG	5.20	127.25	115.30
1	B	3835	LEU	CA-CB-CG	5.19	127.24	115.30
1	D	3835	LEU	CA-CB-CG	5.18	127.22	115.30
1	A	3835	LEU	CA-CB-CG	5.17	127.20	115.30
1	C	3158	LEU	CA-CB-CG	5.17	127.19	115.30
1	B	3158	LEU	CA-CB-CG	5.16	127.17	115.30
1	D	3158	LEU	CA-CB-CG	5.16	127.17	115.30
1	B	3296	LEU	CA-CB-CG	5.14	127.13	115.30
1	D	3296	LEU	CA-CB-CG	5.14	127.12	115.30
1	A	3158	LEU	CA-CB-CG	5.14	127.11	115.30
1	A	3296	LEU	CA-CB-CG	5.13	127.09	115.30
1	C	3296	LEU	CA-CB-CG	5.12	127.07	115.30
1	A	2332	LEU	CB-CG-CD1	5.11	119.69	111.00
1	C	2332	LEU	CB-CG-CD1	5.11	119.69	111.00
1	D	2332	LEU	CB-CG-CD1	5.09	119.65	111.00
1	B	2332	LEU	CB-CG-CD1	5.09	119.65	111.00
1	A	3638	MET	CA-CB-CG	5.03	121.86	113.30
1	B	3638	MET	CA-CB-CG	5.03	121.84	113.30
1	C	3638	MET	CA-CB-CG	5.02	121.83	113.30
1	D	3638	MET	CA-CB-CG	5.02	121.83	113.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	34929	0	34552	426	0
1	B	34929	0	34552	434	0
1	C	34929	0	34552	436	0
1	D	34929	0	34552	442	0
2	E	818	0	824	18	0
2	F	818	0	824	20	0
2	G	818	0	824	20	0
2	H	818	0	824	18	0
3	A	27	0	12	1	0
3	B	27	0	12	1	0
3	C	27	0	12	1	0
3	D	27	0	12	1	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
All	All	143100	0	141552	1777	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 6.

All (1777) 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:2248:ARG:HB3	1:B:2286:LEU:HD11	1.72	0.71
1:B:4978:HIS:HA	1:B:4982:GLU:HG3	1.72	0.71
1:C:4978:HIS:HA	1:C:4982:GLU:HG3	1.72	0.71
1:D:2248:ARG:HB3	1:D:2286:LEU:HD11	1.72	0.71
1:A:2248:ARG:HB3	1:A:2286:LEU:HD11	1.72	0.71
1:A:4978:HIS:HA	1:A:4982:GLU:HG3	1.72	0.71
1:C:2248:ARG:HB3	1:C:2286:LEU:HD11	1.72	0.71
1:D:4978:HIS:HA	1:D:4982:GLU:HG3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ARG:HG2	1:D:3935:TRP:HB3	1.72	0.70
1:B:1520:VAL:HG12	1:B:1527:MET:HG3	1.76	0.68
1:D:1520:VAL:HG12	1:D:1527:MET:HG3	1.75	0.68
1:C:1520:VAL:HG12	1:C:1527:MET:HG3	1.76	0.68
1:A:1520:VAL:HG12	1:A:1527:MET:HG3	1.76	0.67
1:C:3935:TRP:HB3	1:D:76:ARG:HG2	1.77	0.66
1:B:3935:TRP:HB3	1:C:76:ARG:HG2	1.77	0.66
1:D:3980:LEU:HD12	1:D:3985:LEU:HD22	1.77	0.66
1:A:3454:GLU:HA	1:A:3457:ASN:HB2	1.78	0.66
1:A:3935:TRP:HB3	1:B:76:ARG:HG2	1.77	0.66
1:C:3980:LEU:HD12	1:C:3985:LEU:HD22	1.77	0.66
1:B:3454:GLU:HA	1:B:3457:ASN:HB2	1.78	0.65
1:C:3454:GLU:HA	1:C:3457:ASN:HB2	1.78	0.65
1:D:3454:GLU:HA	1:D:3457:ASN:HB2	1.78	0.65
1:B:475:GLN:NE2	1:B:528:SER:O	2.30	0.65
1:C:981:GLN:HG2	1:C:1047:LEU:HD11	1.78	0.65
1:D:981:GLN:HG2	1:D:1047:LEU:HD11	1.78	0.65
1:A:3980:LEU:HD12	1:A:3985:LEU:HD22	1.77	0.65
1:B:3980:LEU:HD12	1:B:3985:LEU:HD22	1.77	0.65
1:A:475:GLN:NE2	1:A:528:SER:O	2.30	0.65
1:D:475:GLN:NE2	1:D:528:SER:O	2.30	0.65
1:C:475:GLN:NE2	1:C:528:SER:O	2.30	0.64
1:A:34:LYS:H	1:A:53:SER:HB3	1.63	0.64
1:A:981:GLN:HG2	1:A:1047:LEU:HD11	1.78	0.64
1:C:3395:ARG:HE	1:C:3453:ARG:HH12	1.45	0.64
1:B:3395:ARG:HE	1:B:3453:ARG:HH12	1.45	0.64
1:C:1024:TYR:O	1:C:1032:LYS:NZ	2.31	0.64
1:B:34:LYS:H	1:B:53:SER:HB3	1.63	0.64
1:B:981:GLN:HG2	1:B:1047:LEU:HD11	1.78	0.64
1:B:1024:TYR:O	1:B:1032:LYS:NZ	2.31	0.64
1:C:3362:ILE:HD11	1:C:3408:LEU:HD22	1.80	0.64
1:D:3395:ARG:HE	1:D:3453:ARG:HH12	1.45	0.64
1:D:3362:ILE:HD11	1:D:3408:LEU:HD22	1.80	0.63
1:A:3362:ILE:HD11	1:A:3408:LEU:HD22	1.79	0.63
1:C:34:LYS:H	1:C:53:SER:HB3	1.63	0.63
1:D:1024:TYR:O	1:D:1032:LYS:NZ	2.31	0.63
1:B:728:ARG:NH2	1:B:1489:CYS:SG	2.72	0.63
1:B:745:SER:HB2	1:B:758:ARG:HB2	1.80	0.63
1:D:1064:GLU:O	1:D:1071:ARG:NH2	2.32	0.63
1:A:728:ARG:NH2	1:A:1489:CYS:SG	2.72	0.63
1:C:3753:PHE:HA	1:C:3756:LYS:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:745:SER:HB2	1:A:758:ARG:HB2	1.80	0.63
1:C:4878:ASP:HB3	1:C:4881:THR:HG22	1.81	0.63
1:D:1432:THR:HA	1:D:1520:VAL:O	1.99	0.63
1:B:1432:THR:HA	1:B:1520:VAL:O	1.99	0.62
1:D:745:SER:HB2	1:D:758:ARG:HB2	1.80	0.62
1:A:1024:TYR:O	1:A:1032:LYS:NZ	2.31	0.62
1:B:1078:GLU:OE2	1:B:1237:TRP:NE1	2.32	0.62
1:B:3362:ILE:HD11	1:B:3408:LEU:HD22	1.80	0.62
1:C:745:SER:HB2	1:C:758:ARG:HB2	1.80	0.62
1:C:1078:GLU:OE2	1:C:1237:TRP:NE1	2.32	0.62
1:D:1078:GLU:OE2	1:D:1237:TRP:NE1	2.32	0.62
1:B:3753:PHE:HA	1:B:3756:LYS:HB3	1.81	0.62
1:D:34:LYS:H	1:D:53:SER:HB3	1.63	0.62
1:A:1432:THR:HA	1:A:1520:VAL:O	1.99	0.62
1:A:3395:ARG:HE	1:A:3453:ARG:HH12	1.45	0.62
1:C:728:ARG:NH2	1:C:1489:CYS:SG	2.72	0.62
1:A:3875:MET:HB3	1:A:3878:ASP:HB3	1.82	0.62
1:A:4878:ASP:HB3	1:A:4881:THR:HG22	1.81	0.62
2:H:20:GLN:HG3	2:H:106:LEU:HD13	1.82	0.62
1:C:35:LEU:HD13	1:C:49:LEU:HD13	1.82	0.62
1:A:1078:GLU:OE2	1:A:1237:TRP:NE1	2.32	0.62
1:B:3659:ALA:HA	1:B:3663:LEU:HD12	1.82	0.62
1:B:3875:MET:HB3	1:B:3878:ASP:HB3	1.82	0.62
1:D:4878:ASP:HB3	1:D:4881:THR:HG22	1.81	0.62
2:G:20:GLN:HG3	2:G:106:LEU:HD13	1.82	0.62
1:A:978:THR:OG1	1:A:981:GLN:OE1	2.18	0.62
1:A:3753:PHE:HA	1:A:3756:LYS:HB3	1.81	0.62
1:B:1064:GLU:O	1:B:1071:ARG:NH2	2.32	0.62
1:B:978:THR:OG1	1:B:981:GLN:OE1	2.18	0.61
1:B:3414:ARG:O	1:B:3418:ASN:ND2	2.33	0.61
1:C:3114:LYS:HD3	1:C:3116:SER:H	1.66	0.61
1:A:580:GLU:HG3	1:A:584:LYS:HZ2	1.65	0.61
1:C:3659:ALA:HA	1:C:3663:LEU:HD12	1.82	0.61
1:D:728:ARG:NH2	1:D:1489:CYS:SG	2.72	0.61
1:A:3659:ALA:HA	1:A:3663:LEU:HD12	1.82	0.61
1:B:2018:GLU:OE1	1:B:2028:ARG:NH1	2.34	0.61
1:B:35:LEU:HD13	1:B:49:LEU:HD13	1.82	0.61
1:B:4878:ASP:HB3	1:B:4881:THR:HG22	1.81	0.61
1:C:1432:THR:HA	1:C:1520:VAL:O	1.99	0.61
1:A:3414:ARG:O	1:A:3418:ASN:ND2	2.33	0.61
1:B:1289:LEU:HD22	1:B:1562:ILE:HD11	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3680:ALA:HB2	1:B:3696:ASP:HB3	1.83	0.61
1:B:4823:LEU:HD22	1:C:4843:LEU:HD22	1.82	0.61
1:A:3842:LEU:HB2	1:A:3929:SER:HB3	1.83	0.61
1:C:3875:MET:HB3	1:C:3878:ASP:HB3	1.82	0.61
2:E:20:GLN:HG3	2:E:106:LEU:HD13	1.82	0.61
1:A:3114:LYS:HD3	1:A:3116:SER:H	1.66	0.61
1:D:3680:ALA:HB2	1:D:3696:ASP:HB3	1.83	0.61
1:A:1568:LYS:HE2	1:A:1574:PRO:HD3	1.83	0.61
1:D:3875:MET:HB3	1:D:3878:ASP:HB3	1.82	0.61
2:F:20:GLN:HG3	2:F:106:LEU:HD13	1.82	0.61
1:C:580:GLU:HG3	1:C:584:LYS:HZ2	1.65	0.61
1:C:4823:LEU:HD22	1:D:4843:LEU:HD22	1.82	0.61
1:D:2018:GLU:OE1	1:D:2028:ARG:NH1	2.33	0.61
1:D:3659:ALA:HA	1:D:3663:LEU:HD12	1.82	0.61
1:A:35:LEU:HD13	1:A:49:LEU:HD13	1.82	0.60
1:C:1064:GLU:O	1:C:1071:ARG:NH2	2.32	0.60
1:C:978:THR:OG1	1:C:981:GLN:OE1	2.18	0.60
1:C:1289:LEU:HD22	1:C:1562:ILE:HD11	1.83	0.60
1:C:2018:GLU:OE1	1:C:2028:ARG:NH1	2.34	0.60
1:D:978:THR:OG1	1:D:981:GLN:OE1	2.18	0.60
1:D:3753:PHE:HA	1:D:3756:LYS:HB3	1.81	0.60
1:D:3733:CYS:O	1:D:3766:GLN:NE2	2.34	0.60
1:D:3842:LEU:HB2	1:D:3929:SER:HB3	1.83	0.60
1:D:3114:LYS:HD3	1:D:3116:SER:H	1.65	0.60
1:B:3114:LYS:HD3	1:B:3116:SER:H	1.65	0.60
1:C:3414:ARG:O	1:C:3418:ASN:ND2	2.33	0.60
1:D:35:LEU:HD13	1:D:49:LEU:HD13	1.82	0.60
1:D:2630:VAL:HG12	1:D:2682:ILE:HD11	1.84	0.60
1:A:3680:ALA:HB2	1:A:3696:ASP:HB3	1.83	0.60
1:C:633:LEU:HD13	1:C:1639:LEU:HD21	1.83	0.60
1:D:1568:LYS:HE2	1:D:1574:PRO:HD3	1.83	0.60
1:A:2018:GLU:OE1	1:A:2028:ARG:NH1	2.33	0.60
1:A:2630:VAL:HG12	1:A:2682:ILE:HD11	1.84	0.60
1:B:3350:ARG:HE	1:B:3351:PRO:HD2	1.67	0.60
1:C:317:ARG:NH1	1:C:349:GLN:OE1	2.35	0.60
1:D:317:ARG:NH1	1:D:349:GLN:OE1	2.35	0.60
1:D:3350:ARG:HE	1:D:3351:PRO:HD2	1.67	0.60
1:A:1289:LEU:HD22	1:A:1562:ILE:HD11	1.83	0.60
1:A:3350:ARG:HE	1:A:3351:PRO:HD2	1.67	0.60
1:A:3733:CYS:O	1:A:3766:GLN:NE2	2.35	0.60
1:B:882:TRP:O	1:B:886:ARG:NH1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2630:VAL:HG12	1:C:2682:ILE:HD11	1.84	0.60
1:C:3842:LEU:HB2	1:C:3929:SER:HB3	1.83	0.60
1:A:1064:GLU:O	1:A:1071:ARG:NH2	2.32	0.60
1:B:3733:CYS:O	1:B:3766:GLN:NE2	2.35	0.60
1:C:3769:ARG:O	1:C:3773:ARG:NH1	2.35	0.60
1:A:3769:ARG:O	1:A:3773:ARG:NH1	2.35	0.60
1:C:882:TRP:O	1:C:886:ARG:NH1	2.34	0.60
1:D:882:TRP:O	1:D:886:ARG:NH1	2.34	0.60
1:B:633:LEU:HD13	1:B:1639:LEU:HD21	1.84	0.59
1:C:3350:ARG:HE	1:C:3351:PRO:HD2	1.67	0.59
1:C:3733:CYS:O	1:C:3766:GLN:NE2	2.34	0.59
1:B:3872:GLU:HG3	1:B:3874:VAL:H	1.68	0.59
1:C:3680:ALA:HB2	1:C:3696:ASP:HB3	1.83	0.59
1:D:633:LEU:HD13	1:D:1639:LEU:HD21	1.84	0.59
1:A:882:TRP:O	1:A:886:ARG:NH1	2.34	0.59
1:C:1232:ARG:NH2	1:C:1828:ASP:O	2.35	0.59
1:C:3872:GLU:HG3	1:C:3874:VAL:H	1.67	0.59
1:D:3872:GLU:HG3	1:D:3874:VAL:H	1.68	0.59
1:D:4244:GLU:HG3	1:D:4668:LEU:HD13	1.84	0.59
1:A:317:ARG:NH1	1:A:349:GLN:OE1	2.35	0.59
1:A:1545:ASN:HD21	2:E:32:ASN:HA	1.67	0.59
1:D:688:LEU:HD23	1:D:690:GLU:H	1.68	0.59
1:D:1289:LEU:HD22	1:D:1562:ILE:HD11	1.83	0.59
1:B:317:ARG:NH1	1:B:349:GLN:OE1	2.35	0.59
1:B:1175:SER:OG	1:B:1180:ARG:NH2	2.36	0.59
1:C:2310:CYS:HB3	1:C:2313:LEU:HB2	1.84	0.59
1:C:4244:GLU:HG3	1:C:4668:LEU:HD13	1.84	0.59
1:D:2000:SER:O	1:D:2005:GLN:NE2	2.31	0.59
1:A:897:ARG:HB2	1:A:903:LEU:HD11	1.85	0.59
1:B:1568:LYS:HE2	1:B:1574:PRO:HD3	1.83	0.59
1:C:4039:MET:SD	1:C:4043:GLN:NE2	2.76	0.59
1:A:2974:ILE:HD13	1:A:3049:LEU:HD12	1.85	0.59
1:A:4039:MET:SD	1:A:4043:GLN:NE2	2.76	0.59
1:B:3769:ARG:O	1:B:3773:ARG:NH1	2.35	0.59
1:D:1476:MET:HB3	1:D:1485:SER:HB2	1.85	0.59
1:D:2583:LEU:HD13	1:D:2622:LEU:HB2	1.85	0.59
1:B:1232:ARG:NH2	1:B:1828:ASP:O	2.35	0.59
1:B:2974:ILE:HD13	1:B:3049:LEU:HD12	1.85	0.59
1:C:2380:ILE:HG21	1:C:2469:ILE:HG12	1.85	0.59
1:C:2974:ILE:HD13	1:C:3049:LEU:HD12	1.85	0.59
1:D:1175:SER:OG	1:D:1180:ARG:NH2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1694:LEU:HB3	1:A:1715:LEU:HD12	1.85	0.59
1:A:2380:ILE:HG21	1:A:2469:ILE:HG12	1.85	0.59
1:A:3872:GLU:HG3	1:A:3874:VAL:H	1.67	0.59
1:D:897:ARG:HB2	1:D:903:LEU:HD11	1.85	0.59
1:D:2380:ILE:HG21	1:D:2469:ILE:HG12	1.85	0.59
1:D:3769:ARG:O	1:D:3773:ARG:NH1	2.35	0.59
1:A:4244:GLU:HG3	1:A:4668:LEU:HD13	1.84	0.59
1:B:2630:VAL:HG12	1:B:2682:ILE:HD11	1.84	0.59
1:C:4904:PRO:HB3	1:C:4913:ARG:HG2	1.85	0.59
1:D:580:GLU:HG3	1:D:584:LYS:HZ2	1.66	0.59
1:D:2974:ILE:HD13	1:D:3049:LEU:HD12	1.85	0.59
1:B:3842:LEU:HB2	1:B:3929:SER:HB3	1.83	0.58
1:B:4039:MET:SD	1:B:4043:GLN:NE2	2.76	0.58
1:B:4244:GLU:HG3	1:B:4668:LEU:HD13	1.84	0.58
1:A:2310:CYS:HB3	1:A:2313:LEU:HB2	1.84	0.58
1:B:551:LEU:HB2	1:B:589:LEU:HD21	1.85	0.58
1:B:1694:LEU:HB3	1:B:1715:LEU:HD12	1.85	0.58
1:B:2380:ILE:HG21	1:B:2469:ILE:HG12	1.85	0.58
1:C:1476:MET:HB3	1:C:1485:SER:HB2	1.85	0.58
1:C:1568:LYS:HE2	1:C:1574:PRO:HD3	1.83	0.58
1:D:1232:ARG:NH2	1:D:1828:ASP:O	2.35	0.58
1:A:551:LEU:HB2	1:A:589:LEU:HD21	1.85	0.58
1:A:2583:LEU:HD13	1:A:2622:LEU:HB2	1.84	0.58
1:B:688:LEU:HD23	1:B:690:GLU:H	1.68	0.58
1:A:1476:MET:HB3	1:A:1485:SER:HB2	1.85	0.58
1:D:355:LEU:HD22	1:D:380:GLN:HA	1.86	0.58
1:D:3414:ARG:O	1:D:3418:ASN:ND2	2.33	0.58
2:G:17:LYS:HG2	2:G:20:GLN:HE22	1.69	0.58
1:A:355:LEU:HD22	1:A:380:GLN:HA	1.86	0.58
1:B:1296:GLN:NE2	1:B:1545:ASN:OD1	2.37	0.58
1:D:4039:MET:SD	1:D:4043:GLN:NE2	2.76	0.58
1:A:1175:SER:OG	1:A:1180:ARG:NH2	2.36	0.58
1:A:2095:GLN:HA	1:A:2127:GLN:HE21	1.69	0.58
1:D:2310:CYS:HB3	1:D:2313:LEU:HB2	1.84	0.58
2:E:38:SER:O	2:E:42:ARG:NH2	2.37	0.58
2:G:38:SER:O	2:G:42:ARG:NH2	2.37	0.58
1:A:25:SER:HA	1:A:33:LEU:O	2.04	0.58
1:C:1296:GLN:NE2	1:C:1545:ASN:OD1	2.37	0.58
1:C:2978:GLU:OE2	1:C:3053:ARG:NH1	2.36	0.58
1:D:1296:GLN:NE2	1:D:1545:ASN:OD1	2.37	0.58
1:D:2095:GLN:HA	1:D:2127:GLN:HE21	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3322:ILE:O	1:D:3326:ASN:ND2	2.36	0.58
1:D:4904:PRO:HB3	1:D:4913:ARG:HG2	1.85	0.58
2:F:17:LYS:HG2	2:F:20:GLN:HE22	1.69	0.58
1:A:688:LEU:HD23	1:A:690:GLU:H	1.68	0.58
1:A:2470:ILE:HG22	1:A:2525:GLY:HA3	1.86	0.58
1:B:2583:LEU:HD13	1:B:2622:LEU:HB2	1.84	0.58
1:B:3322:ILE:O	1:B:3326:ASN:ND2	2.36	0.58
1:C:355:LEU:HD22	1:C:380:GLN:HA	1.86	0.58
1:C:688:LEU:HD23	1:C:690:GLU:H	1.67	0.58
1:C:2095:GLN:HA	1:C:2127:GLN:HE21	1.69	0.58
1:D:1694:LEU:HB3	1:D:1715:LEU:HD12	1.85	0.58
1:B:1476:MET:HB3	1:B:1485:SER:HB2	1.85	0.58
1:B:4904:PRO:HB3	1:B:4913:ARG:HG2	1.85	0.58
1:D:25:SER:HA	1:D:33:LEU:O	2.04	0.58
1:C:181:HIS:HD1	1:C:198:THR:HG1	1.51	0.58
1:C:2583:LEU:HD13	1:C:2622:LEU:HB2	1.84	0.58
1:D:551:LEU:HB2	1:D:589:LEU:HD21	1.85	0.58
1:A:886:ARG:HE	1:A:904:HIS:HB2	1.69	0.57
1:C:1694:LEU:HB3	1:C:1715:LEU:HD12	1.85	0.57
1:A:633:LEU:HD13	1:A:1639:LEU:HD21	1.84	0.57
1:A:1296:GLN:NE2	1:A:1545:ASN:OD1	2.37	0.57
1:B:23:GLN:OE1	1:B:203:ASN:ND2	2.38	0.57
1:B:1545:ASN:HD21	2:F:32:ASN:HA	1.69	0.57
1:C:25:SER:HA	1:C:33:LEU:O	2.04	0.57
1:C:886:ARG:HE	1:C:904:HIS:HB2	1.69	0.57
1:B:2310:CYS:HB3	1:B:2313:LEU:HB2	1.84	0.57
1:C:551:LEU:HB2	1:C:589:LEU:HD21	1.85	0.57
1:C:1175:SER:OG	1:C:1180:ARG:NH2	2.36	0.57
1:B:1297:PHE:HD1	1:B:1522:LEU:HA	1.70	0.57
1:B:2095:GLN:HA	1:B:2127:GLN:HE21	1.69	0.57
1:C:1545:ASN:HD21	2:G:32:ASN:HA	1.69	0.57
1:D:23:GLN:OE1	1:D:203:ASN:ND2	2.38	0.57
1:D:886:ARG:HE	1:D:904:HIS:HB2	1.69	0.57
1:D:1545:ASN:HD21	2:H:32:ASN:HA	1.69	0.57
2:H:17:LYS:HG2	2:H:20:GLN:HE22	1.69	0.57
1:B:886:ARG:HE	1:B:904:HIS:HB2	1.69	0.57
1:C:897:ARG:HB2	1:C:903:LEU:HD11	1.85	0.57
1:A:3020:THR:HG23	1:A:3023:LYS:H	1.70	0.57
1:A:3051:ARG:O	1:A:3053:ARG:NE	2.37	0.57
1:B:355:LEU:HD22	1:B:380:GLN:HA	1.86	0.57
1:B:2470:ILE:HG22	1:B:2525:GLY:HA3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1252:HIS:O	1:C:1275:ARG:NH1	2.38	0.57
2:F:38:SER:O	2:F:42:ARG:NH2	2.37	0.57
1:A:4904:PRO:HB3	1:A:4913:ARG:HG2	1.85	0.57
1:B:1712:TYR:OH	1:B:1814:MET:SD	2.63	0.57
1:C:1712:TYR:OH	1:C:1814:MET:SD	2.63	0.57
2:H:38:SER:O	2:H:42:ARG:NH2	2.37	0.57
1:A:498:THR:HA	1:A:553:ARG:HH12	1.70	0.57
1:B:897:ARG:HB2	1:B:903:LEU:HD11	1.85	0.57
1:D:1252:HIS:O	1:D:1275:ARG:NH1	2.38	0.57
1:D:3020:THR:HG23	1:D:3023:LYS:H	1.70	0.57
1:B:25:SER:HA	1:B:33:LEU:O	2.04	0.57
1:B:1252:HIS:O	1:B:1275:ARG:NH1	2.38	0.57
1:C:2470:ILE:HG22	1:C:2525:GLY:HA3	1.86	0.57
1:A:1255:TYR:O	1:A:1275:ARG:NH1	2.38	0.56
1:A:1259:ARG:NH2	1:A:1595:LEU:O	2.39	0.56
1:C:1297:PHE:HD1	1:C:1522:LEU:HA	1.70	0.56
1:C:3051:ARG:O	1:C:3053:ARG:NE	2.37	0.56
1:D:4570:ALA:O	1:D:4574:ASN:ND2	2.38	0.56
2:E:17:LYS:HG2	2:E:20:GLN:HE22	1.69	0.56
1:A:23:GLN:OE1	1:A:203:ASN:ND2	2.38	0.56
1:A:1252:HIS:O	1:A:1275:ARG:NH1	2.38	0.56
1:A:3997:ALA:HB1	1:A:4057:MET:HG2	1.86	0.56
1:A:4823:LEU:HD22	1:B:4843:LEU:HD22	1.86	0.56
1:B:498:THR:HA	1:B:553:ARG:HH12	1.70	0.56
1:B:1255:TYR:O	1:B:1275:ARG:NH1	2.38	0.56
1:B:3051:ARG:O	1:B:3053:ARG:NE	2.37	0.56
1:C:23:GLN:OE1	1:C:203:ASN:ND2	2.38	0.56
1:C:2000:SER:O	1:C:2005:GLN:NE2	2.31	0.56
1:C:3997:ALA:HB1	1:C:4057:MET:HG2	1.86	0.56
1:A:2871:LEU:HG	1:A:2927:LEU:HD11	1.88	0.56
1:B:3020:THR:HG23	1:B:3023:LYS:H	1.70	0.56
1:B:3997:ALA:HB1	1:B:4057:MET:HG2	1.86	0.56
1:C:299:LEU:HD22	1:C:378:LEU:HB2	1.88	0.56
1:C:1259:ARG:NH2	1:C:1595:LEU:O	2.39	0.56
1:C:1277:TRP:HD1	1:C:1559:GLN:HG3	1.71	0.56
1:D:355:LEU:HB2	1:D:378:LEU:HG	1.88	0.56
1:D:1259:ARG:NH2	1:D:1595:LEU:O	2.39	0.56
1:D:2871:LEU:HG	1:D:2927:LEU:HD11	1.88	0.56
2:G:40:ARG:NH2	2:G:102:GLU:OE1	2.39	0.56
1:A:355:LEU:HB2	1:A:378:LEU:HG	1.88	0.56
1:A:1297:PHE:HD1	1:A:1522:LEU:HA	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1423:ASP:HB3	1:A:1426:ILE:HB	1.87	0.56
1:A:4570:ALA:O	1:A:4574:ASN:ND2	2.38	0.56
1:B:2000:SER:O	1:B:2005:GLN:NE2	2.31	0.56
1:D:299:LEU:HD22	1:D:378:LEU:HB2	1.88	0.56
1:D:1297:PHE:HD1	1:D:1522:LEU:HA	1.70	0.56
1:D:3997:ALA:HB1	1:D:4057:MET:HG2	1.86	0.56
1:A:233:ILE:HD12	1:A:242:ARG:HB3	1.88	0.56
1:C:498:THR:HA	1:C:553:ARG:HH12	1.70	0.56
1:C:1451:GLY:HA3	1:C:1494:MET:HA	1.88	0.56
1:D:1712:TYR:OH	1:D:1814:MET:SD	2.63	0.56
1:D:2978:GLU:OE2	1:D:3053:ARG:NH1	2.36	0.56
1:D:3051:ARG:O	1:D:3053:ARG:NE	2.37	0.56
1:B:355:LEU:HB2	1:B:378:LEU:HG	1.88	0.56
1:B:2273:LEU:HD23	1:B:2330:ARG:HG2	1.88	0.56
1:C:2745:VAL:HG11	1:C:2818:ALA:HB2	1.88	0.56
1:D:2745:VAL:HG11	1:D:2818:ALA:HB2	1.88	0.56
1:B:1277:TRP:HD1	1:B:1559:GLN:HG3	1.71	0.56
1:B:1423:ASP:HB3	1:B:1426:ILE:HB	1.87	0.56
1:B:1780:PRO:O	2:F:42:ARG:NH1	2.39	0.56
1:C:1255:TYR:O	1:C:1275:ARG:NH1	2.38	0.56
1:C:3850:GLN:NE2	1:C:3872:GLU:OE1	2.39	0.56
1:A:1780:PRO:O	2:E:42:ARG:NH1	2.39	0.56
1:B:3850:GLN:NE2	1:B:3872:GLU:OE1	2.39	0.56
1:C:4570:ALA:O	1:C:4574:ASN:ND2	2.38	0.56
1:D:181:HIS:HD1	1:D:198:THR:HG1	1.54	0.56
1:D:498:THR:HA	1:D:553:ARG:HH12	1.70	0.56
1:D:1255:TYR:O	1:D:1275:ARG:NH1	2.38	0.56
1:D:1780:PRO:O	2:H:42:ARG:NH1	2.39	0.56
2:F:40:ARG:NH2	2:F:102:GLU:OE1	2.39	0.56
1:B:299:LEU:HD22	1:B:378:LEU:HB2	1.88	0.56
1:B:3752:SER:OG	1:B:3755:GLU:OE1	2.24	0.56
1:C:4172:GLU:HG3	1:C:4175:ARG:HE	1.71	0.56
1:D:1423:ASP:HB3	1:D:1426:ILE:HB	1.87	0.56
1:A:2978:GLU:OE2	1:A:3053:ARG:NH1	2.36	0.56
1:B:1451:GLY:HA3	1:B:1494:MET:HA	1.88	0.56
1:A:829:TYR:HB3	1:A:1073:ARG:HH11	1.72	0.55
1:B:2003:GLN:O	1:B:2007:ASN:ND2	2.40	0.55
1:B:4172:GLU:HG3	1:B:4175:ARG:HE	1.71	0.55
1:A:1712:TYR:OH	1:A:1814:MET:SD	2.63	0.55
1:A:3075:LEU:O	1:A:3146:HIS:NE2	2.37	0.55
1:C:829:TYR:HB3	1:C:1073:ARG:HH11	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2871:LEU:HG	1:C:2927:LEU:HD11	1.88	0.55
1:D:1277:TRP:HD1	1:D:1559:GLN:HG3	1.71	0.55
1:D:1451:GLY:HA3	1:D:1494:MET:HA	1.88	0.55
1:A:867:LEU:HD13	1:A:929:LEU:HB3	1.89	0.55
1:A:1232:ARG:NH2	1:A:1828:ASP:O	2.35	0.55
1:C:355:LEU:HB2	1:C:378:LEU:HG	1.88	0.55
1:C:1423:ASP:HB3	1:C:1426:ILE:HB	1.87	0.55
1:D:2470:ILE:HG22	1:D:2525:GLY:HA3	1.86	0.55
1:A:299:LEU:HD22	1:A:378:LEU:HB2	1.88	0.55
1:A:3752:SER:OG	1:A:3755:GLU:OE1	2.24	0.55
1:B:2871:LEU:HG	1:B:2927:LEU:HD11	1.88	0.55
1:B:4570:ALA:O	1:B:4574:ASN:ND2	2.38	0.55
1:C:233:ILE:HD12	1:C:242:ARG:HB3	1.88	0.55
1:C:1780:PRO:O	2:G:42:ARG:NH1	2.39	0.55
1:B:233:ILE:HD12	1:B:242:ARG:HB3	1.88	0.55
1:B:2745:VAL:HG11	1:B:2818:ALA:HB2	1.88	0.55
1:C:867:LEU:HD13	1:C:929:LEU:HB3	1.89	0.55
1:C:2273:LEU:HD23	1:C:2330:ARG:HG2	1.88	0.55
1:D:233:ILE:HD12	1:D:242:ARG:HB3	1.88	0.55
1:D:3850:GLN:NE2	1:D:3872:GLU:OE1	2.39	0.55
1:B:1259:ARG:NH2	1:B:1595:LEU:O	2.39	0.55
1:C:1131:ARG:NH1	1:C:1178:ALA:O	2.40	0.55
1:D:2003:GLN:O	1:D:2007:ASN:ND2	2.40	0.55
2:E:40:ARG:NH2	2:E:102:GLU:OE1	2.39	0.55
2:H:40:ARG:NH2	2:H:102:GLU:OE1	2.39	0.55
1:A:2745:VAL:HG11	1:A:2818:ALA:HB2	1.88	0.55
1:A:2788:HIS:NE2	1:A:2790:MET:SD	2.80	0.55
1:A:2788:HIS:HD2	1:A:2791:LEU:HB2	1.72	0.55
1:B:632:LEU:O	1:B:634:GLN:NE2	2.40	0.55
1:B:829:TYR:HB3	1:B:1073:ARG:HH11	1.71	0.55
1:B:2371:GLU:HG2	1:C:129:ASP:HA	1.88	0.55
1:C:632:LEU:O	1:C:634:GLN:NE2	2.40	0.55
1:D:867:LEU:HD13	1:D:929:LEU:HB3	1.89	0.55
1:D:4172:GLU:HG3	1:D:4175:ARG:HE	1.71	0.55
1:D:4864:ASN:ND2	1:D:4874:MET:SD	2.80	0.55
1:A:2611:CYS:HA	1:A:2614:ILE:HG22	1.89	0.55
1:A:4843:LEU:HD22	1:D:4823:LEU:HD22	1.89	0.55
1:C:2371:GLU:HG2	1:D:129:ASP:HA	1.88	0.55
1:C:3020:THR:HG23	1:C:3023:LYS:H	1.70	0.55
1:A:49:LEU:HD12	1:A:189:LEU:HB3	1.89	0.55
1:A:4172:GLU:HG3	1:A:4175:ARG:HE	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2788:HIS:NE2	1:C:2790:MET:SD	2.80	0.55
1:C:4864:ASN:ND2	1:C:4874:MET:SD	2.80	0.55
1:D:1131:ARG:NH1	1:D:1178:ALA:O	2.40	0.55
1:D:1561:VAL:HG12	1:D:1562:ILE:HG23	1.89	0.55
1:A:3850:GLN:NE2	1:A:3872:GLU:OE1	2.39	0.54
1:B:1152:MET:HB2	1:B:1161:ILE:HB	1.89	0.54
1:B:3846:ALA:HB1	1:B:3873:LYS:HG3	1.90	0.54
1:D:3752:SER:OG	1:D:3755:GLU:OE1	2.24	0.54
1:A:1152:MET:HB2	1:A:1161:ILE:HB	1.89	0.54
1:A:1277:TRP:HD1	1:A:1559:GLN:HG3	1.71	0.54
1:A:3322:ILE:O	1:A:3326:ASN:ND2	2.36	0.54
1:B:867:LEU:HD13	1:B:929:LEU:HB3	1.89	0.54
1:D:49:LEU:HD12	1:D:189:LEU:HB3	1.89	0.54
2:E:73:LYS:HE2	2:E:98:ILE:HG23	1.90	0.54
1:A:1451:GLY:HA3	1:A:1494:MET:HA	1.88	0.54
1:C:1152:MET:HB2	1:C:1161:ILE:HB	1.89	0.54
1:D:1653:LEU:O	1:D:1660:GLN:NE2	2.40	0.54
1:D:2273:LEU:HD23	1:D:2330:ARG:HG2	1.88	0.54
1:D:3846:ALA:HB1	1:D:3873:LYS:HG3	1.90	0.54
1:A:1131:ARG:NH1	1:A:1178:ALA:O	2.40	0.54
1:A:2003:GLN:O	1:A:2007:ASN:ND2	2.39	0.54
1:B:1653:LEU:O	1:B:1660:GLN:NE2	2.40	0.54
1:C:2003:GLN:O	1:C:2007:ASN:ND2	2.40	0.54
1:B:2788:HIS:NE2	1:B:2790:MET:SD	2.80	0.54
1:C:1561:VAL:HG12	1:C:1562:ILE:HG23	1.89	0.54
1:C:2788:HIS:HD2	1:C:2791:LEU:HB2	1.72	0.54
1:B:2611:CYS:HA	1:B:2614:ILE:HG22	1.88	0.54
1:B:3696:ASP:OD1	1:B:3696:ASP:N	2.41	0.54
1:B:4864:ASN:ND2	1:B:4874:MET:SD	2.80	0.54
1:D:632:LEU:O	1:D:634:GLN:NE2	2.40	0.54
1:C:707:VAL:HG13	1:C:713:SER:HB2	1.90	0.54
1:A:632:LEU:O	1:A:634:GLN:NE2	2.40	0.54
1:B:2978:GLU:OE2	1:B:3053:ARG:NH1	2.36	0.54
1:D:829:TYR:HB3	1:D:1073:ARG:HH11	1.71	0.54
1:D:1152:MET:HB2	1:D:1161:ILE:HB	1.90	0.54
1:D:2021:CYS:O	1:D:2028:ARG:NH2	2.41	0.54
1:D:2788:HIS:NE2	1:D:2790:MET:SD	2.80	0.54
1:D:3990:VAL:HG23	1:D:4051:SER:HB3	1.89	0.54
1:A:1561:VAL:HG12	1:A:1562:ILE:HG23	1.90	0.54
1:A:4864:ASN:ND2	1:A:4874:MET:SD	2.80	0.54
1:B:707:VAL:HG13	1:B:713:SER:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1612:PHE:O	1:B:1614:GLN:NE2	2.41	0.54
1:B:3990:VAL:HG23	1:B:4051:SER:HB3	1.89	0.54
1:C:3846:ALA:HB1	1:C:3873:LYS:HG3	1.90	0.54
1:D:1612:PHE:O	1:D:1614:GLN:NE2	2.41	0.54
2:H:73:LYS:HE2	2:H:98:ILE:HG23	1.90	0.54
1:A:3846:ALA:HB1	1:A:3873:LYS:HG3	1.90	0.54
1:B:2788:HIS:HD2	1:B:2791:LEU:HB2	1.72	0.54
1:C:3322:ILE:O	1:C:3326:ASN:ND2	2.36	0.54
1:D:23:GLN:HE21	1:D:34:LYS:HB3	1.72	0.54
1:D:4689:THR:OG1	1:D:4690:GLU:N	2.41	0.54
1:A:181:HIS:HD1	1:A:198:THR:HG1	1.53	0.53
1:B:3075:LEU:O	1:B:3146:HIS:NE2	2.37	0.53
1:D:2788:HIS:HD2	1:D:2791:LEU:HB2	1.72	0.53
1:A:2371:GLU:HG2	1:B:129:ASP:HA	1.88	0.53
1:A:2888:ARG:HD2	1:A:2891:LYS:HE3	1.90	0.53
1:B:1131:ARG:NH1	1:B:1178:ALA:O	2.40	0.53
1:C:707:VAL:HG23	1:C:782:SER:HB3	1.90	0.53
1:C:2021:CYS:O	1:C:2028:ARG:NH2	2.41	0.53
1:C:3990:VAL:HG23	1:C:4051:SER:HB3	1.89	0.53
2:F:73:LYS:HE2	2:F:98:ILE:HG23	1.90	0.53
1:A:2021:CYS:O	1:A:2028:ARG:NH2	2.41	0.53
1:A:3540:TYR:HE1	1:A:3549:VAL:HG21	1.74	0.53
1:A:4242:ILE:HG12	1:A:4993:MET:HG2	1.90	0.53
1:B:23:GLN:HE21	1:B:34:LYS:HB3	1.72	0.53
1:D:707:VAL:HG23	1:D:782:SER:HB3	1.90	0.53
1:D:4242:ILE:HG12	1:D:4993:MET:HG2	1.89	0.53
1:A:129:ASP:HA	1:D:2371:GLU:HG2	1.91	0.53
1:A:2273:LEU:HD23	1:A:2330:ARG:HG2	1.88	0.53
1:A:4689:THR:OG1	1:A:4690:GLU:N	2.41	0.53
1:C:3414:ARG:NH1	1:C:3417:ASP:OD2	2.41	0.53
1:D:3540:TYR:HE1	1:D:3549:VAL:HG21	1.74	0.53
1:C:2611:CYS:HA	1:C:2614:ILE:HG22	1.88	0.53
1:C:3075:LEU:O	1:C:3146:HIS:NE2	2.37	0.53
1:C:4242:ILE:HG12	1:C:4993:MET:HG2	1.89	0.53
1:D:2611:CYS:HA	1:D:2614:ILE:HG22	1.89	0.53
1:A:707:VAL:HG13	1:A:713:SER:HB2	1.90	0.53
1:A:2000:SER:O	1:A:2005:GLN:NE2	2.31	0.53
1:B:2021:CYS:O	1:B:2028:ARG:NH2	2.41	0.53
1:B:3540:TYR:HE1	1:B:3549:VAL:HG21	1.74	0.53
1:B:4242:ILE:HG12	1:B:4993:MET:HG2	1.89	0.53
1:C:23:GLN:HE21	1:C:34:LYS:HB3	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1612:PHE:O	1:C:1614:GLN:NE2	2.41	0.53
1:C:3540:TYR:HE1	1:C:3549:VAL:HG21	1.74	0.53
1:D:173:SER:HB3	1:D:178:ARG:H	1.73	0.53
1:A:23:GLN:HE21	1:A:34:LYS:HB3	1.72	0.53
1:B:1561:VAL:HG12	1:B:1562:ILE:HG23	1.89	0.53
1:B:2888:ARG:HD2	1:B:2891:LYS:HE3	1.90	0.53
1:B:3180:ASN:HB2	1:B:3183:VAL:HG23	1.91	0.53
1:C:173:SER:HB3	1:C:178:ARG:H	1.73	0.53
1:C:2888:ARG:HD2	1:C:2891:LYS:HE3	1.90	0.53
1:D:707:VAL:HG13	1:D:713:SER:HB2	1.89	0.53
1:B:580:GLU:HG3	1:B:584:LYS:HZ2	1.73	0.53
1:B:2867:LEU:HD21	1:B:2871:LEU:HD23	1.91	0.53
2:G:73:LYS:HE2	2:G:98:ILE:HG23	1.90	0.53
1:A:1612:PHE:O	1:A:1614:GLN:NE2	2.41	0.53
1:A:3990:VAL:HG23	1:A:4051:SER:HB3	1.89	0.53
1:B:49:LEU:HD12	1:B:189:LEU:HB3	1.89	0.53
1:C:266:ARG:NH2	1:C:331:VAL:O	2.40	0.53
1:D:2872:GLN:NE2	1:D:2924:GLN:OE1	2.42	0.53
1:A:1153:ILE:HG13	1:A:1160:ILE:HG12	1.91	0.53
1:B:173:SER:HB3	1:B:178:ARG:H	1.73	0.53
1:C:49:LEU:HD12	1:C:189:LEU:HB3	1.89	0.53
1:C:2867:LEU:HD21	1:C:2871:LEU:HD23	1.91	0.53
1:A:708:GLY:HA3	1:A:722:TRP:HB3	1.90	0.52
1:C:2971:GLN:NE2	1:C:3045:LYS:O	2.43	0.52
1:D:3414:ARG:NH1	1:D:3417:ASP:OD2	2.41	0.52
1:A:2872:GLN:NE2	1:A:2924:GLN:OE1	2.42	0.52
1:A:3414:ARG:NH1	1:A:3417:ASP:OD2	2.41	0.52
1:C:1153:ILE:HG13	1:C:1160:ILE:HG12	1.91	0.52
1:A:2971:GLN:NE2	1:A:3045:LYS:O	2.43	0.52
1:C:708:GLY:HA3	1:C:722:TRP:HB3	1.90	0.52
1:C:3078:ARG:NH2	1:C:3151:GLN:O	2.40	0.52
1:A:173:SER:HB3	1:A:178:ARG:H	1.73	0.52
1:A:3940:LYS:O	1:A:4002:LYS:NZ	2.42	0.52
1:B:4818:MET:N	1:B:4818:MET:SD	2.83	0.52
1:C:2974:ILE:HD12	1:C:3053:ARG:HH12	1.75	0.52
1:C:4818:MET:SD	1:C:4818:MET:N	2.83	0.52
1:D:3065:VAL:O	1:D:3069:HIS:ND1	2.43	0.52
1:D:3180:ASN:HB2	1:D:3183:VAL:HG23	1.91	0.52
2:G:7:ILE:HD11	2:G:73:LYS:HB2	1.92	0.52
1:A:2653:LYS:HB3	1:A:2657:LEU:HG	1.92	0.52
1:B:2971:GLN:NE2	1:B:3045:LYS:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3078:ARG:NH2	1:B:3151:GLN:O	2.41	0.52
1:C:3219:TYR:OH	1:C:3239:MET:SD	2.60	0.52
1:D:451:TYR:O	1:D:474:ARG:NH1	2.43	0.52
1:D:1112:ASP:HB3	1:D:1603:VAL:HB	1.92	0.52
2:H:7:ILE:HD11	2:H:73:LYS:HB2	1.92	0.52
1:A:3924:LEU:HD21	1:A:3984:ARG:HH21	1.75	0.52
1:C:2538:THR:HG23	1:C:2540:THR:H	1.75	0.52
1:C:2626:LEU:HD22	1:C:2640:PRO:HB3	1.92	0.52
1:C:2872:GLN:NE2	1:C:2924:GLN:OE1	2.42	0.52
1:C:3065:VAL:O	1:C:3069:HIS:ND1	2.43	0.52
1:D:708:GLY:HA3	1:D:722:TRP:HB3	1.90	0.52
1:A:707:VAL:HG23	1:A:782:SER:HB3	1.90	0.52
1:A:1652:GLU:OE2	1:A:1656:ARG:NH1	2.43	0.52
1:B:2653:LYS:HB3	1:B:2657:LEU:HG	1.92	0.52
1:C:575:LEU:HD22	1:C:609:CYS:HB3	1.92	0.52
1:A:1653:LEU:O	1:A:1660:GLN:NE2	2.40	0.52
1:B:707:VAL:HG23	1:B:782:SER:HB3	1.90	0.52
1:B:3065:VAL:O	1:B:3069:HIS:ND1	2.43	0.52
1:B:3889:GLN:HG3	1:B:3967:GLU:HG3	1.92	0.52
1:C:451:TYR:O	1:C:474:ARG:NH1	2.43	0.52
1:C:3180:ASN:HB2	1:C:3183:VAL:HG23	1.91	0.52
1:C:3889:GLN:HG3	1:C:3967:GLU:HG3	1.92	0.52
1:D:2653:LYS:HB3	1:D:2657:LEU:HG	1.92	0.52
1:D:2971:GLN:NE2	1:D:3045:LYS:O	2.42	0.52
1:A:932:LEU:HB3	1:A:937:CYS:HB3	1.92	0.52
1:A:4818:MET:N	1:A:4818:MET:SD	2.83	0.52
1:B:666:VAL:HG21	1:B:684:VAL:HG11	1.92	0.52
1:B:932:LEU:HB3	1:B:937:CYS:HB3	1.92	0.52
1:C:2653:LYS:HB3	1:C:2657:LEU:HG	1.92	0.52
1:D:3075:LEU:O	1:D:3146:HIS:NE2	2.37	0.52
1:D:3924:LEU:HD21	1:D:3984:ARG:HH21	1.75	0.52
1:A:3065:VAL:O	1:A:3069:HIS:ND1	2.43	0.52
1:B:451:TYR:O	1:B:474:ARG:NH1	2.43	0.52
1:B:708:GLY:HA3	1:B:722:TRP:HB3	1.90	0.52
1:B:1153:ILE:HG13	1:B:1160:ILE:HG12	1.91	0.52
1:B:3414:ARG:NH1	1:B:3417:ASP:OD2	2.41	0.52
1:B:4689:THR:OG1	1:B:4690:GLU:N	2.41	0.52
1:D:2595:LEU:O	1:D:2600:ARG:NH2	2.43	0.52
1:D:2888:ARG:HD2	1:D:2891:LYS:HE3	1.90	0.52
1:B:3757:GLU:OE2	1:B:4718:LYS:NZ	2.44	0.51
1:C:4689:THR:OG1	1:C:4690:GLU:N	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1652:GLU:OE2	1:D:1656:ARG:NH1	2.43	0.51
1:D:2538:THR:HG23	1:D:2540:THR:H	1.75	0.51
1:D:2867:LEU:HD21	1:D:2871:LEU:HD23	1.91	0.51
1:A:643:SER:HA	1:A:781:VAL:O	2.11	0.51
1:A:1112:ASP:HB3	1:A:1603:VAL:HB	1.92	0.51
1:B:218:HIS:HD1	1:B:341:TYR:HH	1.58	0.51
1:B:2538:THR:HG23	1:B:2540:THR:H	1.75	0.51
1:B:2626:LEU:HD22	1:B:2640:PRO:HB3	1.92	0.51
1:B:2974:ILE:HD12	1:B:3053:ARG:HH12	1.75	0.51
1:C:1652:GLU:OE2	1:C:1656:ARG:NH1	2.43	0.51
1:C:2595:LEU:O	1:C:2600:ARG:NH2	2.43	0.51
1:D:666:VAL:HG21	1:D:684:VAL:HG11	1.92	0.51
1:D:932:LEU:HB3	1:D:937:CYS:HB3	1.92	0.51
1:D:2974:ILE:HD12	1:D:3053:ARG:HH12	1.75	0.51
1:A:666:VAL:HG21	1:A:684:VAL:HG11	1.92	0.51
1:A:3180:ASN:HB2	1:A:3183:VAL:HG23	1.91	0.51
1:A:3757:GLU:OE2	1:A:4718:LYS:NZ	2.44	0.51
1:B:3924:LEU:HD21	1:B:3984:ARG:HH21	1.75	0.51
1:C:932:LEU:HB3	1:C:937:CYS:HB3	1.92	0.51
1:C:1112:ASP:HB3	1:C:1603:VAL:HB	1.92	0.51
1:D:643:SER:HA	1:D:781:VAL:O	2.11	0.51
1:D:1007:TYR:O	1:D:1017:ARG:NH2	2.43	0.51
1:D:1153:ILE:HG13	1:D:1160:ILE:HG12	1.91	0.51
1:D:2299:VAL:HG11	1:D:2356:LEU:HB3	1.93	0.51
1:D:4818:MET:N	1:D:4818:MET:SD	2.83	0.51
2:F:7:ILE:HD11	2:F:73:LYS:HB2	1.92	0.51
1:A:451:TYR:O	1:A:474:ARG:NH1	2.43	0.51
1:B:534:ARG:HD2	1:B:570:GLU:HG2	1.93	0.51
1:B:2872:GLN:NE2	1:B:2924:GLN:OE1	2.42	0.51
1:C:666:VAL:HG21	1:C:684:VAL:HG11	1.92	0.51
1:D:2591:ARG:HH12	1:D:2634:ASN:HD21	1.58	0.51
1:A:2595:LEU:O	1:A:2600:ARG:NH2	2.43	0.51
1:A:2867:LEU:HD21	1:A:2871:LEU:HD23	1.91	0.51
1:B:575:LEU:HD22	1:B:609:CYS:HB3	1.92	0.51
1:C:3157:ILE:HA	1:C:3161:VAL:HB	1.93	0.51
1:D:1238:PHE:HB3	1:D:1608:MET:HE1	1.93	0.51
1:A:231:LEU:HA	1:A:246:TYR:O	2.11	0.51
1:A:1007:TYR:O	1:A:1017:ARG:NH2	2.43	0.51
1:A:3889:GLN:HG3	1:A:3967:GLU:HG3	1.92	0.51
1:C:1116:GLY:HA3	1:C:1132:TRP:HB3	1.92	0.51
1:C:1658:ASP:N	1:C:1658:ASP:OD1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2299:VAL:HG11	1:C:2356:LEU:HB3	1.93	0.51
1:D:2626:LEU:HD22	1:D:2640:PRO:HB3	1.92	0.51
1:D:3757:GLU:OE2	1:D:4718:LYS:NZ	2.44	0.51
1:A:534:ARG:HD2	1:A:570:GLU:HG2	1.93	0.51
1:B:231:LEU:HA	1:B:246:TYR:O	2.11	0.51
1:B:1112:ASP:HB3	1:B:1603:VAL:HB	1.92	0.51
1:B:1524:THR:O	1:B:1541:GLN:NE2	2.38	0.51
1:C:3270:ILE:HA	1:C:3274:LEU:HD12	1.93	0.51
2:E:7:ILE:HD11	2:E:73:LYS:HB2	1.92	0.51
1:A:575:LEU:HD22	1:A:609:CYS:HB3	1.92	0.51
1:A:1116:GLY:HA3	1:A:1132:TRP:HB3	1.92	0.51
1:B:643:SER:HA	1:B:781:VAL:O	2.11	0.51
1:B:1652:GLU:OE2	1:B:1656:ARG:NH1	2.43	0.51
1:B:2299:VAL:HG11	1:B:2356:LEU:HB3	1.93	0.51
1:B:2948:THR:OG1	1:B:2952:GLU:OE2	2.25	0.51
1:B:3270:ILE:HA	1:B:3274:LEU:HD12	1.93	0.51
1:B:4634:GLU:OE1	1:B:4637:GLY:N	2.42	0.51
1:C:485:SER:HA	1:C:488:LEU:HD12	1.93	0.51
1:C:4068:LEU:HA	1:C:4071:ILE:HB	1.93	0.51
1:D:275:ARG:NH2	1:D:328:LYS:O	2.44	0.51
1:B:181:HIS:HD1	1:B:198:THR:HG1	1.53	0.51
1:C:1784:ALA:HA	2:G:55:VAL:HA	1.93	0.51
1:D:534:ARG:HD2	1:D:570:GLU:HG2	1.93	0.51
1:A:2974:ILE:HD12	1:A:3053:ARG:HH12	1.75	0.51
1:C:643:SER:HA	1:C:781:VAL:O	2.11	0.51
1:C:3324:VAL:HA	1:C:3327:LEU:HB2	1.93	0.51
1:D:3270:ILE:HA	1:D:3274:LEU:HD12	1.93	0.51
1:D:3324:VAL:HA	1:D:3327:LEU:HB2	1.93	0.51
1:B:3157:ILE:HA	1:B:3161:VAL:HB	1.93	0.50
1:C:231:LEU:HA	1:C:246:TYR:O	2.11	0.50
1:D:4112:LEU:O	1:D:4115:SER:OG	2.29	0.50
1:A:485:SER:HA	1:A:488:LEU:HD12	1.93	0.50
1:A:3270:ILE:HA	1:A:3274:LEU:HD12	1.93	0.50
1:B:2591:ARG:HH12	1:B:2634:ASN:HD21	1.58	0.50
1:B:3463:GLU:HA	1:B:3502:ARG:HH22	1.76	0.50
1:C:2339:VAL:HG12	1:C:2349:ASN:HB3	1.93	0.50
1:C:3757:GLU:OE2	1:C:4718:LYS:NZ	2.44	0.50
1:C:4165:GLU:HA	1:C:4168:GLU:HG2	1.93	0.50
1:D:3157:ILE:HA	1:D:3161:VAL:HB	1.93	0.50
1:A:2299:VAL:HG11	1:A:2356:LEU:HB3	1.93	0.50
1:A:2538:THR:HG23	1:A:2540:THR:H	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2591:ARG:HH12	1:A:2634:ASN:HD21	1.58	0.50
1:A:2626:LEU:HD22	1:A:2640:PRO:HB3	1.92	0.50
1:B:1116:GLY:HA3	1:B:1132:TRP:HB3	1.92	0.50
1:B:1270:LEU:HB2	1:B:1564:PHE:HB2	1.94	0.50
1:C:1007:TYR:O	1:C:1017:ARG:NH2	2.43	0.50
1:D:1658:ASP:N	1:D:1658:ASP:OD1	2.44	0.50
1:B:4165:GLU:HA	1:B:4168:GLU:HG2	1.93	0.50
1:C:534:ARG:HD2	1:C:570:GLU:HG2	1.93	0.50
1:C:758:ARG:HG2	1:C:763:PRO:HA	1.94	0.50
1:C:3634:ALA:O	1:C:3638:MET:HB2	2.11	0.50
1:D:231:LEU:HA	1:D:246:TYR:O	2.11	0.50
1:D:575:LEU:HD22	1:D:609:CYS:HB3	1.92	0.50
1:D:3634:ALA:O	1:D:3638:MET:HB2	2.11	0.50
1:A:3607:GLU:HA	1:A:3610:GLU:HG2	1.93	0.50
1:A:4165:GLU:HA	1:A:4168:GLU:HG2	1.93	0.50
1:B:2595:LEU:O	1:B:2600:ARG:NH2	2.43	0.50
1:C:275:ARG:NH2	1:C:328:LYS:O	2.44	0.50
1:C:3940:LYS:O	1:C:4002:LYS:NZ	2.42	0.50
1:D:758:ARG:HG2	1:D:763:PRO:HA	1.94	0.50
1:B:485:SER:HA	1:B:488:LEU:HD12	1.93	0.50
1:B:3607:GLU:HA	1:B:3610:GLU:HG2	1.93	0.50
1:D:218:HIS:ND1	1:D:341:TYR:OH	2.44	0.50
1:D:485:SER:HA	1:D:488:LEU:HD12	1.93	0.50
1:D:3607:GLU:HA	1:D:3610:GLU:HG2	1.93	0.50
1:D:3889:GLN:HG3	1:D:3967:GLU:HG3	1.92	0.50
1:D:4068:LEU:HA	1:D:4071:ILE:HB	1.93	0.50
1:A:758:ARG:HG2	1:A:763:PRO:HA	1.94	0.50
1:A:2716:ASP:OD1	1:A:2716:ASP:N	2.45	0.50
1:A:3157:ILE:HA	1:A:3161:VAL:HB	1.93	0.50
1:A:3634:ALA:O	1:A:3638:MET:HB2	2.11	0.50
1:B:758:ARG:HG2	1:B:763:PRO:HA	1.94	0.50
1:B:1007:TYR:O	1:B:1017:ARG:NH2	2.43	0.50
1:B:1658:ASP:OD1	1:B:1658:ASP:N	2.44	0.50
1:D:1116:GLY:HA3	1:D:1132:TRP:HB3	1.93	0.50
1:A:275:ARG:NH2	1:A:328:LYS:O	2.44	0.50
1:B:2534:ALA:HB2	1:B:2589:LEU:HG	1.94	0.50
1:B:1784:ALA:HA	2:F:55:VAL:HA	1.93	0.50
1:B:2339:VAL:HG12	1:B:2349:ASN:HB3	1.93	0.50
1:B:3634:ALA:O	1:B:3638:MET:HB2	2.11	0.50
1:C:1270:LEU:HB2	1:C:1564:PHE:HB2	1.94	0.50
1:C:2591:ARG:HH12	1:C:2634:ASN:HD21	1.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3924:LEU:HD21	1:C:3984:ARG:HH21	1.75	0.50
1:D:4165:GLU:HA	1:D:4168:GLU:HG2	1.93	0.50
1:B:275:ARG:NH2	1:B:328:LYS:O	2.44	0.49
1:C:3752:SER:OG	1:C:3755:GLU:OE1	2.24	0.49
1:C:4634:GLU:OE1	1:C:4637:GLY:N	2.42	0.49
1:D:3459:VAL:HG13	1:D:3464:ILE:HB	1.94	0.49
1:D:3463:GLU:HA	1:D:3502:ARG:HH22	1.76	0.49
1:C:2144:ILE:HG12	1:C:2152:THR:HG21	1.94	0.49
1:C:3459:VAL:HG13	1:C:3464:ILE:HB	1.94	0.49
1:D:2128:TYR:OH	1:D:3676:ASP:OD2	2.30	0.49
1:A:546:TRP:CE2	1:A:550:LYS:HE2	2.48	0.49
1:A:1808:ARG:NH1	1:A:1853:ILE:O	2.45	0.49
1:B:4112:LEU:O	1:B:4115:SER:OG	2.29	0.49
1:C:2534:ALA:HB2	1:C:2589:LEU:HG	1.94	0.49
1:C:3463:GLU:HA	1:C:3502:ARG:HH22	1.76	0.49
1:C:3607:GLU:HA	1:C:3610:GLU:HG2	1.93	0.49
1:D:1270:LEU:HB2	1:D:1564:PHE:HB2	1.94	0.49
1:D:1784:ALA:HA	2:H:55:VAL:HA	1.93	0.49
1:D:3078:ARG:NH2	1:D:3151:GLN:O	2.40	0.49
1:A:218:HIS:ND1	1:A:341:TYR:OH	2.44	0.49
1:A:2339:VAL:HG12	1:A:2349:ASN:HB3	1.93	0.49
1:A:2960:LEU:HD23	1:A:2963:LEU:HD12	1.94	0.49
1:A:3463:GLU:HA	1:A:3502:ARG:HH22	1.76	0.49
1:D:266:ARG:NH2	1:D:331:VAL:O	2.40	0.49
1:A:870:ILE:HG13	1:A:874:LEU:HD23	1.94	0.49
1:A:1658:ASP:N	1:A:1658:ASP:OD1	2.44	0.49
1:A:4068:LEU:HA	1:A:4071:ILE:HB	1.93	0.49
1:B:546:TRP:CE2	1:B:550:LYS:HE2	2.48	0.49
1:B:870:ILE:HG13	1:B:874:LEU:HD23	1.94	0.49
1:B:939:VAL:HB	1:B:1051:TYR:HB3	1.95	0.49
1:B:1864:LYS:NZ	1:B:1873:GLU:OE1	2.37	0.49
1:C:2531:ARG:HG2	1:C:2585:THR:HG21	1.94	0.49
1:C:4112:LEU:O	1:C:4115:SER:OG	2.29	0.49
1:D:939:VAL:HB	1:D:1051:TYR:HB3	1.95	0.49
1:D:2144:ILE:HG12	1:D:2152:THR:HG21	1.94	0.49
1:A:939:VAL:HB	1:A:1051:TYR:HB3	1.95	0.49
1:A:1270:LEU:HB2	1:A:1564:PHE:HB2	1.94	0.49
1:A:2519:LEU:HD13	1:A:2522:LEU:HD12	1.95	0.49
1:A:3324:VAL:HA	1:A:3327:LEU:HB2	1.93	0.49
1:B:2519:LEU:HD13	1:B:2522:LEU:HD12	1.95	0.49
1:B:3324:VAL:HA	1:B:3327:LEU:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1238:PHE:HB3	1:C:1608:MET:HE1	1.93	0.49
1:D:2531:ARG:HG2	1:D:2585:THR:HG21	1.95	0.49
1:A:2534:ALA:HB2	1:A:2589:LEU:HG	1.94	0.49
1:B:2960:LEU:HD23	1:B:2963:LEU:HD12	1.94	0.49
1:C:475:GLN:OE1	1:C:533:ASN:ND2	2.41	0.49
1:C:2960:LEU:HD23	1:C:2963:LEU:HD12	1.94	0.49
1:D:3768:SER:HA	1:D:3771:HIS:CD2	2.48	0.49
1:A:3405:LEU:O	1:A:3409:TYR:HB2	2.13	0.49
1:C:870:ILE:HG13	1:C:874:LEU:HD23	1.94	0.49
1:C:939:VAL:HB	1:C:1051:TYR:HB3	1.95	0.49
1:C:3696:ASP:OD1	1:C:3696:ASP:N	2.41	0.49
1:D:43:GLY:N	1:D:447:ASP:OD2	2.46	0.49
1:D:875:ALA:O	1:D:879:HIS:ND1	2.46	0.49
1:A:414:PHE:HE1	1:A:436:LEU:HD13	1.77	0.49
1:A:1524:THR:O	1:A:1541:GLN:NE2	2.38	0.49
1:B:2144:ILE:HG12	1:B:2152:THR:HG21	1.94	0.49
1:B:3405:LEU:O	1:B:3409:TYR:HB2	2.13	0.49
1:B:3459:VAL:HG13	1:B:3464:ILE:HB	1.94	0.49
1:C:4190:ILE:H	1:C:5031:GLN:HE22	1.61	0.49
1:C:4818:MET:O	1:C:4824:ARG:NH1	2.46	0.49
1:D:3219:TYR:OH	1:D:3239:MET:SD	2.60	0.49
1:D:3537:LYS:HG3	1:D:3604:TYR:HB2	1.95	0.49
1:D:4190:ILE:H	1:D:5031:GLN:HE22	1.61	0.49
1:A:2144:ILE:HG12	1:A:2152:THR:HG21	1.94	0.48
1:A:4818:MET:O	1:A:4824:ARG:NH1	2.46	0.48
1:B:414:PHE:HE1	1:B:436:LEU:HD13	1.77	0.48
1:B:667:MET:HB3	1:B:790:ARG:HB2	1.95	0.48
1:B:3768:SER:HA	1:B:3771:HIS:CD2	2.48	0.48
1:C:875:ALA:O	1:C:879:HIS:ND1	2.46	0.48
1:C:3768:SER:HA	1:C:3771:HIS:CD2	2.48	0.48
1:D:660:GLY:HA2	1:D:750:LEU:HB2	1.95	0.48
1:D:2339:VAL:HG12	1:D:2349:ASN:HB3	1.93	0.48
1:D:4818:MET:O	1:D:4824:ARG:NH1	2.46	0.48
1:A:43:GLY:N	1:A:447:ASP:OD2	2.46	0.48
1:A:648:ILE:HG23	1:A:814:ALA:HB3	1.95	0.48
1:A:3078:ARG:NH2	1:A:3151:GLN:O	2.41	0.48
1:B:232:THR:HG22	1:B:258:SER:HB3	1.94	0.48
1:B:875:ALA:O	1:B:879:HIS:ND1	2.46	0.48
1:C:408:ALA:O	1:C:412:ASN:HB2	2.14	0.48
1:D:232:THR:HG22	1:D:258:SER:HB3	1.94	0.48
1:D:546:TRP:CE2	1:D:550:LYS:HE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ARG:NH2	1:A:331:VAL:O	2.40	0.48
1:B:1089:TYR:HA	1:B:1151:CYS:O	2.14	0.48
1:B:3537:LYS:HG3	1:B:3604:TYR:HB2	1.95	0.48
1:C:667:MET:HB3	1:C:790:ARG:HB2	1.95	0.48
1:D:2534:ALA:HB2	1:D:2589:LEU:HG	1.94	0.48
1:D:2960:LEU:HD23	1:D:2963:LEU:HD12	1.94	0.48
1:A:1089:TYR:HA	1:A:1151:CYS:O	2.14	0.48
1:A:2013:LYS:NZ	1:A:3661:TRP:O	2.39	0.48
1:A:2531:ARG:HG2	1:A:2585:THR:HG21	1.95	0.48
1:A:3459:VAL:HG13	1:A:3464:ILE:HB	1.94	0.48
1:B:1189:LEU:HD12	1:B:1190:PRO:HD2	1.96	0.48
1:D:1089:TYR:HA	1:D:1151:CYS:O	2.14	0.48
1:D:1189:LEU:HD12	1:D:1190:PRO:HD2	1.96	0.48
1:D:3940:LYS:O	1:D:4002:LYS:NZ	2.42	0.48
1:A:232:THR:HG22	1:A:258:SER:HB3	1.94	0.48
1:B:4068:LEU:HA	1:B:4071:ILE:HB	1.93	0.48
1:C:232:THR:HG22	1:C:258:SER:HB3	1.94	0.48
1:C:4152:GLU:OE1	1:C:4192:ARG:NH1	2.47	0.48
1:D:408:ALA:O	1:D:412:ASN:HB2	2.14	0.48
1:A:3768:SER:HA	1:A:3771:HIS:CD2	2.48	0.48
1:A:4190:ILE:H	1:A:5031:GLN:HE22	1.61	0.48
1:C:56:GLN:O	1:C:309:THR:OG1	2.28	0.48
1:C:546:TRP:CE2	1:C:550:LYS:HE2	2.48	0.48
1:C:1154:ASP:OD1	1:C:1156:THR:OG1	2.28	0.48
1:C:1653:LEU:O	1:C:1660:GLN:NE2	2.40	0.48
1:C:3405:LEU:O	1:C:3409:TYR:HB2	2.13	0.48
1:D:3329:ILE:O	1:D:3403:ARG:NH2	2.42	0.48
1:A:660:GLY:HA2	1:A:750:LEU:HB2	1.95	0.48
1:A:667:MET:HB3	1:A:790:ARG:HB2	1.95	0.48
1:B:56:GLN:O	1:B:309:THR:OG1	2.28	0.48
1:B:648:ILE:HG23	1:B:814:ALA:HB3	1.95	0.48
1:B:1238:PHE:HB3	1:B:1608:MET:HE1	1.94	0.48
1:B:3817:LEU:HD13	1:B:3899:PHE:HD1	1.79	0.48
1:B:4152:GLU:OE1	1:B:4192:ARG:NH1	2.47	0.48
1:B:4190:ILE:H	1:B:5031:GLN:HE22	1.61	0.48
1:D:56:GLN:O	1:D:309:THR:OG1	2.28	0.48
1:D:648:ILE:HG23	1:D:814:ALA:HB3	1.95	0.48
1:D:3405:LEU:O	1:D:3409:TYR:HB2	2.13	0.48
1:A:1189:LEU:HD12	1:A:1190:PRO:HD2	1.96	0.48
1:A:4152:GLU:OE1	1:A:4192:ARG:NH1	2.47	0.48
1:C:2519:LEU:HD13	1:C:2522:LEU:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:875:ALA:O	1:A:879:HIS:ND1	2.46	0.48
1:A:2856:ASN:ND2	1:A:2858:GLN:OE1	2.43	0.48
1:B:179:TYR:HD2	1:B:197:GLN:HA	1.79	0.48
1:B:660:GLY:HA2	1:B:750:LEU:HB2	1.95	0.48
1:C:443:GLY:N	1:C:447:ASP:OD2	2.46	0.48
1:C:660:GLY:HA2	1:C:750:LEU:HB2	1.95	0.48
1:C:1189:LEU:HD12	1:C:1190:PRO:HD2	1.96	0.48
1:D:414:PHE:HE1	1:D:436:LEU:HD13	1.77	0.48
1:A:15:ARG:HE	1:A:100:THR:HG22	1.79	0.48
1:A:818:ARG:NH2	1:A:1025:ARG:O	2.47	0.48
1:A:2869:ARG:NH2	1:A:2870[B]:GLU:OE2	2.47	0.48
1:C:414:PHE:HE1	1:C:436:LEU:HD13	1.77	0.48
1:C:2869:ARG:NH2	1:C:2870[B]:GLU:OE2	2.47	0.48
1:D:870:ILE:HG13	1:D:874:LEU:HD23	1.94	0.48
1:D:2869:ARG:NH2	1:D:2870[B]:GLU:OE2	2.47	0.48
1:D:3788:GLY:HA2	1:D:3835:LEU:HD12	1.96	0.48
1:A:3523:ASN:OD1	1:A:3582:ARG:NH2	2.46	0.47
1:A:3537:LYS:HG3	1:A:3604:TYR:HB2	1.95	0.47
1:A:3817:LEU:HD13	1:A:3899:PHE:HD1	1.79	0.47
1:B:15:ARG:HE	1:B:100:THR:HG22	1.79	0.47
1:B:2531:ARG:HG2	1:B:2585:THR:HG21	1.94	0.47
1:B:2869:ARG:NH2	1:B:2870[B]:GLU:OE2	2.47	0.47
1:C:3788:GLY:HA2	1:C:3835:LEU:HD12	1.96	0.47
1:D:1808:ARG:NH1	1:D:1853:ILE:O	2.45	0.47
1:B:218:HIS:ND1	1:B:341:TYR:OH	2.44	0.47
1:C:1116:GLY:O	1:C:1134:LEU:N	2.47	0.47
1:D:1116:GLY:O	1:D:1134:LEU:N	2.47	0.47
1:D:2519:LEU:HD13	1:D:2522:LEU:HD12	1.95	0.47
1:A:2792:ARG:HB2	1:A:2797:PHE:HD1	1.79	0.47
1:B:1116:GLY:O	1:B:1134:LEU:N	2.47	0.47
1:B:4818:MET:O	1:B:4824:ARG:NH1	2.46	0.47
1:C:179:TYR:HD2	1:C:197:GLN:HA	1.79	0.47
1:C:2856:ASN:ND2	1:C:2858:GLN:OE1	2.43	0.47
1:D:3817:LEU:HD13	1:D:3899:PHE:HD1	1.79	0.47
1:A:299:LEU:HD13	1:A:378:LEU:HD22	1.96	0.47
1:A:1238:PHE:HB3	1:A:1608:MET:HE1	1.95	0.47
1:B:408:ALA:O	1:B:412:ASN:HB2	2.14	0.47
1:B:3940:LYS:O	1:B:4002:LYS:NZ	2.42	0.47
1:C:3046:LEU:HB3	1:C:3068:LEU:HD21	1.96	0.47
1:C:3537:LYS:HG3	1:C:3604:TYR:HB2	1.95	0.47
1:C:4583:SER:HB2	1:C:4631:PHE:HE1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:27:THR:HB	2:E:100:ASP:HB3	1.97	0.47
1:A:3548:GLU:HA	1:A:3551:GLU:HG3	1.96	0.47
1:A:3801:GLY:O	1:A:3805:LEU:HB2	2.14	0.47
1:B:3046:LEU:HB3	1:B:3068:LEU:HD21	1.97	0.47
1:B:3329:ILE:O	1:B:3403:ARG:NH2	2.42	0.47
1:B:3788:GLY:HA2	1:B:3835:LEU:HD12	1.96	0.47
1:C:1089:TYR:HA	1:C:1151:CYS:O	2.14	0.47
1:C:3801:GLY:O	1:C:3805:LEU:HB2	2.14	0.47
1:D:179:TYR:HD2	1:D:197:GLN:HA	1.79	0.47
1:D:667:MET:HB3	1:D:790:ARG:HB2	1.95	0.47
1:D:818:ARG:NH2	1:D:1025:ARG:O	2.47	0.47
1:D:3204:ALA:HB1	1:D:3207:GLU:HB2	1.97	0.47
1:D:4190:ILE:N	1:D:5031:GLN:HE22	2.12	0.47
1:A:408:ALA:O	1:A:412:ASN:HB2	2.14	0.47
1:A:1116:GLY:O	1:A:1134:LEU:N	2.47	0.47
1:A:3788:GLY:HA2	1:A:3835:LEU:HD12	1.96	0.47
1:A:4112:LEU:O	1:A:4115:SER:OG	2.29	0.47
1:A:4190:ILE:N	1:A:5031:GLN:HE22	2.12	0.47
1:A:4583:SER:HB2	1:A:4631:PHE:HE1	1.79	0.47
1:A:4634:GLU:OE1	1:A:4637:GLY:N	2.42	0.47
1:B:551:LEU:HD21	1:B:585:SER:HB3	1.97	0.47
1:C:15:ARG:HE	1:C:100:THR:HG22	1.79	0.47
1:C:818:ARG:NH2	1:C:1025:ARG:O	2.47	0.47
1:C:3809:ASN:HB3	1:C:3812:VAL:HB	1.96	0.47
1:C:3817:LEU:HD13	1:C:3899:PHE:HD1	1.79	0.47
1:C:4182:GLU:HG3	1:C:4192:ARG:HG3	1.97	0.47
1:D:15:ARG:HE	1:D:100:THR:HG22	1.79	0.47
1:D:551:LEU:HD21	1:D:585:SER:HB3	1.97	0.47
1:A:2507:ASP:HB3	1:A:2561:LEU:HD13	1.97	0.47
1:A:3062:PRO:HA	1:A:3065:VAL:HG22	1.97	0.47
1:A:4182:GLU:HG3	1:A:4192:ARG:HG3	1.97	0.47
1:B:299:LEU:HD13	1:B:378:LEU:HD22	1.96	0.47
1:B:622:THR:HA	1:B:626:LEU:HD23	1.96	0.47
1:B:818:ARG:NH2	1:B:1025:ARG:O	2.47	0.47
1:B:1076:ARG:NH1	1:B:1077:ALA:O	2.48	0.47
1:B:2740:VAL:HG21	1:B:2819:TRP:HE1	1.80	0.47
1:B:2863:SER:HB2	1:B:2924:GLN:HB3	1.96	0.47
1:B:3062:PRO:HA	1:B:3065:VAL:HG22	1.97	0.47
1:B:4679:ARG:O	1:B:4683:PHE:HB2	2.15	0.47
1:C:648:ILE:HG23	1:C:814:ALA:HB3	1.95	0.47
1:C:2948:THR:OG1	1:C:2952:GLU:OE2	2.25	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4190:ILE:N	1:C:5031:GLN:HE22	2.12	0.47
1:C:4679:ARG:O	1:C:4683:PHE:HB2	2.15	0.47
1:D:2716:ASP:OD1	1:D:2716:ASP:N	2.45	0.47
1:D:2792:ARG:HB2	1:D:2797:PHE:HD1	1.79	0.47
1:D:3548:GLU:HA	1:D:3551:GLU:HG3	1.97	0.47
1:D:4182:GLU:HG3	1:D:4192:ARG:HG3	1.97	0.47
2:H:27:THR:HB	2:H:100:ASP:HB3	1.97	0.47
1:A:551:LEU:HD21	1:A:585:SER:HB3	1.97	0.47
1:A:1864:LYS:NZ	1:A:1873:GLU:OE1	2.37	0.47
1:A:3046:LEU:HB3	1:A:3068:LEU:HD21	1.97	0.47
1:A:4853:VAL:O	1:A:4857:ASN:ND2	2.48	0.47
1:B:1927:LEU:HD13	1:B:2101:MET:HG3	1.97	0.47
1:B:2507:ASP:HB3	1:B:2561:LEU:HD13	1.97	0.47
1:B:3548:GLU:HA	1:B:3551:GLU:HG3	1.97	0.47
1:B:4011:GLU:O	1:B:4014:LYS:N	2.48	0.47
1:A:475:GLN:OE1	1:A:533:ASN:ND2	2.41	0.47
1:A:3219:TYR:OH	1:A:3239:MET:SD	2.60	0.47
1:A:4011:GLU:O	1:A:4014:LYS:N	2.48	0.47
1:B:3801:GLY:O	1:B:3805:LEU:HB2	2.15	0.47
1:B:4626:ASN:OD1	1:B:4626:ASN:N	2.48	0.47
1:C:1927:LEU:HD13	1:C:2101:MET:HG3	1.97	0.47
1:C:2128:TYR:OH	1:C:3676:ASP:OD2	2.30	0.47
1:C:2585:THR:HG22	1:C:2588:ARG:HH12	1.80	0.47
1:C:4680:LYS:HE3	1:C:4680:LYS:HB3	1.66	0.47
1:D:179:TYR:N	1:D:194:SER:O	2.48	0.47
1:D:3801:GLY:O	1:D:3805:LEU:HB2	2.14	0.47
1:A:1147:ASP:HB3	1:A:1164:LEU:HD11	1.97	0.47
1:A:2740:VAL:HG21	1:A:2819:TRP:HE1	1.80	0.47
1:B:1154:ASP:OD1	1:B:1156:THR:OG1	2.28	0.47
1:C:179:TYR:N	1:C:194:SER:O	2.48	0.47
1:C:2507:ASP:HB3	1:C:2561:LEU:HD13	1.97	0.47
1:D:1147:ASP:HB3	1:D:1164:LEU:HD11	1.97	0.47
1:D:3046:LEU:HB3	1:D:3068:LEU:HD21	1.97	0.47
1:D:3603:LEU:HA	1:D:3606:LEU:HD12	1.97	0.47
1:A:3206:LEU:HB2	1:A:3280:TYR:CZ	2.50	0.46
1:B:103:TYR:HE2	1:B:157:ARG:HG2	1.81	0.46
1:B:475:GLN:OE1	1:B:533:ASN:ND2	2.41	0.46
1:B:1769:THR:N	1:B:1956:GLU:OE2	2.48	0.46
1:B:2585:THR:HG22	1:B:2588:ARG:HH12	1.80	0.46
1:B:4190:ILE:N	1:B:5031:GLN:HE22	2.12	0.46
1:B:4583:SER:HB2	1:B:4631:PHE:HE1	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:LEU:HD13	1:C:378:LEU:HD22	1.96	0.46
1:A:2573:GLU:OE2	1:A:2615:ARG:NE	2.49	0.46
1:B:2716:ASP:OD1	1:B:2716:ASP:N	2.45	0.46
1:D:1154:ASP:OD1	1:D:1156:THR:OG1	2.28	0.46
1:D:1769:THR:N	1:D:1956:GLU:OE2	2.48	0.46
1:D:2573:GLU:OE2	1:D:2615:ARG:NE	2.49	0.46
1:D:2863:SER:HB2	1:D:2924:GLN:HB3	1.96	0.46
1:D:4011:GLU:O	1:D:4014:LYS:N	2.48	0.46
1:D:4976:GLU:H	1:D:4976:GLU:HG2	1.50	0.46
1:A:2863:SER:HB2	1:A:2924:GLN:HB3	1.96	0.46
1:A:3204:ALA:HB1	1:A:3207:GLU:HB2	1.96	0.46
1:B:14:LEU:HB2	1:B:163:VAL:HG13	1.97	0.46
1:B:1036:ARG:O	1:B:1040:CYS:HB2	2.15	0.46
1:B:1147:ASP:HB3	1:B:1164:LEU:HD11	1.97	0.46
1:C:1036:ARG:O	1:C:1040:CYS:HB2	2.15	0.46
1:C:1147:ASP:HB3	1:C:1164:LEU:HD11	1.97	0.46
1:C:2522:LEU:HD23	1:C:2526:PHE:HD2	1.80	0.46
1:C:4878:ASP:OD1	1:C:4879:MET:N	2.49	0.46
1:D:4878:ASP:OD1	1:D:4879:MET:N	2.49	0.46
1:A:179:TYR:HD2	1:A:197:GLN:HA	1.79	0.46
1:A:179:TYR:N	1:A:194:SER:O	2.48	0.46
1:A:350:HIS:HB2	1:A:378:LEU:HD21	1.98	0.46
1:A:1111:PRO:HB2	1:A:1603:VAL:HG12	1.98	0.46
1:A:1769:THR:N	1:A:1956:GLU:OE2	2.49	0.46
1:A:3592:ILE:HA	1:A:3595:ARG:HG2	1.97	0.46
1:B:2522:LEU:HD23	1:B:2526:PHE:HD2	1.80	0.46
1:B:3051:ARG:HA	1:B:3131:TYR:CZ	2.50	0.46
1:B:3523:ASN:OD1	1:B:3582:ARG:NH2	2.46	0.46
1:C:622:THR:HA	1:C:626:LEU:HD23	1.96	0.46
1:C:1769:THR:N	1:C:1956:GLU:OE2	2.48	0.46
1:D:299:LEU:HD13	1:D:378:LEU:HD22	1.96	0.46
1:D:2522:LEU:HD23	1:D:2526:PHE:HD2	1.80	0.46
2:F:27:THR:HB	2:F:100:ASP:HB3	1.97	0.46
1:A:3282:PRO:HA	1:A:3285:TRP:HB2	1.98	0.46
1:B:2792:ARG:HB2	1:B:2797:PHE:HD1	1.79	0.46
1:B:4182:GLU:HG3	1:B:4192:ARG:HG3	1.97	0.46
1:C:103:TYR:HE2	1:C:157:ARG:HG2	1.81	0.46
1:D:350:HIS:HB2	1:D:378:LEU:HD21	1.98	0.46
1:D:622:THR:HA	1:D:626:LEU:HD23	1.96	0.46
1:D:1569:GLN:HB2	1:D:1572:ILE:HD12	1.97	0.46
1:D:1927:LEU:HD13	1:D:2101:MET:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2507:ASP:HB3	1:D:2561:LEU:HD13	1.97	0.46
1:D:3206:LEU:HB2	1:D:3280:TYR:CZ	2.50	0.46
1:A:2128:TYR:OH	1:A:3676:ASP:OD2	2.30	0.46
1:A:2288:LEU:HD13	1:A:2346:VAL:HG21	1.98	0.46
1:A:2522:LEU:HD23	1:A:2526:PHE:HD2	1.80	0.46
1:A:3051:ARG:HA	1:A:3131:TYR:CZ	2.50	0.46
1:A:3603:LEU:HA	1:A:3606:LEU:HD12	1.97	0.46
1:A:4878:ASP:OD1	1:A:4879:MET:N	2.49	0.46
1:B:350:HIS:HB2	1:B:378:LEU:HD21	1.98	0.46
1:B:1808:ARG:NH1	1:B:1853:ILE:O	2.45	0.46
1:B:2013:LYS:NZ	1:B:3661:TRP:O	2.39	0.46
1:B:3282:PRO:HA	1:B:3285:TRP:HB2	1.98	0.46
1:B:3809:ASN:HB3	1:B:3812:VAL:HB	1.96	0.46
1:B:4878:ASP:OD1	1:B:4879:MET:N	2.49	0.46
1:C:1116:GLY:H	1:C:1121:ALA:HB3	1.81	0.46
1:C:3282:PRO:HA	1:C:3285:TRP:HB2	1.98	0.46
1:C:3523:ASN:OD1	1:C:3582:ARG:NH2	2.46	0.46
1:D:1111:PRO:HB2	1:D:1603:VAL:HG12	1.98	0.46
1:D:3282:PRO:HA	1:D:3285:TRP:HB2	1.98	0.46
1:D:3592:ILE:HA	1:D:3595:ARG:HG2	1.97	0.46
1:D:4583:SER:HB2	1:D:4631:PHE:HE1	1.79	0.46
1:D:4679:ARG:O	1:D:4683:PHE:HB2	2.15	0.46
1:A:622:THR:HA	1:A:626:LEU:HD23	1.96	0.46
1:B:179:TYR:N	1:B:194:SER:O	2.48	0.46
1:B:266:ARG:NH2	1:B:331:VAL:O	2.40	0.46
1:B:3206:LEU:HB2	1:B:3280:TYR:CZ	2.50	0.46
1:C:551:LEU:HD21	1:C:585:SER:HB3	1.97	0.46
1:C:1291:LEU:HB3	1:C:1595:LEU:HD11	1.98	0.46
1:C:2740:VAL:HG21	1:C:2819:TRP:HE1	1.80	0.46
1:C:2863:SER:HB2	1:C:2924:GLN:HB3	1.96	0.46
1:C:3051:ARG:HA	1:C:3131:TYR:CZ	2.50	0.46
1:C:3062:PRO:HA	1:C:3065:VAL:HG22	1.97	0.46
1:C:3204:ALA:HB1	1:C:3207:GLU:HB2	1.96	0.46
1:C:3548:GLU:HA	1:C:3551:GLU:HG3	1.97	0.46
1:C:3592:ILE:HA	1:C:3595:ARG:HG2	1.97	0.46
1:C:4063:ASP:OD1	1:C:4064:MET:N	2.49	0.46
1:D:1036:ARG:O	1:D:1040:CYS:HB2	2.15	0.46
1:D:2948:THR:OG1	1:D:2952:GLU:OE2	2.25	0.46
1:D:3062:PRO:HA	1:D:3065:VAL:HG22	1.97	0.46
1:D:3809:ASN:HB3	1:D:3812:VAL:HB	1.96	0.46
1:D:4152:GLU:OE1	1:D:4192:ARG:NH1	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4634:GLU:OE1	1:D:4637:GLY:N	2.42	0.46
1:A:14:LEU:HB2	1:A:163:VAL:HG13	1.97	0.46
1:A:103:TYR:HE2	1:A:157:ARG:HG2	1.81	0.46
1:A:3809:ASN:HB3	1:A:3812:VAL:HB	1.96	0.46
1:C:218:HIS:ND1	1:C:341:TYR:OH	2.44	0.46
1:C:350:HIS:HB2	1:C:378:LEU:HD21	1.98	0.46
1:C:1111:PRO:HB2	1:C:1603:VAL:HG12	1.98	0.46
1:C:4011:GLU:O	1:C:4014:LYS:N	2.48	0.46
1:D:585:SER:O	1:D:588:SER:OG	2.28	0.46
1:D:629:ARG:NH1	2:H:90:VAL:O	2.45	0.46
1:A:4679:ARG:O	1:A:4683:PHE:HB2	2.15	0.46
1:B:2128:TYR:OH	1:B:3676:ASP:OD2	2.30	0.46
1:B:3862:ASP:OD1	1:B:3862:ASP:N	2.49	0.46
1:C:2792:ARG:HB2	1:C:2797:PHE:HD1	1.79	0.46
1:C:3206:LEU:HB2	1:C:3280:TYR:CZ	2.50	0.46
1:C:3603:LEU:HA	1:C:3606:LEU:HD12	1.97	0.46
1:D:475:GLN:OE1	1:D:533:ASN:ND2	2.41	0.46
1:D:1093:GLU:HB3	1:D:1201:HIS:HB3	1.98	0.46
1:D:2585:THR:HG22	1:D:2588:ARG:HH12	1.80	0.46
1:D:2740:VAL:HG21	1:D:2819:TRP:HE1	1.80	0.46
1:D:3610:GLU:HG3	1:D:3611:HIS:CE1	2.51	0.46
1:D:3696:ASP:OD1	1:D:3696:ASP:N	2.41	0.46
2:G:27:THR:HB	2:G:100:ASP:HB3	1.97	0.46
1:A:868:GLU:HA	1:A:871:ARG:HB2	1.98	0.46
1:A:1927:LEU:HD13	1:A:2101:MET:HG3	1.97	0.46
1:A:2437:ALA:O	1:A:2508:ARG:NH2	2.49	0.46
1:A:4063:ASP:OD1	1:A:4064:MET:N	2.49	0.46
1:B:2437:ALA:O	1:B:2508:ARG:NH2	2.49	0.46
1:B:3610:GLU:HG3	1:B:3611:HIS:CE1	2.51	0.46
1:C:14:LEU:HB2	1:C:163:VAL:HG13	1.97	0.46
1:C:4853:VAL:O	1:C:4857:ASN:ND2	2.48	0.46
1:D:499:THR:HG23	1:D:502:HIS:H	1.81	0.46
1:D:1116:GLY:H	1:D:1121:ALA:HB3	1.81	0.46
1:D:4063:ASP:OD1	1:D:4064:MET:N	2.49	0.46
2:E:66:MET:HG2	2:E:72:ALA:HB2	1.98	0.46
2:G:66:MET:HG2	2:G:72:ALA:HB2	1.98	0.46
1:A:1036:ARG:O	1:A:1040:CYS:HB2	2.15	0.45
1:A:1569:GLN:HB2	1:A:1572:ILE:HD12	1.98	0.45
1:A:1784:ALA:HA	2:E:55:VAL:HA	1.98	0.45
1:B:2573:GLU:OE2	1:B:2615:ARG:NE	2.49	0.45
1:C:472:ARG:NH2	1:C:531:ARG:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:936:GLY:HA3	1:C:1056:PRO:HB3	1.98	0.45
1:C:2573:GLU:OE2	1:C:2615:ARG:NE	2.49	0.45
1:C:3329:ILE:O	1:C:3403:ARG:NH2	2.42	0.45
1:D:3051:ARG:HA	1:D:3131:TYR:CZ	2.50	0.45
2:F:66:MET:HG2	2:F:72:ALA:HB2	1.98	0.45
1:A:2928:LYS:HD3	1:A:2928:LYS:HA	1.79	0.45
1:A:3868:ARG:HH11	1:A:3870:ASN:HB3	1.82	0.45
1:A:4630:TYR:OH	1:B:4860:ARG:NH2	2.49	0.45
1:B:1093:GLU:HB3	1:B:1201:HIS:HB3	1.98	0.45
1:B:1116:GLY:H	1:B:1121:ALA:HB3	1.81	0.45
1:B:1291:LEU:HB3	1:B:1595:LEU:HD11	1.98	0.45
1:B:2288:LEU:HD13	1:B:2346:VAL:HG21	1.98	0.45
1:B:4983:HIS:O	3:B:5101:ADP:N6	2.50	0.45
1:C:868:GLU:HA	1:C:871:ARG:HB2	1.98	0.45
1:C:4983:HIS:O	3:C:5101:ADP:N6	2.50	0.45
1:D:868:GLU:HA	1:D:871:ARG:HB2	1.98	0.45
1:D:4626:ASN:N	1:D:4626:ASN:OD1	2.48	0.45
1:D:4853:VAL:O	1:D:4857:ASN:ND2	2.48	0.45
1:B:1569:GLN:HB2	1:B:1572:ILE:HD12	1.98	0.45
1:C:1569:GLN:HB2	1:C:1572:ILE:HD12	1.97	0.45
1:C:2437:ALA:O	1:C:2508:ARG:NH2	2.49	0.45
1:C:2928:LYS:HD3	1:C:2928:LYS:HA	1.79	0.45
1:D:1291:LEU:HB3	1:D:1595:LEU:HD11	1.98	0.45
1:A:1990:GLU:HG2	1:A:1994:ARG:HH21	1.81	0.45
1:A:2585:THR:HG22	1:A:2588:ARG:HH12	1.80	0.45
1:A:3329:ILE:O	1:A:3403:ARG:NH2	2.42	0.45
1:B:257:ARG:O	1:B:284:HIS:NE2	2.49	0.45
1:B:277:GLY:HA2	1:B:315:CYS:HB3	1.98	0.45
1:B:585:SER:O	1:B:588:SER:OG	2.28	0.45
1:B:1990:GLU:HG2	1:B:1994:ARG:HH21	1.81	0.45
1:B:3204:ALA:HB1	1:B:3207:GLU:HB2	1.96	0.45
1:D:1079:LYS:HG2	1:D:1107:PRO:HB3	1.97	0.45
1:D:1096:THR:OG1	1:D:1198:GLN:OE1	2.34	0.45
1:D:2437:ALA:O	1:D:2508:ARG:NH2	2.49	0.45
1:A:1079:LYS:HG2	1:A:1107:PRO:HB3	1.97	0.45
1:A:1116:GLY:H	1:A:1121:ALA:HB3	1.81	0.45
1:A:1291:LEU:HB3	1:A:1595:LEU:HD11	1.98	0.45
1:A:1469:VAL:HG13	1:A:1492:CYS:HB3	1.98	0.45
1:A:1753:LYS:HB3	1:A:1758:ARG:HG3	1.99	0.45
1:A:2516:ASP:OD1	1:A:2517:PHE:N	2.50	0.45
1:A:2584[B]:HIS:HE1	1:A:2625:ARG:HB2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4983:HIS:O	3:A:5101:ADP:N6	2.50	0.45
1:B:868:GLU:HA	1:B:871:ARG:HB2	1.98	0.45
1:B:1079:LYS:HG2	1:B:1107:PRO:HB3	1.97	0.45
1:C:289:ARG:HG2	1:C:303:ASP:HA	1.98	0.45
1:C:499:THR:HG23	1:C:502:HIS:H	1.81	0.45
1:C:1577:ALA:O	1:C:1584:ARG:NE	2.46	0.45
1:C:1808:ARG:NH1	1:C:1853:ILE:O	2.45	0.45
1:C:2584[B]:HIS:HE1	1:C:2625:ARG:HB2	1.82	0.45
1:C:3610:GLU:HG3	1:C:3611:HIS:CE1	2.51	0.45
1:D:1864:LYS:NZ	1:D:1873:GLU:OE1	2.37	0.45
1:D:4983:HIS:O	3:D:5101:ADP:N6	2.50	0.45
1:B:3592:ILE:HA	1:B:3595:ARG:HG2	1.97	0.45
1:C:1469:VAL:HG13	1:C:1492:CYS:HB3	1.98	0.45
1:C:1653:LEU:HD23	1:C:1660:GLN:HA	1.99	0.45
1:C:1753:LYS:HB3	1:C:1758:ARG:HG3	1.99	0.45
1:C:3157:ILE:HG22	1:C:3162:GLN:HG2	1.98	0.45
1:D:472:ARG:NH2	1:D:531:ARG:O	2.49	0.45
1:D:1076:ARG:NH1	1:D:1077:ALA:O	2.48	0.45
1:D:1990:GLU:HG2	1:D:1994:ARG:HH21	1.81	0.45
1:D:2584[B]:HIS:HE1	1:D:2625:ARG:HB2	1.82	0.45
1:A:1093:GLU:HB3	1:A:1201:HIS:HB3	1.98	0.45
1:A:3610:GLU:HG3	1:A:3611:HIS:CE1	2.51	0.45
1:B:289:ARG:HG2	1:B:303:ASP:HA	1.98	0.45
1:B:499:THR:HG23	1:B:502:HIS:H	1.81	0.45
1:B:3603:LEU:HA	1:B:3606:LEU:HD12	1.97	0.45
1:C:1943:LEU:HD13	1:C:2098:VAL:HG22	1.99	0.45
1:C:1990:GLU:HG2	1:C:1994:ARG:HH21	1.81	0.45
1:C:2288:LEU:HD13	1:C:2346:VAL:HG21	1.98	0.45
1:D:884:LEU:HB2	1:D:969:PRO:HD3	1.99	0.45
1:D:3862:ASP:OD1	1:D:3862:ASP:N	2.49	0.45
1:A:499:THR:HG23	1:A:502:HIS:H	1.81	0.45
1:A:4976:GLU:H	1:A:4976:GLU:HG2	1.49	0.45
1:B:1111:PRO:HB2	1:B:1603:VAL:HG12	1.98	0.45
1:B:1753:LYS:HB3	1:B:1758:ARG:HG3	1.99	0.45
1:C:629:ARG:NH1	2:G:90:VAL:O	2.45	0.45
1:C:863:LEU:HA	1:C:864:PRO:HD3	1.84	0.45
1:C:1093:GLU:HB3	1:C:1201:HIS:HB3	1.98	0.45
1:D:1943:LEU:HD13	1:D:2098:VAL:HG22	1.99	0.45
1:A:1577:ALA:O	1:A:1584:ARG:NE	2.46	0.45
1:A:3157:ILE:HG22	1:A:3162:GLN:HG2	1.98	0.45
1:B:3868:ARG:HH11	1:B:3870:ASN:HB3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4063:ASP:OD1	1:B:4064:MET:N	2.49	0.45
1:B:4658:ILE:HD11	1:B:4793:GLY:HA2	1.99	0.45
1:C:4626:ASN:OD1	1:C:4626:ASN:N	2.48	0.45
1:C:4976:GLU:H	1:C:4976:GLU:HG2	1.49	0.45
1:D:2516:ASP:OD1	1:D:2517:PHE:N	2.50	0.45
1:A:1228:ILE:HG12	1:D:3571:TRP:CE2	2.52	0.45
1:A:1436:SER:HA	1:A:1517:GLY:HA2	1.99	0.45
1:A:2677:LYS:HE2	1:A:2677:LYS:HB3	1.74	0.45
1:A:4626:ASN:N	1:A:4626:ASN:OD1	2.48	0.45
1:A:4721:LYS:HD3	1:A:4741:LEU:HB3	1.99	0.45
1:B:884:LEU:HB2	1:B:969:PRO:HD3	1.99	0.45
1:B:1653:LEU:HD23	1:B:1660:GLN:HA	1.99	0.45
1:B:3157:ILE:HG22	1:B:3162:GLN:HG2	1.98	0.45
1:B:4188:ARG:HE	1:B:4188:ARG:HB3	1.73	0.45
1:C:3433:GLU:OE1	1:C:3436:ARG:NH1	2.49	0.45
1:C:4721:LYS:HD3	1:C:4741:LEU:HB3	1.99	0.45
1:D:936:GLY:HA3	1:D:1056:PRO:HB3	1.98	0.45
1:D:2856:ASN:ND2	1:D:2858:GLN:OE1	2.43	0.45
1:D:3868:ARG:HH11	1:D:3870:ASN:HB3	1.82	0.45
1:D:4861:LYS:H	1:D:4861:LYS:HG2	1.53	0.45
2:G:62:GLY:HA3	2:G:74:LEU:HD21	1.99	0.45
1:A:1076:ARG:NH1	1:A:1077:ALA:O	2.48	0.44
1:A:4677:LEU:HD11	1:A:4687:TYR:HE2	1.82	0.44
1:B:43:GLY:N	1:B:447:ASP:OD2	2.46	0.44
1:B:3579:LEU:HD23	1:B:3582:ARG:HG2	1.99	0.44
1:B:4721:LYS:HD3	1:B:4741:LEU:HB3	1.99	0.44
1:C:1079:LYS:HG2	1:C:1107:PRO:HB3	1.97	0.44
1:C:4243:PHE:HD2	1:C:4668:LEU:HD12	1.83	0.44
1:D:103:TYR:HE2	1:D:157:ARG:HG2	1.81	0.44
1:D:2013:LYS:NZ	1:D:3661:TRP:O	2.39	0.44
1:A:277:GLY:HA2	1:A:315:CYS:HB3	1.98	0.44
1:B:472:ARG:NH2	1:B:531:ARG:O	2.50	0.44
1:B:1784:ALA:O	2:F:82:TYR:OH	2.36	0.44
1:B:2208:MET:SD	1:B:2253:HIS:ND1	2.91	0.44
1:D:277:GLY:HA2	1:D:315:CYS:HB3	1.98	0.44
1:D:289:ARG:HG2	1:D:303:ASP:HA	1.98	0.44
1:D:1436:SER:HA	1:D:1517:GLY:HA2	1.99	0.44
1:D:3523:ASN:OD1	1:D:3582:ARG:NH2	2.46	0.44
1:A:936:GLY:HA3	1:A:1056:PRO:HB3	1.98	0.44
1:A:1154:ASP:OD1	1:A:1156:THR:OG1	2.28	0.44
1:A:4107:GLU:O	1:A:4111:LEU:HG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4243:PHE:HD2	1:B:4668:LEU:HD12	1.83	0.44
1:B:4853:VAL:O	1:B:4857:ASN:ND2	2.48	0.44
1:C:277:GLY:HA2	1:C:315:CYS:HB3	1.98	0.44
1:C:2516:ASP:OD1	1:C:2517:PHE:N	2.50	0.44
1:C:3579:LEU:HD23	1:C:3582:ARG:HG2	1.99	0.44
1:C:3862:ASP:N	1:C:3862:ASP:OD1	2.49	0.44
1:D:3157:ILE:HG22	1:D:3162:GLN:HG2	1.98	0.44
1:C:2208:MET:SD	1:C:2253:HIS:ND1	2.91	0.44
1:D:14:LEU:HB2	1:D:163:VAL:HG13	1.97	0.44
1:D:2288:LEU:HD13	1:D:2346:VAL:HG21	1.98	0.44
1:D:4721:LYS:HD3	1:D:4741:LEU:HB3	1.99	0.44
2:E:62:GLY:HA3	2:E:74:LEU:HD21	1.99	0.44
2:H:66:MET:HG2	2:H:72:ALA:HB2	1.98	0.44
1:A:289:ARG:HG2	1:A:303:ASP:HA	1.98	0.44
1:A:472:ARG:NH2	1:A:531:ARG:O	2.50	0.44
1:A:3579:LEU:HD23	1:A:3582:ARG:HG2	1.99	0.44
1:B:936:GLY:HA3	1:B:1056:PRO:HB3	1.98	0.44
1:B:2516:ASP:OD1	1:B:2517:PHE:N	2.50	0.44
1:B:2970:SER:OG	1:B:2971:GLN:OE1	2.36	0.44
1:D:1653:LEU:HD23	1:D:1660:GLN:HA	1.99	0.44
1:D:2135:LEU:HD23	1:D:2135:LEU:HA	1.86	0.44
2:H:74:LEU:HB2	2:H:99:PHE:HB2	2.00	0.44
1:A:4658:ILE:HD11	1:A:4793:GLY:HA2	1.99	0.44
1:B:1469:VAL:HG13	1:B:1492:CYS:HB3	1.98	0.44
1:B:3433:GLU:OE1	1:B:3436:ARG:NH1	2.49	0.44
1:B:4090:LYS:HE2	1:B:4090:LYS:HB3	1.84	0.44
1:B:4861:LYS:H	1:B:4861:LYS:HG2	1.53	0.44
1:C:2616:PRO:HA	1:C:2619:LEU:HD12	2.00	0.44
1:D:1753:LYS:HB3	1:D:1758:ARG:HG3	1.99	0.44
1:D:2616:PRO:HA	1:D:2619:LEU:HD12	2.00	0.44
1:A:2891:LYS:HA	1:A:2894:LEU:HB3	2.00	0.44
1:B:1943:LEU:HD13	1:B:2098:VAL:HG22	1.99	0.44
1:C:2355:ARG:HA	1:C:2358:ILE:HG22	2.00	0.44
1:D:1469:VAL:HG13	1:D:1492:CYS:HB3	1.98	0.44
1:A:884:LEU:HB2	1:A:969:PRO:HD3	1.99	0.44
1:A:1782:PHE:O	2:E:82:TYR:OH	2.35	0.44
1:A:4243:PHE:HD2	1:A:4668:LEU:HD12	1.83	0.44
1:B:581:ASN:HA	1:B:584:LYS:HZ3	1.83	0.44
1:B:2891:LYS:HA	1:B:2894:LEU:HB3	2.00	0.44
1:B:4680:LYS:HE3	1:B:4680:LYS:HB3	1.66	0.44
1:C:1076:ARG:NH1	1:C:1077:ALA:O	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2013:LYS:NZ	1:C:3661:TRP:O	2.39	0.44
1:C:2813:LEU:HA	1:C:2816:MET:HE3	2.00	0.44
1:C:3533:ILE:HD13	1:C:3596:VAL:HG13	2.00	0.44
1:D:1577:ALA:O	1:D:1584:ARG:NE	2.46	0.44
1:D:4243:PHE:HD2	1:D:4668:LEU:HD12	1.83	0.44
2:E:74:LEU:HB2	2:E:99:PHE:HB2	2.00	0.44
1:A:585:SER:O	1:A:588:SER:OG	2.28	0.44
1:A:1943:LEU:HD13	1:A:2098:VAL:HG22	1.99	0.44
1:A:3335:MET:SD	1:A:3403:ARG:NH1	2.91	0.44
1:A:4092:ASP:HA	1:A:4095:LYS:HG2	2.00	0.44
1:A:4647:SER:O	1:A:4651:THR:OG1	2.35	0.44
1:B:1436:SER:HA	1:B:1517:GLY:HA2	1.99	0.44
1:B:2584[B]:HIS:HE1	1:B:2625:ARG:HB2	1.82	0.44
1:C:1784:ALA:O	2:G:82:TYR:OH	2.36	0.44
1:C:4107:GLU:O	1:C:4111:LEU:HG	2.18	0.44
1:D:257:ARG:O	1:D:284:HIS:NE2	2.49	0.44
1:D:2970:SER:OG	1:D:2971:GLN:OE1	2.36	0.44
1:A:56:GLN:O	1:A:309:THR:OG1	2.28	0.43
1:A:4971:THR:HG22	1:A:4972:PRO:HD2	2.00	0.43
1:B:2377:LEU:HA	1:B:2380:ILE:HG22	2.00	0.43
1:B:3194:LEU:HA	1:B:3197:LEU:HG	2.00	0.43
1:C:2377:LEU:HA	1:C:2380:ILE:HG22	2.00	0.43
1:C:3868:ARG:HH11	1:C:3870:ASN:HB3	1.82	0.43
1:C:4639:MET:O	1:C:4643:LEU:N	2.47	0.43
1:C:4647:SER:O	1:C:4651:THR:OG1	2.35	0.43
1:C:4658:ILE:HD11	1:C:4793:GLY:HA2	1.99	0.43
1:D:4647:SER:O	1:D:4651:THR:OG1	2.35	0.43
2:F:62:GLY:HA3	2:F:74:LEU:HD21	1.99	0.43
1:A:2044:ILE:HD11	1:A:2131:LEU:HD23	2.00	0.43
1:A:2911:LEU:HD13	1:A:2915:GLU:HG3	2.00	0.43
1:B:3335:MET:SD	1:B:3403:ARG:NH1	2.91	0.43
1:C:884:LEU:HB2	1:C:969:PRO:HD3	1.99	0.43
1:C:1864:LYS:NZ	1:C:1873:GLU:OE1	2.37	0.43
1:C:2891:LYS:HA	1:C:2894:LEU:HB3	2.00	0.43
1:D:2911:LEU:HD13	1:D:2915:GLU:HG3	2.00	0.43
1:D:4092:ASP:HA	1:D:4095:LYS:HG2	2.00	0.43
1:D:4107:GLU:O	1:D:4111:LEU:HG	2.18	0.43
1:D:4181:ILE:HD12	1:D:4183:ILE:HG23	2.00	0.43
1:D:4677:LEU:HD11	1:D:4687:TYR:HE2	1.82	0.43
1:D:4971:THR:HG22	1:D:4972:PRO:HD2	2.00	0.43
2:F:74:LEU:HB2	2:F:99:PHE:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:24:VAL:HG12	2:G:103:LEU:HA	2.00	0.43
1:A:1653:LEU:HD23	1:A:1660:GLN:HA	1.99	0.43
1:A:2377:LEU:HA	1:A:2380:ILE:HG22	2.00	0.43
1:B:876:GLU:HG2	1:B:910:PHE:CE2	2.53	0.43
1:B:2689:LYS:O	1:B:2993:GLN:NE2	2.51	0.43
1:B:4107:GLU:O	1:B:4111:LEU:HG	2.18	0.43
1:C:876:GLU:HG2	1:C:910:PHE:CE2	2.53	0.43
1:C:1436:SER:HA	1:C:1517:GLY:HA2	1.99	0.43
1:C:4874:MET:H	1:C:4874:MET:HG2	1.61	0.43
1:D:2208:MET:SD	1:D:2253:HIS:ND1	2.91	0.43
1:D:3579:LEU:HD23	1:D:3582:ARG:HG2	1.99	0.43
1:D:3823:LYS:HA	1:D:3823:LYS:HD3	1.78	0.43
1:D:4035:VAL:HG13	1:D:5032:TYR:HE2	1.84	0.43
2:G:74:LEU:HB2	2:G:99:PHE:HB2	2.00	0.43
1:A:257:ARG:O	1:A:284:HIS:NE2	2.49	0.43
1:A:2208:MET:SD	1:A:2253:HIS:ND1	2.91	0.43
1:A:4035:VAL:HG13	1:A:5032:TYR:HE2	1.84	0.43
1:A:4750:ILE:H	1:A:4750:ILE:HG13	1.60	0.43
1:B:260:TRP:HA	1:B:283:ARG:O	2.19	0.43
1:B:1724:CYS:SG	1:B:1728:ARG:NH1	2.92	0.43
1:B:2001:PRO:HG2	1:B:3864:THR:HB	2.01	0.43
1:B:2813:LEU:HA	1:B:2816:MET:HE3	2.00	0.43
1:B:3523:ASN:O	1:B:3582:ARG:NH2	2.51	0.43
1:B:4677:LEU:HD11	1:B:4687:TYR:HE2	1.82	0.43
1:B:4976:GLU:H	1:B:4976:GLU:HG2	1.50	0.43
1:C:2689:LYS:O	1:C:2993:GLN:NE2	2.51	0.43
1:C:3194:LEU:HA	1:C:3197:LEU:HG	2.00	0.43
1:C:4035:VAL:HG13	1:C:5032:TYR:HE2	1.84	0.43
1:D:2377:LEU:HA	1:D:2380:ILE:HG22	2.00	0.43
1:D:2638:LYS:NZ	1:D:2694:GLU:OE2	2.47	0.43
1:D:3245:VAL:HG23	1:D:3248:ARG:H	1.84	0.43
1:D:4658:ILE:HD11	1:D:4793:GLY:HA2	1.99	0.43
1:A:260:TRP:HA	1:A:283:ARG:O	2.19	0.43
1:A:1724:CYS:SG	1:A:1728:ARG:NH1	2.92	0.43
1:A:2002:PRO:HB3	1:A:3641:LEU:HD13	2.00	0.43
1:A:2377:LEU:HA	1:A:2377:LEU:HD23	1.90	0.43
1:A:2970:SER:OG	1:A:2971:GLN:OE1	2.36	0.43
1:A:3533:ILE:HD13	1:A:3596:VAL:HG13	2.00	0.43
1:B:69:LEU:HD12	1:B:69:LEU:HA	1.87	0.43
1:B:150:MET:O	1:B:151:HIS:ND1	2.52	0.43
1:B:3524:MET:HA	1:B:3582:ARG:HH22	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3533:ILE:HD13	1:B:3596:VAL:HG13	2.00	0.43
1:B:4971:THR:HG22	1:B:4972:PRO:HD2	2.00	0.43
1:C:1699:GLU:OE2	1:C:1813:ARG:NH1	2.45	0.43
1:C:1782:PHE:O	2:G:82:TYR:OH	2.30	0.43
1:C:2002:PRO:HB3	1:C:3641:LEU:HD13	2.00	0.43
1:C:2742:THR:HB	1:C:2814:LYS:HG3	2.01	0.43
1:D:260:TRP:HA	1:D:283:ARG:O	2.19	0.43
1:D:1524:THR:O	1:D:1541:GLN:NE2	2.38	0.43
1:D:3523:ASN:O	1:D:3582:ARG:NH2	2.51	0.43
1:D:3582:ARG:HD3	1:D:3582:ARG:HA	1.84	0.43
1:A:150:MET:O	1:A:151:HIS:ND1	2.52	0.43
1:A:2355:ARG:HA	1:A:2358:ILE:HG22	2.00	0.43
1:A:2742:THR:HB	1:A:2814:LYS:HG3	2.01	0.43
1:A:3523:ASN:O	1:A:3582:ARG:NH2	2.51	0.43
1:C:1724:CYS:SG	1:C:1728:ARG:NH1	2.92	0.43
1:C:2044:ILE:HD11	1:C:2131:LEU:HD23	2.00	0.43
1:C:2962:GLN:HA	1:C:2965:ARG:HG2	2.01	0.43
1:C:3524:MET:HA	1:C:3582:ARG:HH22	1.84	0.43
1:D:1724:CYS:SG	1:D:1728:ARG:NH1	2.92	0.43
1:D:4874:MET:H	1:D:4874:MET:HG2	1.61	0.43
1:A:2689:LYS:O	1:A:2993:GLN:NE2	2.51	0.43
1:A:2755:ILE:HD12	1:A:2813:LEU:HG	2.01	0.43
1:A:2963:LEU:O	1:A:2967:MET:HB2	2.19	0.43
1:B:2355:ARG:HA	1:B:2358:ILE:HG22	2.00	0.43
1:C:260:TRP:HA	1:C:283:ARG:O	2.19	0.43
1:C:3245:VAL:HG23	1:C:3248:ARG:H	1.84	0.43
1:C:3335:MET:SD	1:C:3403:ARG:NH1	2.91	0.43
1:D:1110:ARG:HE	1:D:1110:ARG:HB3	1.70	0.43
1:D:2742:THR:HB	1:D:2814:LYS:HG3	2.01	0.43
1:D:2891:LYS:HA	1:D:2894:LEU:HB3	2.00	0.43
1:D:3354:LEU:HA	1:D:3358:PHE:HD2	1.84	0.43
1:D:4639:MET:O	1:D:4643:LEU:N	2.47	0.43
1:A:2616:PRO:HA	1:A:2619:LEU:HD12	2.00	0.43
1:B:2742:THR:HB	1:B:2814:LYS:HG3	2.01	0.43
1:B:2963:LEU:O	1:B:2967:MET:HB2	2.19	0.43
1:B:3354:LEU:HA	1:B:3358:PHE:HD2	1.84	0.43
1:B:4035:VAL:HG13	1:B:5032:TYR:HE2	1.84	0.43
1:B:4639:MET:O	1:B:4643:LEU:N	2.47	0.43
1:B:4647:SER:O	1:B:4651:THR:OG1	2.35	0.43
1:C:1096:THR:OG1	1:C:1198:GLN:OE1	2.34	0.43
1:C:2001:PRO:HG2	1:C:3864:THR:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2476:ILE:HG23	1:C:2536:LEU:HD21	2.01	0.43
1:D:1784:ALA:O	2:H:82:TYR:OH	2.36	0.43
1:D:2755:ILE:HD12	1:D:2813:LEU:HG	2.01	0.43
1:D:4675:LYS:HG3	1:D:4715:TYR:CE1	2.54	0.43
1:A:876:GLU:HG2	1:A:910:PHE:CE2	2.53	0.43
1:A:1101:ARG:NH1	1:A:1115:LEU:O	2.52	0.43
1:A:1158:ASN:HB3	1:A:1182:ILE:H	1.84	0.43
1:A:3862:ASP:OD1	1:A:3862:ASP:N	2.49	0.43
1:A:4675:LYS:HG3	1:A:4715:TYR:CE1	2.54	0.43
1:B:118:LEU:HA	1:B:137:LEU:HD23	2.01	0.43
1:B:2616:PRO:HA	1:B:2619:LEU:HD12	2.00	0.43
1:C:531:ARG:NH1	1:C:562:GLU:OE2	2.52	0.43
1:C:3523:ASN:O	1:C:3582:ARG:NH2	2.51	0.43
1:C:4181:ILE:HD12	1:C:4183:ILE:HG23	2.00	0.43
1:D:873:LYS:HG2	1:D:970:LEU:HD13	2.01	0.43
1:D:2689:LYS:O	1:D:2993:GLN:NE2	2.51	0.43
2:F:24:VAL:HG12	2:F:103:LEU:HA	2.00	0.43
1:A:3354:LEU:HA	1:A:3358:PHE:HD2	1.84	0.43
1:A:4181:ILE:HD12	1:A:4183:ILE:HG23	2.00	0.43
1:B:1454:THR:OG1	1:B:1456:ASP:OD1	2.27	0.43
1:B:2044:ILE:HD11	1:B:2131:LEU:HD23	2.00	0.43
1:B:2476:ILE:HG23	1:B:2536:LEU:HD21	2.01	0.43
1:B:2911:LEU:HD13	1:B:2915:GLU:HG3	2.00	0.43
1:B:2962:GLN:HA	1:B:2965:ARG:HG2	2.01	0.43
1:D:876:GLU:HG2	1:D:910:PHE:CE2	2.53	0.43
1:D:1158:ASN:HB3	1:D:1182:ILE:H	1.84	0.43
1:D:3533:ILE:HD13	1:D:3596:VAL:HG13	2.00	0.43
2:E:20:GLN:HB2	2:E:107:GLU:HG2	2.01	0.43
2:H:24:VAL:HG12	2:H:103:LEU:HA	2.00	0.43
2:H:62:GLY:HA3	2:H:74:LEU:HD21	1.99	0.43
1:A:1000:ARG:HA	1:A:1000:ARG:HD3	1.86	0.42
1:A:3524:MET:HA	1:A:3582:ARG:HH22	1.84	0.42
1:B:157:ARG:HG3	1:B:158:SER:H	1.84	0.42
1:C:69:LEU:HD12	1:C:69:LEU:HA	1.87	0.42
1:C:873:LYS:HG2	1:C:970:LEU:HD13	2.01	0.42
1:C:1842:LEU:HD23	1:C:1842:LEU:HA	1.88	0.42
1:C:2355:ARG:O	1:C:2359:ARG:HG2	2.19	0.42
1:C:2963:LEU:O	1:C:2967:MET:HB2	2.19	0.42
1:C:3756:LYS:HG3	1:C:3760:LYS:NZ	2.34	0.42
1:D:2002:PRO:HB3	1:D:3641:LEU:HD13	2.00	0.42
1:D:2608:MET:HG3	1:D:2642:LYS:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2859:PRO:HA	1:D:2860:PRO:HD3	1.94	0.42
2:H:20:GLN:HB2	2:H:107:GLU:HG2	2.01	0.42
1:A:846:LEU:HD22	1:A:846:LEU:HA	1.92	0.42
1:A:2476:ILE:HG23	1:A:2536:LEU:HD21	2.01	0.42
1:A:3245:VAL:HG23	1:A:3248:ARG:H	1.84	0.42
1:B:2319:PRO:HG3	1:B:2392:ARG:HA	2.01	0.42
1:B:2355:ARG:O	1:B:2359:ARG:HG2	2.19	0.42
1:B:4092:ASP:HA	1:B:4095:LYS:HG2	2.00	0.42
1:C:150:MET:O	1:C:151:HIS:ND1	2.52	0.42
1:C:1271:ARG:HA	1:C:1563:GLN:HA	2.01	0.42
1:C:1454:THR:OG1	1:C:1456:ASP:OD1	2.27	0.42
1:C:2970:SER:OG	1:C:2971:GLN:OE1	2.36	0.42
1:C:3354:LEU:HA	1:C:3358:PHE:HD2	1.84	0.42
1:C:4677:LEU:HD11	1:C:4687:TYR:HE2	1.82	0.42
1:C:4971:THR:HG22	1:C:4972:PRO:HD2	2.00	0.42
1:D:3335:MET:SD	1:D:3403:ARG:NH1	2.91	0.42
1:A:2319:PRO:HG3	1:A:2392:ARG:HA	2.01	0.42
1:A:2608:MET:HG3	1:A:2642:LYS:HE3	2.01	0.42
1:A:2813:LEU:HA	1:A:2816:MET:HE3	2.00	0.42
1:A:2909:ASP:OD1	1:A:2909:ASP:N	2.52	0.42
1:B:2002:PRO:HB3	1:B:3641:LEU:HD13	2.00	0.42
1:B:2339:VAL:HG11	1:B:2353:VAL:HG11	2.01	0.42
1:B:2677:LYS:HB3	1:B:2677:LYS:HE2	1.74	0.42
1:C:257:ARG:O	1:C:284:HIS:NE2	2.49	0.42
1:C:4675:LYS:HG3	1:C:4715:TYR:CE1	2.54	0.42
1:D:39:ALA:HB2	1:D:47:CYS:HA	2.02	0.42
1:D:1231[B]:GLN:H	1:D:1231[B]:GLN:HG3	1.44	0.42
1:D:1253:PRO:HG2	1:D:1254:HIS:CD2	2.54	0.42
1:D:2813:LEU:HA	1:D:2816:MET:HE3	2.00	0.42
1:A:873:LYS:HG2	1:A:970:LEU:HD13	2.01	0.42
1:A:2001:PRO:HG2	1:A:3864:THR:HB	2.01	0.42
1:A:2962:GLN:HA	1:A:2965:ARG:HG2	2.01	0.42
1:B:145:ALA:HA	1:B:175:SER:HB3	2.02	0.42
1:B:873:LYS:HG2	1:B:970:LEU:HD13	2.01	0.42
1:B:1815:LEU:HD22	1:B:1845:VAL:HG21	2.02	0.42
1:B:3756:LYS:HG3	1:B:3760:LYS:NZ	2.35	0.42
1:C:1253:PRO:HG2	1:C:1254:HIS:CD2	2.54	0.42
1:C:2339:VAL:HG11	1:C:2353:VAL:HG11	2.01	0.42
1:C:2755:ILE:HD12	1:C:2813:LEU:HG	2.01	0.42
1:C:2911:LEU:HD13	1:C:2915:GLU:HG3	2.00	0.42
1:D:150:MET:O	1:D:151:HIS:ND1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2355:ARG:HA	1:D:2358:ILE:HG22	2.00	0.42
1:D:3524:MET:HA	1:D:3582:ARG:HH22	1.84	0.42
1:A:157:ARG:HG3	1:A:158:SER:H	1.84	0.42
1:A:596:ASN:HD21	1:A:598:LYS:HE2	1.85	0.42
1:A:863:LEU:HA	1:A:864:PRO:HD3	1.84	0.42
1:A:3756:LYS:HG3	1:A:3760:LYS:NZ	2.35	0.42
1:B:1158:ASN:HB3	1:B:1182:ILE:H	1.84	0.42
1:B:2755:ILE:HD12	1:B:2813:LEU:HG	2.01	0.42
1:B:2997:PHE:O	1:B:3001:ILE:HB	2.19	0.42
1:B:3245:VAL:HG23	1:B:3248:ARG:H	1.84	0.42
1:B:4685:GLY:HA3	1:B:4689:THR:HG23	2.01	0.42
1:C:1158:ASN:HB3	1:C:1182:ILE:H	1.84	0.42
1:D:771:PHE:HB3	1:D:1472:VAL:HG23	2.02	0.42
1:D:1619:ARG:NH2	1:D:1622:GLU:OE1	2.53	0.42
1:D:2963:LEU:O	1:D:2967:MET:HB2	2.19	0.42
1:D:3852:LYS:HE3	1:D:3852:LYS:HB3	1.97	0.42
1:A:1619:ARG:NH2	1:A:1622:GLU:OE1	2.53	0.42
1:A:1815:LEU:HD22	1:A:1845:VAL:HG21	2.02	0.42
1:A:1842:LEU:HD23	1:A:1842:LEU:HA	1.88	0.42
1:A:2309:SER:HB2	1:A:2314:LEU:HD11	2.02	0.42
1:A:3194:LEU:HA	1:A:3197:LEU:HG	2.00	0.42
1:A:4138:ASP:O	1:A:4142:ASN:ND2	2.34	0.42
1:B:1253:PRO:HG2	1:B:1254:HIS:CD2	2.54	0.42
1:B:2765:LYS:HD3	1:B:2765:LYS:HA	1.81	0.42
1:B:3219:TYR:OH	1:B:3239:MET:SD	2.60	0.42
1:C:2725:LYS:HZ3	1:C:2738:ARG:HH22	1.68	0.42
1:C:3007:ASN:O	1:C:3011:THR:OG1	2.27	0.42
1:C:4092:ASP:HA	1:C:4095:LYS:HG2	2.00	0.42
1:D:2001:PRO:HG2	1:D:3864:THR:HB	2.00	0.42
1:D:2453:ILE:HD13	1:D:2456:ILE:HD12	2.02	0.42
1:D:3046:LEU:O	1:D:3049:LEU:HB3	2.20	0.42
1:D:3756:LYS:HG3	1:D:3760:LYS:NZ	2.34	0.42
2:E:24:VAL:HG12	2:E:103:LEU:HA	2.00	0.42
1:A:2017:ASP:N	1:A:2017:ASP:OD1	2.53	0.42
1:A:2948:THR:OG1	1:A:2952:GLU:OE2	2.25	0.42
1:A:4685:GLY:HA3	1:A:4689:THR:HG23	2.01	0.42
1:B:1271:ARG:HA	1:B:1563:GLN:HA	2.01	0.42
1:B:2909:ASP:N	1:B:2909:ASP:OD1	2.52	0.42
1:B:4181:ILE:HD12	1:B:4183:ILE:HG23	2.00	0.42
1:B:4675:LYS:HG3	1:B:4715:TYR:CE1	2.54	0.42
1:C:492:ASP:OD1	1:C:546:TRP:NE1	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:775:GLY:H	1:C:848:HIS:CE1	2.38	0.42
1:C:1101:ARG:NH1	1:C:1115:LEU:O	2.52	0.42
1:C:1231[B]:GLN:H	1:C:1231[B]:GLN:HG3	1.44	0.42
1:C:1289:LEU:HD23	1:C:1597:VAL:HG11	2.01	0.42
1:C:2017:ASP:OD1	1:C:2017:ASP:N	2.53	0.42
1:C:3582:ARG:HD3	1:C:3582:ARG:HA	1.84	0.42
1:D:1000:ARG:HA	1:D:1000:ARG:HD3	1.85	0.42
1:D:1101:ARG:NH1	1:D:1115:LEU:O	2.52	0.42
1:D:1289:LEU:HD23	1:D:1597:VAL:HG11	2.01	0.42
1:D:2319:PRO:HG3	1:D:2392:ARG:HA	2.01	0.42
1:D:3194:LEU:HA	1:D:3197:LEU:HG	2.00	0.42
1:A:2453:ILE:HD13	1:A:2456:ILE:HD12	2.02	0.42
1:A:2997:PHE:O	1:A:3001:ILE:HB	2.19	0.42
1:B:1101:ARG:NH1	1:B:1115:LEU:O	2.52	0.42
1:B:1110:ARG:HE	1:B:1110:ARG:HB3	1.70	0.42
1:B:2309:SER:HB2	1:B:2314:LEU:HD11	2.02	0.42
1:B:2453:ILE:HD13	1:B:2456:ILE:HD12	2.02	0.42
1:B:2614:ILE:O	1:B:2650:ARG:NH2	2.43	0.42
1:C:771:PHE:HB3	1:C:1472:VAL:HG23	2.02	0.42
1:C:3046:LEU:O	1:C:3049:LEU:HB3	2.20	0.42
1:D:1815:LEU:HD22	1:D:1845:VAL:HG21	2.02	0.42
1:D:2017:ASP:OD1	1:D:2017:ASP:N	2.53	0.42
1:A:145:ALA:HA	1:A:175:SER:HB3	2.02	0.42
1:A:1149:VAL:HG22	1:A:1164:LEU:HD13	2.01	0.42
1:A:1231[B]:GLN:H	1:A:1231[B]:GLN:HG3	1.44	0.42
1:A:2801:ASP:OD1	1:A:2801:ASP:N	2.53	0.42
1:B:596:ASN:HD21	1:B:598:LYS:HE2	1.85	0.42
1:B:637:LEU:HD23	1:B:637:LEU:HA	1.93	0.42
1:B:884:LEU:HD13	1:B:968:ALA:H	1.85	0.42
1:B:1448:VAL:HG22	1:B:1554:VAL:HG23	2.02	0.42
1:B:2017:ASP:N	1:B:2017:ASP:OD1	2.53	0.42
1:B:2965:ARG:HG3	1:B:2966:TRP:CD1	2.55	0.42
1:C:1815:LEU:HD22	1:C:1845:VAL:HG21	2.02	0.42
1:C:2319:PRO:HG3	1:C:2392:ARG:HA	2.01	0.42
1:C:2499:LYS:O	1:C:2503:VAL:HG23	2.20	0.42
1:C:2997:PHE:O	1:C:3001:ILE:HB	2.19	0.42
1:D:775:GLY:H	1:D:848:HIS:CE1	2.38	0.42
1:D:1448:VAL:HG22	1:D:1554:VAL:HG23	2.02	0.42
1:D:1698:LEU:HD21	1:D:1715:LEU:HD13	2.02	0.42
1:D:2245:GLN:HA	1:D:2248:ARG:HG2	2.02	0.42
1:D:2962:GLN:HA	1:D:2965:ARG:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3616:LYS:HD3	1:D:3616:LYS:HA	1.91	0.42
1:A:838:HIS:CE1	1:A:1201:HIS:HB2	2.55	0.42
1:A:2965:ARG:HG3	1:A:2966:TRP:CD1	2.55	0.42
1:B:3888:LEU:HD23	1:B:3888:LEU:HA	1.88	0.42
1:B:4734:ARG:HB3	1:B:4745:LEU:HD11	2.02	0.42
1:C:1619:ARG:NH2	1:C:1622:GLU:OE1	2.53	0.42
1:D:2377:LEU:HA	1:D:2377:LEU:HD23	1.90	0.42
1:D:2677:LYS:HB3	1:D:2677:LYS:HE2	1.74	0.42
1:D:2765:LYS:HD3	1:D:2765:LYS:HA	1.81	0.42
1:D:2909:ASP:OD1	1:D:2909:ASP:N	2.52	0.42
1:D:3433:GLU:OE1	1:D:3436:ARG:NH1	2.49	0.42
1:D:3888:LEU:HD23	1:D:3888:LEU:HA	1.88	0.42
1:D:4685:GLY:HA3	1:D:4689:THR:HG23	2.01	0.42
1:A:1110:ARG:HE	1:A:1110:ARG:HB3	1.70	0.41
1:A:2355:ARG:O	1:A:2359:ARG:HG2	2.19	0.41
1:C:157:ARG:HG3	1:C:158:SER:H	1.85	0.41
1:C:2309:SER:HB2	1:C:2314:LEU:HD11	2.02	0.41
1:C:2879:ALA:HB2	1:C:2923:ALA:HB2	2.02	0.41
1:D:2339:VAL:HG11	1:D:2353:VAL:HG11	2.01	0.41
1:D:2965:ARG:HG3	1:D:2966:TRP:CD1	2.55	0.41
1:D:3330:ASP:O	1:D:3403:ARG:NH2	2.45	0.41
1:D:4998:LYS:HD3	1:D:5003:HIS:HD2	1.85	0.41
1:A:687:ALA:HA	1:A:713:SER:HA	2.02	0.41
1:A:884:LEU:HD13	1:A:968:ALA:H	1.85	0.41
1:A:1087:ARG:NH1	1:A:1221:GLU:O	2.53	0.41
1:A:1096:THR:OG1	1:A:1198:GLN:OE1	2.34	0.41
1:A:1289:LEU:HD23	1:A:1597:VAL:HG11	2.01	0.41
1:A:3046:LEU:O	1:A:3049:LEU:HB3	2.20	0.41
1:B:629:ARG:NH1	2:F:90:VAL:O	2.45	0.41
1:B:1488:LYS:HE3	1:B:1488:LYS:HB2	1.88	0.41
1:B:2608:MET:HG3	1:B:2642:LYS:HE3	2.01	0.41
1:C:2453:ILE:HD13	1:C:2456:ILE:HD12	2.02	0.41
1:C:2677:LYS:HB3	1:C:2677:LYS:HE2	1.74	0.41
1:C:2965:ARG:HG3	1:C:2966:TRP:CD1	2.55	0.41
1:D:2309:SER:HB2	1:D:2314:LEU:HD11	2.02	0.41
1:D:2476:ILE:HG23	1:D:2536:LEU:HD21	2.01	0.41
1:D:2879:ALA:HB2	1:D:2923:ALA:HB2	2.02	0.41
1:D:2997:PHE:O	1:D:3001:ILE:HB	2.19	0.41
1:D:4734:ARG:HB3	1:D:4745:LEU:HD11	2.02	0.41
1:A:497:TYR:HD2	1:A:503:PHE:HD1	1.69	0.41
1:A:1488:LYS:HE3	1:A:1488:LYS:HB2	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3186:LEU:HB3	1:A:3190:LEU:HD23	2.02	0.41
1:A:4998:LYS:HD3	1:A:5003:HIS:HD2	1.85	0.41
1:B:1289:LEU:HD23	1:B:1597:VAL:HG11	2.01	0.41
1:B:3046:LEU:O	1:B:3049:LEU:HB3	2.20	0.41
1:B:4843:LEU:O	1:B:4847:VAL:HG13	2.20	0.41
1:C:497:TYR:HD2	1:C:503:PHE:HD1	1.69	0.41
1:C:838:HIS:CE1	1:C:1201:HIS:HB2	2.55	0.41
1:C:1149:VAL:HG22	1:C:1164:LEU:HD13	2.01	0.41
1:C:2608:MET:HG3	1:C:2642:LYS:HE3	2.01	0.41
1:C:4239:GLU:OE2	1:C:5014:TYR:OH	2.33	0.41
1:C:4685:GLY:HA3	1:C:4689:THR:HG23	2.01	0.41
1:D:838:HIS:CE1	1:D:1201:HIS:HB2	2.55	0.41
1:D:2814:LYS:HA	1:D:2817:ILE:HG22	2.03	0.41
1:D:2928:LYS:HA	1:D:2928:LYS:HD3	1.79	0.41
1:D:3107:VAL:HG11	1:D:3171:SER:HB2	2.03	0.41
1:D:4013:LEU:HD12	1:D:4013:LEU:HA	1.94	0.41
1:A:1271:ARG:HA	1:A:1563:GLN:HA	2.01	0.41
1:A:1698:LEU:HD21	1:A:1715:LEU:HD13	2.02	0.41
1:A:3652:MET:HA	1:A:3655:GLU:HG2	2.03	0.41
1:B:497:TYR:HD2	1:B:503:PHE:HD1	1.69	0.41
1:B:1087:ARG:NH1	1:B:1221:GLU:O	2.53	0.41
1:B:1619:ARG:NH2	1:B:1622:GLU:OE1	2.53	0.41
1:B:2245:GLN:HA	1:B:2248:ARG:HG2	2.02	0.41
1:B:2499:LYS:O	1:B:2503:VAL:HG23	2.20	0.41
1:C:1448:VAL:HG22	1:C:1554:VAL:HG23	2.02	0.41
1:C:4003:LEU:HD22	1:C:4009:GLN:HG2	2.02	0.41
1:C:4998:LYS:HD3	1:C:5003:HIS:HD2	1.85	0.41
1:D:207:SER:H	1:D:334:MET:HE2	1.84	0.41
1:D:884:LEU:HD13	1:D:968:ALA:H	1.85	0.41
1:D:1077:ALA:HB3	1:D:1189:LEU:HD11	2.02	0.41
1:D:4989:MET:HE3	1:D:4989:MET:HB3	1.87	0.41
1:A:771:PHE:HB3	1:A:1472:VAL:HG23	2.02	0.41
1:A:1253:PRO:HG2	1:A:1254:HIS:CD2	2.54	0.41
1:A:1448:VAL:HG22	1:A:1554:VAL:HG23	2.02	0.41
1:A:2499:LYS:O	1:A:2503:VAL:HG23	2.20	0.41
1:A:2654:TYR:HA	1:A:2661:TRP:H	1.86	0.41
1:A:3571:TRP:CE2	1:B:1228:ILE:HG12	2.56	0.41
1:A:4843:LEU:O	1:A:4847:VAL:HG13	2.20	0.41
1:B:39:ALA:HB2	1:B:47:CYS:HA	2.02	0.41
1:B:771:PHE:HB3	1:B:1472:VAL:HG23	2.02	0.41
1:B:775:GLY:H	1:B:848:HIS:CE1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1249:PRO:HA	1:B:1250:PRO:HD3	1.96	0.41
1:B:2023:LEU:O	1:B:2028:ARG:NE	2.54	0.41
1:B:4138:ASP:O	1:B:4142:ASN:ND2	2.34	0.41
1:B:4646:LEU:HD23	1:B:4646:LEU:HA	1.87	0.41
1:C:118:LEU:HA	1:C:137:LEU:HD23	2.01	0.41
1:C:1698:LEU:HD21	1:C:1715:LEU:HD13	2.02	0.41
1:D:118:LEU:HA	1:D:137:LEU:HD23	2.01	0.41
1:D:266:ARG:CZ	1:D:330:ASP:HB2	2.51	0.41
1:D:858:THR:OG1	1:D:927:GLU:OE2	2.31	0.41
1:D:1149:VAL:HG22	1:D:1164:LEU:HD13	2.01	0.41
1:D:2355:ARG:O	1:D:2359:ARG:HG2	2.19	0.41
1:D:2782:ASP:N	1:D:2782:ASP:OD1	2.53	0.41
1:A:39:ALA:HB2	1:A:47:CYS:HA	2.02	0.41
1:A:118:LEU:HA	1:A:137:LEU:HD23	2.01	0.41
1:A:266:ARG:CZ	1:A:330:ASP:HB2	2.51	0.41
1:A:308:HIS:HD2	1:A:310:LYS:HB3	1.86	0.41
1:A:2245:GLN:HA	1:A:2248:ARG:HG2	2.02	0.41
1:A:2622:LEU:O	1:A:2626:LEU:HG	2.21	0.41
1:A:4054:ASN:O	1:A:4058:ILE:HG12	2.21	0.41
1:B:663:TYR:OH	1:B:665:GLU:OE2	2.36	0.41
1:B:4003:LEU:HD22	1:B:4009:GLN:HG2	2.03	0.41
1:B:4630:TYR:OH	1:C:4860:ARG:NH2	2.54	0.41
1:C:1249:PRO:HA	1:C:1250:PRO:HD3	1.96	0.41
1:C:2814:LYS:HA	1:C:2817:ILE:HG22	2.03	0.41
1:C:4630:TYR:OH	1:D:4860:ARG:NH2	2.54	0.41
1:D:497:TYR:HD2	1:D:503:PHE:HD1	1.69	0.41
1:D:596:ASN:HD21	1:D:598:LYS:HE2	1.85	0.41
1:D:2499:LYS:O	1:D:2503:VAL:HG23	2.20	0.41
1:D:4800:LEU:HD23	1:D:4800:LEU:HA	1.89	0.41
2:E:37:ASP:OD1	2:E:42:ARG:NH2	2.54	0.41
1:A:1072:VAL:HA	1:A:1194:LEU:O	2.21	0.41
1:A:1077:ALA:HB3	1:A:1189:LEU:HD11	2.02	0.41
1:A:1699:GLU:OE2	1:A:1813:ARG:NH1	2.45	0.41
1:A:2879:ALA:HB2	1:A:2923:ALA:HB2	2.02	0.41
1:A:3568:SER:HA	1:A:3571:TRP:HE1	1.85	0.41
1:B:838:HIS:CE1	1:B:1201:HIS:HB2	2.55	0.41
1:B:932:LEU:HD22	1:B:984:LEU:HD21	2.03	0.41
1:B:1155:LEU:HD12	1:B:1184:ILE:HD13	2.02	0.41
1:B:2782:ASP:OD1	1:B:2782:ASP:N	2.53	0.41
1:C:39:ALA:HB2	1:C:47:CYS:HA	2.02	0.41
1:C:145:ALA:HA	1:C:175:SER:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:HIS:HD2	1:C:310:LYS:HB3	1.86	0.41
1:C:932:LEU:HD22	1:C:984:LEU:HD21	2.03	0.41
1:C:1573:MET:SD	1:C:1574:PRO:HD2	2.61	0.41
1:C:3652:MET:HA	1:C:3655:GLU:HG2	2.03	0.41
1:D:145:ALA:HA	1:D:175:SER:HB3	2.02	0.41
1:D:2044:ILE:HD11	1:D:2131:LEU:HD23	2.00	0.41
2:F:20:GLN:HB2	2:F:107:GLU:HG2	2.01	0.41
2:F:87:HIS:HA	2:F:88:PRO:HD3	1.96	0.41
2:G:20:GLN:HB2	2:G:107:GLU:HG2	2.01	0.41
1:A:69:LEU:HA	1:A:69:LEU:HD12	1.87	0.41
1:A:775:GLY:H	1:A:848:HIS:CE1	2.38	0.41
1:A:2584[B]:HIS:CE1	1:A:2625:ARG:HB2	2.56	0.41
1:B:869:ARG:CZ	1:B:870:ILE:HB	2.51	0.41
1:B:1072:VAL:HA	1:B:1194:LEU:O	2.21	0.41
1:B:1149:VAL:HG22	1:B:1164:LEU:HD13	2.01	0.41
1:B:1743[A]:ARG:HE	1:B:1743[A]:ARG:HB2	1.67	0.41
1:B:3652:MET:HA	1:B:3655:GLU:HG2	2.03	0.41
1:C:663:TYR:HE1	1:C:745:SER:HB3	1.85	0.41
1:C:1773:PRO:HA	1:C:1774:PRO:HD3	1.93	0.41
1:C:4734:ARG:HB3	1:C:4745:LEU:HD11	2.02	0.41
1:D:1087:ARG:NH1	1:D:1221:GLU:O	2.54	0.41
1:D:2474:LEU:HD23	1:D:2494:PHE:HD2	1.86	0.41
1:D:4090:LYS:HE2	1:D:4090:LYS:HB3	1.84	0.41
2:G:37:ASP:OD1	2:G:42:ARG:NH2	2.54	0.41
1:A:1155:LEU:HD12	1:A:1184:ILE:HD13	2.02	0.41
1:A:2814:LYS:HA	1:A:2817:ILE:HG22	2.03	0.41
1:A:3433:GLU:OE1	1:A:3436:ARG:NH1	2.49	0.41
1:A:3460:VAL:HA	1:A:3502:ARG:CZ	2.51	0.41
1:A:3823:LYS:HD3	1:A:3823:LYS:HA	1.78	0.41
1:A:4865:LYS:HD2	1:A:4865:LYS:HA	1.82	0.41
1:B:661:LYS:HB3	1:B:808:TYR:HA	2.02	0.41
1:B:687:ALA:HA	1:B:713:SER:HA	2.03	0.41
1:B:1573:MET:SD	1:B:1574:PRO:HD2	2.61	0.41
1:B:1773:PRO:HA	1:B:1774:PRO:HD3	1.93	0.41
1:B:2500:ALA:HB2	1:B:2553:TYR:HD1	1.86	0.41
1:B:3186:LEU:HB3	1:B:3190:LEU:HD23	2.02	0.41
1:C:884:LEU:HD13	1:C:968:ALA:H	1.85	0.41
1:C:1087:ARG:NH1	1:C:1221:GLU:O	2.54	0.41
1:C:1524:THR:O	1:C:1541:GLN:NE2	2.38	0.41
1:C:1577:ALA:HB1	1:C:1584:ARG:HA	2.03	0.41
1:C:2023:LEU:O	1:C:2028:ARG:NE	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2500:ALA:HB2	1:C:2553:TYR:HD1	1.86	0.41
1:C:3107:VAL:HG11	1:C:3171:SER:HB2	2.03	0.41
1:C:3186:LEU:HB3	1:C:3190:LEU:HD23	2.02	0.41
1:D:863:LEU:HA	1:D:864:PRO:HD3	1.84	0.41
1:D:869:ARG:CZ	1:D:870:ILE:HB	2.51	0.41
1:D:932:LEU:HD22	1:D:984:LEU:HD21	2.03	0.41
1:D:1271:ARG:HA	1:D:1563:GLN:HA	2.01	0.41
1:D:1849:LEU:HA	1:D:1849:LEU:HD23	1.88	0.41
1:D:2023:LEU:O	1:D:2028:ARG:NE	2.54	0.41
1:D:2584[B]:HIS:CE1	1:D:2625:ARG:HB2	2.56	0.41
1:D:2654:TYR:HA	1:D:2661:TRP:H	1.86	0.41
1:D:3186:LEU:HB3	1:D:3190:LEU:HD23	2.02	0.41
1:D:3420:ARG:NH1	1:D:3516:LYS:O	2.52	0.41
1:D:3460:VAL:HA	1:D:3502:ARG:CZ	2.51	0.41
1:D:3568:SER:HA	1:D:3571:TRP:HE1	1.85	0.41
1:D:3652:MET:HA	1:D:3655:GLU:HG2	2.03	0.41
1:D:4843:LEU:O	1:D:4847:VAL:HG13	2.20	0.41
1:A:2339:VAL:HG11	1:A:2353:VAL:HG11	2.01	0.41
1:A:2474:LEU:HD23	1:A:2494:PHE:HD2	1.86	0.41
1:A:4734:ARG:HB3	1:A:4745:LEU:HD11	2.02	0.41
1:B:2288:LEU:HD23	1:B:2288:LEU:HA	1.91	0.41
1:B:2879:ALA:HB2	1:B:2923:ALA:HB2	2.02	0.41
1:C:2245:GLN:HA	1:C:2248:ARG:HG2	2.02	0.41
1:C:2309:SER:OG	1:C:2321:ILE:O	2.28	0.41
1:C:4090:LYS:HE2	1:C:4090:LYS:HB3	1.83	0.41
1:D:826:ILE:HG22	1:D:827:LYS:HG2	2.03	0.41
1:D:1577:ALA:HB1	1:D:1584:ARG:HA	2.03	0.41
1:D:2500:ALA:HB2	1:D:2553:TYR:HD1	1.86	0.41
2:F:37:ASP:OD1	2:F:42:ARG:NH2	2.54	0.41
1:A:932:LEU:HD22	1:A:984:LEU:HD21	2.03	0.40
1:A:2023:LEU:O	1:A:2028:ARG:NE	2.54	0.40
1:A:4748:LEU:HD23	1:A:4748:LEU:HA	1.96	0.40
1:B:266:ARG:CZ	1:B:330:ASP:HB2	2.51	0.40
1:B:2584[B]:HIS:CE1	1:B:2625:ARG:HB2	2.56	0.40
1:B:2814:LYS:HA	1:B:2817:ILE:HG22	2.03	0.40
1:B:2978:GLU:HA	1:B:2981:VAL:HG12	2.03	0.40
1:B:3460:VAL:HA	1:B:3502:ARG:CZ	2.51	0.40
1:B:3568:SER:HA	1:B:3571:TRP:HE1	1.85	0.40
1:B:4054:ASN:O	1:B:4058:ILE:HG12	2.21	0.40
1:C:266:ARG:CZ	1:C:330:ASP:HB2	2.51	0.40
1:C:661:LYS:HB3	1:C:808:TYR:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2716:ASP:OD1	1:C:2716:ASP:N	2.45	0.40
1:C:2782:ASP:OD1	1:C:2782:ASP:N	2.53	0.40
1:C:3460:VAL:HA	1:C:3502:ARG:CZ	2.51	0.40
1:D:1155:LEU:HD12	1:D:1184:ILE:HD13	2.02	0.40
1:D:1488:LYS:HE3	1:D:1488:LYS:HB2	1.88	0.40
2:G:99:PHE:HB3	2:G:101:VAL:HG23	2.03	0.40
1:A:2978:GLU:HA	1:A:2981:VAL:HG12	2.03	0.40
1:B:663:TYR:HE1	1:B:745:SER:HB3	1.85	0.40
1:B:1231[B]:GLN:H	1:B:1231[B]:GLN:HG3	1.44	0.40
1:B:1698:LEU:HD21	1:B:1715:LEU:HD13	2.02	0.40
1:B:3823:LYS:HA	1:B:3823:LYS:HD3	1.78	0.40
1:B:4692:PRO:HG3	1:B:4703:ARG:HD2	2.03	0.40
1:C:878:ILE:HD11	1:C:925:SER:HB2	2.04	0.40
1:C:1077:ALA:HB3	1:C:1189:LEU:HD11	2.02	0.40
1:C:1431:THR:HG21	1:C:1523:ALA:HB2	2.03	0.40
1:C:2283:ASN:HD21	1:C:2286:LEU:HD13	1.86	0.40
1:C:2575:ARG:HA	1:C:2575:ARG:HD2	1.95	0.40
1:C:2978:GLU:HA	1:C:2981:VAL:HG12	2.03	0.40
1:C:3249:LEU:HD12	1:C:3249:LEU:HA	1.91	0.40
1:C:3891:LEU:HB3	1:C:3899:PHE:CE2	2.57	0.40
1:D:663:TYR:HE1	1:D:745:SER:HB3	1.85	0.40
1:D:1573:MET:SD	1:D:1574:PRO:HD2	2.61	0.40
1:D:4155:PRO:HG3	1:D:5036:LEU:HD23	2.04	0.40
1:A:826:ILE:HG22	1:A:827:LYS:HG2	2.03	0.40
1:A:1578:ALA:O	1:A:1584:ARG:NH2	2.53	0.40
1:A:2004:GLU:HA	1:A:2007:ASN:HD22	1.87	0.40
1:A:2336:ARG:HG2	1:A:2435:ARG:HD2	2.04	0.40
1:A:2752:ASP:HA	1:A:2755:ILE:HG12	2.03	0.40
1:A:2782:ASP:OD1	1:A:2782:ASP:N	2.53	0.40
1:A:3696:ASP:OD1	1:A:3696:ASP:N	2.41	0.40
1:A:3891:LEU:HB3	1:A:3899:PHE:CE2	2.57	0.40
1:B:1077:ALA:HB3	1:B:1189:LEU:HD11	2.02	0.40
1:B:2136:ARG:O	1:B:2140:ARG:NH2	2.55	0.40
1:B:2622:LEU:O	1:B:2626:LEU:HG	2.21	0.40
1:B:2654:TYR:HA	1:B:2661:TRP:H	1.86	0.40
1:B:3330:ASP:O	1:B:3403:ARG:NH2	2.45	0.40
1:C:107:ILE:HD13	1:C:107:ILE:HA	1.92	0.40
1:C:596:ASN:HD21	1:C:598:LYS:HE2	1.85	0.40
1:C:2280:VAL:HA	1:C:2287:ALA:HB1	2.04	0.40
1:C:2296:GLU:HA	1:C:2299:VAL:HG12	2.03	0.40
1:C:2474:LEU:HD23	1:C:2494:PHE:HD2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2909:ASP:OD1	1:C:2909:ASP:N	2.52	0.40
1:C:3995:VAL:O	1:C:3999:MET:HG2	2.22	0.40
1:C:4800:LEU:HD23	1:C:4800:LEU:HA	1.89	0.40
1:D:157:ARG:HG3	1:D:158:SER:H	1.84	0.40
1:D:687:ALA:HA	1:D:713:SER:HA	2.02	0.40
1:D:2283:ASN:HD21	1:D:2286:LEU:HD13	1.86	0.40
1:D:2752:ASP:HA	1:D:2755:ILE:HG12	2.03	0.40
1:D:2978:GLU:HA	1:D:2981:VAL:HG12	2.03	0.40
1:D:5008:SER:O	1:D:5012:LYS:HD2	2.21	0.40
1:A:16:THR:HA	1:A:69:LEU:HD23	2.04	0.40
1:B:1699:GLU:OE2	1:B:1813:ARG:NH1	2.45	0.40
1:B:2283:ASN:HD21	1:B:2286:LEU:HD13	1.86	0.40
1:B:3159:ASP:OD1	1:B:3159:ASP:N	2.54	0.40
1:B:3995:VAL:O	1:B:3999:MET:HG2	2.22	0.40
1:B:4998:LYS:HD3	1:B:5003:HIS:HD2	1.85	0.40
1:C:1155:LEU:HD12	1:C:1184:ILE:HD13	2.02	0.40
1:C:2622:LEU:O	1:C:2626:LEU:HG	2.21	0.40
1:C:4059:LEU:HD13	1:C:4059:LEU:HA	1.96	0.40
1:C:4155:PRO:HG3	1:C:5036:LEU:HD23	2.04	0.40
1:D:1225:PRO:HG2	1:D:1228:ILE:HD13	2.03	0.40
1:D:1695:LEU:HB3	1:D:1810:LYS:NZ	2.37	0.40
1:D:2136:ARG:O	1:D:2140:ARG:NH2	2.55	0.40
1:D:4054:ASN:O	1:D:4058:ILE:HG12	2.21	0.40
2:F:99:PHE:HB3	2:F:101:VAL:HG23	2.03	0.40
1:A:1573:MET:SD	1:A:1574:PRO:HD2	2.61	0.40
1:A:1969:LEU:HD21	1:A:2009:LEU:HD13	2.04	0.40
1:A:3290:GLU:OE1	1:A:3309:SER:N	2.54	0.40
1:A:3995:VAL:O	1:A:3999:MET:HG2	2.22	0.40
1:A:4155:PRO:HG3	1:A:5036:LEU:HD23	2.04	0.40
1:B:494:LEU:HD12	1:B:515:TRP:CD1	2.57	0.40
1:B:2336:ARG:HG2	1:B:2435:ARG:HD2	2.04	0.40
1:B:3891:LEU:HB3	1:B:3899:PHE:CE2	2.57	0.40
1:B:4750:ILE:H	1:B:4750:ILE:HG13	1.60	0.40
1:C:2584[B]:HIS:CE1	1:C:2625:ARG:HB2	2.56	0.40
1:C:2801:ASP:OD1	1:C:2801:ASP:N	2.53	0.40
1:C:4054:ASN:O	1:C:4058:ILE:HG12	2.21	0.40
1:C:4706:LEU:H	1:C:4706:LEU:HG	1.73	0.40
1:C:5008:SER:O	1:C:5012:LYS:HD2	2.21	0.40
1:C:5012:LYS:O	1:C:5016:GLU:HG2	2.21	0.40
1:D:308:HIS:HD2	1:D:310:LYS:HB3	1.86	0.40
1:D:378:LEU:HD12	1:D:378:LEU:HA	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:733:PRO:HG2	1:D:762:CYS:HB3	2.04	0.40
1:D:878:ILE:HD11	1:D:925:SER:HB2	2.04	0.40
1:D:3995:VAL:O	1:D:3999:MET:HG2	2.22	0.40
1:D:4003:LEU:HD22	1:D:4009:GLN:HG2	2.02	0.40
2:E:23:VAL:HG22	2:E:47:LYS:HG2	2.04	0.40
2:H:23:VAL:HG22	2:H:47:LYS:HG2	2.04	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	4356/5037 (86%)	4216 (97%)	137 (3%)	3 (0%)	48	79
1	B	4356/5037 (86%)	4216 (97%)	137 (3%)	3 (0%)	48	79
1	C	4356/5037 (86%)	4216 (97%)	137 (3%)	3 (0%)	48	79
1	D	4356/5037 (86%)	4216 (97%)	137 (3%)	3 (0%)	48	79
2	E	105/350 (30%)	102 (97%)	3 (3%)	0	100	100
2	F	105/350 (30%)	102 (97%)	3 (3%)	0	100	100
2	G	105/350 (30%)	102 (97%)	3 (3%)	0	100	100
2	H	105/350 (30%)	102 (97%)	3 (3%)	0	100	100
All	All	17844/21548 (83%)	17272 (97%)	560 (3%)	12 (0%)	50	79

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3615	SER
1	A	4712	PRO
1	B	3615	SER
1	B	4712	PRO

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Mol	Chain	Res	Type
1	C	3615	SER
1	C	4712	PRO
1	D	3615	SER
1	D	4712	PRO
1	A	3692	GLU
1	B	3692	GLU
1	C	3692	GLU
1	D	3692	GLU

### 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	3808/4276 (89%)	3691 (97%)	117 (3%)	35	62
1	B	3808/4276 (89%)	3691 (97%)	117 (3%)	35	62
1	C	3808/4276 (89%)	3691 (97%)	117 (3%)	35	62
1	D	3808/4276 (89%)	3691 (97%)	117 (3%)	35	62
2	E	88/304 (29%)	88 (100%)	0	100	100
2	F	88/304 (29%)	88 (100%)	0	100	100
2	G	88/304 (29%)	88 (100%)	0	100	100
2	H	88/304 (29%)	88 (100%)	0	100	100
All	All	15584/18320 (85%)	15116 (97%)	468 (3%)	39	63

All (468) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	373	LYS
1	A	392	ARG
1	A	846	LEU
1	A	1462	MET
1	A	1534	LYS
1	A	1743[A]	ARG
1	A	1743[B]	ARG

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Mol	Chain	Res	Type
1	A	1752	ARG
1	A	1758	ARG
1	A	2100[A]	HIS
1	A	2100[B]	HIS
1	A	2268[A]	GLN
1	A	2268[B]	GLN
1	A	2336	ARG
1	A	2369[A]	ARG
1	A	2369[B]	ARG
1	A	2786	LYS
1	A	2806	ARG
1	A	2827	ARG
1	A	2985	ARG
1	A	3053	ARG
1	A	3185	LYS
1	A	3225	ARG
1	A	3614	LYS
1	A	3622	LYS
1	A	3652	MET
1	A	3692	GLU
1	A	4178	LEU
1	A	4180	ARG
1	A	4184	MET
1	A	4188	ARG
1	A	4189	ARG
1	A	4192	ARG
1	A	4200	THR
1	A	4206	GLU
1	A	4209	GLN
1	A	4211	LYS
1	A	4212	GLU
1	A	4221	VAL
1	A	4224	GLU
1	A	4227	GLU
1	A	4231	MET
1	A	4252	SER
1	A	4541	TRP
1	A	4543	GLU
1	A	4544	LEU
1	A	4550	LYS
1	A	4555	LEU
1	A	4556	SER

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Mol	Chain	Res	Type
1	A	4561	THR
1	A	4569	LEU
1	A	4577	LEU
1	A	4580	TYR
1	A	4581	LYS
1	A	4583	SER
1	A	4584	ASP
1	A	4627	MET
1	A	4628	VAL
1	A	4632	LEU
1	A	4633	GLU
1	A	4635	SER
1	A	4636	THR
1	A	4651	THR
1	A	4662	ASN
1	A	4665	LYS
1	A	4666	VAL
1	A	4676	GLU
1	A	4679	ARG
1	A	4680	LYS
1	A	4682	GLU
1	A	4689	THR
1	A	4694	ASP
1	A	4696	ASP
1	A	4697	VAL
1	A	4704	LEU
1	A	4705	VAL
1	A	4706	LEU
1	A	4710	SER
1	A	4716	TRP
1	A	4720	VAL
1	A	4722	ARG
1	A	4736	ARG
1	A	4743	MET
1	A	4748	LEU
1	A	4750	ILE
1	A	4779	LYS
1	A	4809	PHE
1	A	4818	MET
1	A	4835	LYS
1	A	4836	GLN
1	A	4837	LEU

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Mol	Chain	Res	Type
1	A	4844	LEU
1	A	4861	LYS
1	A	4870	ASP
1	A	4874	MET
1	A	4884	LEU
1	A	4889	VAL
1	A	4911	LEU
1	A	4927	ILE
1	A	4932	ILE
1	A	4933	GLN
1	A	4948	GLU
1	A	4966	ASP
1	A	4971	THR
1	A	4976	GLU
1	A	4982	GLU
1	A	4989	MET
1	A	4992	LEU
1	A	4993	MET
1	A	4995	LEU
1	A	4997	ASN
1	A	5002	GLU
1	A	5012	LYS
1	A	5013	MET
1	A	5027	CYS
1	A	5028	PHE
1	A	5034	ASP
1	B	373	LYS
1	B	392	ARG
1	B	846	LEU
1	B	1462	MET
1	B	1534	LYS
1	B	1743[A]	ARG
1	B	1743[B]	ARG
1	B	1752	ARG
1	B	1758	ARG
1	B	2100[A]	HIS
1	B	2100[B]	HIS
1	B	2268[A]	GLN
1	B	2268[B]	GLN
1	B	2336	ARG
1	B	2369[A]	ARG
1	B	2369[B]	ARG

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Mol	Chain	Res	Type
1	B	2786	LYS
1	B	2806	ARG
1	B	2827	ARG
1	B	2985	ARG
1	B	3053	ARG
1	B	3185	LYS
1	B	3225	ARG
1	B	3614	LYS
1	B	3622	LYS
1	B	3652	MET
1	B	3692	GLU
1	B	4178	LEU
1	B	4180	ARG
1	B	4184	MET
1	B	4188	ARG
1	B	4189	ARG
1	B	4192	ARG
1	B	4200	THR
1	B	4206	GLU
1	B	4209	GLN
1	B	4211	LYS
1	B	4212	GLU
1	B	4221	VAL
1	B	4224	GLU
1	B	4227	GLU
1	B	4231	MET
1	B	4252	SER
1	B	4541	TRP
1	B	4543	GLU
1	B	4544	LEU
1	B	4550	LYS
1	B	4555	LEU
1	B	4556	SER
1	B	4561	THR
1	B	4569	LEU
1	B	4577	LEU
1	B	4580	TYR
1	B	4581	LYS
1	B	4583	SER
1	B	4584	ASP
1	B	4627	MET
1	B	4628	VAL

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Mol	Chain	Res	Type
1	B	4632	LEU
1	B	4633	GLU
1	B	4635	SER
1	B	4636	THR
1	B	4651	THR
1	B	4662	ASN
1	B	4665	LYS
1	B	4666	VAL
1	B	4676	GLU
1	B	4679	ARG
1	B	4680	LYS
1	B	4682	GLU
1	B	4689	THR
1	B	4694	ASP
1	B	4696	ASP
1	B	4697	VAL
1	B	4704	LEU
1	B	4705	VAL
1	B	4706	LEU
1	B	4710	SER
1	B	4716	TRP
1	B	4720	VAL
1	B	4722	ARG
1	B	4736	ARG
1	B	4743	MET
1	B	4748	LEU
1	B	4750	ILE
1	B	4779	LYS
1	B	4809	PHE
1	B	4818	MET
1	B	4835	LYS
1	B	4836	GLN
1	B	4837	LEU
1	B	4844	LEU
1	B	4861	LYS
1	B	4870	ASP
1	B	4874	MET
1	B	4884	LEU
1	B	4889	VAL
1	B	4911	LEU
1	B	4927	ILE
1	B	4932	ILE

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Mol	Chain	Res	Type
1	B	4933	GLN
1	B	4948	GLU
1	B	4966	ASP
1	B	4971	THR
1	B	4976	GLU
1	B	4982	GLU
1	B	4989	MET
1	B	4992	LEU
1	B	4993	MET
1	B	4995	LEU
1	B	4997	ASN
1	B	5002	GLU
1	B	5012	LYS
1	B	5013	MET
1	B	5027	CYS
1	B	5028	PHE
1	B	5034	ASP
1	C	373	LYS
1	C	392	ARG
1	C	846	LEU
1	C	1462	MET
1	C	1534	LYS
1	C	1743[A]	ARG
1	C	1743[B]	ARG
1	C	1752	ARG
1	C	1758	ARG
1	C	2100[A]	HIS
1	C	2100[B]	HIS
1	C	2268[A]	GLN
1	C	2268[B]	GLN
1	C	2336	ARG
1	C	2369[A]	ARG
1	C	2369[B]	ARG
1	C	2786	LYS
1	C	2806	ARG
1	C	2827	ARG
1	C	2985	ARG
1	C	3053	ARG
1	C	3185	LYS
1	C	3225	ARG
1	C	3614	LYS
1	C	3622	LYS

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Mol	Chain	Res	Type
1	C	3652	MET
1	C	3692	GLU
1	C	4178	LEU
1	C	4180	ARG
1	C	4184	MET
1	C	4188	ARG
1	C	4189	ARG
1	C	4192	ARG
1	C	4200	THR
1	C	4206	GLU
1	C	4209	GLN
1	C	4211	LYS
1	C	4212	GLU
1	C	4221	VAL
1	C	4224	GLU
1	C	4227	GLU
1	C	4231	MET
1	C	4252	SER
1	C	4541	TRP
1	C	4543	GLU
1	C	4544	LEU
1	C	4550	LYS
1	C	4555	LEU
1	C	4556	SER
1	C	4561	THR
1	C	4569	LEU
1	C	4577	LEU
1	C	4580	TYR
1	C	4581	LYS
1	C	4583	SER
1	C	4584	ASP
1	C	4627	MET
1	C	4628	VAL
1	C	4632	LEU
1	C	4633	GLU
1	C	4635	SER
1	C	4636	THR
1	C	4651	THR
1	C	4662	ASN
1	C	4665	LYS
1	C	4666	VAL
1	C	4676	GLU

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Mol	Chain	Res	Type
1	C	4679	ARG
1	C	4680	LYS
1	C	4682	GLU
1	C	4689	THR
1	C	4694	ASP
1	C	4696	ASP
1	C	4697	VAL
1	C	4704	LEU
1	C	4705	VAL
1	C	4706	LEU
1	C	4710	SER
1	C	4716	TRP
1	C	4720	VAL
1	C	4722	ARG
1	C	4736	ARG
1	C	4743	MET
1	C	4748	LEU
1	C	4750	ILE
1	C	4779	LYS
1	C	4809	PHE
1	C	4818	MET
1	C	4835	LYS
1	C	4836	GLN
1	C	4837	LEU
1	C	4844	LEU
1	C	4861	LYS
1	C	4870	ASP
1	C	4874	MET
1	C	4884	LEU
1	C	4889	VAL
1	C	4911	LEU
1	C	4927	ILE
1	C	4932	ILE
1	C	4933	GLN
1	C	4948	GLU
1	C	4966	ASP
1	C	4971	THR
1	C	4976	GLU
1	C	4982	GLU
1	C	4989	MET
1	C	4992	LEU
1	C	4993	MET

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Mol	Chain	Res	Type
1	C	4995	LEU
1	C	4997	ASN
1	C	5002	GLU
1	C	5012	LYS
1	C	5013	MET
1	C	5027	CYS
1	C	5028	PHE
1	C	5034	ASP
1	D	373	LYS
1	D	392	ARG
1	D	846	LEU
1	D	1462	MET
1	D	1534	LYS
1	D	1743[A]	ARG
1	D	1743[B]	ARG
1	D	1752	ARG
1	D	1758	ARG
1	D	2100[A]	HIS
1	D	2100[B]	HIS
1	D	2268[A]	GLN
1	D	2268[B]	GLN
1	D	2336	ARG
1	D	2369[A]	ARG
1	D	2369[B]	ARG
1	D	2786	LYS
1	D	2806	ARG
1	D	2827	ARG
1	D	2985	ARG
1	D	3053	ARG
1	D	3185	LYS
1	D	3225	ARG
1	D	3614	LYS
1	D	3622	LYS
1	D	3652	MET
1	D	3692	GLU
1	D	4178	LEU
1	D	4180	ARG
1	D	4184	MET
1	D	4188	ARG
1	D	4189	ARG
1	D	4192	ARG
1	D	4200	THR

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Mol	Chain	Res	Type
1	D	4206	GLU
1	D	4209	GLN
1	D	4211	LYS
1	D	4212	GLU
1	D	4221	VAL
1	D	4224	GLU
1	D	4227	GLU
1	D	4231	MET
1	D	4252	SER
1	D	4541	TRP
1	D	4543	GLU
1	D	4544	LEU
1	D	4550	LYS
1	D	4555	LEU
1	D	4556	SER
1	D	4561	THR
1	D	4569	LEU
1	D	4577	LEU
1	D	4580	TYR
1	D	4581	LYS
1	D	4583	SER
1	D	4584	ASP
1	D	4627	MET
1	D	4628	VAL
1	D	4632	LEU
1	D	4633	GLU
1	D	4635	SER
1	D	4636	THR
1	D	4651	THR
1	D	4662	ASN
1	D	4665	LYS
1	D	4666	VAL
1	D	4676	GLU
1	D	4679	ARG
1	D	4680	LYS
1	D	4682	GLU
1	D	4689	THR
1	D	4694	ASP
1	D	4696	ASP
1	D	4697	VAL
1	D	4704	LEU
1	D	4705	VAL

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Mol	Chain	Res	Type
1	D	4706	LEU
1	D	4710	SER
1	D	4716	TRP
1	D	4720	VAL
1	D	4722	ARG
1	D	4736	ARG
1	D	4743	MET
1	D	4748	LEU
1	D	4750	ILE
1	D	4779	LYS
1	D	4809	PHE
1	D	4818	MET
1	D	4835	LYS
1	D	4836	GLN
1	D	4837	LEU
1	D	4844	LEU
1	D	4861	LYS
1	D	4870	ASP
1	D	4874	MET
1	D	4884	LEU
1	D	4889	VAL
1	D	4911	LEU
1	D	4927	ILE
1	D	4932	ILE
1	D	4933	GLN
1	D	4948	GLU
1	D	4966	ASP
1	D	4971	THR
1	D	4976	GLU
1	D	4982	GLU
1	D	4989	MET
1	D	4992	LEU
1	D	4993	MET
1	D	4995	LEU
1	D	4997	ASN
1	D	5002	GLU
1	D	5012	LYS
1	D	5013	MET
1	D	5027	CYS
1	D	5028	PHE
1	D	5034	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	203	ASN
1	A	597	HIS
1	A	624	ASN
1	A	1614	GLN
1	A	1631	GLN
1	A	2127	GLN
1	A	2872	GLN
1	A	2924	GLN
1	A	3325	ASN
1	A	3611	HIS
1	A	3766	GLN
1	A	3895	HIS
1	A	4201	ASN
1	A	4626	ASN
1	A	4836	GLN
1	A	4997	ASN
1	A	5031	GLN
1	B	23	GLN
1	B	203	ASN
1	B	597	HIS
1	B	1631	GLN
1	B	2127	GLN
1	B	2634	ASN
1	B	2872	GLN
1	B	2924	GLN
1	B	3325	ASN
1	B	3611	HIS
1	B	3766	GLN
1	B	3895	HIS
1	B	4201	ASN
1	B	4626	ASN
1	B	4836	GLN
1	B	4997	ASN
1	B	5031	GLN
1	C	23	GLN
1	C	203	ASN
1	C	597	HIS
1	C	877	ASN
1	C	1614	GLN
1	C	1631	GLN
1	C	2127	GLN

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Mol	Chain	Res	Type
1	C	2634	ASN
1	C	2872	GLN
1	C	2924	GLN
1	C	3611	HIS
1	C	3766	GLN
1	C	3895	HIS
1	C	4201	ASN
1	C	4626	ASN
1	C	4836	GLN
1	C	4997	ASN
1	C	5031	GLN
1	D	23	GLN
1	D	203	ASN
1	D	597	HIS
1	D	877	ASN
1	D	1631	GLN
1	D	2127	GLN
1	D	2634	ASN
1	D	2872	GLN
1	D	2924	GLN
1	D	3325	ASN
1	D	3611	HIS
1	D	3766	GLN
1	D	3895	HIS
1	D	4201	ASN
1	D	4626	ASN
1	D	4836	GLN
1	D	4997	ASN
1	D	5031	GLN
2	E	20	GLN
2	F	20	GLN
2	G	20	GLN
2	H	20	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
3	ADP	A	5101	-	24,29,29	0.85	1 (4%)	29,45,45	1.36	4 (13%)
3	ADP	B	5101	-	24,29,29	0.85	1 (4%)	29,45,45	1.36	4 (13%)
3	ADP	D	5101	-	24,29,29	0.85	1 (4%)	29,45,45	1.36	4 (13%)
3	ADP	C	5101	-	24,29,29	0.85	1 (4%)	29,45,45	1.36	4 (13%)

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
3	ADP	A	5101	-	-	4/12/32/32	0/3/3/3
3	ADP	B	5101	-	-	4/12/32/32	0/3/3/3
3	ADP	D	5101	-	-	4/12/32/32	0/3/3/3
3	ADP	C	5101	-	-	4/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5101	ADP	PA-O3A	2.17	1.61	1.59
3	D	5101	ADP	PA-O3A	2.17	1.61	1.59
3	C	5101	ADP	PA-O3A	2.16	1.61	1.59
3	B	5101	ADP	PA-O3A	2.16	1.61	1.59

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	5101	ADP	C4'-O4'-C1'	-3.85	106.40	109.92
3	A	5101	ADP	C4'-O4'-C1'	-3.84	106.40	109.92
3	B	5101	ADP	C4'-O4'-C1'	-3.84	106.41	109.92
3	C	5101	ADP	C4'-O4'-C1'	-3.84	106.41	109.92
3	D	5101	ADP	N3-C2-N1	-3.71	123.63	128.67
3	C	5101	ADP	N3-C2-N1	-3.71	123.63	128.67
3	A	5101	ADP	N3-C2-N1	-3.71	123.64	128.67
3	B	5101	ADP	N3-C2-N1	-3.71	123.64	128.67
3	B	5101	ADP	O4'-C1'-N9	2.10	111.53	108.75
3	D	5101	ADP	O4'-C1'-N9	2.10	111.53	108.75
3	A	5101	ADP	O4'-C1'-N9	2.10	111.53	108.75
3	C	5101	ADP	O4'-C1'-N9	2.10	111.53	108.75
3	B	5101	ADP	C4-C5-N7	-2.09	107.13	109.34
3	D	5101	ADP	C4-C5-N7	-2.09	107.13	109.34
3	C	5101	ADP	C4-C5-N7	-2.09	107.13	109.34
3	A	5101	ADP	C4-C5-N7	-2.09	107.13	109.34

There are no chirality outliers.

All (16) torsion outliers are listed below:

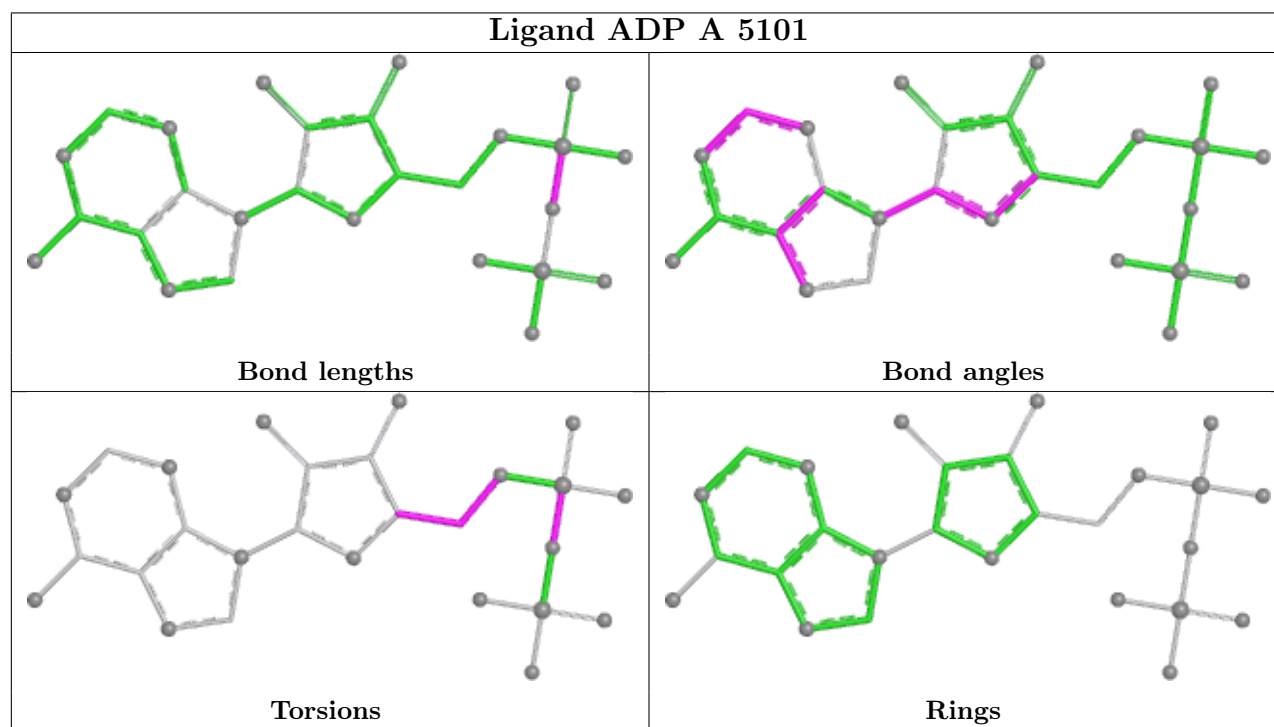
Mol	Chain	Res	Type	Atoms
3	A	5101	ADP	PB-O3A-PA-O5'
3	B	5101	ADP	PB-O3A-PA-O5'
3	C	5101	ADP	PB-O3A-PA-O5'
3	D	5101	ADP	PB-O3A-PA-O5'
3	A	5101	ADP	O4'-C4'-C5'-O5'
3	B	5101	ADP	O4'-C4'-C5'-O5'
3	C	5101	ADP	O4'-C4'-C5'-O5'
3	D	5101	ADP	O4'-C4'-C5'-O5'
3	A	5101	ADP	C3'-C4'-C5'-O5'
3	B	5101	ADP	C3'-C4'-C5'-O5'
3	C	5101	ADP	C3'-C4'-C5'-O5'
3	D	5101	ADP	C3'-C4'-C5'-O5'
3	A	5101	ADP	C4'-C5'-O5'-PA
3	B	5101	ADP	C4'-C5'-O5'-PA
3	C	5101	ADP	C4'-C5'-O5'-PA
3	D	5101	ADP	C4'-C5'-O5'-PA

There are no ring outliers.

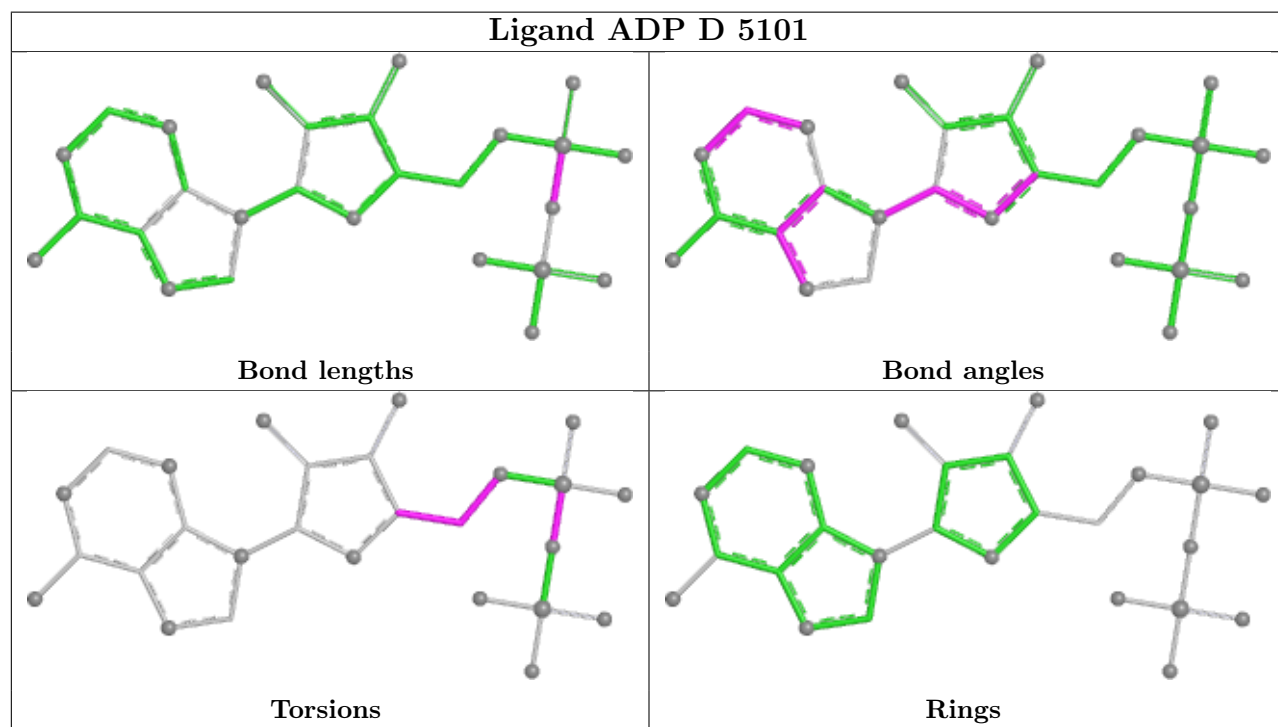
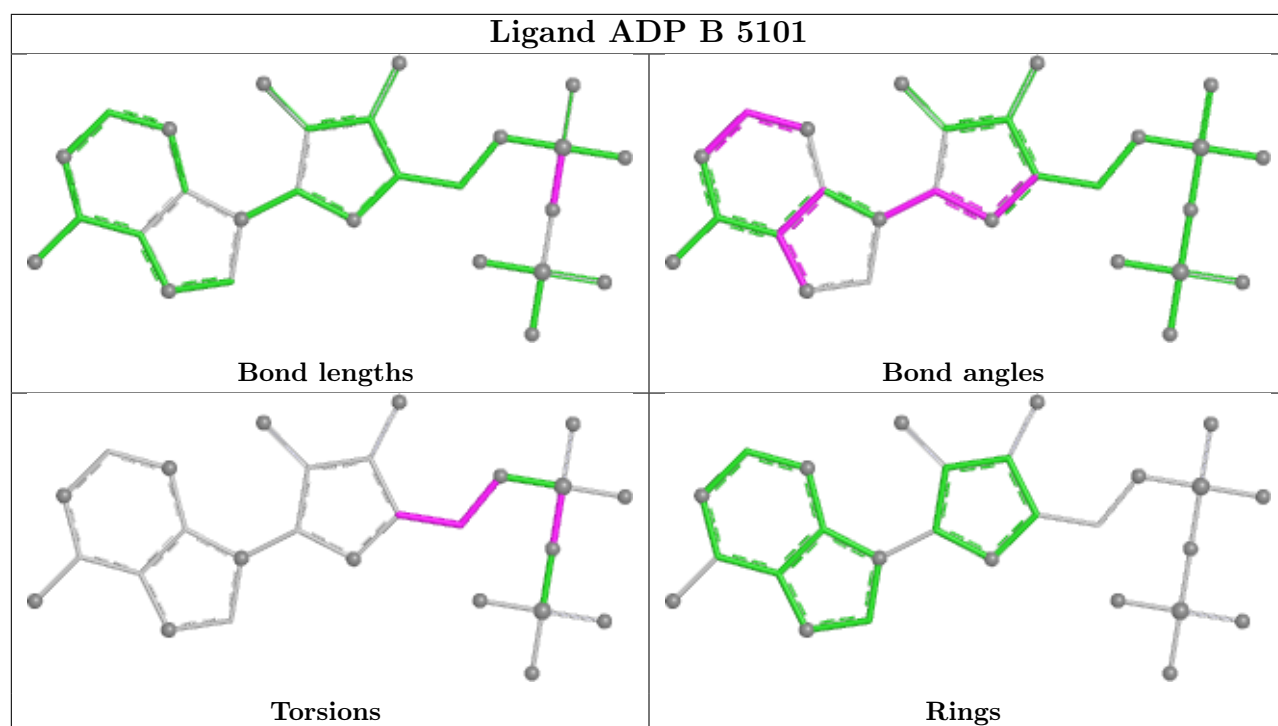
4 monomers are involved in 4 short contacts:

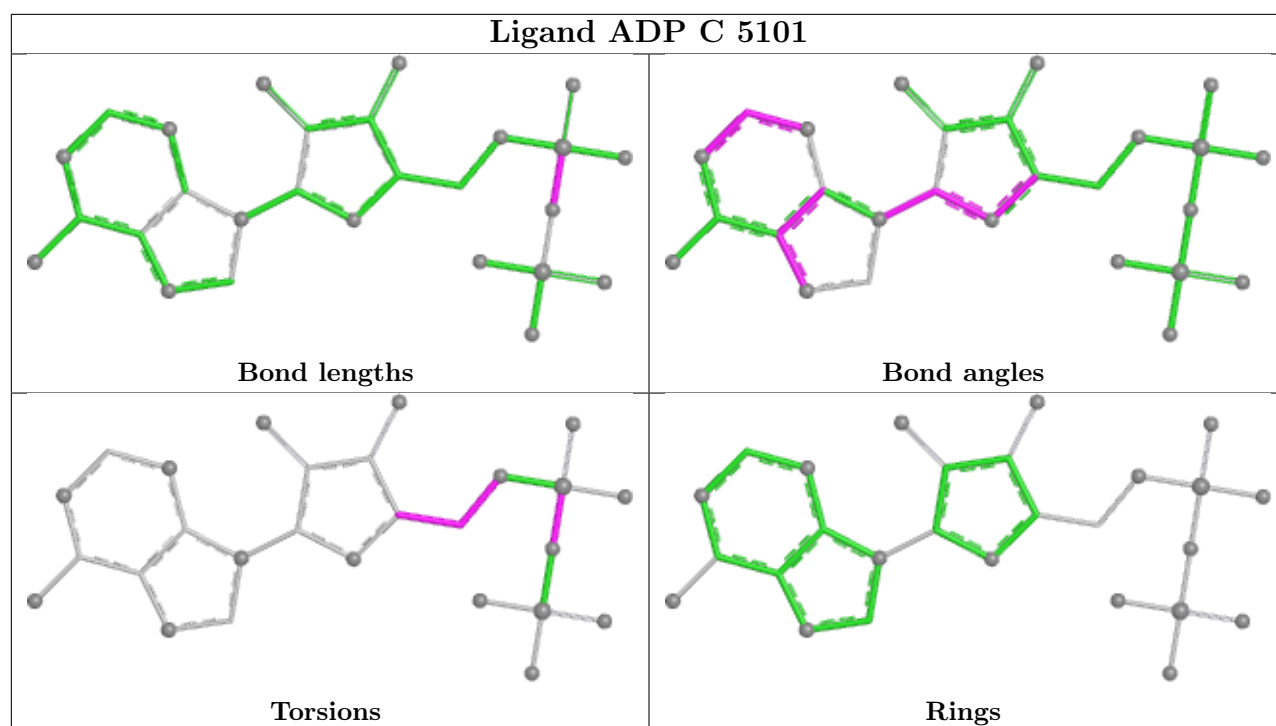
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	5101	ADP	1	0
3	B	5101	ADP	1	0
3	D	5101	ADP	1	0
3	C	5101	ADP	1	0

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.

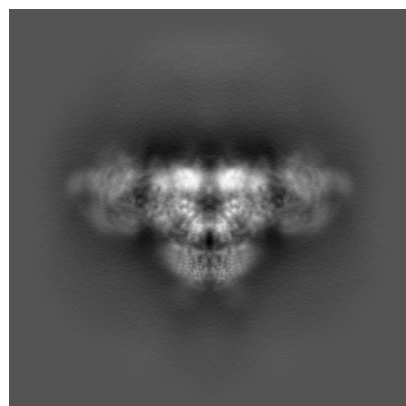
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40424. These allow visual inspection of the internal detail of the map and identification of artifacts.

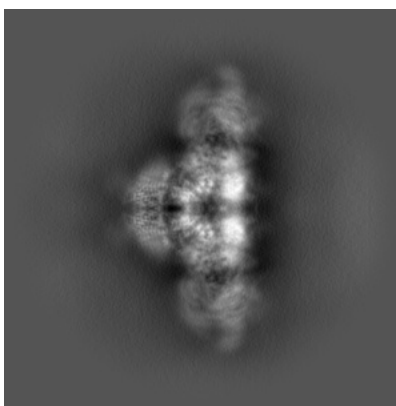
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

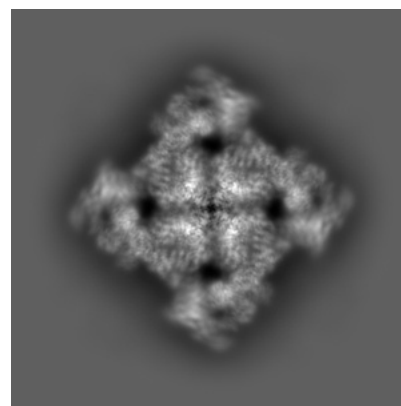
#### 6.1.1 Primary map



X

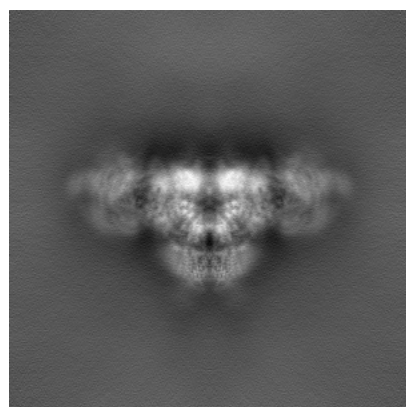


Y

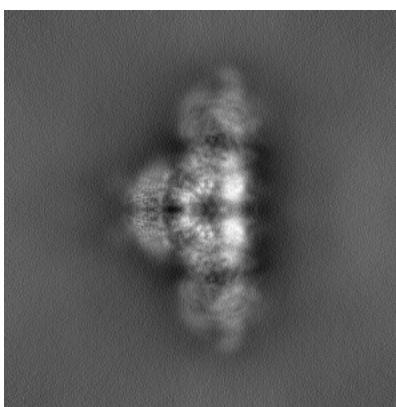


Z

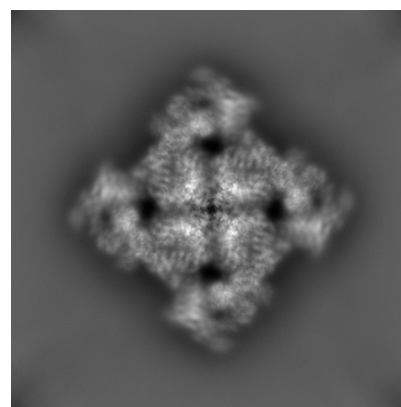
#### 6.1.2 Raw map



X



Y

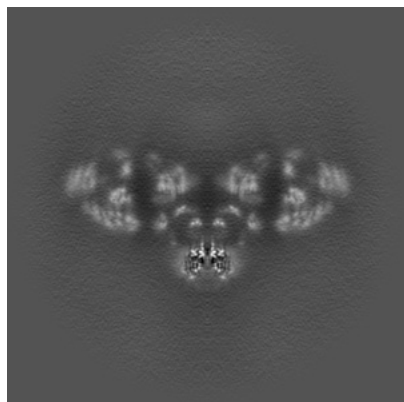


Z

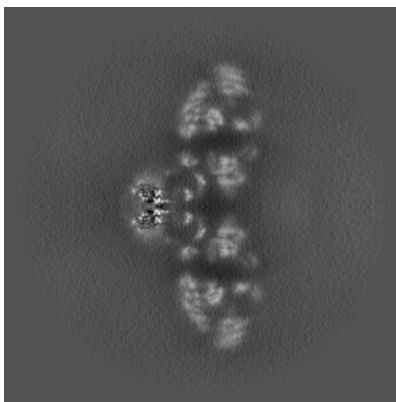
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

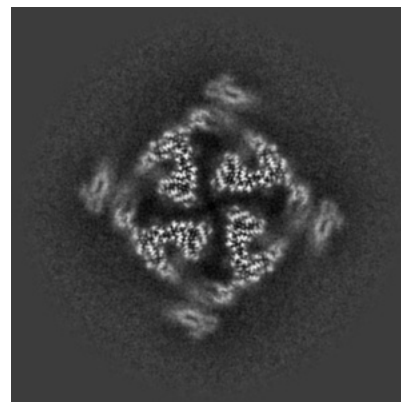
### 6.2.1 Primary map



X Index: 200

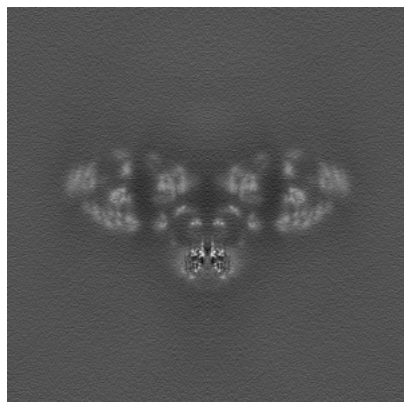


Y Index: 200

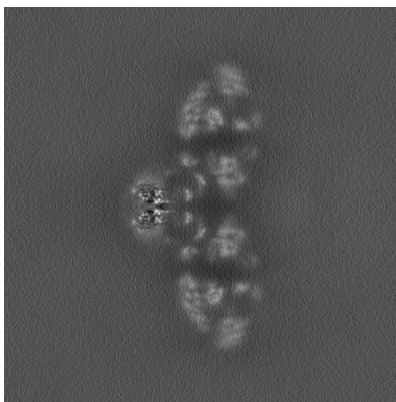


Z Index: 200

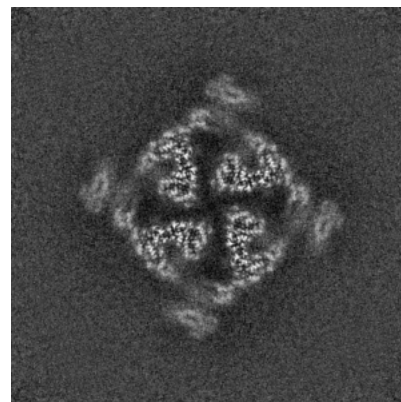
### 6.2.2 Raw map



X Index: 200



Y Index: 200

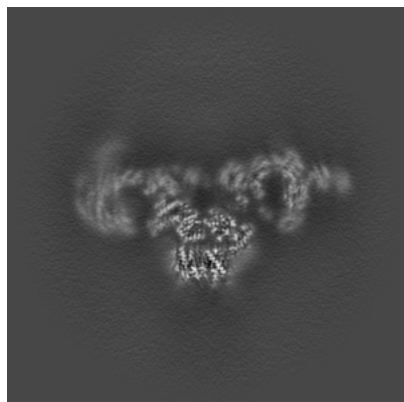


Z Index: 200

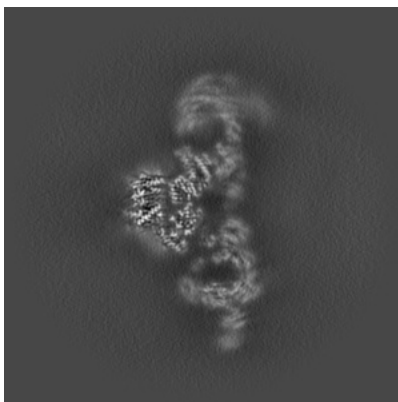
The images above show central slices of the map in three orthogonal directions.

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

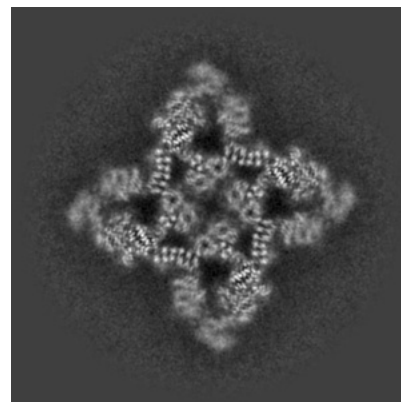
### 6.3.1 Primary map



X Index: 186

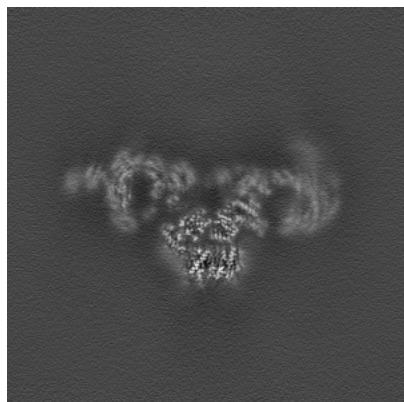


Y Index: 186

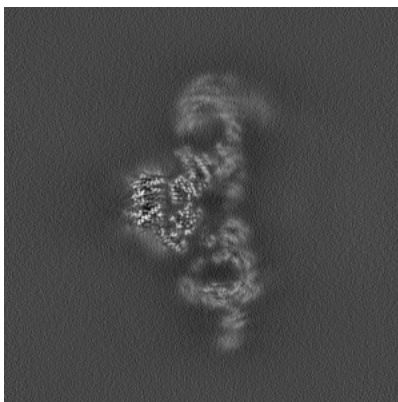


Z Index: 223

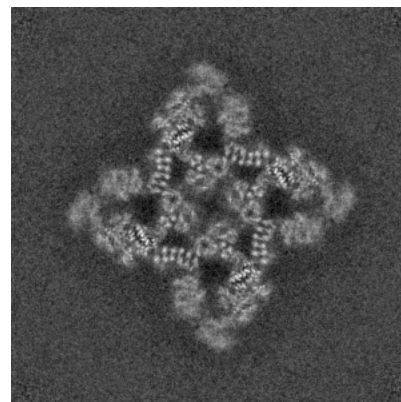
### 6.3.2 Raw map



X Index: 214



Y Index: 186



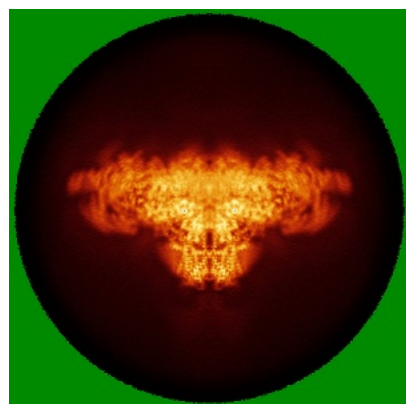
Z Index: 223

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

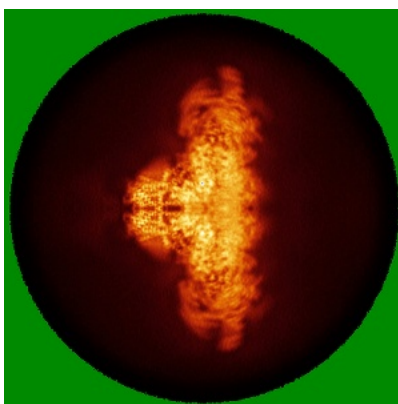


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

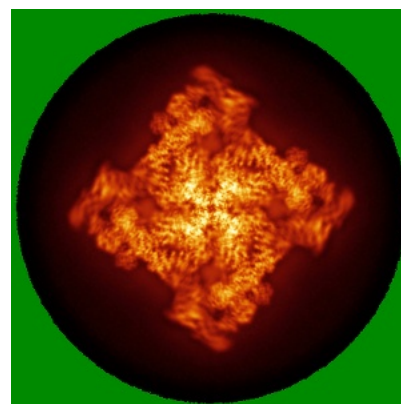
### 6.4.1 Primary map



X

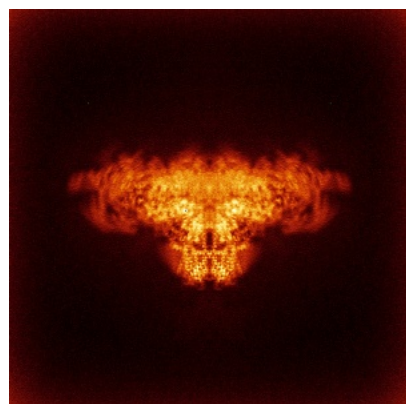


Y

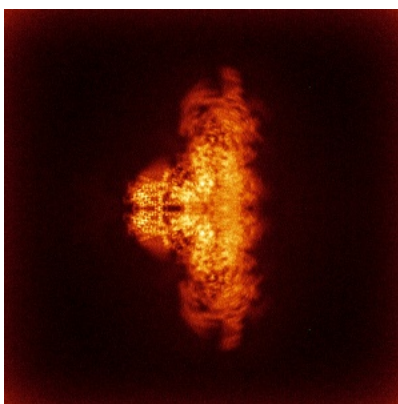


Z

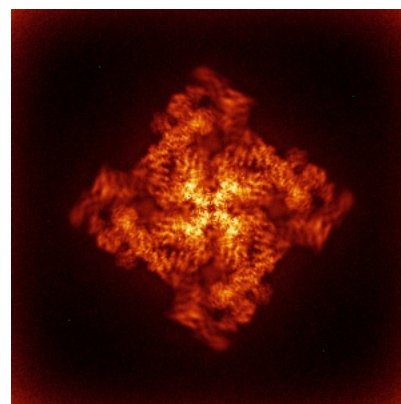
### 6.4.2 Raw map



X



Y

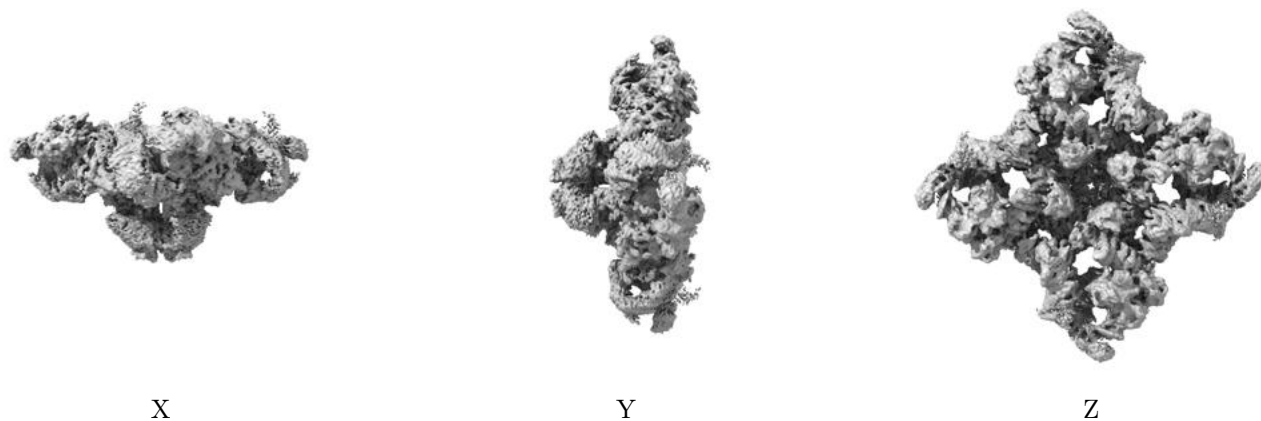


Z

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

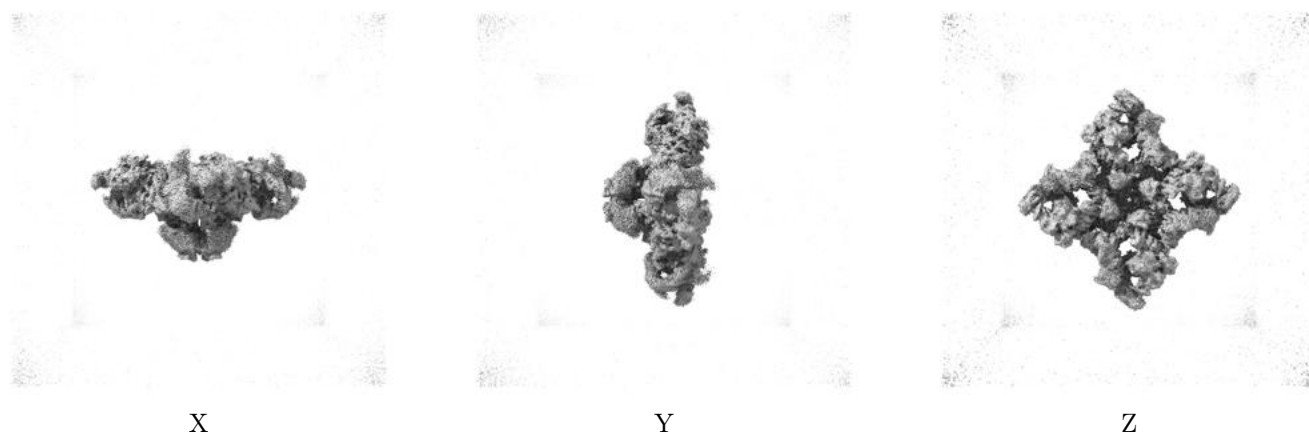
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.263. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

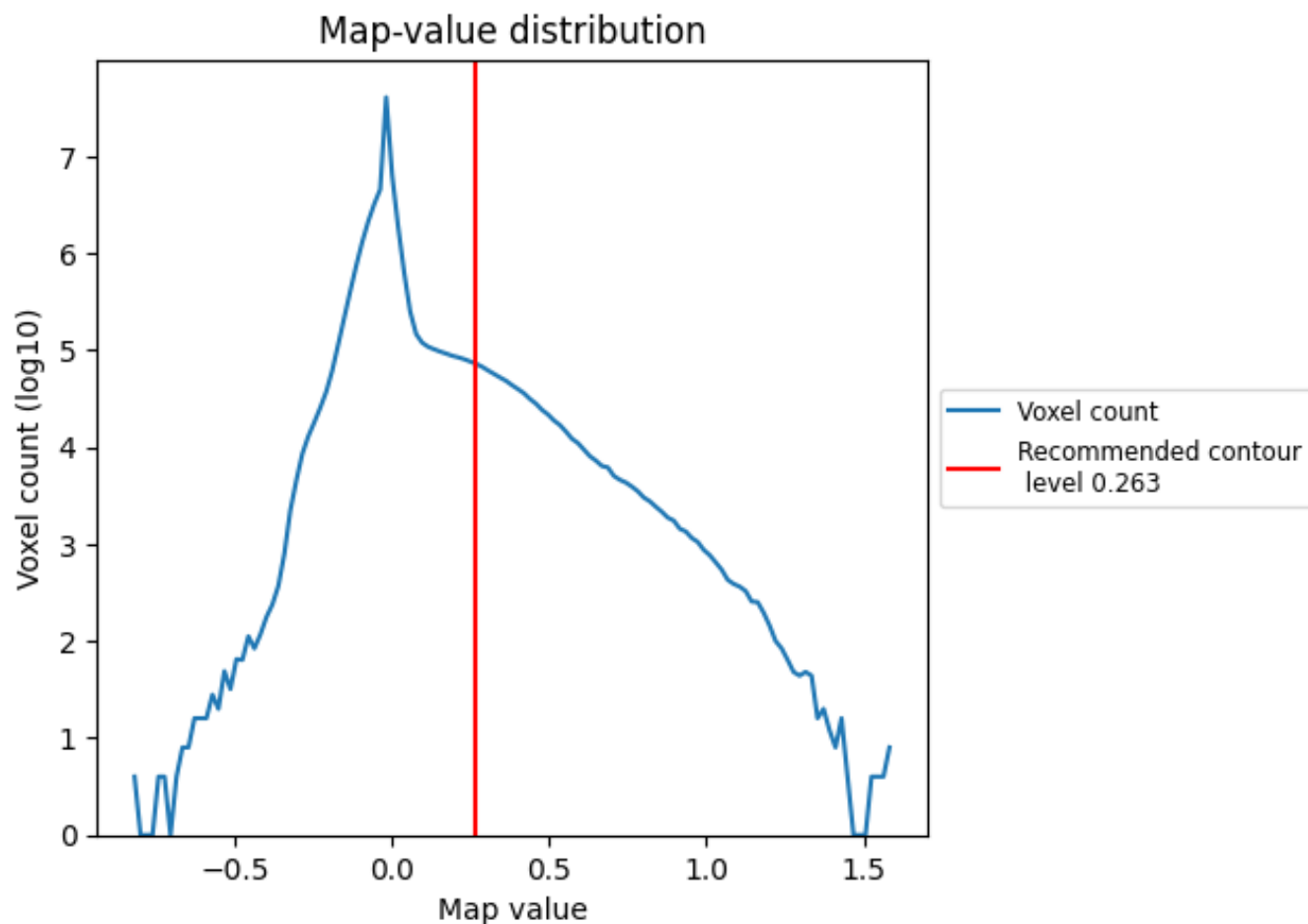
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

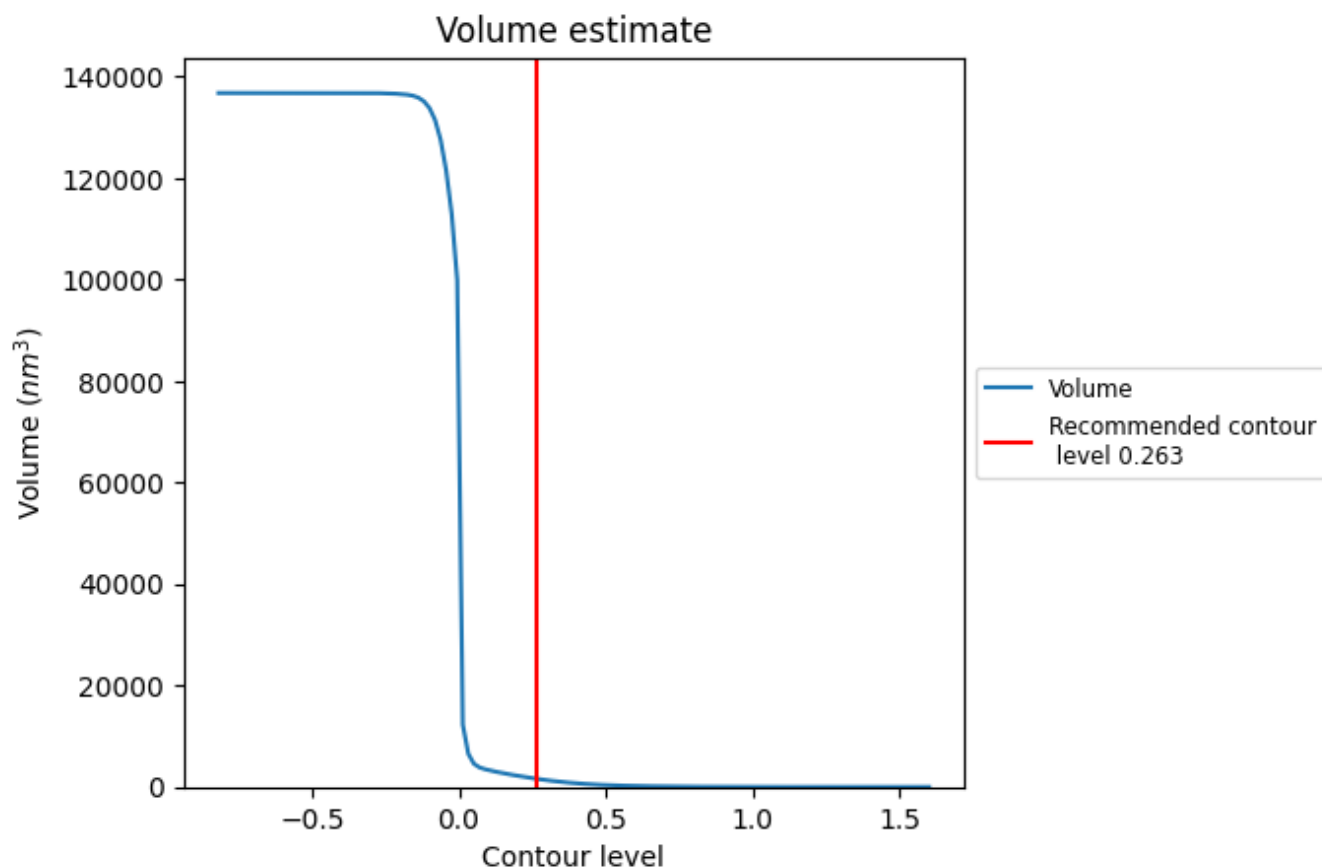
### 7.1 Map-value distribution [i](#)



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



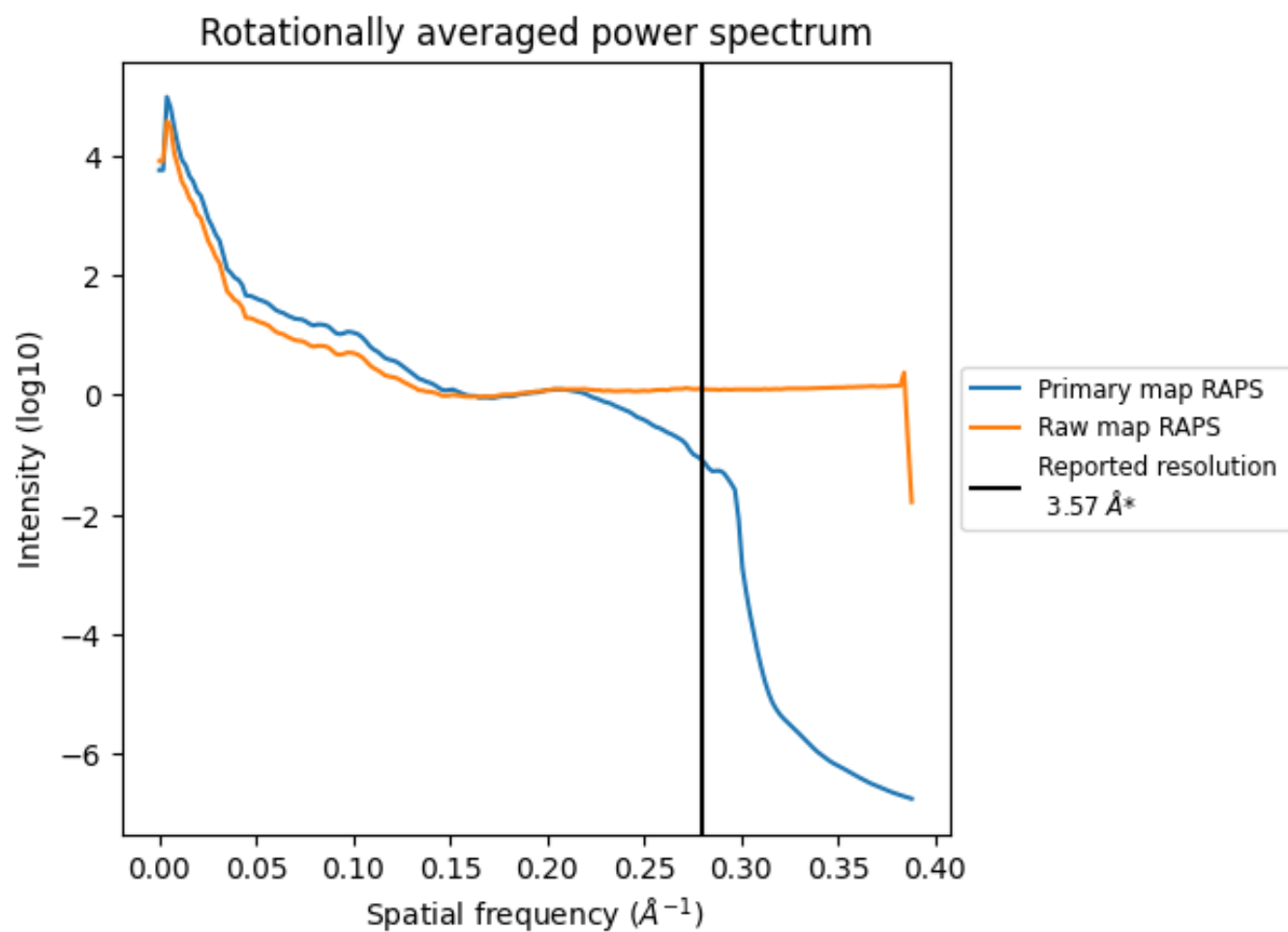
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1622 nm<sup>3</sup>; this corresponds to an approximate mass of 1465 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 ⓘ

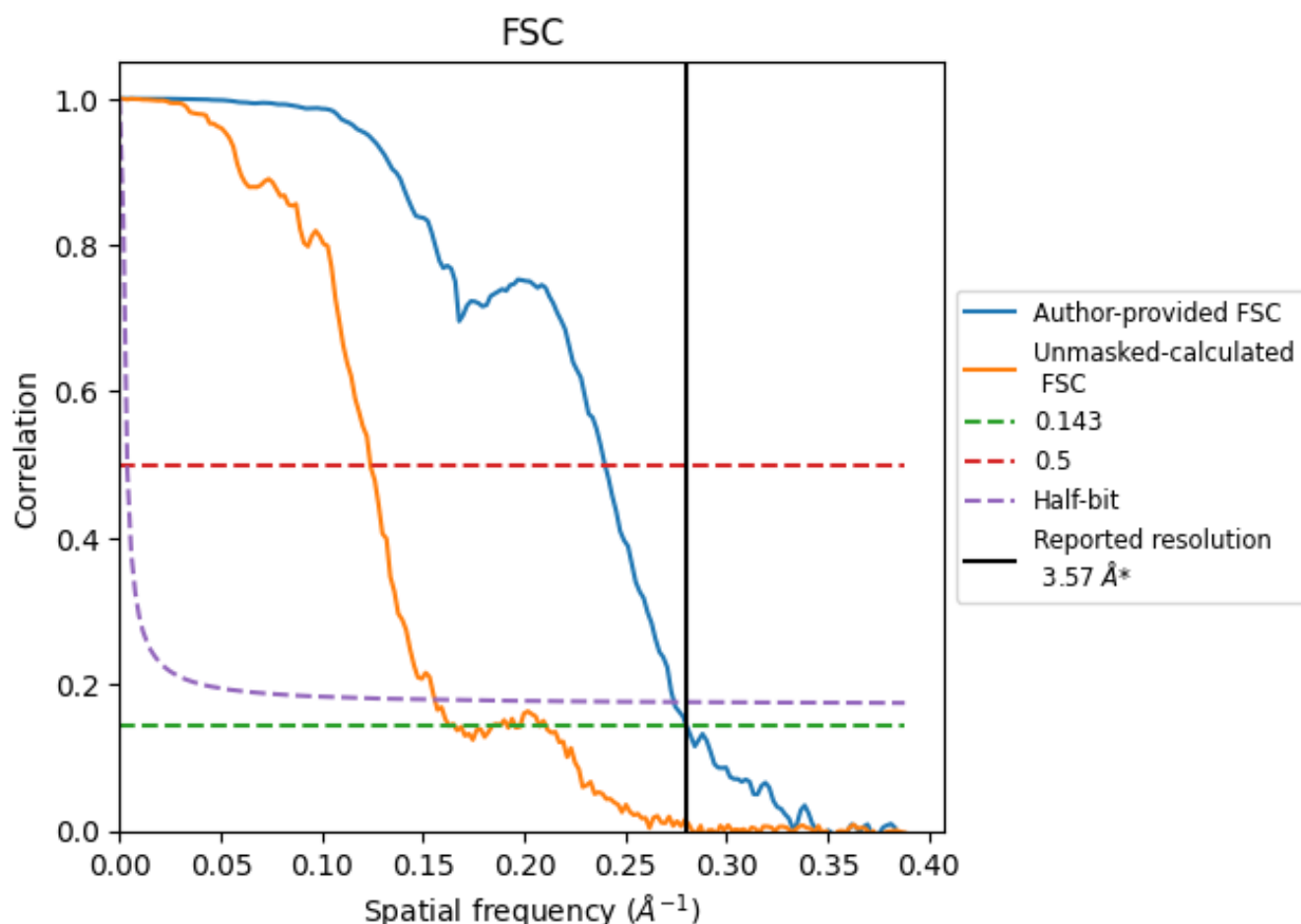


\*Reported resolution corresponds to spatial frequency of 0.280  $\text{\AA}^{-1}$

## 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 0.280  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

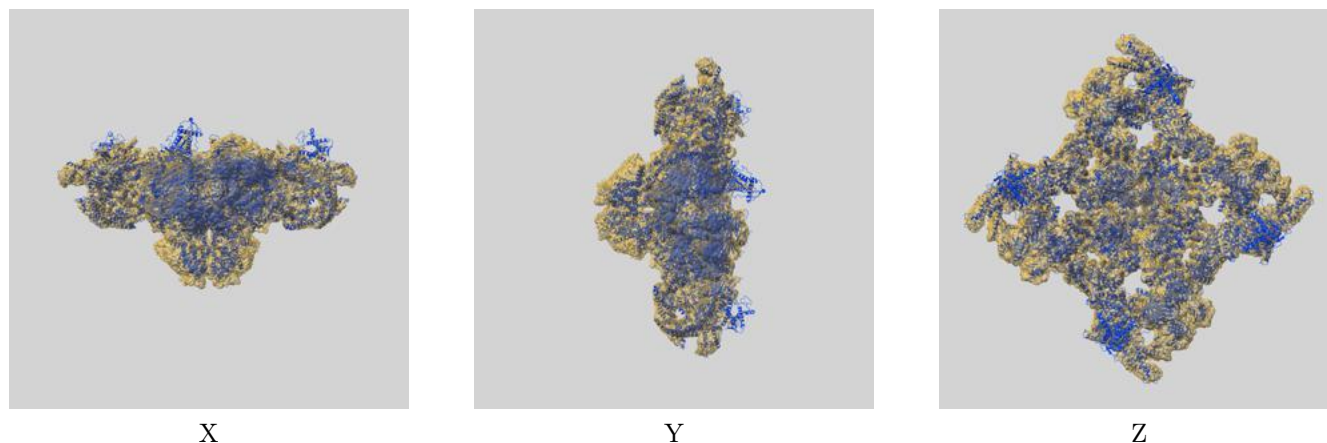
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.57	-	-
Author-provided FSC curve	3.57	4.17	3.65
Unmasked-calculated*	6.04	8.06	6.41

\*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 6.04 differs from the reported value 3.57 by more than 10 %

## 9 Map-model fit [i](#)

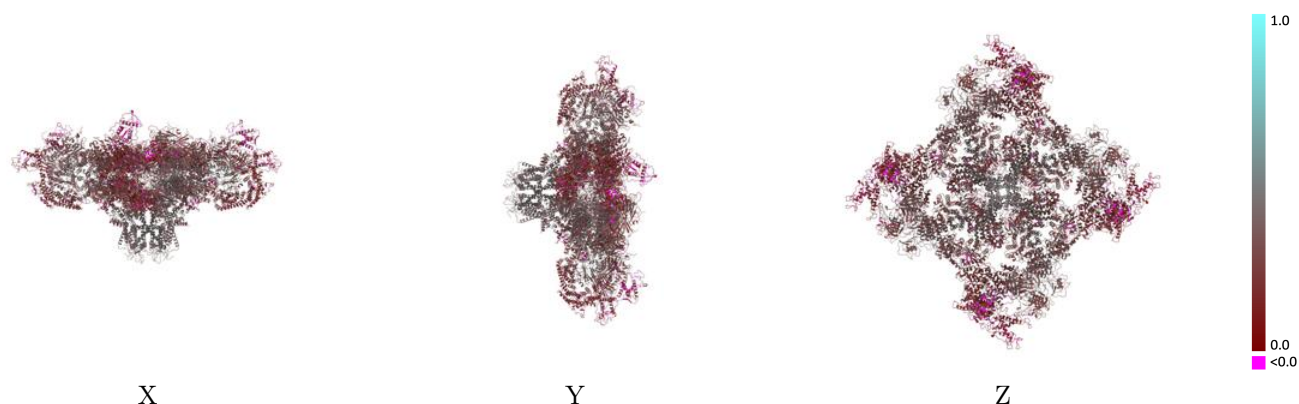
This section contains information regarding the fit between EMDB map EMD-40424 and PDB model 8SEP. Per-residue inclusion information can be found in section [3](#) on page [8](#).

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



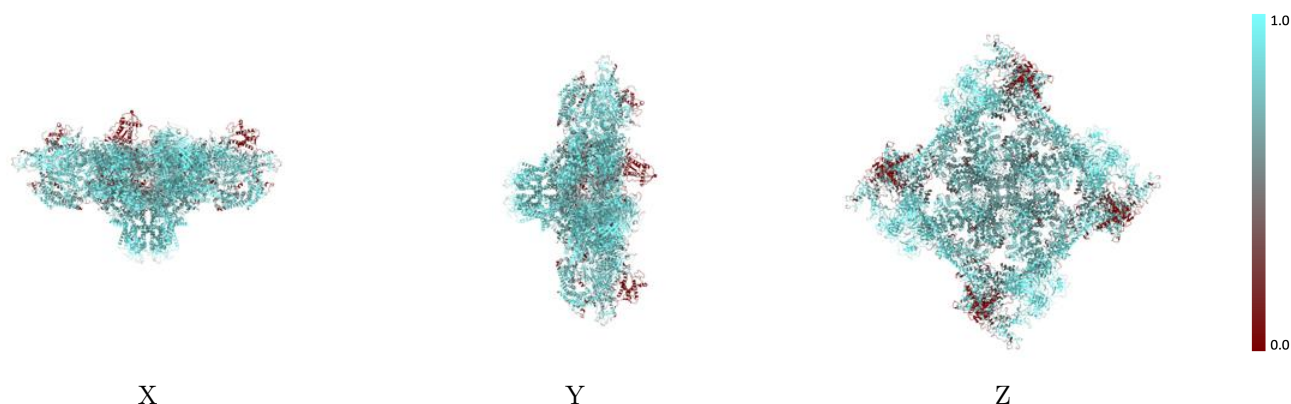
The images above show the 3D surface view of the map at the recommended contour level 0.263 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



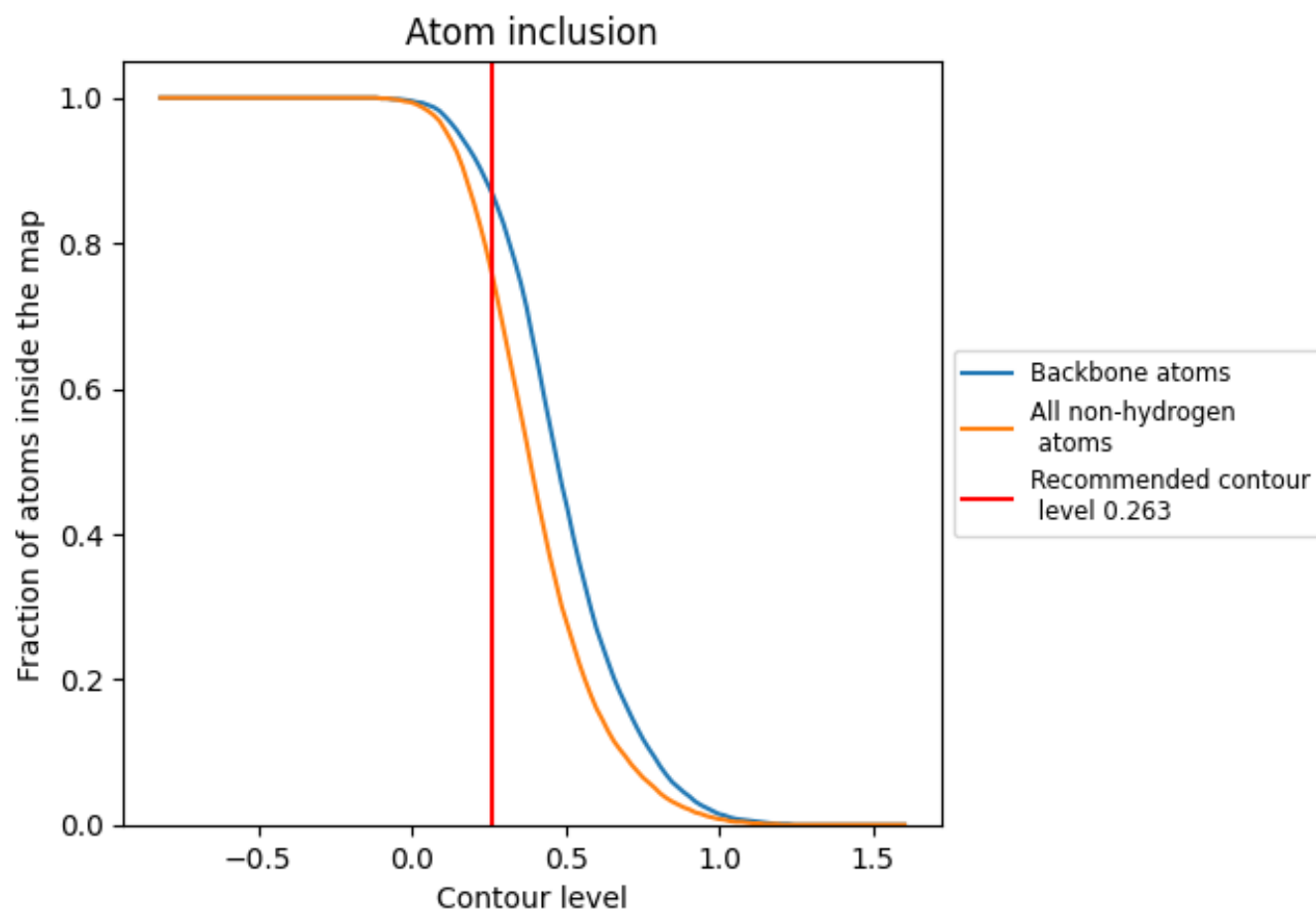
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.263).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 75% 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 (0.263) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7520	<div></div> 0.2890
A	<div></div> 0.7480	<div></div> 0.2870
B	<div></div> 0.7490	<div></div> 0.2880
C	<div></div> 0.7490	<div></div> 0.2880
D	<div></div> 0.7490	<div></div> 0.2880
E	<div></div> 0.9160	<div></div> 0.3620
F	<div></div> 0.9160	<div></div> 0.3620
G	<div></div> 0.9160	<div></div> 0.3620
H	<div></div> 0.9160	<div></div> 0.3620

1.0

0.0

<0.0