



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 12:04 AM UTC

PDB ID : 5TAZ / pdb_00005taz
EMDB ID : EMD-8390
Title : Structure of rabbit RyR1 (ryanodine dataset, class 3)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on : 2016-09-10
Resolution : 4.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

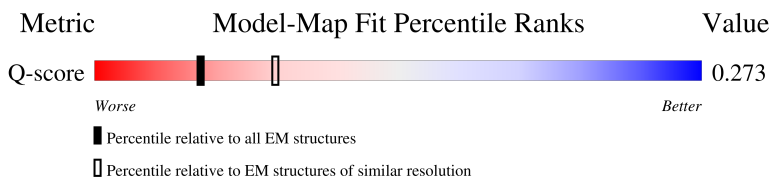
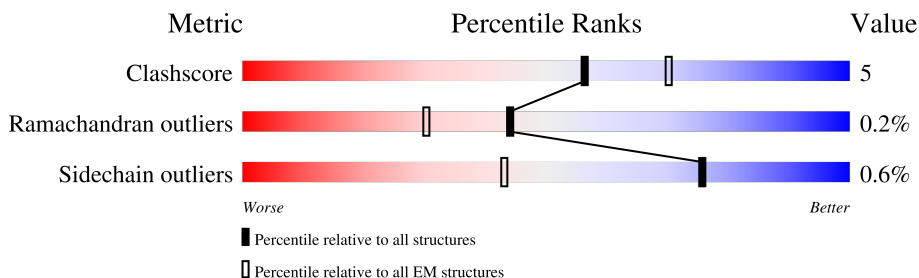
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4585 (3.80 - 4.80)

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

Mol	Chain	Length	Quality of chain
1	A	108	31% 87% 12% .
1	F	108	31% 89% 10% .
1	H	108	31% 88% 11% .
1	J	108	31% 89% 10% .

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Mol	Chain	Length	Quality of chain			
2	B	4416		38%	84%	10% 5%
2	E	4416		38%	84%	10% 5%
2	G	4416		38%	84%	10% 5%
2	I	4416		38%	84%	10% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 121276 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	J	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

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

Mol	Chain	Residues	Atoms		AltConf
3	B	1	Total	Zn	0
			1	1	
3	I	1	Total	Zn	0
			1	1	
3	G	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	

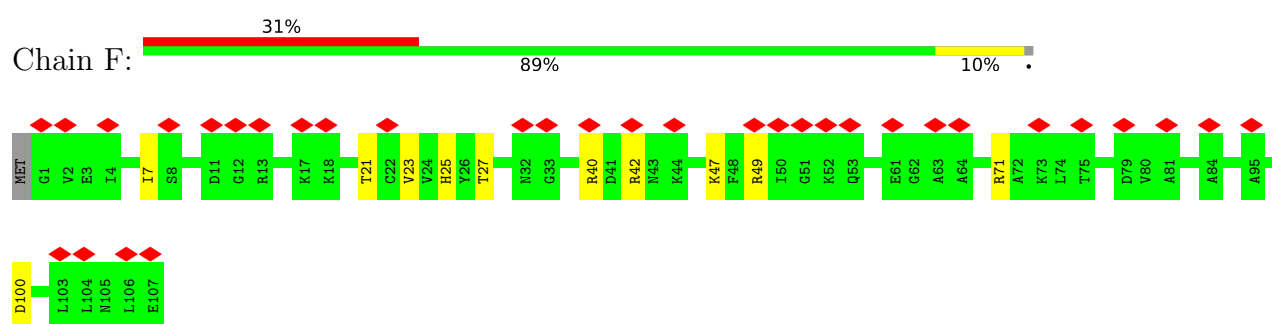
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total 1	Ca 1	0
4	I	1	Total 1	Ca 1	0
4	G	1	Total 1	Ca 1	0
4	E	1	Total 1	Ca 1	0

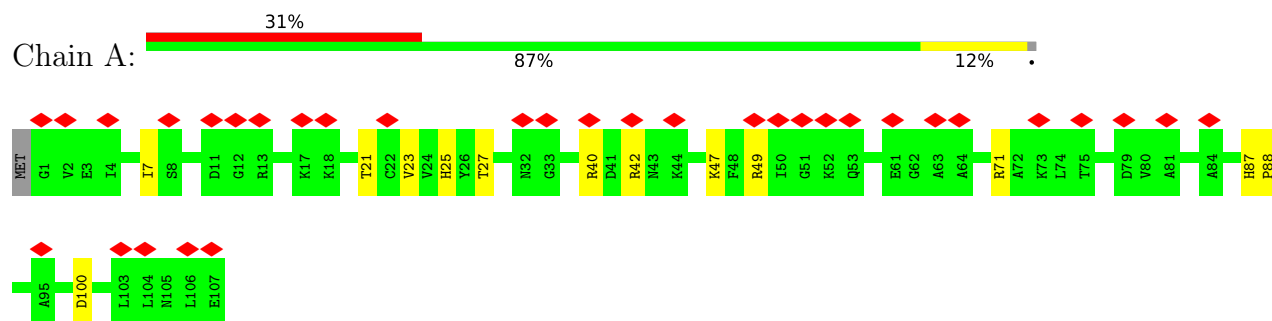
3 Residue-property plots [i](#)

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

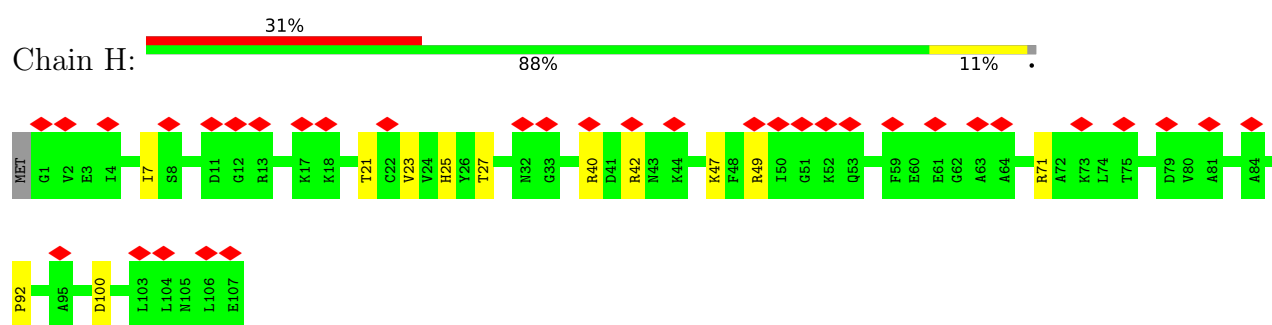
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



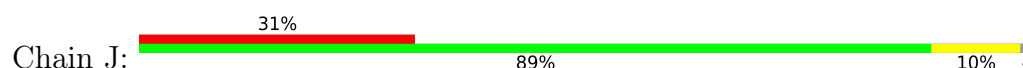
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

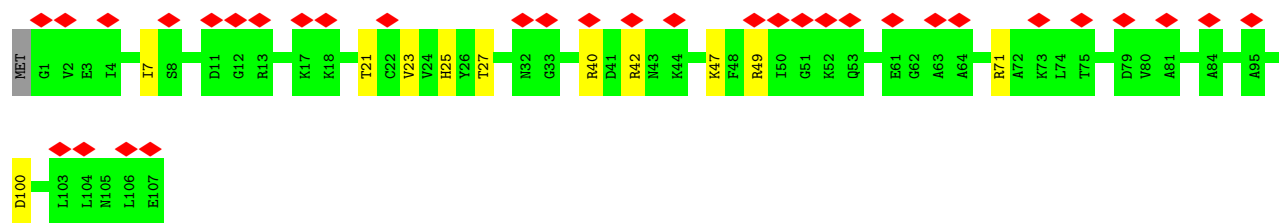


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

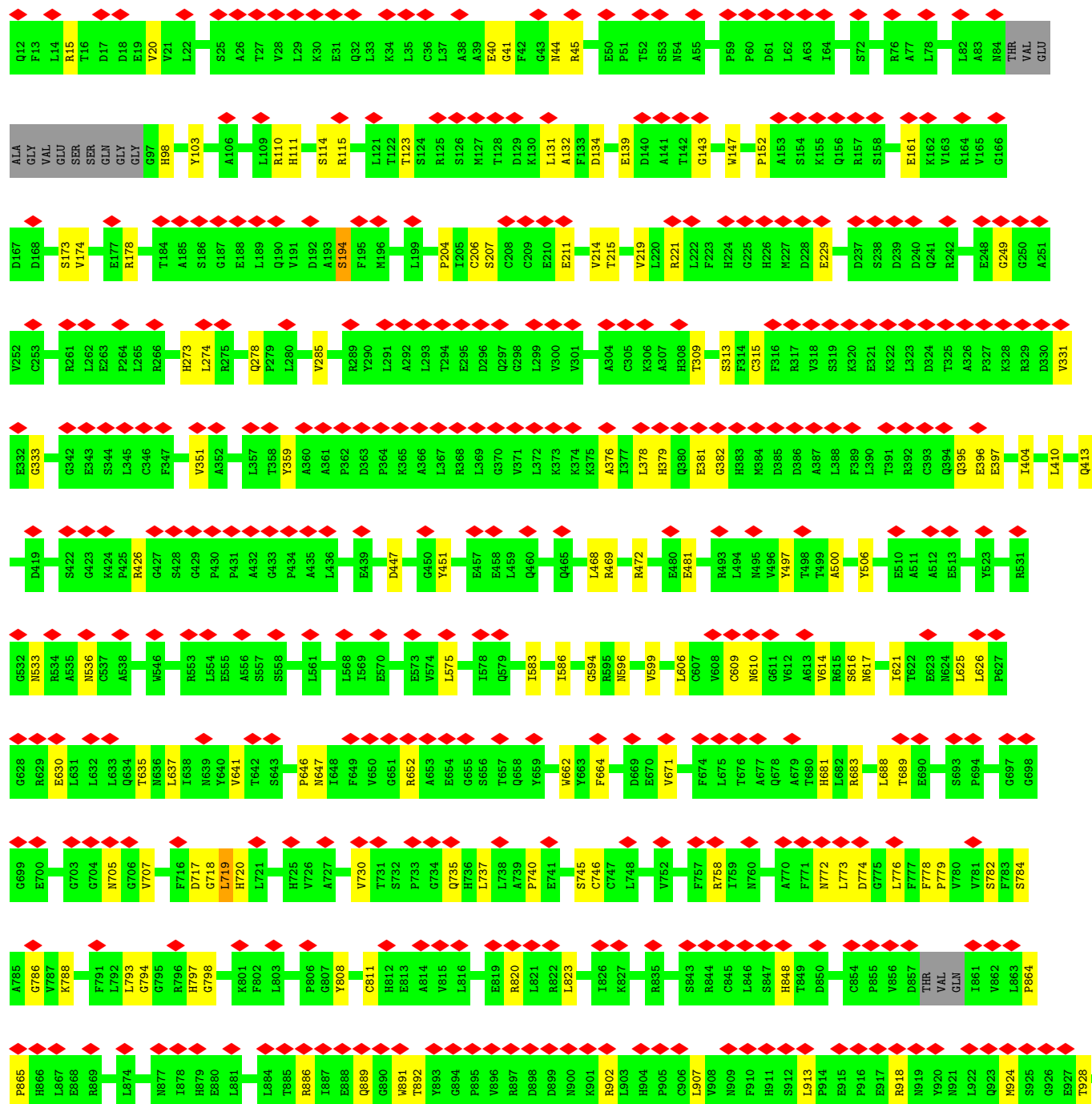
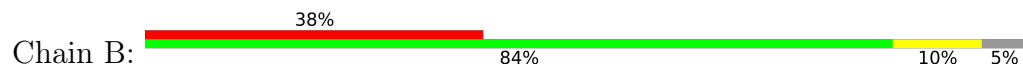


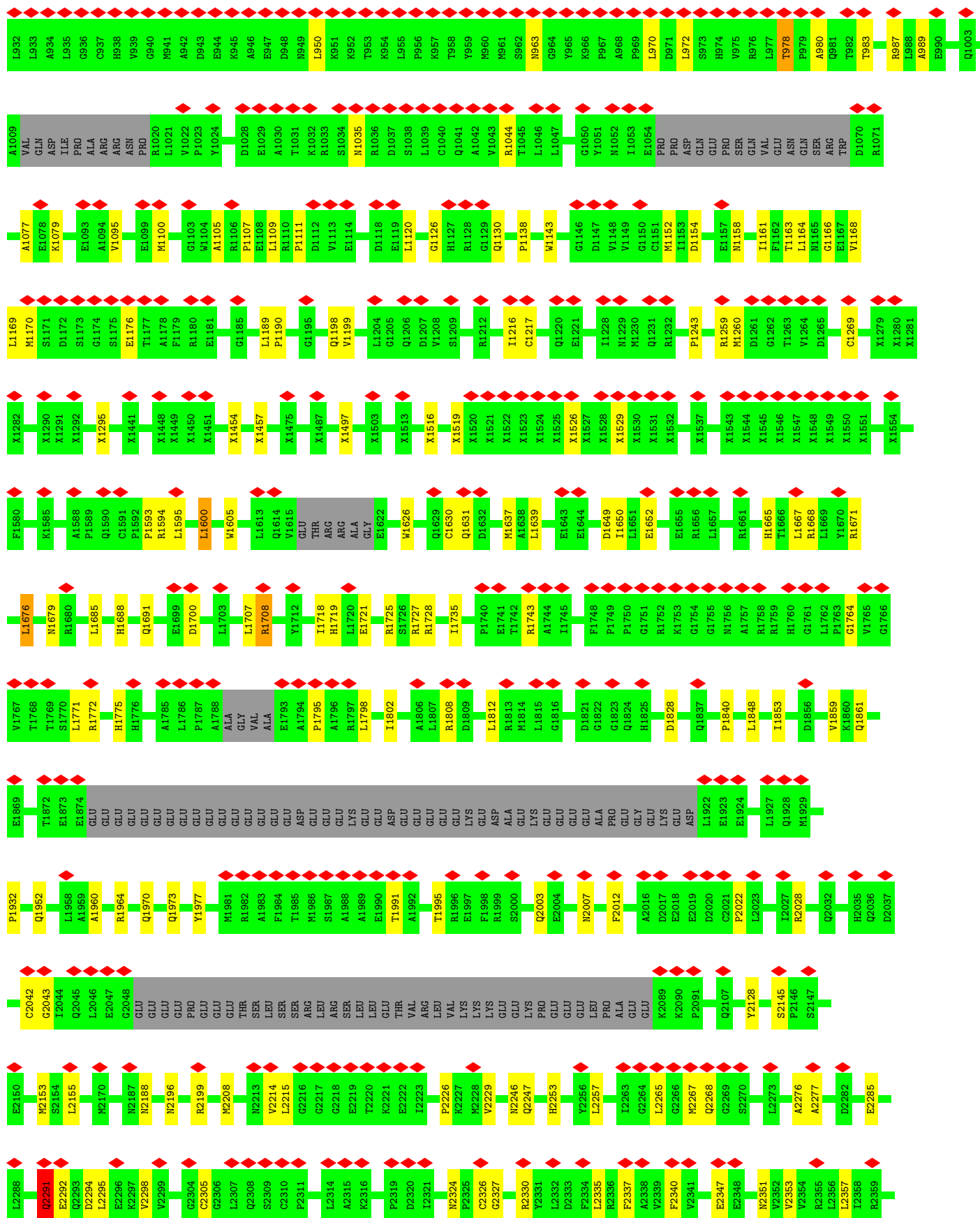
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



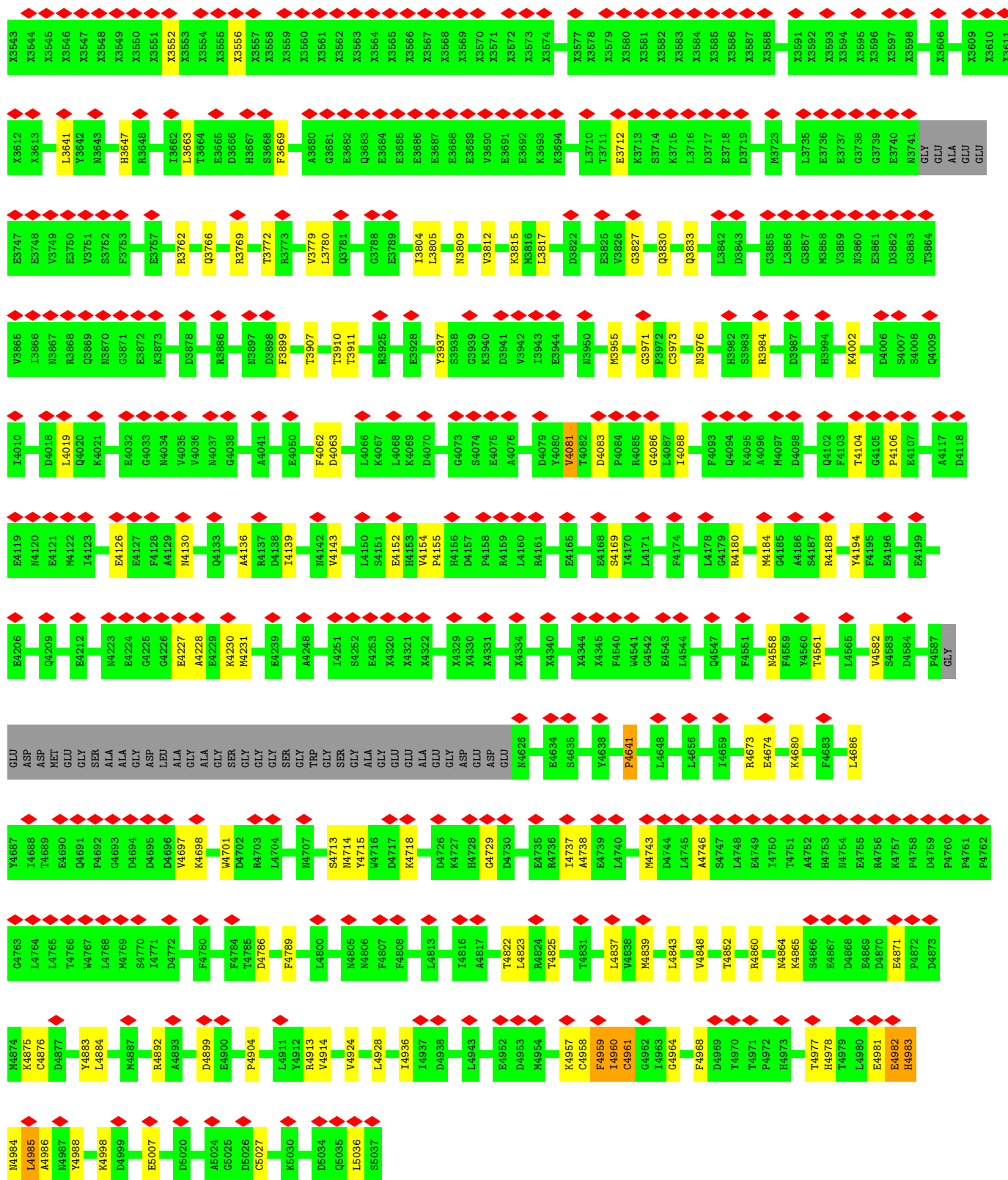


• Molecule 2: Ryanodine receptor 1

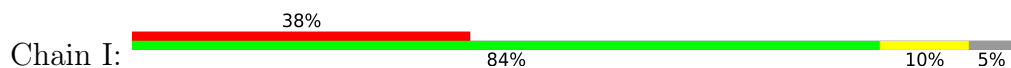


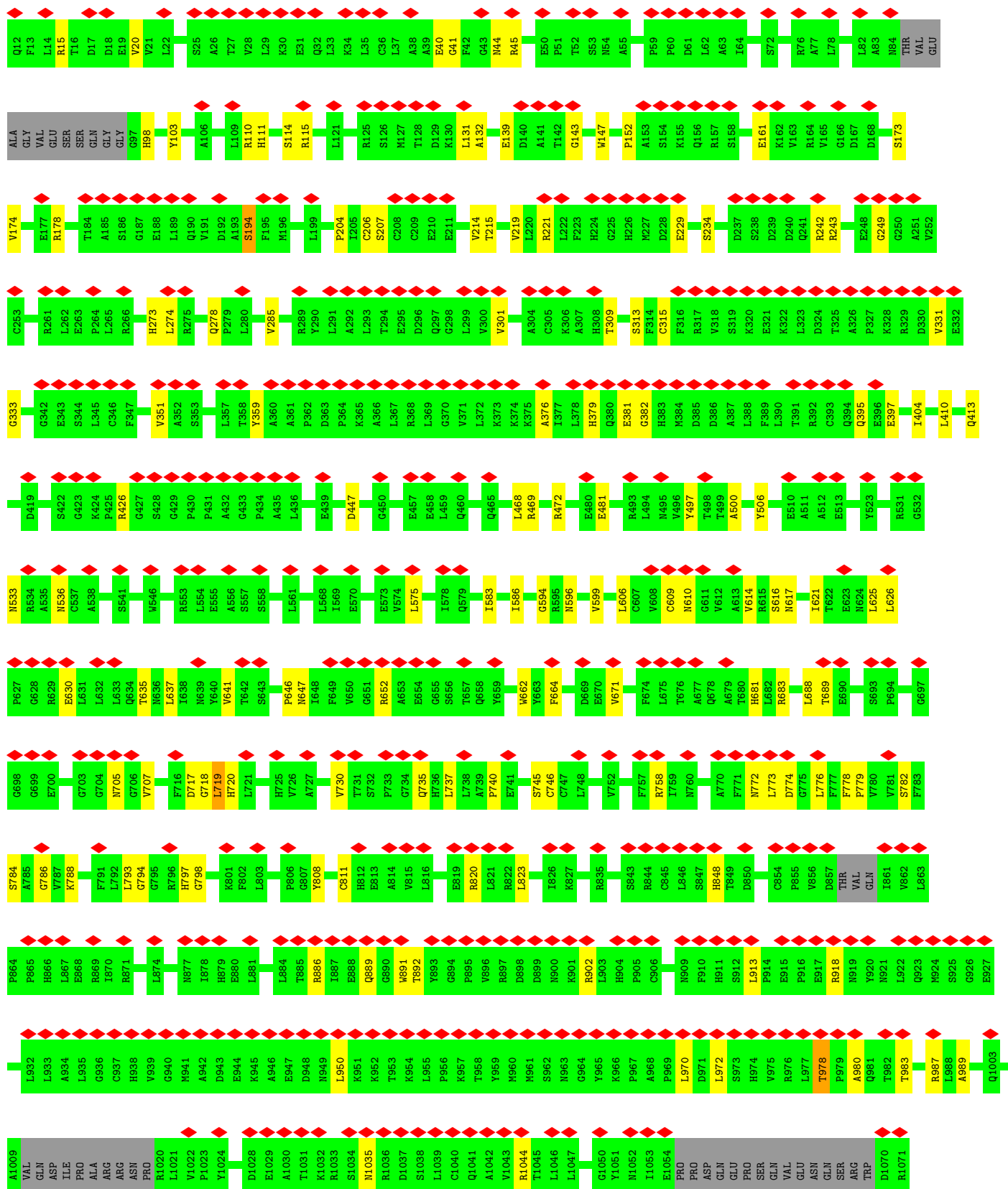


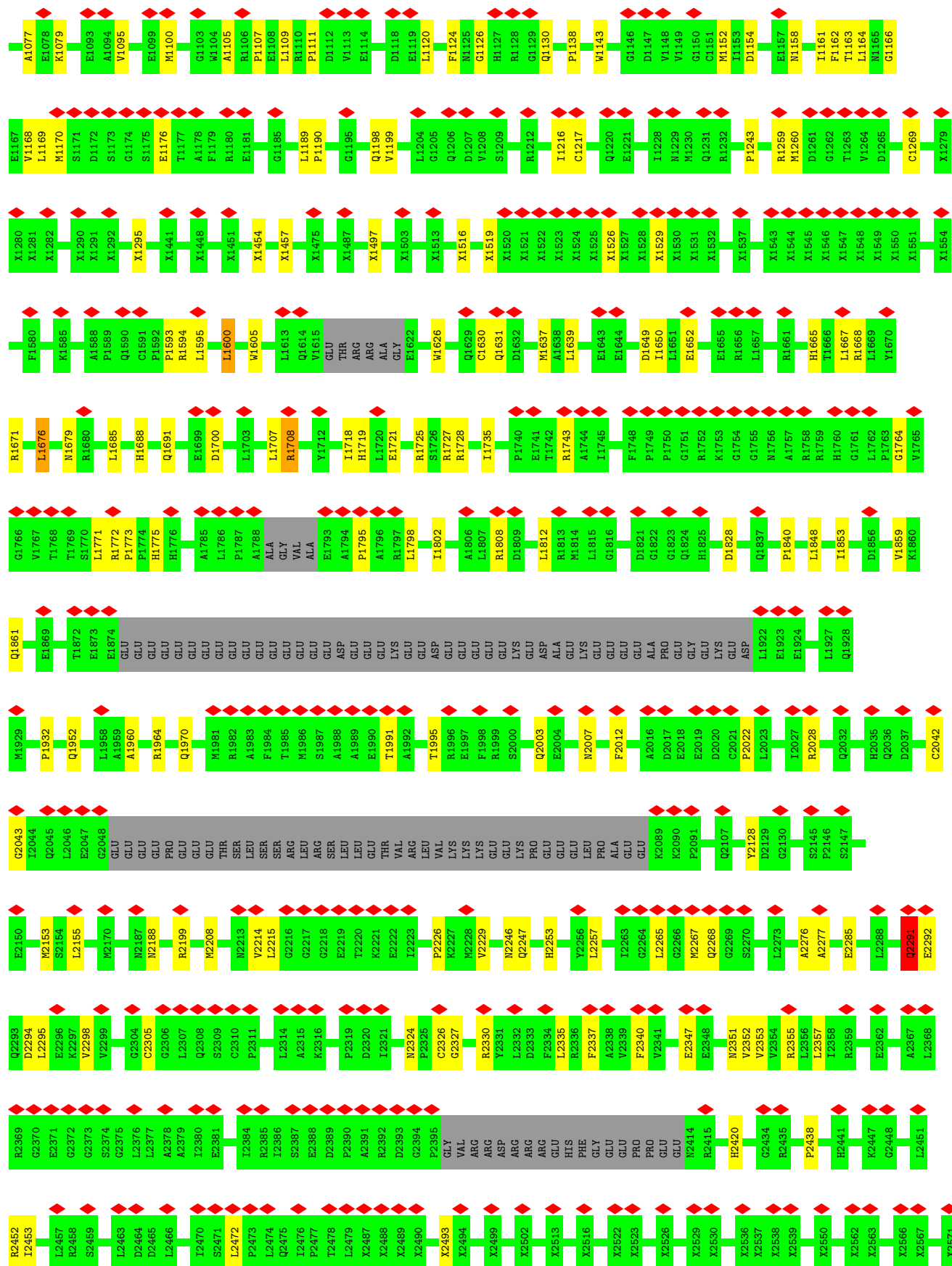
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E2362	A2367	L2368	R2369	G2370	E2371	G2372	G2373	S2374	G2375	L2376	L2377	A2378	A2379	L2380	E2381	L2384	R2385	L2386	S2387	E2388	D2389	P2390	A2391	R2392	D2393	G2394	P2395	GLY	VAL	ARG	ARG	ASP	ARG	ARG	ARG	ARG	HIS	PHE	GLY	GLU	GLU	PRO	PRO	GLU	GLU	N2414	R2415	H2420	L2430	G2434	R2435	C2436	A2437	P2438					



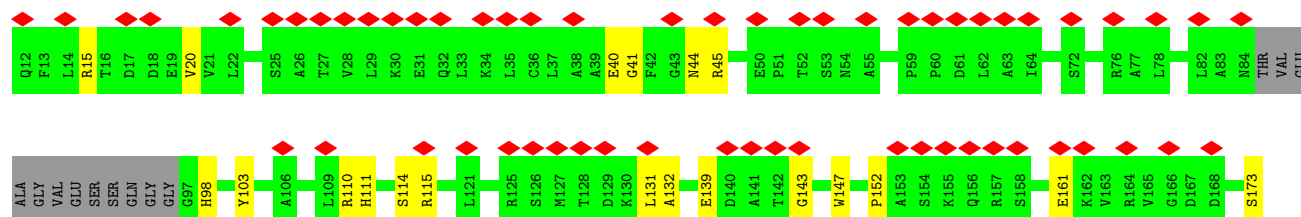
• Molecule 2: Ryanodine receptor 1







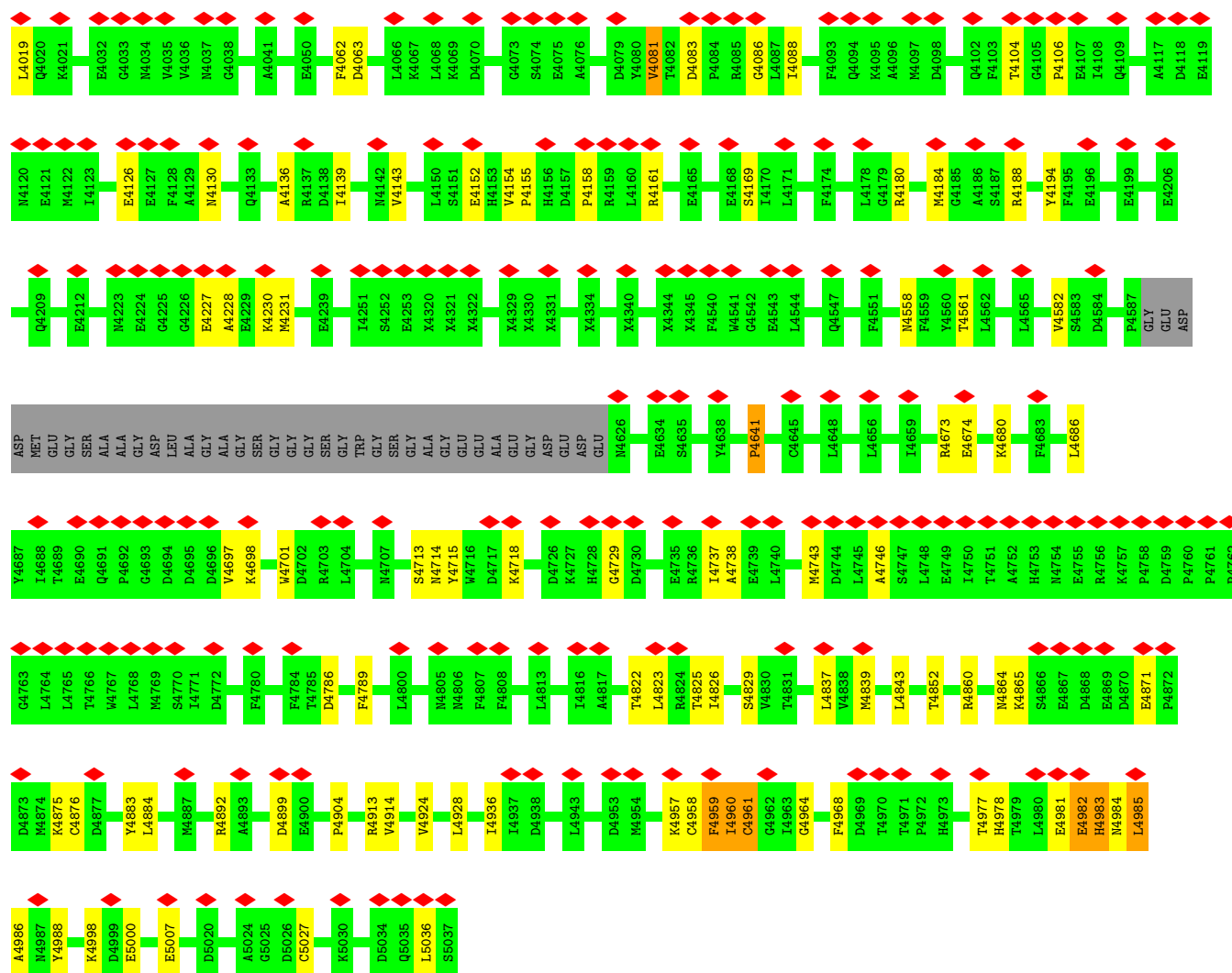
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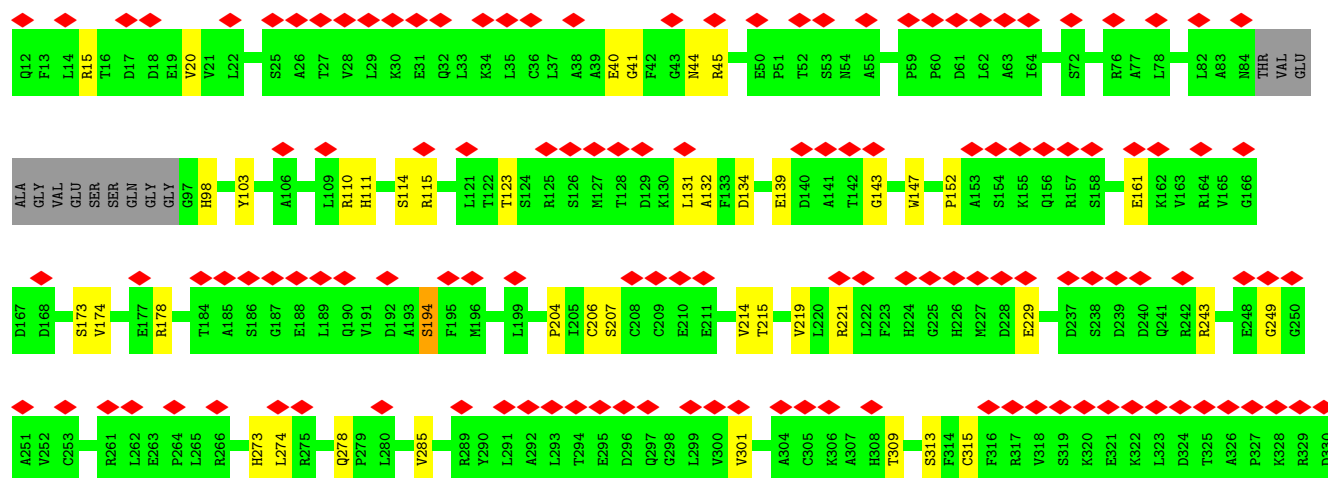
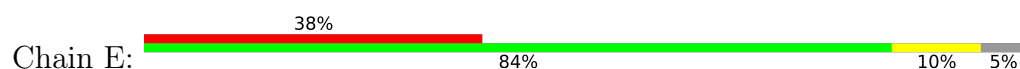


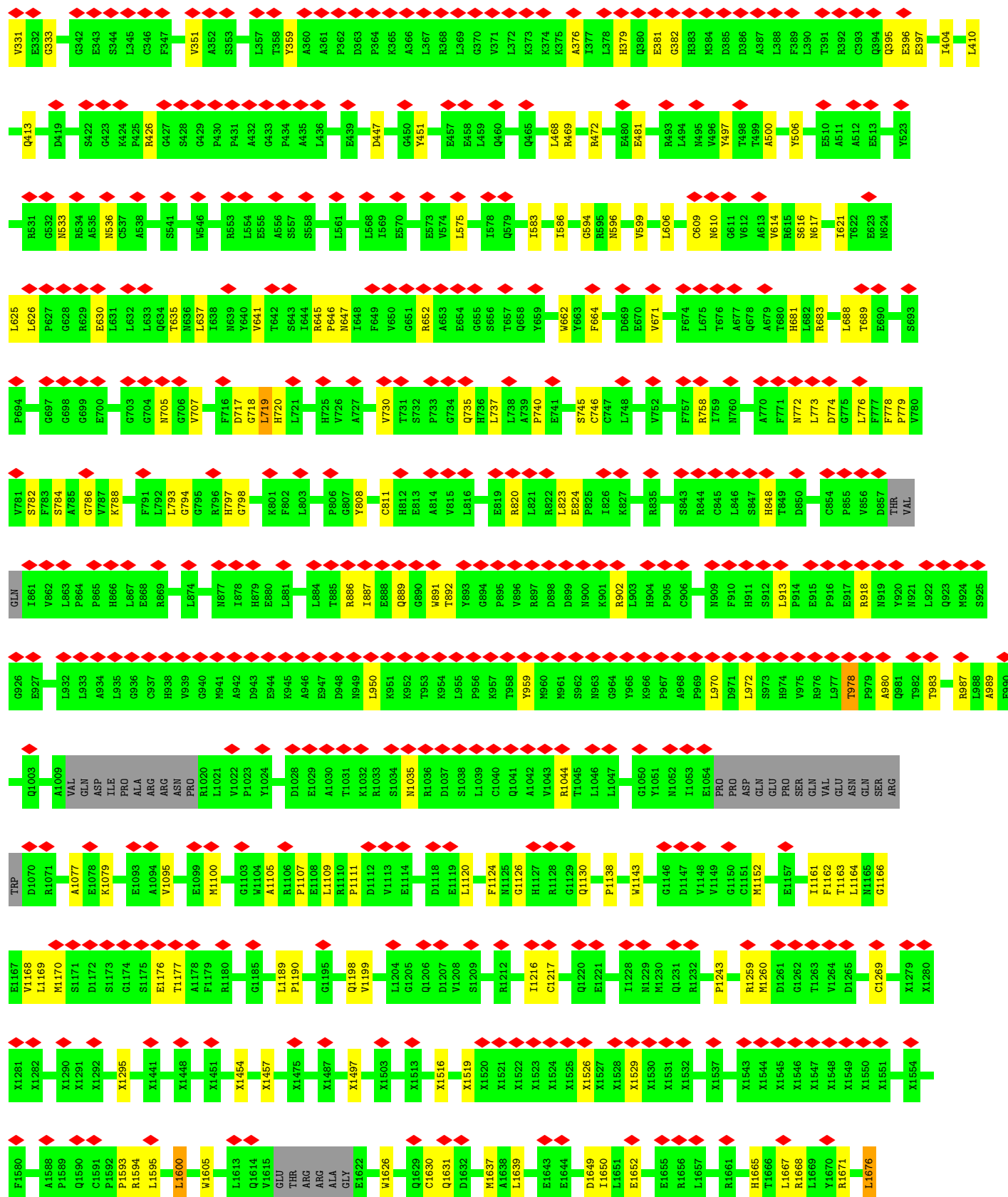


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• Molecule 2: Ryanodine receptor 1







N2884	X2946	X3049	X3215	X3286	X3360	X3436	X3548	N3643	V3749	V3865	K4021	N4122
T2885	X2947	X3050	X3216	X3287	X3361	X3437	X3549	H3647	E3750	I3866	E4032	I4123
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G2887	X2949	X3062	X3218	X3289	X3363	X3442	X3551	I3652	S3752	R3868	N4034	E4127
R2888	X2950	X3063	X3219	X3290	X3364	X3443	X3552	L3653	F3753	Q3869	V4035	F4128
R2889	X2951	X3062	X3220	X3291	X3365	X3444	X3553	L3654	E3757	N3870	V4036	A4129
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Q2892	X2954	X3062	X3223	X3294	X3368	X3447	X3556	E3666	K3761	K3873	A4041	A4136
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K2897	X2959	X3062	X3228	X3299	X3373	X3452	X3561	A3680	T3772	N3887	D4065	V4143
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F2929	X2991	X3062	X3260	X3331	X3405	X3484	X3593	GLY	G3863	L4018	D4118	Q4209
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G2933	X2995	X3062	X3264	X3335	X3409	X3488	X3597	GLU				
G2934	X2996	X3062	X3265	X3336	X3410	X3489	X3598					
Y2935	X2997	X3062	X3266	X3337	X3411	X3490	X3599					
A2936	X2998	X3062	X3267	X3338	X3412	X3491	X3600					
R2937	X2999	X3062	X3268	X3339	X3413	X3492	X3601					
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R2939	X3001	X3062	X3270	X3341	X3415	X3494	X3603					
X2942	X3002	X3062	X3271	X3342	X3416	X3495	X3604					
X2943	X3003	X3062	X3272	X3343	X3417	X3496	X3605					
X2944	X3004	X3062	X3273	X3344	X3418	X3497	X3606					
X2945	X3005	X3062	X3274	X3345	X3419	X3498	X3607					
	X3006	X3062	X3275	X3346	X3420	X3499	X3608					
	X3007	X3062	X3276	X3347	X3421	X3500	X3609					
	X3008	X3062	X3277	X3348	X3422	X3501	X3610					
	X3009	X3062	X3278	X3349	X3423	X3502	X3611					
	X3010	X3062	X3279	X3350	X3424	X3503	X3612					
	X3011	X3062	X3280	X3351	X3425	X3504	X3613					
	X3012	X3062	X3281	X3352	X3426	X3505	X3614					
	X3013	X3062	X3282	X3353	X3427	X3506	X3615					
	X3014	X3062	X3283	X3354	X3428	X3507	X3616					
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	X3016	X3062	X3285	X3356	X3430	X3509	X3618					
	X3017	X3062	X3286	X3357	X3431	X3510	X3619					
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	X3025	X3062	X3294	X3365	X3439	X3518	X3627					
	X3026	X3062	X3295	X3366	X3440	X3519	X3628					
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	X3031	X3062	X3300	X3371	X3445	X3524	X3633					
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	X3033	X3062	X3302	X3373	X3447	X3526	X3635					
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	X3038	X3062	X3307	X3378	X3452	X3531	X3640					
	X3039	X3062	X3308	X3379	X3453	X3532	X3641					
	X3040	X3062	X3309	X3380	X3454	X3533	X3642					
	X3041	X3062	X3310	X3381	X3455	X3534	X3643					
	X3042	X3062	X3311	X3382	X3456	X3535	X3644					
	X3043	X3062	X3312	X3383	X3457	X3536	X3645					
	X3044	X3062	X3313	X3384	X3458	X3537	X3646					
	X3045	X3062	X3314	X3385	X3459	X3538	X3647					
	X3046	X3062	X3315	X3386	X3460	X3539	X3648					
	X3047	X3062	X3316	X3387	X3461	X3540	X3649					
	X3048	X3062	X3317	X3388	X3462	X3541	X3650					
		X3062	X3318	X3389	X3463	X3542	X3651					
		X3062	X3319	X3390	X3464	X3543	X3652					
		X3062	X3320	X3391	X3465	X3544	X3653					
		X3062	X3321	X3392	X3466	X3545	X3654					
		X3062	X3322	X3393	X3467	X3546	X3655					
		X3062	X3323	X3394	X3468	X3547	X3656					
		X3062	X3324	X3395	X3469	X3548	X3657					
		X3062	X3325	X3396	X3470	X3549	X3658					
		X3062	X3326	X3397	X3471	X3550	X3659					
		X3062	X3327	X3398	X3472	X3551	X3660					
		X3062	X3328	X3399	X3473	X3552	X3661					
		X3062	X3329	X3400	X3474	X3553	X3662					
		X3062	X3330	X3401	X3475	X3554	X3663					
		X3062	X3331	X3402	X3476	X3555	X3664					
		X3062	X3332	X3403	X3477	X3556	X3665					
		X3062	X3333	X3404	X3478	X3557	X3666					



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.147	Depositor
Minimum map value	-0.068	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.19	0/834	0.48	0/1123
1	F	0.19	0/834	0.48	0/1123
1	H	0.19	0/834	0.48	0/1123
1	J	0.19	0/834	0.48	0/1123
2	B	0.20	0/25428	0.51	3/34534 (0.0%)
2	E	0.20	0/25428	0.51	3/34534 (0.0%)
2	G	0.20	0/25428	0.51	3/34534 (0.0%)
2	I	0.20	0/25428	0.51	3/34534 (0.0%)
All	All	0.20	0/105048	0.51	12/142628 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	11
2	E	0	11
2	G	0	11
2	I	0	11
All	All	0	44

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	4960	ILE	N-CA-C	-6.71	105.30	111.67
2	B	4960	ILE	N-CA-C	-6.68	105.33	111.67
2	I	4960	ILE	N-CA-C	-6.68	105.33	111.67
2	E	4960	ILE	N-CA-C	-6.68	105.33	111.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2291	GLN	CA-C-N	5.70	132.43	121.54
2	B	2291	GLN	C-N-CA	5.70	132.43	121.54
2	I	2291	GLN	CA-C-N	5.70	132.43	121.54
2	I	2291	GLN	C-N-CA	5.70	132.43	121.54
2	G	2291	GLN	CA-C-N	5.69	132.42	121.54
2	G	2291	GLN	C-N-CA	5.69	132.42	121.54
2	E	2291	GLN	CA-C-N	5.69	132.41	121.54
2	E	2291	GLN	C-N-CA	5.69	132.41	121.54

There are no chirality outliers.

All (44) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	194	SER	Peptide
2	B	2291	GLN	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	3971	GLY	Peptide
2	B	4641	PRO	Peptide
2	B	808	TYR	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide
2	E	194	SER	Peptide
2	E	2291	GLN	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	3971	GLY	Peptide
2	E	4641	PRO	Peptide
2	E	808	TYR	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	Peptide
2	G	194	SER	Peptide
2	G	2291	GLN	Peptide
2	G	2472	LEU	Peptide

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Mol	Chain	Res	Type	Group
2	G	2807	TRP	Peptide
2	G	3971	GLY	Peptide
2	G	4641	PRO	Peptide
2	G	808	TYR	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1795	PRO	Peptide
2	I	1828	ASP	Peptide
2	I	194	SER	Peptide
2	I	2291	GLN	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	3971	GLY	Peptide
2	I	4641	PRO	Peptide
2	I	808	TYR	Peptide

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	818	0	824	7	0
1	F	818	0	824	6	0
1	H	818	0	824	7	0
1	J	818	0	824	6	0
2	B	29499	0	24749	274	0
2	E	29499	0	24749	272	0
2	G	29499	0	24749	275	0
2	I	29499	0	24748	272	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
All	All	121276	0	102291	1086	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (1086) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4968:PHE:CE2	2:E:4978:HIS:CE1	2.18	1.32
2:B:4968:PHE:CE2	2:B:4978:HIS:CE1	2.18	1.32
2:I:4968:PHE:CE2	2:I:4978:HIS:CE1	2.18	1.30
2:G:4968:PHE:CE2	2:G:4978:HIS:CE1	2.18	1.30
2:B:4968:PHE:HE2	2:B:4978:HIS:CE1	1.67	1.02
2:I:4968:PHE:HE2	2:I:4978:HIS:CE1	1.67	0.96
2:G:4968:PHE:CE2	2:G:4978:HIS:HE1	1.81	0.95
2:I:4968:PHE:CE2	2:I:4978:HIS:HE1	1.81	0.94
2:E:4968:PHE:HE2	2:E:4978:HIS:CE1	1.67	0.93
2:E:4968:PHE:CE2	2:E:4978:HIS:HE1	1.81	0.92
2:G:4968:PHE:HE2	2:G:4978:HIS:CE1	1.67	0.91
2:B:4968:PHE:CE2	2:B:4978:HIS:HE1	1.81	0.91
2:I:4968:PHE:CE2	2:I:4978:HIS:ND1	2.43	0.87
2:I:4982:GLU:HG3	2:I:5027:CYS:SG	2.15	0.86
2:E:4968:PHE:CE2	2:E:4978:HIS:ND1	2.43	0.86
2:E:4982:GLU:HG3	2:E:5027:CYS:SG	2.15	0.86
2:G:4982:GLU:HG3	2:G:5027:CYS:SG	2.15	0.85
2:B:4982:GLU:HG3	2:B:5027:CYS:SG	2.15	0.85
2:B:4968:PHE:CE2	2:B:4978:HIS:ND1	2.43	0.85
2:G:4968:PHE:CE2	2:G:4978:HIS:ND1	2.43	0.84
2:G:4968:PHE:CD2	2:G:4978:HIS:ND1	2.52	0.78
2:E:4960:ILE:HD11	2:E:4985:LEU:HD23	1.66	0.77
2:I:4968:PHE:CD2	2:I:4978:HIS:ND1	2.52	0.77
2:B:4960:ILE:HD11	2:B:4985:LEU:HD23	1.66	0.77
2:B:4968:PHE:CD2	2:B:4978:HIS:ND1	2.52	0.77
2:E:4968:PHE:CD2	2:E:4978:HIS:ND1	2.52	0.76
2:I:4960:ILE:HD11	2:I:4985:LEU:HD23	1.66	0.76
2:G:4960:ILE:HD11	2:G:4985:LEU:HD23	1.66	0.76
2:B:4230:LYS:HD2	2:B:4959:PHE:CD1	2.25	0.72
2:I:4230:LYS:HD2	2:I:4959:PHE:CD1	2.25	0.71
2:E:4230:LYS:HD2	2:E:4959:PHE:CD1	2.25	0.70
2:G:4230:LYS:HD2	2:G:4959:PHE:CD1	2.25	0.70
2:E:379:HIS:HD2	2:E:382:GLY:H	1.39	0.69
2:B:379:HIS:HD2	2:B:382:GLY:H	1.39	0.68
2:I:4230:LYS:HG3	2:I:4959:PHE:HE1	1.57	0.68
2:G:4230:LYS:HG3	2:G:4959:PHE:HE1	1.57	0.68
2:G:379:HIS:HD2	2:G:382:GLY:H	1.39	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4230:LYS:HG3	2:B:4959:PHE:HE1	1.57	0.67
2:E:4230:LYS:HG3	2:E:4959:PHE:HE1	1.57	0.67
2:I:379:HIS:HD2	2:I:382:GLY:H	1.39	0.67
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.77	0.67
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.77	0.67
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.77	0.66
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.77	0.66
2:I:4984:ASN:C	2:I:4986:ALA:H	2.04	0.66
2:G:4984:ASN:C	2:G:4986:ALA:H	2.04	0.66
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.61	0.65
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.61	0.65
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.61	0.65
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.79	0.65
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.79	0.65
2:B:4983:HIS:HD2	2:B:4988:TYR:OH	1.80	0.65
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.61	0.64
2:B:4984:ASN:C	2:B:4986:ALA:H	2.04	0.64
2:B:3762:ARG:O	2:B:3766:GLN:NE2	2.30	0.64
2:I:3762:ARG:O	2:I:3766:GLN:NE2	2.30	0.64
2:G:3762:ARG:O	2:G:3766:GLN:NE2	2.30	0.64
2:I:4957:LYS:HE2	2:I:4964:GLY:CA	2.27	0.64
2:E:4984:ASN:C	2:E:4986:ALA:H	2.04	0.64
2:B:4957:LYS:HE2	2:B:4964:GLY:CA	2.27	0.64
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.80	0.64
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.79	0.63
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.79	0.63
2:E:3762:ARG:O	2:E:3766:GLN:NE2	2.30	0.63
2:E:4957:LYS:HE2	2:E:4964:GLY:CA	2.27	0.63
2:E:4983:HIS:HD2	2:E:4988:TYR:OH	1.80	0.63
2:I:4983:HIS:HD2	2:I:4988:TYR:OH	1.80	0.63
2:G:4957:LYS:HE2	2:G:4964:GLY:CA	2.27	0.63
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.80	0.63
2:G:4983:HIS:HD2	2:G:4988:TYR:OH	1.80	0.63
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.80	0.63
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.81	0.63
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.81	0.63
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.80	0.62
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.81	0.62
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.81	0.62
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.81	0.62
2:B:313:SER:HB3	2:B:351:VAL:HB	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1637:MET:SD	2:E:1708:ARG:NH1	2.73	0.61
2:B:1637:MET:SD	2:B:1708:ARG:NH1	2.74	0.61
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.82	0.61
2:G:313:SER:HB3	2:G:351:VAL:HB	1.82	0.61
2:I:313:SER:HB3	2:I:351:VAL:HB	1.82	0.61
2:I:1637:MET:SD	2:I:1708:ARG:NH1	2.74	0.61
2:E:359:TYR:HA	2:E:376:ALA:HA	1.83	0.61
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.34	0.61
2:E:313:SER:HB3	2:E:351:VAL:HB	1.82	0.61
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.34	0.60
2:G:359:TYR:HA	2:G:376:ALA:HA	1.83	0.60
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.83	0.60
2:B:331:VAL:HG12	2:B:333:GLY:H	1.66	0.60
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.34	0.60
2:G:4230:LYS:HD2	2:G:4959:PHE:HD1	1.66	0.60
2:G:1637:MET:SD	2:G:1708:ARG:NH1	2.74	0.60
2:I:331:VAL:HG12	2:I:333:GLY:H	1.66	0.60
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.67	0.60
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.84	0.60
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.83	0.60
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.83	0.60
2:I:4984:ASN:O	2:I:4986:ALA:N	2.35	0.60
2:E:4230:LYS:HD2	2:E:4959:PHE:HD1	1.67	0.60
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.67	0.60
2:G:4582:VAL:HG11	2:E:4860:ARG:HD2	1.82	0.60
2:G:4984:ASN:O	2:G:4986:ALA:N	2.35	0.60
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.67	0.60
2:B:359:TYR:HA	2:B:376:ALA:HA	1.83	0.59
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.84	0.59
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.83	0.59
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.84	0.59
2:I:359:TYR:HA	2:I:376:ALA:HA	1.83	0.59
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.84	0.59
2:E:4904:PRO:HB3	2:E:4913:ARG:HD3	1.85	0.59
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.84	0.59
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.36	0.59
2:B:4904:PRO:HB3	2:B:4913:ARG:HD3	1.85	0.59
2:E:4126:GLU:O	2:E:4130:ASN:ND2	2.35	0.59
2:E:4984:ASN:O	2:E:4986:ALA:N	2.35	0.59
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.85	0.59
2:B:4126:GLU:O	2:B:4130:ASN:ND2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4968:PHE:CZ	2:B:4978:HIS:HE1	2.20	0.59
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.85	0.59
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.67	0.59
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.34	0.59
2:E:331:VAL:HG12	2:E:333:GLY:H	1.66	0.59
2:E:1152:MET:HE1	2:E:1217:CYS:HB3	1.84	0.59
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.84	0.59
2:E:111:HIS:HD2	2:E:114:SER:H	1.50	0.59
2:B:111:HIS:HD2	2:B:114:SER:H	1.50	0.59
2:I:4904:PRO:HB3	2:I:4913:ARG:HD3	1.85	0.59
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.34	0.59
2:E:4968:PHE:CZ	2:E:4978:HIS:HE1	2.20	0.59
2:I:1152:MET:HE1	2:I:1217:CYS:HB3	1.84	0.59
2:G:111:HIS:HD2	2:G:114:SER:H	1.50	0.59
2:G:331:VAL:HG12	2:G:333:GLY:H	1.66	0.59
2:G:1152:MET:HE1	2:G:1217:CYS:HB3	1.84	0.59
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.84	0.59
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.85	0.58
2:I:4126:GLU:O	2:I:4130:ASN:ND2	2.35	0.58
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.34	0.58
2:B:4984:ASN:O	2:B:4986:ALA:N	2.35	0.58
2:I:4230:LYS:HD2	2:I:4959:PHE:HD1	1.67	0.58
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.68	0.58
2:G:978:THR:HB	2:G:980:ALA:H	1.67	0.58
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.83	0.58
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.68	0.58
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.34	0.58
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.36	0.58
2:I:4968:PHE:CZ	2:I:4978:HIS:HE1	2.20	0.58
2:G:4904:PRO:HB3	2:G:4913:ARG:HD3	1.85	0.58
2:G:4968:PHE:CZ	2:G:4978:HIS:HE1	2.20	0.58
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.84	0.58
2:I:978:THR:HB	2:I:980:ALA:H	1.68	0.58
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.34	0.58
2:I:173:SER:HB3	2:I:178:ARG:H	1.69	0.58
2:G:4126:GLU:O	2:G:4130:ASN:ND2	2.35	0.58
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.36	0.58
2:B:978:THR:HB	2:B:980:ALA:H	1.67	0.58
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.85	0.58
2:B:2827:ARG:HH21	2:B:2931:GLN:HG3	1.69	0.58
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.36	0.58
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.85	0.58
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.69	0.58
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.34	0.58
2:I:2827:ARG:HH21	2:I:2931:GLN:HG3	1.69	0.58
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.69	0.57
2:G:173:SER:HB3	2:G:178:ARG:H	1.69	0.57
2:E:978:THR:HB	2:E:980:ALA:H	1.68	0.57
2:B:173:SER:HB3	2:B:178:ARG:H	1.69	0.57
2:B:1152:MET:HE1	2:B:1217:CYS:HB3	1.84	0.57
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.86	0.57
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.86	0.57
2:I:111:HIS:HD2	2:I:114:SER:H	1.50	0.57
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.86	0.57
2:E:173:SER:HB3	2:E:178:ARG:H	1.69	0.57
2:B:4230:LYS:HD2	2:B:4959:PHE:HD1	1.67	0.57
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.68	0.57
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.87	0.57
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.68	0.57
2:G:40:GLU:HB3	2:G:44:ASN:HB3	1.87	0.57
2:G:2827:ARG:HH21	2:G:2931:GLN:HG3	1.69	0.57
2:E:40:GLU:HB3	2:E:44:ASN:HB3	1.87	0.57
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.38	0.57
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.38	0.57
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.38	0.57
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.69	0.57
2:B:4924:VAL:HA	2:B:4928:LEU:HB2	1.87	0.56
2:I:889:GLN:O	2:I:902:ARG:NH1	2.39	0.56
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.86	0.56
2:E:889:GLN:O	2:E:902:ARG:NH1	2.38	0.56
2:E:2827:ARG:HH21	2:E:2931:GLN:HG3	1.69	0.56
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.79	0.56
2:I:4924:VAL:HA	2:I:4928:LEU:HB2	1.87	0.56
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.38	0.56
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.79	0.56
2:B:889:GLN:O	2:B:902:ARG:NH1	2.38	0.56
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.88	0.56
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.87	0.56
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.79	0.56
2:I:40:GLU:HB3	2:I:44:ASN:HB3	1.87	0.56
2:I:2347:GLU:O	2:I:2351:ASN:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:609:CYS:SG	2:B:610:ASN:N	2.79	0.56
2:B:2452:ARG:NH1	2:I:174:VAL:O	2.39	0.56
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.79	0.56
2:E:2347:GLU:O	2:E:2351:ASN:N	2.39	0.56
2:E:4924:VAL:HA	2:E:4928:LEU:HB2	1.87	0.56
2:B:40:GLU:HB3	2:B:44:ASN:HB3	1.87	0.55
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.39	0.55
2:G:889:GLN:O	2:G:902:ARG:NH1	2.38	0.55
2:G:4180:ARG:NH1	2:G:4981:GLU:OE1	2.39	0.55
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.39	0.55
2:G:1170:MET:HE1	2:G:1176:GLU:HG3	1.88	0.55
2:B:174:VAL:O	2:E:2452:ARG:NH1	2.39	0.55
2:B:2347:GLU:O	2:B:2351:ASN:N	2.39	0.55
2:G:4924:VAL:HA	2:G:4928:LEU:HB2	1.87	0.55
2:E:4984:ASN:C	2:E:4986:ALA:N	2.65	0.55
2:B:4180:ARG:NH1	2:B:4981:GLU:OE1	2.39	0.55
2:G:2347:GLU:O	2:G:2351:ASN:N	2.39	0.55
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.72	0.55
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.39	0.55
2:I:609:CYS:SG	2:I:610:ASN:N	2.79	0.55
2:I:2452:ARG:NH1	2:G:174:VAL:O	2.40	0.55
2:G:609:CYS:SG	2:G:610:ASN:N	2.79	0.55
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.39	0.55
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.34	0.55
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.89	0.55
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.89	0.55
2:G:2452:ARG:NH1	2:E:174:VAL:O	2.40	0.55
2:E:609:CYS:SG	2:E:610:ASN:N	2.79	0.55
2:E:4957:LYS:HE2	2:E:4964:GLY:HA2	1.88	0.55
2:B:1170:MET:HE1	2:B:1176:GLU:HG3	1.88	0.54
2:B:4984:ASN:C	2:B:4986:ALA:N	2.64	0.54
1:A:21:THR:HA	1:A:49:ARG:HA	1.89	0.54
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.34	0.54
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.89	0.54
2:I:4957:LYS:HE2	2:I:4964:GLY:HA2	1.88	0.54
2:I:4984:ASN:C	2:I:4986:ALA:N	2.64	0.54
2:E:1170:MET:HE1	2:E:1176:GLU:HG3	1.88	0.54
2:I:4180:ARG:NH1	2:I:4981:GLU:OE1	2.39	0.54
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.89	0.54
1:H:21:THR:HA	1:H:49:ARG:HA	1.89	0.54
2:I:1170:MET:HE1	2:I:1176:GLU:HG3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.89	0.54
2:G:4957:LYS:HE2	2:G:4964:GLY:HA2	1.88	0.54
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.72	0.54
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.72	0.54
1:H:7:ILE:HB	1:H:71:ARG:HB3	1.90	0.54
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.90	0.54
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.89	0.54
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.72	0.54
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.89	0.54
1:F:21:THR:HA	1:F:49:ARG:HA	1.89	0.54
2:B:4957:LYS:HE2	2:B:4964:GLY:HA2	1.88	0.54
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.89	0.54
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.41	0.54
2:E:4180:ARG:NH1	2:E:4981:GLU:OE1	2.39	0.54
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.90	0.53
2:B:4823:LEU:HD23	2:I:4843:LEU:HD12	1.91	0.53
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.89	0.53
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.41	0.53
1:F:7:ILE:HB	1:F:71:ARG:HB3	1.90	0.53
1:J:21:THR:HA	1:J:49:ARG:HA	1.89	0.53
2:I:730:VAL:O	2:I:735:GLN:NE2	2.41	0.53
2:B:730:VAL:O	2:B:735:GLN:NE2	2.41	0.53
2:G:1164:LEU:HB3	2:G:1169:LEU:HD21	1.91	0.53
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.41	0.53
2:B:1164:LEU:HB3	2:B:1169:LEU:HD21	1.91	0.53
2:B:4839:MET:HB3	2:E:4823:LEU:HD11	1.89	0.53
2:G:730:VAL:O	2:G:735:GLN:NE2	2.41	0.53
2:B:4843:LEU:HD12	2:E:4823:LEU:HD23	1.90	0.53
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.89	0.53
2:E:730:VAL:O	2:E:735:GLN:NE2	2.41	0.53
2:E:4865:LYS:HG3	2:E:4875:LYS:HZ3	1.74	0.53
2:B:111:HIS:CD2	2:B:114:SER:H	2.27	0.53
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.42	0.53
2:I:1164:LEU:HB3	2:I:1169:LEU:HD21	1.91	0.53
2:B:1667:LEU:HD23	2:B:1671:ARG:HH12	1.74	0.53
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.42	0.53
2:I:4674:GLU:HG3	2:I:4714:ASN:HB3	1.91	0.52
1:A:7:ILE:HB	1:A:71:ARG:HB3	1.90	0.52
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.89	0.52
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.41	0.52
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4865:LYS:HG3	2:G:4875:LYS:HZ3	1.74	0.52
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.89	0.52
2:E:1164:LEU:HB3	2:E:1169:LEU:HD21	1.91	0.52
2:B:4823:LEU:HD11	2:I:4839:MET:HB3	1.91	0.52
2:I:4823:LEU:HD23	2:G:4843:LEU:HD12	1.91	0.52
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.42	0.52
2:B:1650:ILE:HG13	2:B:1707:LEU:HD21	1.91	0.52
2:B:3804:ILE:O	2:B:3809:ASN:ND2	2.42	0.52
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.42	0.52
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.90	0.52
2:G:4674:GLU:HG3	2:G:4714:ASN:HB3	1.91	0.52
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.43	0.52
2:B:4674:GLU:HG3	2:B:4714:ASN:HB3	1.91	0.52
2:I:1667:LEU:HD23	2:I:1671:ARG:HH12	1.74	0.52
2:G:4823:LEU:HD23	2:E:4843:LEU:HD12	1.92	0.52
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.43	0.52
2:E:1650:ILE:HG13	2:E:1707:LEU:HD21	1.91	0.52
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.90	0.52
2:I:4865:LYS:HG3	2:I:4875:LYS:HZ3	1.74	0.52
2:G:533:ASN:ND2	2:G:536:ASN:OD1	2.40	0.52
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.92	0.52
2:B:469:ARG:HH21	2:B:3712:GLU:HB3	1.75	0.52
2:B:4865:LYS:HG3	2:B:4875:LYS:HZ3	1.75	0.52
2:I:111:HIS:CD2	2:I:114:SER:H	2.27	0.52
2:I:3804:ILE:O	2:I:3809:ASN:ND2	2.42	0.52
2:G:3804:ILE:O	2:G:3809:ASN:ND2	2.42	0.52
2:E:1667:LEU:HD23	2:E:1671:ARG:HH12	1.74	0.52
2:E:3804:ILE:O	2:E:3809:ASN:ND2	2.42	0.52
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.92	0.52
2:B:4230:LYS:HE3	2:B:4231:MET:HE2	1.92	0.52
2:I:4823:LEU:HD11	2:G:4839:MET:HB3	1.91	0.52
2:G:111:HIS:CD2	2:G:114:SER:H	2.27	0.52
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.43	0.52
2:E:2868:SER:O	2:E:2872:GLN:N	2.43	0.52
2:I:823:LEU:HD23	2:I:1626:TRP:HB3	1.92	0.51
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.92	0.51
2:G:132:ALA:HA	2:G:194:SER:HB2	1.92	0.51
2:G:469:ARG:HH21	2:G:3712:GLU:HB3	1.75	0.51
2:G:2868:SER:O	2:G:2872:GLN:N	2.43	0.51
2:E:621:ILE:O	2:E:625:LEU:N	2.40	0.51
2:E:4230:LYS:HE3	2:E:4231:MET:HE2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4998:LYS:NZ	2:E:5007:GLU:OE1	2.43	0.51
2:B:4860:ARG:HG3	2:B:4876:CYS:HB3	1.93	0.51
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.92	0.51
2:G:4860:ARG:HG3	2:G:4876:CYS:HB3	1.92	0.51
2:E:469:ARG:HH21	2:E:3712:GLU:HB3	1.75	0.51
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.92	0.51
1:J:7:ILE:HB	1:J:71:ARG:HB3	1.90	0.51
2:I:132:ALA:HA	2:I:194:SER:HB2	1.92	0.51
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.43	0.51
2:G:823:LEU:HD23	2:G:1626:TRP:HB3	1.92	0.51
2:G:4823:LEU:HD11	2:E:4839:MET:HB3	1.92	0.51
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.43	0.51
2:I:4860:ARG:HG3	2:I:4876:CYS:HB3	1.92	0.51
2:G:1650:ILE:HG13	2:G:1707:LEU:HD21	1.91	0.51
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.40	0.51
2:B:1100:MET:HE2	2:B:1198:GLN:HB3	1.93	0.51
2:E:1100:MET:HE2	2:E:1198:GLN:HB3	1.93	0.51
2:B:132:ALA:HA	2:B:194:SER:HB2	1.92	0.51
2:B:621:ILE:O	2:B:625:LEU:N	2.40	0.51
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.92	0.51
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	1.93	0.51
2:E:111:HIS:CD2	2:E:114:SER:H	2.27	0.51
2:E:132:ALA:HA	2:E:194:SER:HB2	1.92	0.51
2:E:823:LEU:HD23	2:E:1626:TRP:HB3	1.92	0.51
2:B:1516:UNK:N	2:B:1529:UNK:O	2.44	0.51
2:B:2868:SER:O	2:B:2872:GLN:N	2.43	0.51
2:I:469:ARG:HH21	2:I:3712:GLU:HB3	1.75	0.51
2:I:621:ILE:O	2:I:625:LEU:N	2.40	0.51
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.43	0.51
2:G:1516:UNK:N	2:G:1529:UNK:O	2.44	0.51
2:E:2199:ARG:NH2	2:E:2246:ASN:OD1	2.44	0.51
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.43	0.50
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.92	0.50
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	1.93	0.50
2:I:1100:MET:HE2	2:I:1198:GLN:HB3	1.93	0.50
2:I:1650:ILE:HG13	2:I:1707:LEU:HD21	1.91	0.50
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.76	0.50
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	1.93	0.50
2:I:4230:LYS:HE3	2:I:4231:MET:HE2	1.92	0.50
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.93	0.50
2:E:1649:ASP:HB3	2:E:1652:GLU:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.76	0.50
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.93	0.50
2:G:1100:MET:HE2	2:G:1198:GLN:HB3	1.93	0.50
2:E:4860:ARG:HG3	2:E:4876:CYS:HB3	1.93	0.50
2:B:614:VAL:HG22	2:B:616:SER:H	1.76	0.50
2:I:2199:ARG:NH2	2:I:2246:ASN:OD1	2.44	0.50
2:G:2337:PHE:HA	2:G:2340:PHE:HB2	1.94	0.50
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	1.94	0.50
2:E:2337:PHE:HA	2:E:2340:PHE:HB2	1.94	0.50
2:E:4674:GLU:HG3	2:E:4714:ASN:HB3	1.91	0.50
2:I:1516:UNK:N	2:I:1529:UNK:O	2.44	0.50
2:I:2868:SER:O	2:I:2872:GLN:N	2.43	0.50
2:I:4230:LYS:CG	2:I:4959:PHE:HE1	2.24	0.50
2:G:621:ILE:O	2:G:625:LEU:N	2.40	0.50
2:I:278:GLN:N	2:I:315:CYS:SG	2.85	0.50
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	1.94	0.50
2:G:4230:LYS:HE3	2:G:4231:MET:HE2	1.92	0.50
2:E:1516:UNK:N	2:E:1529:UNK:O	2.44	0.50
2:B:823:LEU:HD23	2:B:1626:TRP:HB3	1.92	0.50
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	1.94	0.50
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.94	0.50
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.93	0.50
2:E:614:VAL:HG22	2:E:616:SER:H	1.76	0.50
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.94	0.50
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.42	0.50
2:E:4983:HIS:ND1	2:E:4983:HIS:N	2.60	0.50
2:B:4230:LYS:CG	2:B:4959:PHE:HE1	2.24	0.50
2:I:683:ARG:NH1	2:I:707:VAL:O	2.43	0.50
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	1.94	0.50
2:I:4837:LEU:HD22	2:I:4936:ILE:HD11	1.93	0.50
2:G:1667:LEU:HD23	2:G:1671:ARG:HH12	1.74	0.50
2:B:2199:ARG:NH2	2:B:2246:ASN:OD1	2.44	0.50
2:B:4837:LEU:HD22	2:B:4936:ILE:HD11	1.93	0.50
2:I:3984:ARG:HH22	2:G:161:GLU:HA	1.77	0.50
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	1.94	0.50
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.76	0.50
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.76	0.49
2:I:4983:HIS:ND1	2:I:4983:HIS:N	2.60	0.49
2:G:4786:ASP:OD2	2:G:4789:PHE:N	2.44	0.49
2:G:4837:LEU:HD22	2:G:4936:ILE:HD11	1.93	0.49
2:B:3984:ARG:HH22	2:I:161:GLU:HA	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.93	0.49
2:G:229:GLU:HA	2:G:249:GLY:HA2	1.95	0.49
2:G:1808:ARG:NH1	2:G:1853:ILE:O	2.45	0.49
2:G:2199:ARG:NH2	2:G:2246:ASN:OD1	2.44	0.49
2:G:3984:ARG:HH22	2:E:161:GLU:HA	1.76	0.49
2:B:278:GLN:N	2:B:315:CYS:SG	2.85	0.49
2:B:2337:PHE:HA	2:B:2340:PHE:HB2	1.94	0.49
2:I:229:GLU:HA	2:I:249:GLY:HA2	1.94	0.49
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.94	0.49
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	1.94	0.49
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.92	0.49
2:E:2267:MET:HE3	2:E:2268:GLN:HG2	1.94	0.49
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	1.94	0.49
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.94	0.49
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	1.94	0.49
2:I:1808:ARG:NH1	2:I:1853:ILE:O	2.45	0.49
2:G:2267:MET:HE3	2:G:2268:GLN:HG2	1.94	0.49
2:G:4983:HIS:ND1	2:G:4983:HIS:N	2.60	0.49
2:E:626:LEU:HD23	2:E:630:GLU:H	1.77	0.49
2:E:4837:LEU:HD22	2:E:4936:ILE:HD11	1.93	0.49
2:B:4063:ASP:OD1	2:B:4169:SER:OG	2.29	0.49
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.93	0.49
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.93	0.49
2:B:626:LEU:HD23	2:B:630:GLU:H	1.78	0.49
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.93	0.49
2:B:4958:CYS:SG	2:B:4961:CYS:N	2.85	0.49
2:G:626:LEU:HD23	2:G:630:GLU:H	1.78	0.49
2:E:1808:ARG:NH1	2:E:1853:ILE:O	2.45	0.49
2:E:4786:ASP:OD2	2:E:4789:PHE:N	2.44	0.49
2:I:626:LEU:HD23	2:I:630:GLU:H	1.78	0.49
2:I:2778:GLY:HA3	2:I:2787:THR:HB	1.95	0.49
2:G:2257:LEU:HD11	2:G:2276:ALA:HB2	1.95	0.49
2:E:2257:LEU:HD11	2:E:2276:ALA:HB2	1.95	0.49
2:E:4958:CYS:SG	2:E:4961:CYS:N	2.85	0.49
2:B:229:GLU:HA	2:B:249:GLY:HA2	1.95	0.49
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.93	0.49
2:G:786:GLY:HA2	2:G:1631:GLN:HA	1.95	0.49
2:E:786:GLY:HA2	2:E:1631:GLN:HA	1.95	0.49
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.84	0.49
2:B:4697:VAL:O	2:B:4701:TRP:N	2.46	0.48
2:B:4983:HIS:ND1	2:B:4983:HIS:N	2.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:683:ARG:NH1	2:E:707:VAL:O	2.43	0.48
2:B:2267:MET:HE3	2:B:2268:GLN:HG2	1.94	0.48
2:I:2337:PHE:HA	2:I:2340:PHE:HB2	1.94	0.48
2:E:229:GLU:HA	2:E:249:GLY:HA2	1.95	0.48
2:G:614:VAL:HG22	2:G:616:SER:H	1.76	0.48
2:B:1771:LEU:HD12	2:B:2153:MET:HE3	1.95	0.48
2:B:2214:VAL:HG23	2:B:2215:LEU:HD12	1.96	0.48
2:I:2267:MET:HE3	2:I:2268:GLN:HG2	1.94	0.48
2:G:1259:ARG:HH12	2:G:1593:PRO:HA	1.78	0.48
2:E:396:GLU:OE2	2:E:451:TYR:OH	2.30	0.48
2:E:1991:THR:O	2:E:1995:THR:OG1	2.31	0.48
2:B:2257:LEU:HD11	2:B:2276:ALA:HB2	1.95	0.48
2:I:614:VAL:HG22	2:I:616:SER:H	1.76	0.48
2:E:1259:ARG:HH12	2:E:1593:PRO:HA	1.78	0.48
2:E:2911:LEU:HB2	2:E:2916:LYS:HE3	1.96	0.48
2:B:533:ASN:ND2	2:B:536:ASN:OD1	2.40	0.48
2:B:1808:ARG:NH1	2:B:1853:ILE:O	2.45	0.48
2:I:2911:LEU:HB2	2:I:2916:LYS:HE3	1.96	0.48
2:G:1991:THR:O	2:G:1995:THR:OG1	2.32	0.48
2:G:2778:GLY:HA3	2:G:2787:THR:HB	1.95	0.48
2:B:4914:VAL:HG21	2:E:4884:LEU:HD11	1.96	0.48
2:I:2257:LEU:HD11	2:I:2276:ALA:HB2	1.95	0.48
2:E:278:GLN:N	2:E:315:CYS:SG	2.85	0.48
2:B:396:GLU:OE2	2:B:451:TYR:OH	2.30	0.48
2:B:786:GLY:HA2	2:B:1631:GLN:HA	1.95	0.48
2:I:786:GLY:HA2	2:I:1631:GLN:HA	1.95	0.48
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.96	0.48
2:I:1991:THR:O	2:I:1995:THR:OG1	2.31	0.47
2:G:1771:LEU:HD12	2:G:2153:MET:HE3	1.95	0.47
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.96	0.47
2:B:2911:LEU:HB2	2:B:2916:LYS:HE3	1.96	0.47
2:I:4063:ASP:OD1	2:I:4169:SER:OG	2.29	0.47
2:I:4697:VAL:O	2:I:4701:TRP:N	2.46	0.47
2:E:41:GLY:O	2:E:45:ARG:NH1	2.47	0.47
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.43	0.47
2:E:4697:VAL:O	2:E:4701:TRP:N	2.47	0.47
2:B:41:GLY:O	2:B:45:ARG:NH1	2.47	0.47
2:I:41:GLY:O	2:I:45:ARG:NH1	2.47	0.47
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.84	0.47
2:E:1771:LEU:HD12	2:E:2153:MET:HE3	1.95	0.47
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1991:THR:O	2:B:1995:THR:OG1	2.32	0.47
2:I:1259:ARG:HH12	2:I:1593:PRO:HA	1.78	0.47
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.50	0.47
2:I:2214:VAL:HG23	2:I:2215:LEU:HD12	1.96	0.47
2:G:395:GLN:NE2	2:G:397:GLU:OE1	2.48	0.47
2:G:2214:VAL:HG23	2:G:2215:LEU:HD12	1.96	0.47
2:G:278:GLN:N	2:G:315:CYS:SG	2.85	0.47
2:G:983:THR:O	2:G:987:ARG:N	2.46	0.47
2:E:1457:UNK:N	2:E:1497:UNK:O	2.48	0.47
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.97	0.47
2:B:1772:ARG:HH21	2:B:1952:GLN:HE22	1.63	0.47
2:B:4081:VAL:HB	2:B:4088:ILE:HD12	1.96	0.47
2:G:41:GLY:O	2:G:45:ARG:NH1	2.47	0.47
2:G:214:VAL:HG12	2:G:274:LEU:HD12	1.97	0.47
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.50	0.47
2:E:2214:VAL:HG23	2:E:2215:LEU:HD12	1.96	0.47
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.97	0.47
2:B:4155:PRO:HD2	2:B:5036:LEU:HD23	1.97	0.47
2:I:1771:LEU:HD12	2:I:2153:MET:HE3	1.95	0.47
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.97	0.47
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.48	0.47
2:G:2911:LEU:HB2	2:G:2916:LYS:HE3	1.96	0.47
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.48	0.47
2:E:1772:ARG:HH21	2:E:1952:GLN:HE22	1.63	0.47
2:E:4155:PRO:HD2	2:E:5036:LEU:HD23	1.97	0.47
2:E:4230:LYS:CG	2:E:4959:PHE:HE1	2.24	0.47
2:B:161:GLU:HA	2:E:3984:ARG:HH22	1.79	0.47
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.97	0.47
2:I:983:THR:O	2:I:987:ARG:N	2.46	0.47
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.97	0.47
2:G:4697:VAL:O	2:G:4701:TRP:N	2.46	0.47
2:E:2778:GLY:HA3	2:E:2787:THR:HB	1.95	0.47
2:B:214:VAL:HG12	2:B:274:LEU:HD12	1.97	0.47
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.50	0.47
2:B:4227:GLU:HG3	2:B:4228:ALA:H	1.80	0.47
2:B:4899:ASP:OD1	2:E:4892:ARG:NH2	2.44	0.47
2:I:395:GLN:NE2	2:I:397:GLU:OE1	2.48	0.47
2:I:1457:UNK:N	2:I:1497:UNK:O	2.48	0.47
2:I:1772:ARG:HH21	2:I:1952:GLN:HE22	1.63	0.47
2:I:4081:VAL:HB	2:I:4088:ILE:HD12	1.96	0.47
2:I:4155:PRO:HD2	2:I:5036:LEU:HD23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4227:GLU:HG3	2:I:4228:ALA:H	1.80	0.47
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.96	0.47
2:G:1457:UNK:N	2:G:1497:UNK:O	2.48	0.47
2:G:2265:LEU:HD22	2:G:2330:ARG:HB3	1.97	0.47
2:E:983:THR:O	2:E:987:ARG:N	2.46	0.47
2:E:2265:LEU:HD22	2:E:2330:ARG:HB3	1.97	0.47
2:E:3361:UNK:O	2:E:3365:UNK:N	2.48	0.47
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.97	0.47
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.97	0.47
2:G:4155:PRO:HD2	2:G:5036:LEU:HD23	1.97	0.47
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.80	0.47
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.97	0.47
2:E:4826:ILE:O	2:E:4829:SER:OG	2.31	0.47
2:B:1457:UNK:N	2:B:1497:UNK:O	2.48	0.46
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.96	0.46
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.50	0.46
2:G:1772:ARG:HH21	2:G:1952:GLN:HE22	1.63	0.46
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.97	0.46
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.80	0.46
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.48	0.46
2:B:2778:GLY:HA3	2:B:2787:THR:HB	1.95	0.46
2:B:2869:ARG:HA	2:B:2872:GLN:HB3	1.97	0.46
2:G:2862:LEU:HB3	2:G:2928:LYS:HB3	1.98	0.46
2:G:4884:LEU:HD11	2:E:4914:VAL:HG21	1.97	0.46
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.98	0.46
2:I:2869:ARG:HA	2:I:2872:GLN:HB3	1.97	0.46
2:I:3361:UNK:O	2:I:3365:UNK:N	2.48	0.46
2:E:1130:GLN:HG2	2:E:1138:PRO:HA	1.98	0.46
2:E:1665:HIS:HA	2:E:1668:ARG:HG2	1.98	0.46
2:B:1259:ARG:HH12	2:B:1593:PRO:HA	1.78	0.46
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.84	0.46
2:B:2902:HIS:HB3	2:B:2905:LEU:HG	1.98	0.46
2:B:3361:UNK:O	2:B:3365:UNK:N	2.48	0.46
2:B:4998:LYS:NZ	2:B:5007:GLU:OE1	2.43	0.46
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.98	0.46
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.98	0.46
2:G:1665:HIS:HA	2:G:1668:ARG:HG2	1.98	0.46
2:E:243:ARG:NH1	2:E:301:VAL:O	2.42	0.46
2:E:395:GLN:NE2	2:E:397:GLU:OE1	2.48	0.46
2:E:2277:ALA:HB1	2:E:2337:PHE:HD2	1.81	0.46
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.81	0.46
2:B:1665:HIS:HA	2:B:1668:ARG:HG2	1.98	0.46
2:I:2862:LEU:HB3	2:I:2928:LYS:HB3	1.98	0.46
2:G:2869:ARG:HA	2:G:2872:GLN:HB3	1.97	0.46
2:G:4984:ASN:C	2:G:4986:ALA:N	2.64	0.46
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.81	0.46
2:E:2902:HIS:HB3	2:E:2905:LEU:HG	1.98	0.46
2:I:214:VAL:HG12	2:I:274:LEU:HD12	1.97	0.46
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.42	0.46
2:G:2277:ALA:HB1	2:G:2337:PHE:HD2	1.81	0.46
2:E:214:VAL:HG12	2:E:274:LEU:HD12	1.97	0.46
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.48	0.46
2:I:2810:LYS:O	2:I:2814:LYS:N	2.42	0.46
2:I:4826:ILE:O	2:I:4829:SER:OG	2.31	0.46
2:E:4063:ASP:OD1	2:E:4169:SER:OG	2.29	0.46
2:B:395:GLN:NE2	2:B:397:GLU:OE1	2.48	0.46
2:B:575:LEU:HD22	2:B:609:CYS:HB3	1.98	0.46
2:B:2265:LEU:HD22	2:B:2330:ARG:HB3	1.97	0.46
2:I:913:LEU:O	2:I:918:ARG:NH2	2.49	0.46
2:I:1665:HIS:HA	2:I:1668:ARG:HG2	1.97	0.46
2:I:4884:LEU:HD11	2:G:4914:VAL:HG21	1.97	0.46
2:G:606:LEU:O	2:G:617:ASN:ND2	2.49	0.46
2:G:2810:LYS:O	2:G:2814:LYS:N	2.42	0.46
2:G:3361:UNK:O	2:G:3365:UNK:N	2.48	0.46
2:E:606:LEU:O	2:E:617:ASN:ND2	2.49	0.46
2:E:2869:ARG:HA	2:E:2872:GLN:HB3	1.97	0.46
2:B:1295:UNK:N	2:B:1454:UNK:O	2.49	0.46
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.97	0.46
2:I:575:LEU:HD22	2:I:609:CYS:HB3	1.98	0.46
2:I:606:LEU:O	2:I:617:ASN:ND2	2.49	0.46
2:I:1105:ALA:N	2:I:1189:LEU:O	2.49	0.46
2:G:1295:UNK:N	2:G:1454:UNK:O	2.49	0.46
2:G:2810:LYS:HE2	2:G:2814:LYS:HE3	1.98	0.46
2:E:2810:LYS:HE2	2:E:2814:LYS:HE3	1.98	0.46
2:E:4081:VAL:HB	2:E:4088:ILE:HD12	1.96	0.46
2:B:913:LEU:O	2:B:918:ARG:NH2	2.49	0.46
2:B:1105:ALA:N	2:B:1189:LEU:O	2.49	0.46
2:B:1130:GLN:HG2	2:B:1138:PRO:HA	1.97	0.46
2:I:772:ASN:ND2	2:I:774:ASP:OD2	2.49	0.46
2:I:2265:LEU:HD22	2:I:2330:ARG:HB3	1.97	0.46
2:I:4852:THR:HG21	2:I:4883:TYR:HB2	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2277:ALA:HB1	2:B:2337:PHE:HD2	1.81	0.45
2:I:776:LEU:HG	2:I:848:HIS:HA	1.99	0.45
2:I:2880:GLU:O	2:I:2884:ASN:N	2.49	0.45
2:I:4713:SER:HA	2:I:4718:LYS:HE2	1.99	0.45
2:I:309:THR:O	2:I:313:SER:OG	2.35	0.45
2:I:1295:UNK:N	2:I:1454:UNK:O	2.49	0.45
2:I:2902:HIS:HB3	2:I:2905:LEU:HG	1.98	0.45
2:G:221:ARG:NH2	2:G:397:GLU:OE2	2.48	0.45
2:G:4081:VAL:HB	2:G:4088:ILE:HD12	1.96	0.45
2:G:4998:LYS:NZ	2:G:5007:GLU:OE1	2.43	0.45
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	1.99	0.45
2:B:309:THR:O	2:B:313:SER:OG	2.35	0.45
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	1.99	0.45
2:B:4713:SER:HA	2:B:4718:LYS:HE2	1.98	0.45
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.81	0.45
2:G:575:LEU:HD22	2:G:609:CYS:HB3	1.98	0.45
2:G:776:LEU:HG	2:G:848:HIS:HA	1.98	0.45
2:G:3760:LYS:NZ	2:G:5000:GLU:OE1	2.40	0.45
2:G:4230:LYS:CG	2:G:4959:PHE:HE1	2.25	0.45
2:G:4852:THR:HG21	2:G:4883:TYR:HB2	1.99	0.45
2:E:575:LEU:HD22	2:E:609:CYS:HB3	1.98	0.45
2:E:2862:LEU:HB3	2:E:2928:LYS:HB3	1.98	0.45
2:B:606:LEU:O	2:B:617:ASN:ND2	2.49	0.45
2:B:683:ARG:NH1	2:B:707:VAL:O	2.43	0.45
2:I:243:ARG:NH1	2:I:301:VAL:O	2.42	0.45
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.99	0.45
2:I:1130:GLN:HG2	2:I:1138:PRO:HA	1.98	0.45
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.97	0.45
2:I:3760:LYS:NZ	2:I:5000:GLU:OE1	2.40	0.45
2:G:309:THR:O	2:G:313:SER:OG	2.35	0.45
2:E:913:LEU:O	2:E:918:ARG:NH2	2.49	0.45
2:E:1295:UNK:N	2:E:1454:UNK:O	2.49	0.45
2:B:2456:ILE:O	2:B:2459:SER:OG	2.33	0.45
2:E:776:LEU:HG	2:E:848:HIS:HA	1.99	0.45
2:B:776:LEU:HG	2:B:848:HIS:HA	1.99	0.45
2:I:1735:ILE:HG23	2:I:1771:LEU:HD23	1.99	0.45
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.50	0.45
2:I:2247:GLN:NE2	2:I:2285:GLU:OE2	2.50	0.45
2:I:4738:ALA:HA	2:I:4743:MET:HE3	1.99	0.45
2:G:243:ARG:NH1	2:G:301:VAL:O	2.42	0.45
2:G:1735:ILE:HG23	2:G:1771:LEU:HD23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2902:HIS:HB3	2:G:2905:LEU:HG	1.98	0.45
2:G:3973:CYS:SG	2:G:3976:ASN:ND2	2.90	0.45
2:E:3760:LYS:NZ	2:E:5000:GLU:OE1	2.40	0.45
2:B:2880:GLU:O	2:B:2884:ASN:N	2.49	0.45
2:I:2810:LYS:HE2	2:I:2814:LYS:HE3	1.98	0.45
2:I:3973:CYS:SG	2:I:3976:ASN:ND2	2.90	0.45
2:G:913:LEU:O	2:G:918:ARG:NH2	2.49	0.45
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.81	0.45
2:G:2764:GLU:HG3	2:G:2857:PRO:HB2	1.99	0.45
2:B:3766:GLN:HG3	2:B:3769:ARG:HH12	1.82	0.45
2:E:4852:THR:HG21	2:E:4883:TYR:HB2	1.99	0.45
2:B:2862:LEU:HB3	2:B:2928:LYS:HB3	1.98	0.45
2:B:4738:ALA:HA	2:B:4743:MET:HE3	1.99	0.45
2:I:3766:GLN:HG3	2:I:3769:ARG:HH12	1.82	0.45
2:I:3779:VAL:HG23	2:I:3780:LEU:HD12	1.99	0.45
2:G:647:ASN:ND2	2:G:820:ARG:O	2.49	0.45
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.50	0.45
2:G:2880:GLU:O	2:G:2884:ASN:N	2.49	0.45
2:G:3766:GLN:HG3	2:G:3769:ARG:HH12	1.82	0.45
2:G:4713:SER:HA	2:G:4718:LYS:HE2	1.98	0.45
2:E:647:ASN:ND2	2:E:820:ARG:O	2.49	0.45
2:E:2155:LEU:HD13	2:E:2188:ASN:HD21	1.82	0.45
2:E:4729:GLY:HA2	2:E:4737:ILE:HG13	1.99	0.45
2:B:2247:GLN:NE2	2:B:2285:GLU:OE2	2.50	0.45
2:B:2810:LYS:HE2	2:B:2814:LYS:HE3	1.98	0.45
2:I:2764:GLU:HG3	2:I:2857:PRO:HB2	1.99	0.45
2:G:2247:GLN:NE2	2:G:2285:GLU:OE2	2.50	0.45
2:G:3840:SER:OG	2:G:3875:MET:O	2.34	0.45
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.50	0.45
2:E:2247:GLN:NE2	2:E:2285:GLU:OE2	2.50	0.45
2:E:3766:GLN:HG3	2:E:3769:ARG:HH12	1.82	0.45
2:B:3973:CYS:SG	2:B:3976:ASN:ND2	2.90	0.44
2:B:4852:THR:HG21	2:B:4883:TYR:HB2	1.99	0.44
2:I:2277:ALA:HB1	2:I:2337:PHE:HD2	1.81	0.44
2:I:4848:VAL:O	2:I:4852:THR:OG1	2.27	0.44
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.99	0.44
2:G:2155:LEU:HD13	2:G:2188:ASN:HD21	1.82	0.44
2:G:2305:CYS:HA	2:G:2324:ASN:HD22	1.82	0.44
2:G:3365:UNK:O	2:G:3369:UNK:N	2.51	0.44
2:G:4826:ILE:O	2:G:4829:SER:OG	2.31	0.44
2:B:2155:LEU:HD13	2:B:2188:ASN:HD21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2764:GLU:HG3	2:B:2857:PRO:HB2	1.99	0.44
2:B:2950:UNK:O	2:B:2954:UNK:N	2.50	0.44
2:B:4959:PHE:CD1	2:B:4959:PHE:O	2.70	0.44
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.84	0.44
2:I:2950:UNK:O	2:I:2954:UNK:N	2.50	0.44
2:G:1130:GLN:HG2	2:G:1138:PRO:HA	1.97	0.44
2:E:2950:UNK:O	2:E:2954:UNK:N	2.50	0.44
2:E:3973:CYS:SG	2:E:3976:ASN:ND2	2.90	0.44
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.99	0.44
2:B:1973:GLN:O	2:B:1977:TYR:N	2.46	0.44
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.40	0.44
2:I:2305:CYS:HA	2:I:2324:ASN:HD22	1.82	0.44
2:G:683:ARG:NH1	2:G:707:VAL:O	2.43	0.44
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	1.99	0.44
2:G:4959:PHE:CD1	2:G:4959:PHE:O	2.70	0.44
2:E:1735:ILE:HG23	2:E:1771:LEU:HD23	1.99	0.44
2:E:2880:GLU:O	2:E:2884:ASN:N	2.49	0.44
2:B:647:ASN:ND2	2:B:820:ARG:O	2.49	0.44
2:B:1735:ILE:HG23	2:B:1771:LEU:HD23	1.99	0.44
2:B:2305:CYS:HA	2:B:2324:ASN:HD22	1.82	0.44
2:B:4884:LEU:HD11	2:I:4914:VAL:HG21	1.98	0.44
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.51	0.44
2:G:20:VAL:HG12	2:G:204:PRO:HA	2.00	0.44
2:G:2950:UNK:O	2:G:2954:UNK:N	2.50	0.44
2:G:4729:GLY:HA2	2:G:4737:ILE:HG13	1.99	0.44
2:E:583:ILE:HA	2:E:586:ILE:HD12	1.99	0.44
2:E:1105:ALA:N	2:E:1189:LEU:O	2.49	0.44
2:B:211:GLU:OE2	2:B:3907:THR:OG1	2.32	0.44
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.51	0.44
2:G:379:HIS:CD2	2:G:381:GLU:H	2.36	0.44
2:E:20:VAL:HG12	2:E:204:PRO:HA	2.00	0.44
2:E:379:HIS:CD2	2:E:381:GLU:H	2.36	0.44
2:E:3365:UNK:O	2:E:3369:UNK:N	2.50	0.44
2:B:583:ILE:HA	2:B:586:ILE:HD12	1.99	0.44
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.50	0.44
2:B:4152:GLU:OE1	2:B:4194:TYR:OH	2.36	0.44
2:B:4928:LEU:HD13	2:B:4928:LEU:HA	1.89	0.44
2:I:583:ILE:HA	2:I:586:ILE:HD12	1.99	0.44
2:I:594:GLY:H	2:I:1594:ARG:HD3	1.82	0.44
2:I:3365:UNK:O	2:I:3369:UNK:N	2.51	0.44
2:G:594:GLY:H	2:G:1594:ARG:HD3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.51	0.44
2:E:635:THR:HB	2:E:1639:LEU:HD23	2.00	0.44
2:E:4713:SER:HA	2:E:4718:LYS:HE2	1.98	0.44
2:B:4729:GLY:HA2	2:B:4737:ILE:HG13	1.99	0.44
2:B:4848:VAL:O	2:B:4852:THR:OG1	2.27	0.44
2:I:4998:LYS:NZ	2:I:5007:GLU:OE1	2.43	0.44
2:G:143:GLY:HA3	2:G:147:TRP:HE1	1.83	0.44
2:G:4892:ARG:NH2	2:E:4899:ASP:OD1	2.48	0.44
2:E:594:GLY:H	2:E:1594:ARG:HD3	1.82	0.44
2:E:892:THR:N	2:E:902:ARG:O	2.50	0.44
2:E:2196:ASN:OD1	2:E:2199:ARG:NH1	2.43	0.44
2:E:2305:CYS:HA	2:E:2324:ASN:HD22	1.82	0.44
2:E:4959:PHE:CD1	2:E:4959:PHE:O	2.70	0.44
2:I:143:GLY:HA3	2:I:147:TRP:HE1	1.83	0.44
2:I:1166:GLY:HA3	2:I:1216:ILE:HD13	2.00	0.44
2:I:4959:PHE:CD1	2:I:4959:PHE:O	2.70	0.44
2:G:211:GLU:OE2	2:G:3907:THR:OG1	2.33	0.44
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.51	0.44
2:B:594:GLY:H	2:B:1594:ARG:HD3	1.82	0.44
2:I:20:VAL:HG12	2:I:204:PRO:HA	2.00	0.44
2:I:379:HIS:CD2	2:I:381:GLU:H	2.36	0.44
2:I:4958:CYS:SG	2:I:4961:CYS:N	2.85	0.44
2:G:4152:GLU:OE1	2:G:4194:TYR:OH	2.36	0.44
2:E:772:ASN:ND2	2:E:774:ASP:OD2	2.49	0.44
2:E:4738:ALA:HA	2:E:4743:MET:HE3	1.99	0.44
2:B:635:THR:HB	2:B:1639:LEU:HD23	2.00	0.43
2:B:662:TRP:HZ3	2:B:811:CYS:HA	1.83	0.43
2:B:772:ASN:ND2	2:B:774:ASP:OD2	2.49	0.43
2:B:1166:GLY:HA3	2:B:1216:ILE:HD13	1.99	0.43
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	2.01	0.43
2:B:3365:UNK:O	2:B:3369:UNK:N	2.51	0.43
2:I:219:VAL:HG13	2:I:285:VAL:HG21	2.00	0.43
2:I:2155:LEU:HD13	2:I:2188:ASN:HD21	1.82	0.43
2:I:4892:ARG:NH2	2:G:4899:ASP:OD1	2.47	0.43
2:G:583:ILE:HA	2:G:586:ILE:HD12	1.99	0.43
2:G:1166:GLY:HA3	2:G:1216:ILE:HD13	1.99	0.43
2:G:4063:ASP:OD1	2:G:4169:SER:OG	2.29	0.43
2:E:309:THR:O	2:E:313:SER:OG	2.35	0.43
2:B:1077:ALA:HB3	2:B:1189:LEU:HD11	2.01	0.43
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.83	0.43
2:B:2810:LYS:O	2:B:2814:LYS:N	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1812:LEU:HD21	2:I:1861:GLN:HG2	2.00	0.43
2:I:2012:PHE:CG	2:I:2022:PRO:HD3	2.54	0.43
2:I:4729:GLY:HA2	2:I:4737:ILE:HG13	1.99	0.43
2:E:1077:ALA:HB3	2:E:1189:LEU:HD11	2.00	0.43
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.99	0.43
2:E:2764:GLU:HG3	2:E:2857:PRO:HB2	1.99	0.43
2:E:4680:LYS:HD3	2:E:4686:LEU:HD22	2.01	0.43
2:B:379:HIS:CD2	2:B:381:GLU:H	2.36	0.43
2:I:652:ARG:HB3	2:I:773:LEU:HD13	2.01	0.43
2:I:1126:GLY:HA3	2:I:1143:TRP:CE2	2.53	0.43
2:I:4786:ASP:OD2	2:I:4789:PHE:N	2.44	0.43
2:G:219:VAL:HG13	2:G:285:VAL:HG21	2.00	0.43
2:G:772:ASN:ND2	2:G:774:ASP:OD2	2.49	0.43
2:E:1166:GLY:HA3	2:E:1216:ILE:HD13	2.00	0.43
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.83	0.43
2:B:410:LEU:HD12	2:B:413:GLN:HE21	1.83	0.43
2:B:1812:LEU:HD21	2:B:1861:GLN:HG2	2.01	0.43
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.83	0.43
2:G:2012:PHE:CG	2:G:2022:PRO:HD3	2.54	0.43
2:E:1126:GLY:HA3	2:E:1143:TRP:CE2	2.53	0.43
2:E:4152:GLU:OE1	2:E:4194:TYR:OH	2.36	0.43
1:A:25:HIS:HB3	1:A:40:ARG:HD3	2.01	0.43
2:B:20:VAL:HG12	2:B:204:PRO:HA	2.00	0.43
2:B:143:GLY:HA3	2:B:147:TRP:HE1	1.83	0.43
2:B:652:ARG:HB3	2:B:773:LEU:HD13	2.01	0.43
2:I:647:ASN:ND2	2:I:820:ARG:O	2.49	0.43
2:G:2353:VAL:O	2:G:2357:LEU:N	2.49	0.43
2:G:4738:ALA:HA	2:G:4743:MET:HE3	1.99	0.43
2:E:15:ARG:HD3	2:E:98:HIS:HB3	2.00	0.43
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	2.01	0.43
1:A:27:THR:HB	1:A:100:ASP:HB3	2.01	0.43
2:B:892:THR:N	2:B:902:ARG:O	2.50	0.43
2:I:221:ARG:NH2	2:I:397:GLU:OE2	2.48	0.43
2:I:3362:UNK:O	2:I:3366:UNK:N	2.52	0.43
2:I:4152:GLU:OE1	2:I:4194:TYR:OH	2.35	0.43
2:G:635:THR:HB	2:G:1639:LEU:HD23	2.00	0.43
2:E:3362:UNK:O	2:E:3366:UNK:N	2.52	0.43
2:B:794:GLY:H	2:B:798:GLY:HA3	1.84	0.43
2:B:1126:GLY:HA3	2:B:1143:TRP:CE2	2.53	0.43
2:B:3362:UNK:O	2:B:3366:UNK:N	2.52	0.43
2:I:15:ARG:HD3	2:I:98:HIS:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:410:LEU:HD12	2:G:413:GLN:HE21	1.83	0.43
2:G:1105:ALA:N	2:G:1189:LEU:O	2.49	0.43
2:G:2420:HIS:ND1	2:G:2493:UNK:O	2.38	0.43
2:G:3827:GLY:HA2	2:G:3830:GLN:HE21	1.84	0.43
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	2.01	0.43
2:G:4680:LYS:HD3	2:G:4686:LEU:HD22	2.01	0.43
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.42	0.43
2:E:221:ARG:NH2	2:E:397:GLU:OE2	2.48	0.43
2:I:1077:ALA:HB3	2:I:1189:LEU:HD11	2.01	0.43
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.52	0.43
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	2.01	0.43
2:I:2758:PHE:O	2:I:2762:THR:N	2.51	0.43
2:G:15:ARG:HD3	2:G:98:HIS:HB3	2.00	0.43
2:G:1077:ALA:HB3	2:G:1189:LEU:HD11	2.01	0.43
2:E:596:ASN:HB3	2:E:599:VAL:HG22	2.01	0.43
2:E:652:ARG:HB3	2:E:773:LEU:HD13	2.01	0.43
1:H:25:HIS:HB3	1:H:40:ARG:HD3	2.01	0.43
2:B:924:MET:O	2:B:928:THR:OG1	2.35	0.43
2:I:2208:MET:HE1	2:I:2253:HIS:HB3	2.01	0.43
2:I:4680:LYS:HD3	2:I:4686:LEU:HD22	2.01	0.43
2:G:206:CYS:SG	2:G:207:SER:N	2.92	0.43
2:G:3362:UNK:O	2:G:3366:UNK:N	2.52	0.43
2:E:410:LEU:HD12	2:E:413:GLN:HE21	1.83	0.43
2:E:794:GLY:H	2:E:798:GLY:HA3	1.84	0.43
2:B:404:ILE:HG21	2:B:481:GLU:HG3	2.01	0.43
2:B:2012:PHE:CG	2:B:2022:PRO:HD3	2.54	0.43
2:B:2758:PHE:O	2:B:2762:THR:N	2.51	0.43
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	2.01	0.43
2:I:4928:LEU:HD13	2:I:4928:LEU:HA	1.89	0.43
2:G:664:PHE:HB2	2:G:746:CYS:HB2	2.01	0.43
2:G:4083:ASP:HB3	2:G:4086:GLY:H	1.84	0.43
2:E:662:TRP:HZ3	2:E:811:CYS:HA	1.83	0.43
2:E:4083:ASP:HB3	2:E:4086:GLY:H	1.84	0.43
2:B:206:CYS:SG	2:B:207:SER:N	2.92	0.42
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.52	0.42
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	2.01	0.42
2:B:4680:LYS:HD3	2:B:4686:LEU:HD22	2.01	0.42
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	2.01	0.42
2:B:4786:ASP:OD2	2:B:4789:PHE:N	2.44	0.42
2:I:635:THR:HB	2:I:1639:LEU:HD23	2.00	0.42
2:I:664:PHE:HB2	2:I:746:CYS:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4822:THR:O	2:I:4825:THR:OG1	2.36	0.42
2:G:652:ARG:HB3	2:G:773:LEU:HD13	2.01	0.42
2:E:681:HIS:HB3	2:E:784:SER:HB3	2.01	0.42
2:E:2420:HIS:ND1	2:E:2493:UNK:O	2.38	0.42
2:B:468:LEU:HB3	2:B:472:ARG:HH12	1.85	0.42
2:B:983:THR:O	2:B:987:ARG:N	2.46	0.42
2:B:3804:ILE:HG22	2:B:3812:VAL:HG21	2.02	0.42
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	2.01	0.42
2:I:206:CYS:SG	2:I:207:SER:N	2.92	0.42
2:G:681:HIS:HB3	2:G:784:SER:HB3	2.01	0.42
2:G:3804:ILE:HG22	2:G:3812:VAL:HG21	2.01	0.42
2:G:4558:ASN:HB2	2:G:4561:THR:HB	2.02	0.42
2:E:2012:PHE:CG	2:E:2022:PRO:HD3	2.54	0.42
1:F:27:THR:HB	1:F:100:ASP:HB3	2.01	0.42
2:B:4822:THR:O	2:B:4825:THR:OG1	2.36	0.42
2:I:794:GLY:H	2:I:798:GLY:HA3	1.84	0.42
2:I:4558:ASN:HB2	2:I:4561:THR:HB	2.01	0.42
2:G:794:GLY:H	2:G:798:GLY:HA3	1.84	0.42
2:E:143:GLY:HA3	2:E:147:TRP:HE1	1.83	0.42
2:E:219:VAL:HG13	2:E:285:VAL:HG21	2.00	0.42
2:E:468:LEU:HB3	2:E:472:ARG:HH12	1.85	0.42
2:I:410:LEU:HD12	2:I:413:GLN:HE21	1.83	0.42
2:I:662:TRP:HZ3	2:I:811:CYS:HA	1.83	0.42
2:I:1727:ARG:NH2	2:I:1773:PRO:O	2.53	0.42
2:I:3827:GLY:HA2	2:I:3830:GLN:HE21	1.84	0.42
2:G:596:ASN:HB3	2:G:599:VAL:HG22	2.01	0.42
2:G:1126:GLY:HA3	2:G:1143:TRP:CE2	2.53	0.42
2:G:2208:MET:HE1	2:G:2253:HIS:HB3	2.01	0.42
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	2.01	0.42
2:E:206:CYS:SG	2:E:207:SER:N	2.92	0.42
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.52	0.42
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	2.01	0.42
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	2.01	0.42
1:J:25:HIS:HB3	1:J:40:ARG:HD3	2.01	0.42
2:B:15:ARG:HD3	2:B:98:HIS:HB3	2.00	0.42
2:B:596:ASN:HB3	2:B:599:VAL:HG22	2.01	0.42
2:I:2420:HIS:ND1	2:I:2493:UNK:O	2.38	0.42
2:G:468:LEU:HB3	2:G:472:ARG:HH12	1.85	0.42
2:E:3804:ILE:HG22	2:E:3812:VAL:HG21	2.01	0.42
1:H:27:THR:HB	1:H:100:ASP:HB3	2.01	0.42
1:J:27:THR:HB	1:J:100:ASP:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:219:VAL:HG13	2:B:285:VAL:HG21	2.00	0.42
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.42	0.42
2:I:404:ILE:HG21	2:I:481:GLU:HG3	2.02	0.42
2:I:2128:TYR:HB3	2:I:3669:PHE:HB3	2.02	0.42
2:G:662:TRP:HZ3	2:G:811:CYS:HA	1.83	0.42
2:G:1812:LEU:HD21	2:G:1861:GLN:HG2	2.00	0.42
2:B:2128:TYR:HB3	2:B:3669:PHE:HB3	2.02	0.42
2:B:4083:ASP:HB3	2:B:4086:GLY:H	1.84	0.42
2:G:4822:THR:O	2:G:4825:THR:OG1	2.36	0.42
2:E:2128:TYR:HB3	2:E:3669:PHE:HB3	2.02	0.42
2:E:2208:MET:HE1	2:E:2253:HIS:HB3	2.01	0.42
2:E:2298:VAL:HG21	2:E:2335:LEU:HD21	2.02	0.42
2:E:2758:PHE:O	2:E:2762:THR:N	2.51	0.42
2:B:1163:THR:HG22	2:B:1168:VAL:HA	2.02	0.42
2:B:2353:VAL:O	2:B:2357:LEU:N	2.49	0.42
2:I:596:ASN:HB3	2:I:599:VAL:HG22	2.01	0.42
2:I:1163:THR:HG22	2:I:1168:VAL:HA	2.02	0.42
2:I:3804:ILE:HG22	2:I:3812:VAL:HG21	2.02	0.42
2:I:4083:ASP:HB3	2:I:4086:GLY:H	1.84	0.42
2:G:404:ILE:HG21	2:G:481:GLU:HG3	2.02	0.42
2:E:664:PHE:HB2	2:E:746:CYS:HB2	2.01	0.42
2:E:3827:GLY:HA2	2:E:3830:GLN:HE21	1.84	0.42
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.83	0.42
2:E:404:ILE:HG21	2:E:481:GLU:HG3	2.01	0.42
2:E:719:LEU:HA	2:E:730:VAL:HG22	2.02	0.42
2:E:2353:VAL:O	2:E:2357:LEU:N	2.49	0.42
2:E:4136:ALA:HA	2:E:4139:ILE:HG22	2.02	0.42
2:B:2208:MET:HE1	2:B:2253:HIS:HB3	2.01	0.42
2:B:4892:ARG:NH2	2:I:4899:ASP:OD1	2.48	0.42
2:I:681:HIS:HB3	2:I:784:SER:HB3	2.01	0.42
2:G:1163:THR:HG22	2:G:1168:VAL:HA	2.02	0.42
2:E:1812:LEU:HD21	2:E:1861:GLN:HG2	2.01	0.42
2:B:2291:GLN:HE21	2:B:2294:ASP:H	1.68	0.41
2:B:2420:HIS:ND1	2:B:2493:UNK:O	2.38	0.41
2:B:4136:ALA:HA	2:B:4139:ILE:HG22	2.02	0.41
2:G:396:GLU:OE2	2:G:451:TYR:OH	2.30	0.41
2:G:892:THR:N	2:G:902:ARG:O	2.50	0.41
2:G:2128:TYR:HB3	2:G:3669:PHE:HB3	2.02	0.41
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	2.01	0.41
2:E:2810:LYS:O	2:E:2814:LYS:N	2.42	0.41
2:B:664:PHE:HB2	2:B:746:CYS:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2353:VAL:O	2:I:2357:LEU:N	2.49	0.41
2:I:4184:MET:HE2	2:I:4188:ARG:HA	2.02	0.41
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	2.01	0.41
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.52	0.41
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	2.01	0.41
2:E:1163:THR:HG22	2:E:1168:VAL:HA	2.02	0.41
2:B:1189:LEU:HD12	2:B:1190:PRO:HD2	2.02	0.41
2:I:2291:GLN:HE21	2:I:2294:ASP:H	1.69	0.41
2:G:907:LEU:O	2:G:963:ASN:ND2	2.41	0.41
2:G:1154:ASP:O	2:G:1158:ASN:N	2.53	0.41
2:G:3663:LEU:H	2:G:3663:LEU:HG	1.72	0.41
2:G:4984:ASN:OD1	2:G:4986:ALA:HB3	2.21	0.41
2:E:689:THR:H	2:E:778:PHE:HE2	1.68	0.41
2:E:793:LEU:HB2	2:E:797:HIS:H	1.85	0.41
2:E:1259:ARG:NH2	2:E:1595:LEU:O	2.54	0.41
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.39	0.41
2:B:4184:MET:HE2	2:B:4188:ARG:HA	2.02	0.41
2:I:950:LEU:HB3	2:I:970:LEU:HD22	2.01	0.41
2:G:1973:GLN:O	2:G:1977:TYR:N	2.46	0.41
2:E:950:LEU:HB3	2:E:970:LEU:HD22	2.01	0.41
2:E:2291:GLN:HE21	2:E:2294:ASP:H	1.69	0.41
2:E:3676:ASP:OD1	2:E:3676:ASP:N	2.53	0.41
2:B:719:LEU:HA	2:B:730:VAL:HG22	2.02	0.41
2:I:1189:LEU:HD12	2:I:1190:PRO:HD2	2.02	0.41
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	2.01	0.41
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	2.03	0.41
2:I:4158:PRO:HA	2:I:4161:ARG:HB2	2.02	0.41
2:I:4984:ASN:OD1	2:I:4986:ALA:HB3	2.21	0.41
2:G:395:GLN:HG3	2:G:397:GLU:H	1.86	0.41
2:E:4984:ASN:OD1	2:E:4986:ALA:HB3	2.21	0.41
2:B:221:ARG:NH2	2:B:397:GLU:OE2	2.48	0.41
2:B:689:THR:H	2:B:778:PHE:HE2	1.68	0.41
2:B:3827:GLY:HA2	2:B:3830:GLN:HE21	1.84	0.41
2:B:4062:PHE:HE2	2:B:4143:VAL:HG21	1.86	0.41
2:I:234:SER:O	2:I:242:ARG:NE	2.52	0.41
2:I:2298:VAL:HG21	2:I:2335:LEU:HD21	2.02	0.41
2:I:4062:PHE:HE2	2:I:4143:VAL:HG21	1.86	0.41
2:G:719:LEU:HA	2:G:730:VAL:HG22	2.02	0.41
2:G:2291:GLN:HE21	2:G:2294:ASP:H	1.68	0.41
2:G:2298:VAL:HG21	2:G:2335:LEU:HD21	2.02	0.41
2:G:4136:ALA:HA	2:G:4139:ILE:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4958:CYS:SG	2:G:4961:CYS:N	2.85	0.41
2:E:4558:ASN:HB2	2:E:4561:THR:HB	2.01	0.41
1:F:25:HIS:HB3	1:F:40:ARG:HD3	2.01	0.41
2:B:1259:ARG:NH2	2:B:1595:LEU:O	2.54	0.41
2:B:4673:ARG:HH12	2:B:4698:LYS:HE3	1.86	0.41
2:I:45:ARG:NH2	2:I:447:ASP:OD1	2.54	0.41
2:I:793:LEU:HB2	2:I:797:HIS:H	1.85	0.41
2:I:1970:GLN:HB3	2:I:3641:LEU:HG	2.03	0.41
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	2.02	0.41
2:B:378:LEU:HD23	2:B:378:LEU:HA	1.94	0.41
2:B:4558:ASN:HB2	2:B:4561:THR:HB	2.02	0.41
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.86	0.41
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	2.02	0.41
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	2.01	0.41
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.39	0.41
2:G:1970:GLN:HB3	2:G:3641:LEU:HG	2.03	0.41
2:G:2196:ASN:OD1	2:G:2199:ARG:NH1	2.43	0.41
1:H:92:PRO:HD3	2:G:627:PRO:HB2	2.03	0.41
2:B:215:THR:HG22	2:B:273:HIS:HA	2.03	0.41
2:B:2298:VAL:HG21	2:B:2335:LEU:HD21	2.02	0.41
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	2.03	0.41
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	2.02	0.41
2:I:215:THR:HG22	2:I:273:HIS:HA	2.03	0.41
2:I:468:LEU:HB3	2:I:472:ARG:HH12	1.85	0.41
2:I:719:LEU:HA	2:I:730:VAL:HG22	2.02	0.41
2:I:892:THR:N	2:I:902:ARG:O	2.50	0.41
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.39	0.41
2:I:1848:LEU:HD22	2:I:1853:ILE:HG13	2.03	0.41
2:I:3662:ILE:H	2:I:3662:ILE:HG13	1.77	0.41
2:I:4673:ARG:HH12	2:I:4698:LYS:HE3	1.86	0.41
2:G:793:LEU:HB2	2:G:797:HIS:H	1.85	0.41
2:G:950:LEU:HB3	2:G:970:LEU:HD22	2.01	0.41
2:G:1725:ARG:HH21	2:G:1725:ARG:HD2	1.74	0.41
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	2.02	0.41
2:G:4062:PHE:HE2	2:G:4143:VAL:HG21	1.86	0.41
2:G:4158:PRO:HA	2:G:4161:ARG:HB2	2.02	0.41
2:E:215:THR:HG22	2:E:273:HIS:HA	2.03	0.41
2:E:1189:LEU:HD12	2:E:1190:PRO:HD2	2.02	0.41
2:E:1970:GLN:HB3	2:E:3641:LEU:HG	2.03	0.41
2:E:2430:ILE:HG21	2:E:2502:UNK:HA	2.03	0.41
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4062:PHE:HE2	2:E:4143:VAL:HG21	1.86	0.41
2:E:4158:PRO:HA	2:E:4161:ARG:HB2	2.02	0.41
2:B:793:LEU:HB2	2:B:797:HIS:H	1.85	0.41
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.39	0.41
2:B:1970:GLN:HB3	2:B:3641:LEU:HG	2.03	0.41
2:B:2437:ALA:HA	2:B:2438:PRO:HD3	1.97	0.41
2:B:4984:ASN:OD1	2:B:4986:ALA:HB3	2.21	0.41
2:I:1154:ASP:O	2:I:1158:ASN:N	2.54	0.41
2:I:3840:SER:OG	2:I:3875:MET:O	2.34	0.41
2:G:215:THR:HG22	2:G:273:HIS:HA	2.03	0.41
2:G:1161:ILE:HA	2:G:1177:THR:HB	2.02	0.41
2:G:2145:SER:HB2	2:G:3647:HIS:CE1	2.56	0.41
2:G:4184:MET:HE2	2:G:4188:ARG:HA	2.02	0.41
2:E:645:ARG:N	2:E:824:GLU:O	2.45	0.41
2:E:2145:SER:HB2	2:E:3647:HIS:CE1	2.56	0.41
1:A:87:HIS:HA	1:A:88:PRO:HD3	1.93	0.40
2:B:864:PRO:HA	2:B:865:PRO:HD3	1.94	0.40
2:B:950:LEU:HB3	2:B:970:LEU:HD22	2.01	0.40
2:B:2196:ASN:OD1	2:B:2199:ARG:NH1	2.43	0.40
2:B:2823:ILE:HG12	2:B:2937:VAL:HG22	2.03	0.40
2:I:4136:ALA:HA	2:I:4139:ILE:HG22	2.02	0.40
2:G:1259:ARG:NH2	2:G:1595:LEU:O	2.54	0.40
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	2.03	0.40
2:E:1124:PHE:HB2	2:E:1162:PHE:CE2	2.56	0.40
2:E:1161:ILE:HA	2:E:1177:THR:HB	2.02	0.40
2:E:1243:PRO:HB2	2:E:1600:LEU:HD22	2.03	0.40
2:E:1973:GLN:O	2:E:1977:TYR:N	2.46	0.40
2:B:681:HIS:HB3	2:B:784:SER:HB3	2.01	0.40
2:B:2927:LEU:HA	2:B:2930:LEU:HD12	2.04	0.40
2:I:1243:PRO:HB2	2:I:1600:LEU:HD22	2.03	0.40
2:G:2430:ILE:HG21	2:G:2502:UNK:HA	2.03	0.40
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.86	0.40
2:G:4673:ARG:HH12	2:G:4698:LYS:HE3	1.86	0.40
2:E:123:THR:OG1	2:E:134:ASP:OD1	2.37	0.40
2:E:4184:MET:HE2	2:E:4188:ARG:HA	2.02	0.40
2:B:45:ARG:NH2	2:B:447:ASP:OD1	2.54	0.40
2:B:123:THR:OG1	2:B:134:ASP:OD1	2.37	0.40
2:B:907:LEU:O	2:B:963:ASN:ND2	2.41	0.40
2:B:1154:ASP:O	2:B:1158:ASN:N	2.53	0.40
2:B:1243:PRO:HB2	2:B:1600:LEU:HD22	2.03	0.40
2:B:2430:ILE:HG21	2:B:2502:UNK:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3552:UNK:O	2:B:3556:UNK:N	2.55	0.40
2:I:1124:PHE:HB2	2:I:1162:PHE:CE2	2.56	0.40
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	2.03	0.40
2:G:1973:GLN:HA	2:G:1976:ARG:HB3	2.04	0.40
2:E:395:GLN:HG3	2:E:397:GLU:H	1.86	0.40
2:E:4822:THR:O	2:E:4825:THR:OG1	2.36	0.40
2:B:1848:LEU:HD22	2:B:1853:ILE:HG13	2.03	0.40
2:G:45:ARG:NH2	2:G:447:ASP:OD1	2.54	0.40
2:G:887:ILE:HG21	2:G:959:TYR:HA	2.04	0.40
2:G:1124:PHE:HB2	2:G:1162:PHE:CE2	2.56	0.40
2:B:2145:SER:HB2	2:B:3647:HIS:CE1	2.56	0.40
2:I:689:THR:H	2:I:778:PHE:HE2	1.68	0.40
2:I:1259:ARG:NH2	2:I:1595:LEU:O	2.54	0.40
2:I:2352:VAL:HG12	2:I:2355:ARG:HH11	1.86	0.40
2:I:3552:UNK:O	2:I:3556:UNK:N	2.55	0.40
2:I:3980:LEU:HD22	2:I:3985:LEU:HD22	2.04	0.40
2:G:1848:LEU:HD22	2:G:1853:ILE:HG13	2.03	0.40
2:G:2776:SER:O	2:G:2788:HIS:N	2.55	0.40
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	2.03	0.40
2:E:45:ARG:NH2	2:E:447:ASP:OD1	2.54	0.40
2:E:887:ILE:HG21	2:E:959:TYR:HA	2.04	0.40
2:E:1965:TYR:OH	2:E:2027:ILE:O	2.35	0.40
2:E:2927:LEU:HA	2:E:2930:LEU:HD12	2.04	0.40
2:E:3694:LYS:HA	2:E:3695:PRO:HD3	1.96	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	105/108 (97%)	93 (89%)	12 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	H	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	J	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	B	3235/4416 (73%)	2899 (90%)	330 (10%)	6 (0%)	43	77
2	E	3235/4416 (73%)	2900 (90%)	329 (10%)	6 (0%)	43	77
2	G	3235/4416 (73%)	2900 (90%)	329 (10%)	6 (0%)	43	77
2	I	3235/4416 (73%)	2899 (90%)	330 (10%)	6 (0%)	43	77
All	All	13360/18096 (74%)	11973 (90%)	1363 (10%)	24 (0%)	44	77

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	4985	LEU
2	I	4985	LEU
2	G	4985	LEU
2	E	4985	LEU
2	B	1708	ARG
2	I	1708	ARG
2	G	1708	ARG
2	E	1708	ARG
2	B	1932	PRO
2	B	2292	GLU
2	B	4641	PRO
2	I	1932	PRO
2	I	2292	GLU
2	I	4641	PRO
2	G	1932	PRO
2	G	2292	GLU
2	G	4641	PRO
2	E	1932	PRO
2	E	2292	GLU
2	E	4641	PRO
2	B	1840	PRO
2	I	1840	PRO
2	G	1840	PRO
2	E	1840	PRO

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	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3022 (82%)	2478 (99%)	15 (1%)	78	80
2	E	2493/3022 (82%)	2478 (99%)	15 (1%)	78	80
2	G	2493/3022 (82%)	2478 (99%)	15 (1%)	78	80
2	I	2493/3022 (82%)	2478 (99%)	15 (1%)	78	80
All	All	10324/12444 (83%)	10264 (99%)	60 (1%)	76	80

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	688	LEU
2	B	719	LEU
2	B	978	THR
2	B	1600	LEU
2	B	1676	LEU
2	B	3663	LEU
2	B	3805	LEU
2	B	4081	VAL
2	B	4154	VAL
2	B	4959	PHE
2	B	4961	CYS
2	B	4977	THR
2	B	4982	GLU
2	B	4983	HIS
2	I	131	LEU
2	I	688	LEU
2	I	719	LEU
2	I	978	THR

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Mol	Chain	Res	Type
2	I	1600	LEU
2	I	1676	LEU
2	I	3663	LEU
2	I	3805	LEU
2	I	4081	VAL
2	I	4154	VAL
2	I	4959	PHE
2	I	4961	CYS
2	I	4977	THR
2	I	4982	GLU
2	I	4983	HIS
2	G	131	LEU
2	G	688	LEU
2	G	719	LEU
2	G	978	THR
2	G	1600	LEU
2	G	1676	LEU
2	G	3663	LEU
2	G	3805	LEU
2	G	4081	VAL
2	G	4154	VAL
2	G	4959	PHE
2	G	4961	CYS
2	G	4977	THR
2	G	4982	GLU
2	G	4983	HIS
2	E	131	LEU
2	E	688	LEU
2	E	719	LEU
2	E	978	THR
2	E	1600	LEU
2	E	1676	LEU
2	E	3663	LEU
2	E	3805	LEU
2	E	4081	VAL
2	E	4154	VAL
2	E	4959	PHE
2	E	4961	CYS
2	E	4977	THR
2	E	4982	GLU
2	E	4983	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (234)

such sidechains are listed below:

Mol	Chain	Res	Type
1	F	31	GLN
1	F	43	ASN
1	F	87	HIS
1	A	31	GLN
1	A	43	ASN
1	A	87	HIS
1	H	31	GLN
1	H	43	ASN
1	H	87	HIS
1	J	31	GLN
1	J	43	ASN
1	J	87	HIS
2	B	57	ASN
2	B	105	HIS
2	B	111	HIS
2	B	113	HIS
2	B	201	ASN
2	B	273	HIS
2	B	379	HIS
2	B	399	GLN
2	B	412	ASN
2	B	413	GLN
2	B	489	ASN
2	B	520	ASN
2	B	582	HIS
2	B	725	HIS
2	B	765	GLN
2	B	797	HIS
2	B	838	HIS
2	B	1220	GLN
2	B	1598	GLN
2	B	1679	ASN
2	B	1688	HIS
2	B	1691	GLN
2	B	1719	HIS
2	B	1760	HIS
2	B	1775	HIS
2	B	1861	GLN
2	B	1928	GLN
2	B	1952	GLN
2	B	2005	GLN
2	B	2041	HIS

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Mol	Chain	Res	Type
2	B	2100	HIS
2	B	2127	GLN
2	B	2291	GLN
2	B	2773	ASN
2	B	3704	HIS
2	B	3771	HIS
2	B	3781	GLN
2	B	3809	ASN
2	B	3814	GLN
2	B	3830	GLN
2	B	3896	ASN
2	B	3960	GLN
2	B	3976	ASN
2	B	3994	HIS
2	B	4034	ASN
2	B	4043	GLN
2	B	4102	GLN
2	B	4109	GLN
2	B	4120	ASN
2	B	4130	ASN
2	B	4246	GLN
2	B	4776	GLN
2	B	4806	ASN
2	B	4946	GLN
2	B	4947	GLN
2	B	4983	HIS
2	B	4987	ASN
2	I	57	ASN
2	I	105	HIS
2	I	111	HIS
2	I	113	HIS
2	I	201	ASN
2	I	273	HIS
2	I	379	HIS
2	I	412	ASN
2	I	413	GLN
2	I	489	ASN
2	I	495	ASN
2	I	520	ASN
2	I	582	HIS
2	I	725	HIS
2	I	765	GLN

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Mol	Chain	Res	Type
2	I	797	HIS
2	I	838	HIS
2	I	1220	GLN
2	I	1598	GLN
2	I	1679	ASN
2	I	1688	HIS
2	I	1691	GLN
2	I	1719	HIS
2	I	1760	HIS
2	I	1775	HIS
2	I	1861	GLN
2	I	1952	GLN
2	I	2005	GLN
2	I	2041	HIS
2	I	2100	HIS
2	I	2127	GLN
2	I	2291	GLN
2	I	2773	ASN
2	I	3704	HIS
2	I	3771	HIS
2	I	3781	GLN
2	I	3809	ASN
2	I	3814	GLN
2	I	3830	GLN
2	I	3896	ASN
2	I	3906	GLN
2	I	3960	GLN
2	I	3976	ASN
2	I	3994	HIS
2	I	4034	ASN
2	I	4043	GLN
2	I	4102	GLN
2	I	4109	GLN
2	I	4120	ASN
2	I	4776	GLN
2	I	4806	ASN
2	I	4946	GLN
2	I	4947	GLN
2	I	4983	HIS
2	I	4987	ASN
2	G	57	ASN
2	G	105	HIS

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Mol	Chain	Res	Type
2	G	111	HIS
2	G	113	HIS
2	G	201	ASN
2	G	273	HIS
2	G	379	HIS
2	G	412	ASN
2	G	413	GLN
2	G	489	ASN
2	G	520	ASN
2	G	725	HIS
2	G	765	GLN
2	G	797	HIS
2	G	838	HIS
2	G	1220	GLN
2	G	1598	GLN
2	G	1679	ASN
2	G	1688	HIS
2	G	1691	GLN
2	G	1719	HIS
2	G	1760	HIS
2	G	1775	HIS
2	G	1861	GLN
2	G	1952	GLN
2	G	2005	GLN
2	G	2041	HIS
2	G	2100	HIS
2	G	2127	GLN
2	G	2291	GLN
2	G	2773	ASN
2	G	3704	HIS
2	G	3771	HIS
2	G	3781	GLN
2	G	3809	ASN
2	G	3814	GLN
2	G	3830	GLN
2	G	3896	ASN
2	G	3906	GLN
2	G	3960	GLN
2	G	3976	ASN
2	G	3994	HIS
2	G	4034	ASN
2	G	4043	GLN

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Mol	Chain	Res	Type
2	G	4054	ASN
2	G	4102	GLN
2	G	4109	GLN
2	G	4120	ASN
2	G	4776	GLN
2	G	4806	ASN
2	G	4946	GLN
2	G	4947	GLN
2	G	4983	HIS
2	G	4987	ASN
2	E	57	ASN
2	E	105	HIS
2	E	111	HIS
2	E	113	HIS
2	E	201	ASN
2	E	273	HIS
2	E	379	HIS
2	E	412	ASN
2	E	413	GLN
2	E	489	ASN
2	E	495	ASN
2	E	520	ASN
2	E	582	HIS
2	E	725	HIS
2	E	765	GLN
2	E	797	HIS
2	E	838	HIS
2	E	1220	GLN
2	E	1598	GLN
2	E	1679	ASN
2	E	1688	HIS
2	E	1691	GLN
2	E	1719	HIS
2	E	1760	HIS
2	E	1775	HIS
2	E	1861	GLN
2	E	1952	GLN
2	E	2005	GLN
2	E	2041	HIS
2	E	2100	HIS
2	E	2127	GLN
2	E	2291	GLN

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Mol	Chain	Res	Type
2	E	2773	ASN
2	E	3704	HIS
2	E	3771	HIS
2	E	3781	GLN
2	E	3809	ASN
2	E	3814	GLN
2	E	3830	GLN
2	E	3896	ASN
2	E	3906	GLN
2	E	3960	GLN
2	E	3976	ASN
2	E	3994	HIS
2	E	4034	ASN
2	E	4043	GLN
2	E	4102	GLN
2	E	4109	GLN
2	E	4120	ASN
2	E	4130	ASN
2	E	4246	GLN
2	E	4776	GLN
2	E	4806	ASN
2	E	4946	GLN
2	E	4983	HIS
2	E	4987	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	14
2	I	14
2	G	14
2	E	14

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	73.83
1	I	4345:UNK	C	4540:PHE	N	73.83
1	G	4345:UNK	C	4540:PHE	N	73.83
1	E	4345:UNK	C	4540:PHE	N	73.83
1	B	3613:UNK	C	3639:THR	N	45.16
1	I	3613:UNK	C	3639:THR	N	45.16
1	G	3613:UNK	C	3639:THR	N	45.16
1	E	3613:UNK	C	3639:THR	N	45.16
1	B	4253:GLU	C	4320:UNK	N	28.14
1	I	4253:GLU	C	4320:UNK	N	28.14
1	G	4253:GLU	C	4320:UNK	N	28.14
1	E	4253:GLU	C	4320:UNK	N	28.14
1	B	3163:UNK	C	3170:UNK	N	16.17
1	I	3163:UNK	C	3170:UNK	N	16.17
1	G	3163:UNK	C	3170:UNK	N	16.17
1	E	3163:UNK	C	3170:UNK	N	16.17
1	B	3063:UNK	C	3134:UNK	N	14.94

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	3063:UNK	C	3134:UNK	N	14.94
1	G	3063:UNK	C	3134:UNK	N	14.94
1	E	3063:UNK	C	3134:UNK	N	14.94
1	B	3468:UNK	C	3511:UNK	N	14.40
1	I	3468:UNK	C	3511:UNK	N	14.40
1	G	3468:UNK	C	3511:UNK	N	14.40
1	E	3468:UNK	C	3511:UNK	N	14.40
1	B	2703:UNK	C	2734:ASN	N	13.12
1	I	2703:UNK	C	2734:ASN	N	13.12
1	G	2703:UNK	C	2734:ASN	N	13.12
1	E	2703:UNK	C	2734:ASN	N	13.12
1	B	3236:UNK	C	3241:UNK	N	12.96
1	I	3236:UNK	C	3241:UNK	N	12.96
1	G	3236:UNK	C	3241:UNK	N	12.96
1	E	3236:UNK	C	3241:UNK	N	12.96
1	B	1564:UNK	C	1573:MET	N	12.42
1	I	1564:UNK	C	1573:MET	N	12.42
1	G	1564:UNK	C	1573:MET	N	12.42
1	E	1564:UNK	C	1573:MET	N	12.42
1	B	2976:UNK	C	2995:UNK	N	12.17
1	I	2976:UNK	C	2995:UNK	N	12.17
1	G	2976:UNK	C	2995:UNK	N	12.17
1	E	2976:UNK	C	2995:UNK	N	12.17
1	B	3254:UNK	C	3261:UNK	N	8.29
1	I	3254:UNK	C	3261:UNK	N	8.29
1	G	3254:UNK	C	3261:UNK	N	8.29
1	E	3254:UNK	C	3261:UNK	N	8.29
1	G	1297:UNK	C	1430:UNK	N	6.05
1	B	1297:UNK	C	1430:UNK	N	6.04
1	I	1297:UNK	C	1430:UNK	N	6.04
1	E	1297:UNK	C	1430:UNK	N	6.04
1	I	2939:ARG	C	2942:UNK	N	3.73
1	G	2939:ARG	C	2942:UNK	N	3.73
1	E	2939:ARG	C	2942:UNK	N	3.73
1	B	2939:ARG	C	2942:UNK	N	3.72
1	G	2479:LEU	C	2487:UNK	N	3.51
1	B	2479:LEU	C	2487:UNK	N	3.50
1	I	2479:LEU	C	2487:UNK	N	3.50
1	E	2479:LEU	C	2487:UNK	N	3.50

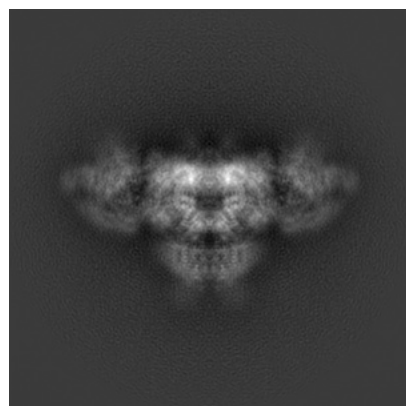
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8390. These allow visual inspection of the internal detail of the map and identification of artifacts.

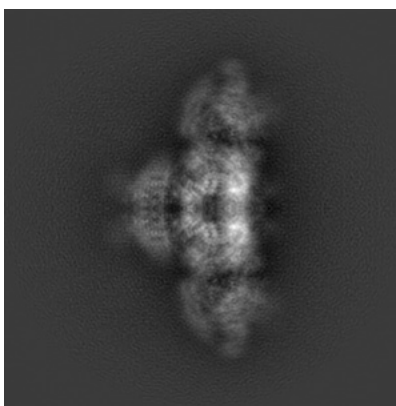
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

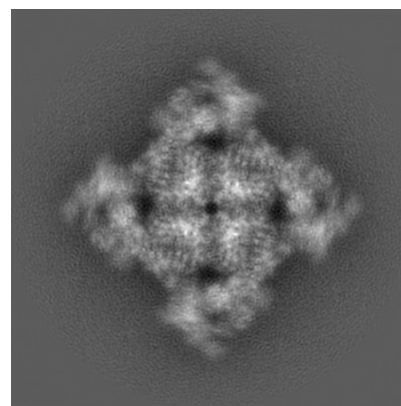
6.1.1 Primary map



X

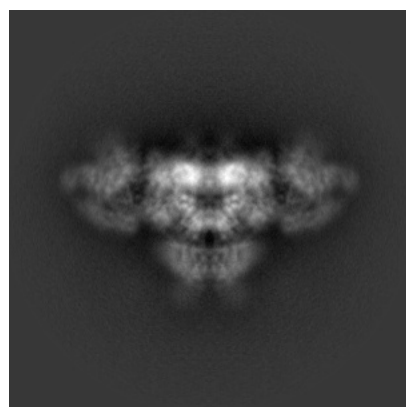


Y

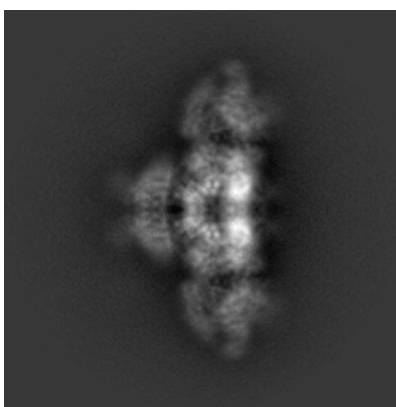


Z

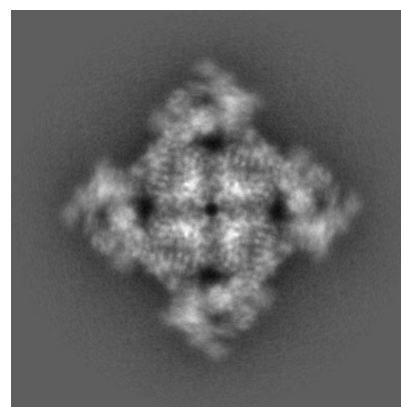
6.1.2 Raw map



X



Y



Z

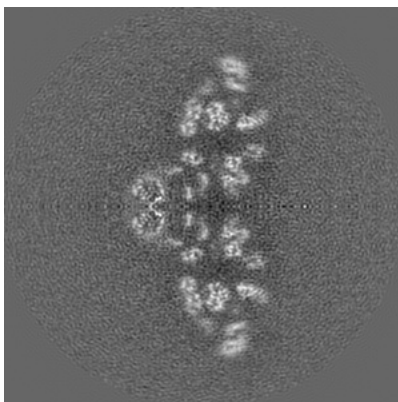
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

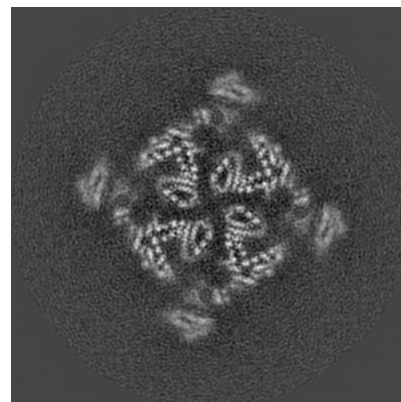
6.2.1 Primary map



X Index: 200

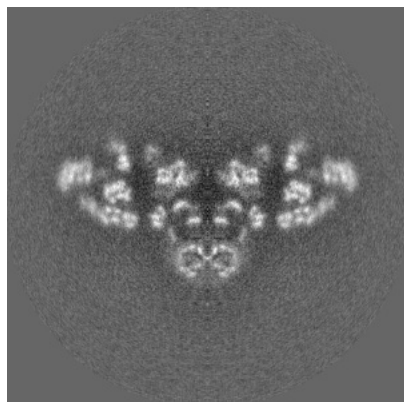


Y Index: 200

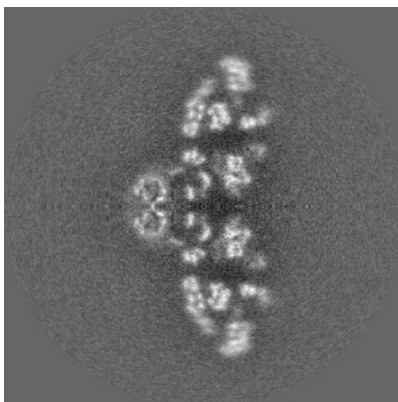


Z Index: 200

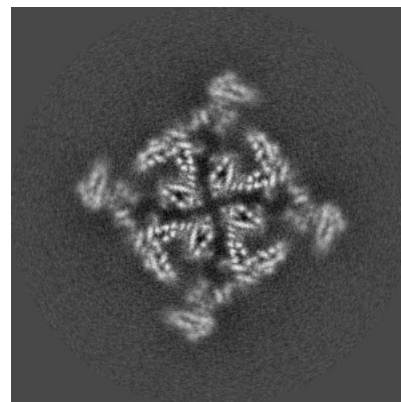
6.2.2 Raw map



X Index: 200



Y Index: 200

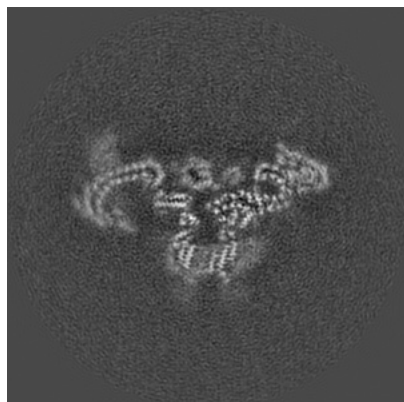


Z Index: 200

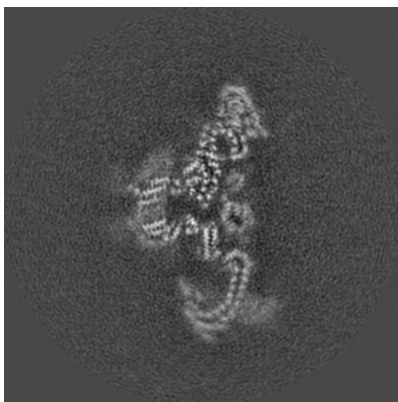
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

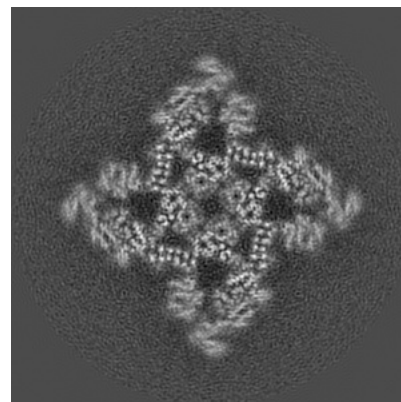
6.3.1 Primary map



X Index: 175

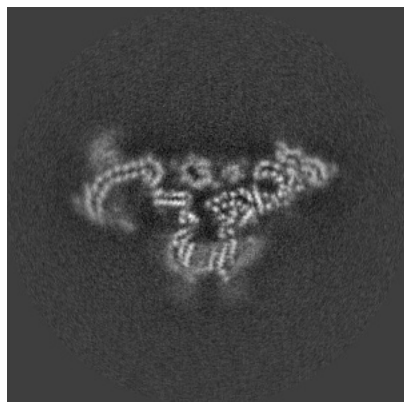


Y Index: 225

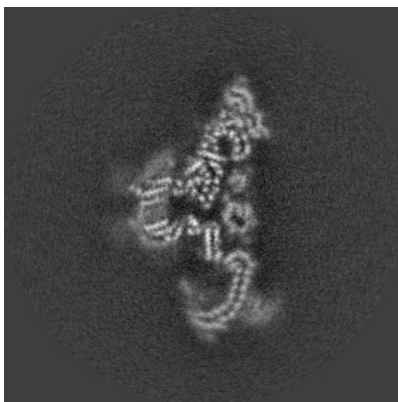


Z Index: 227

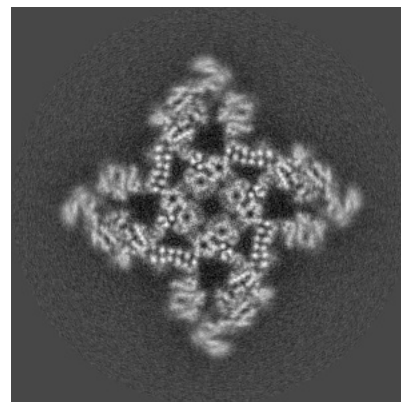
6.3.2 Raw map



X Index: 175



Y Index: 225

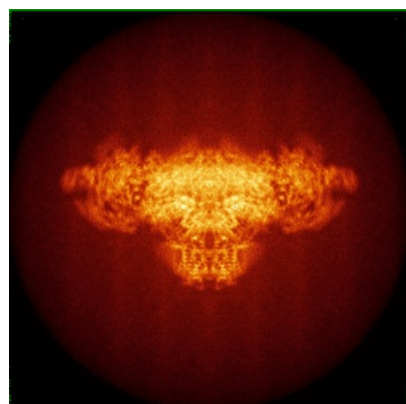


Z Index: 229

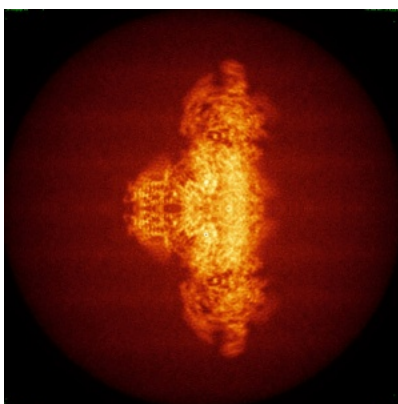
The images above show the largest variance slices of the map in three orthogonal directions.

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

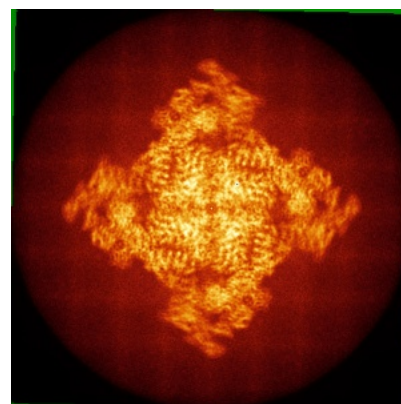
6.4.1 Primary map



X

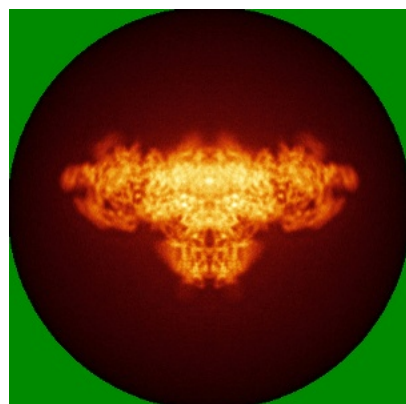


Y

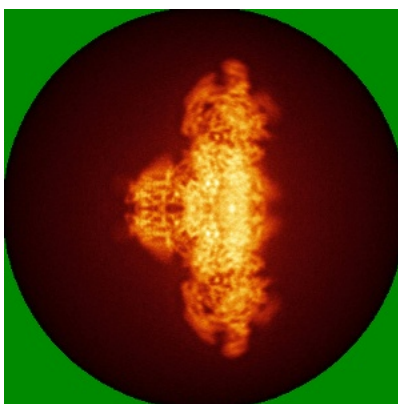


Z

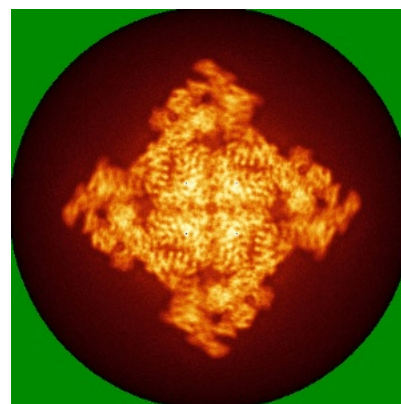
6.4.2 Raw map



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.

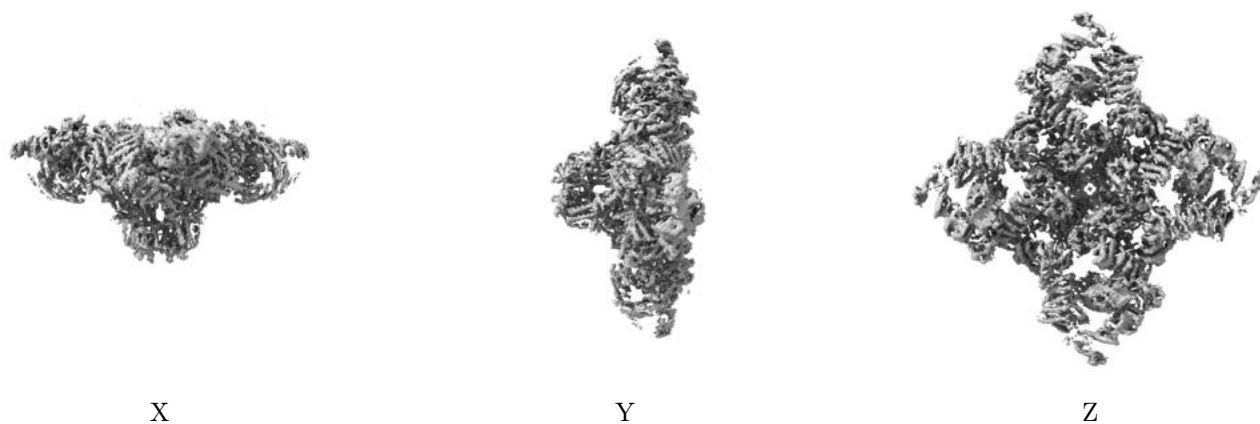
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. 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.

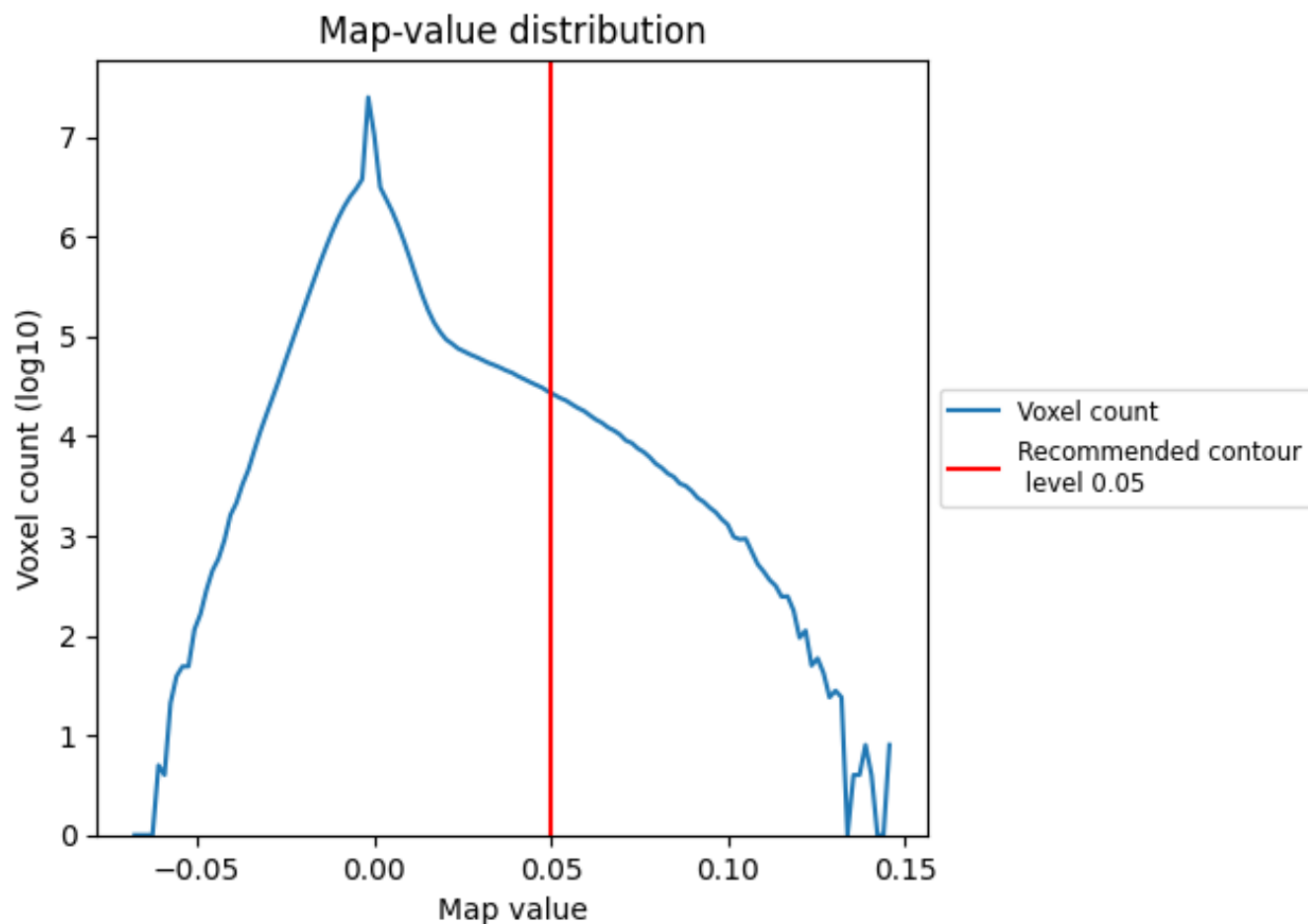
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

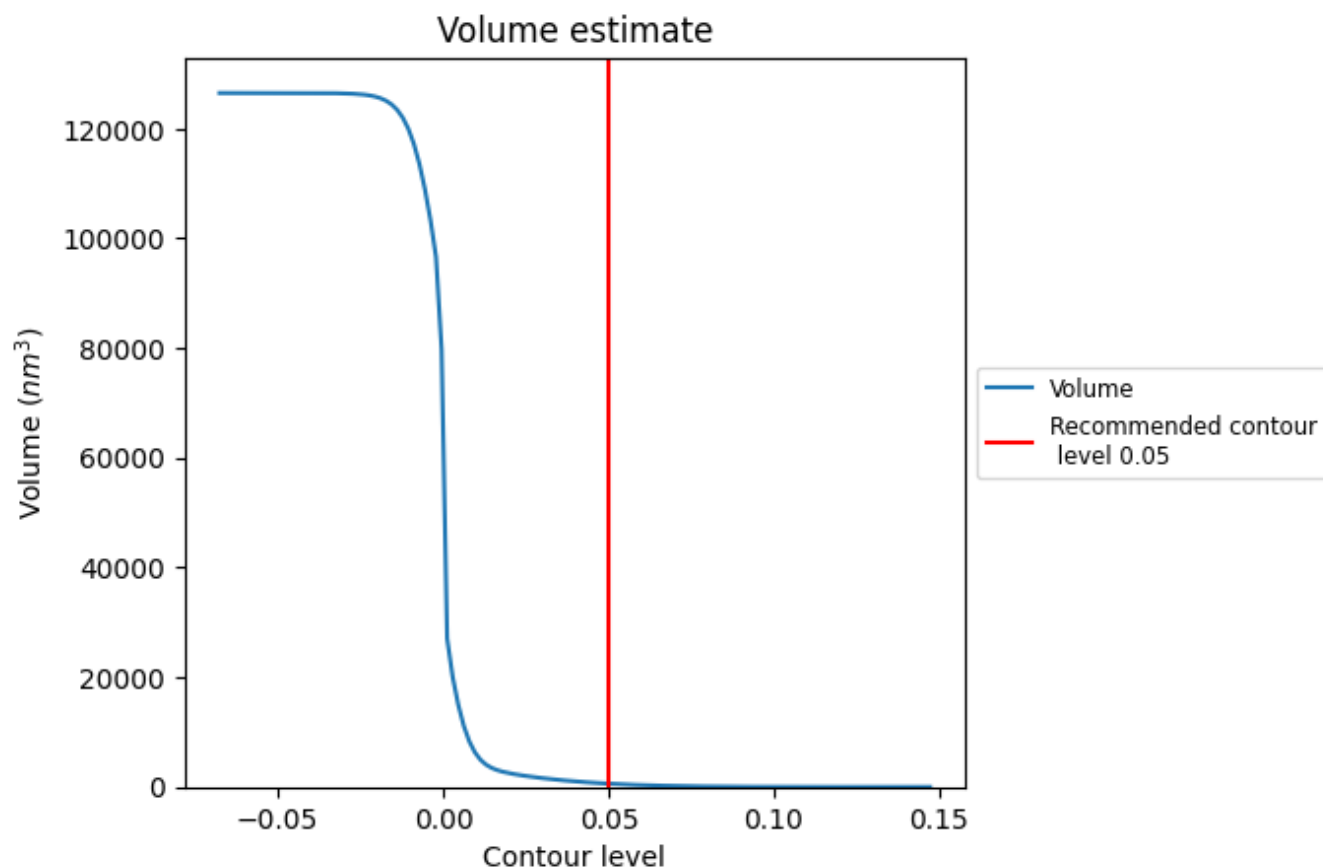
This section contains the results of statistical analysis of the map.

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.

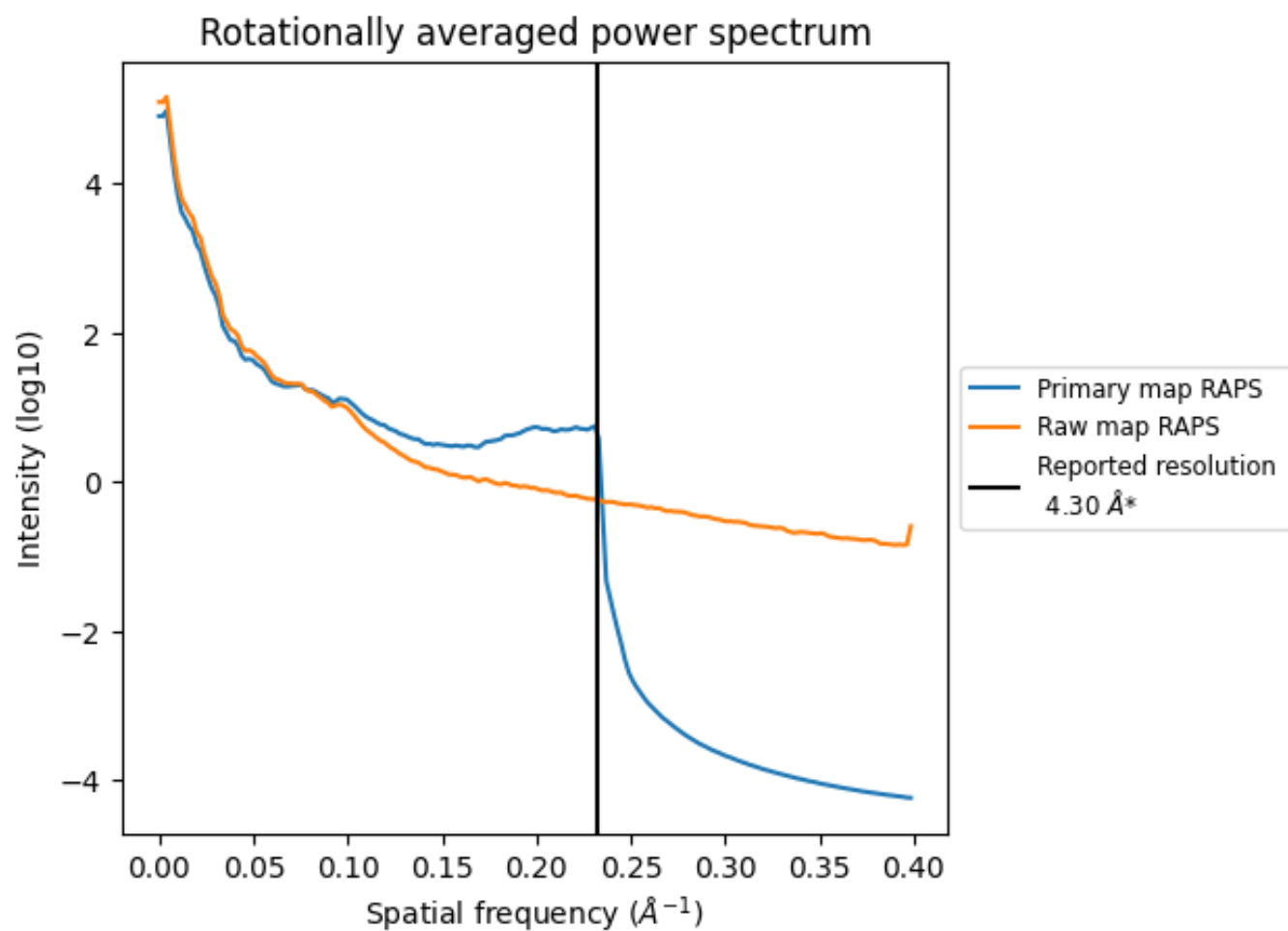
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 603 nm³; this corresponds to an approximate mass of 545 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 ⓘ

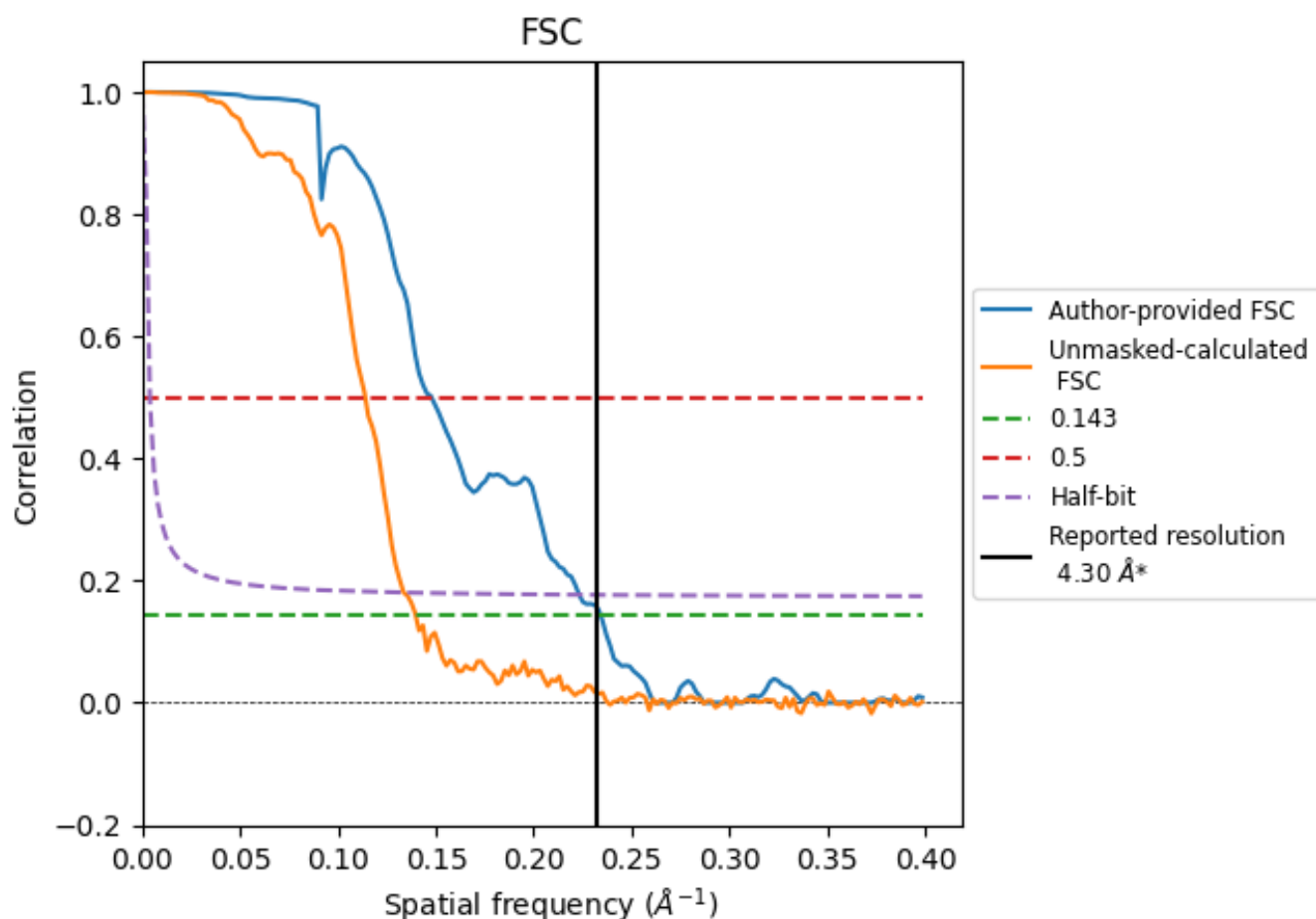


*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

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 $0.233 \text{ \AA}^{-1}$

8.2 Resolution estimates

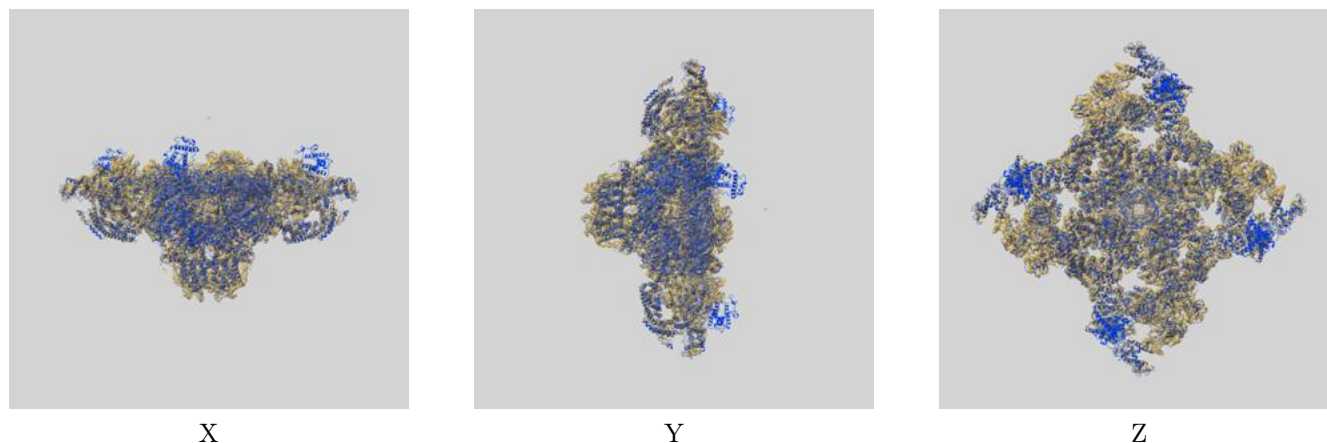
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.27	6.77	4.48
Unmasked-calculated*	7.16	8.77	7.49

*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 7.16 differs from the reported value 4.3 by more than 10 %

9 Map-model fit [i](#)

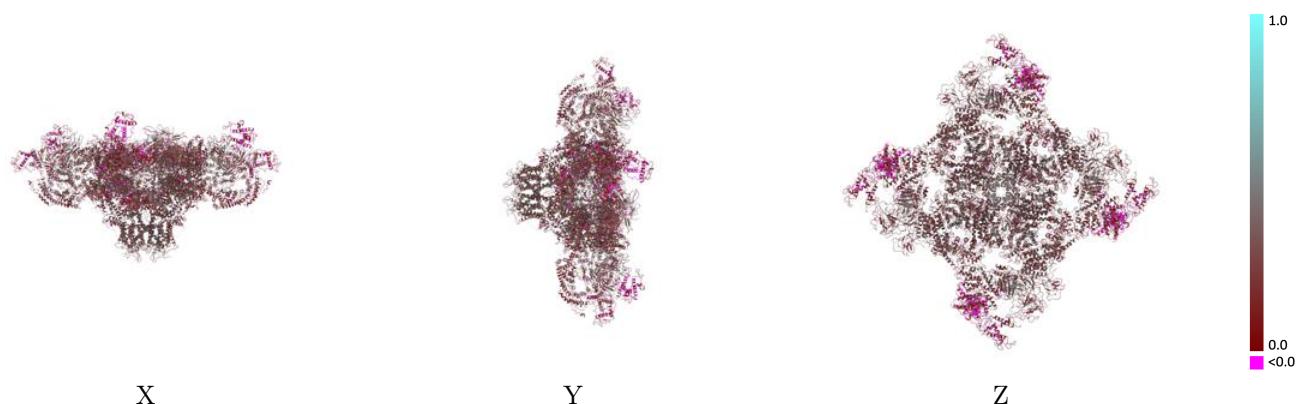
This section contains information regarding the fit between EMDB map EMD-8390 and PDB model 5TAZ. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



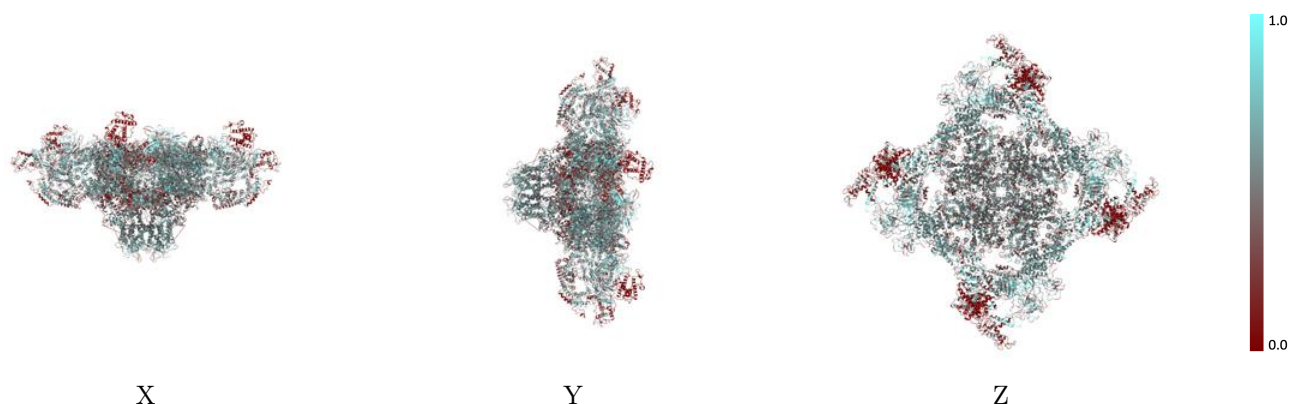
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



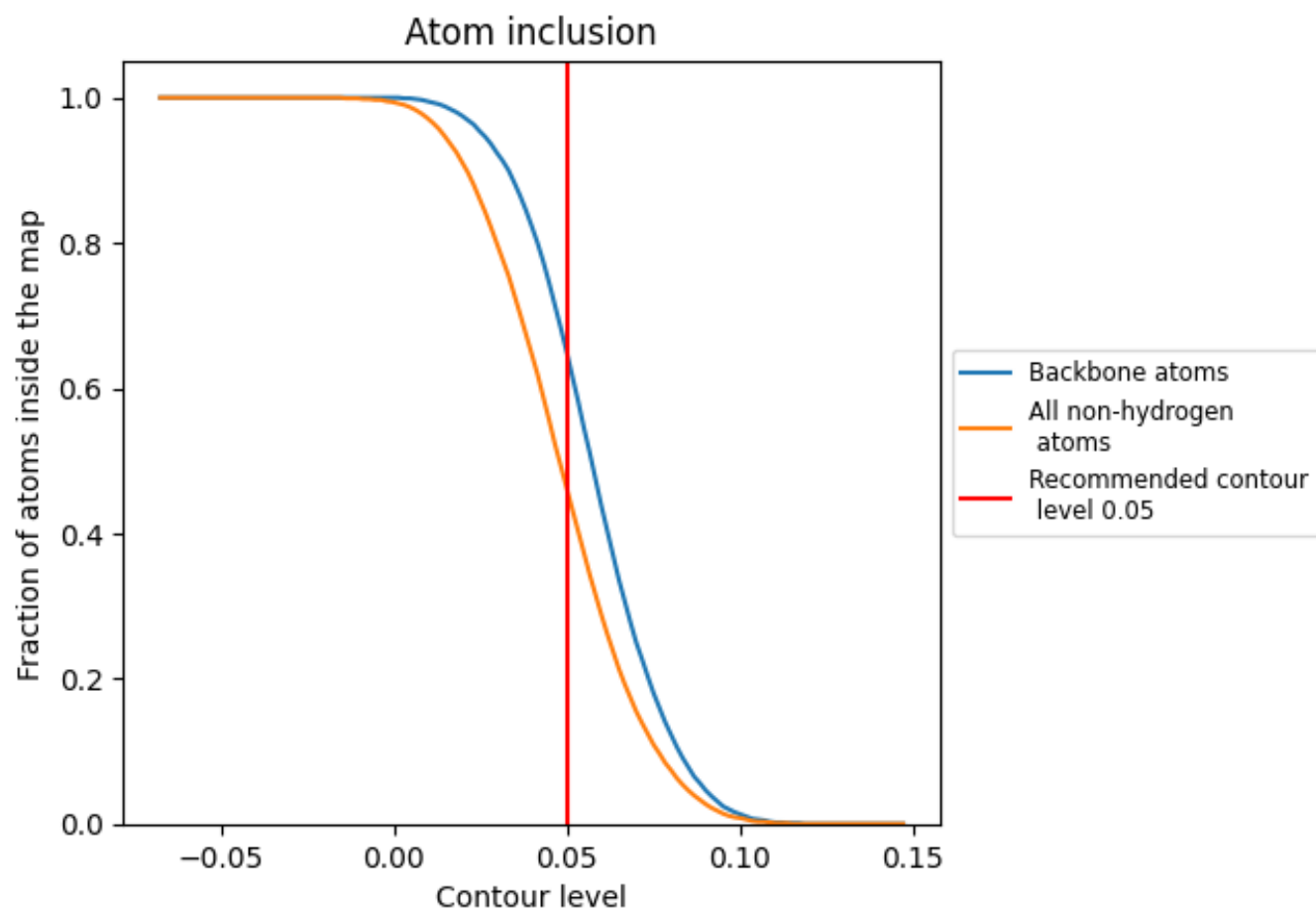
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 46% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4620	0.2730
A	0.4880	0.2880
B	0.4610	0.2730
E	0.4610	0.2730
F	0.4860	0.2930
G	0.4610	0.2730
H	0.4850	0.2930
I	0.4610	0.2730
J	0.4910	0.2910

