



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 04:46 AM UTC

PDB ID : 5TAQ / pdb_00005taq
EMDB ID : EMD-8382
Title : Structure of rabbit RyR1 (Caffeine/ATP/Ca²⁺ dataset, class 3&4)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-10
Resolution : 4.10 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

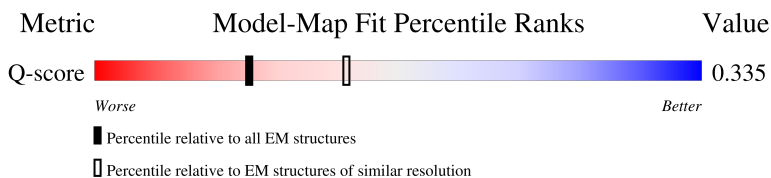
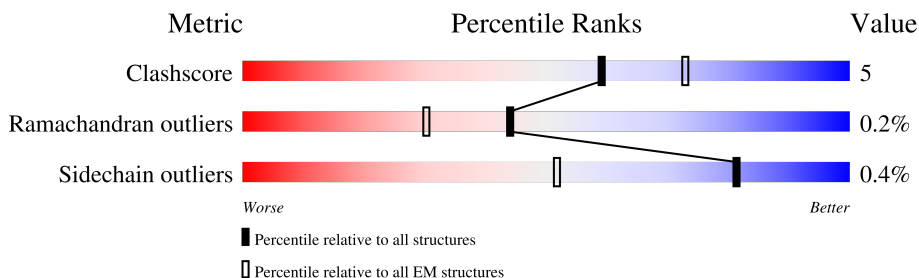
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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.



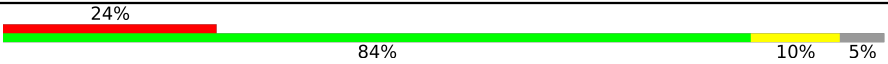
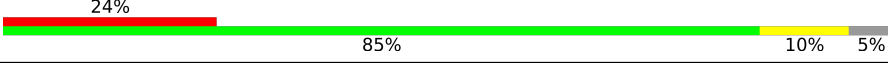
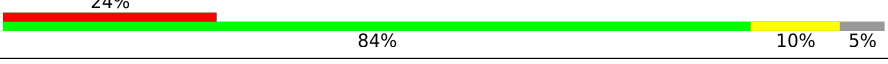
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 (3.60 - 4.60)

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	20% 80% 19% ..
1	F	108	19% 80% 19% ..
1	H	108	21% 80% 19% ..
1	J	108	19% 78% 20% ..

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Mol	Chain	Length	Quality of chain
2	B	4416	
2	E	4416	
2	G	4416	
2	I	4416	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CFF	B	5102	-	X	-	-
4	CFF	E	5102	-	X	-	-
4	CFF	G	5102	-	X	-	-
4	CFF	I	5102	-	X	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 121456 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.

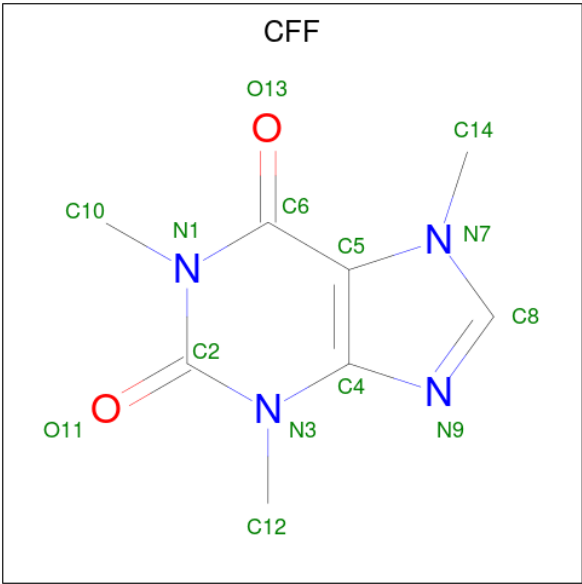
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

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



Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	4	2	
4	E	1	Total	C	N	O	0
			14	8	4	2	
4	I	1	Total	C	N	O	0
			14	8	4	2	
4	G	1	Total	C	N	O	0
			14	8	4	2	

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

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

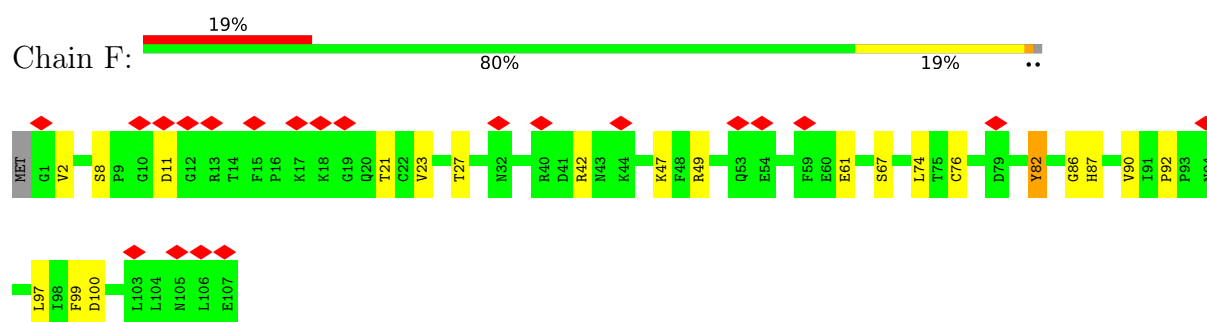
- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

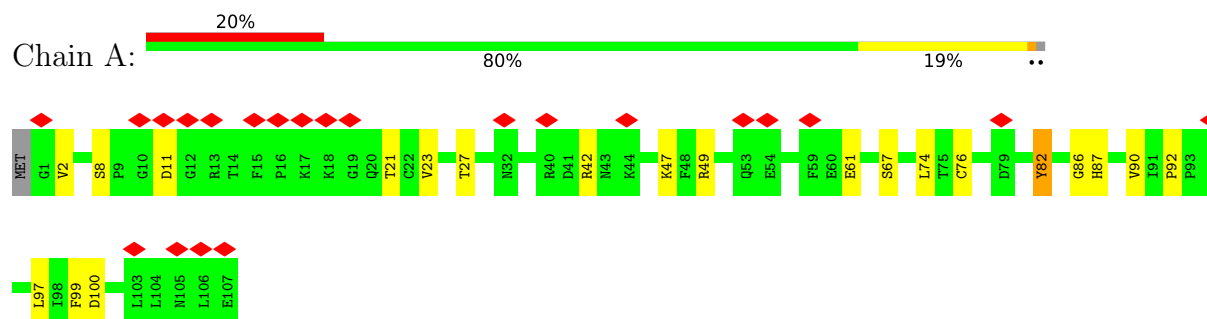
3 Residue-property plots [i](#)

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.

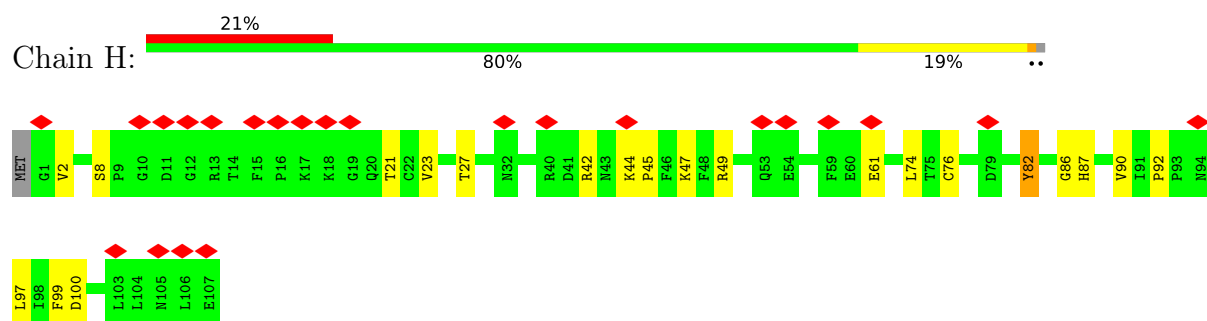
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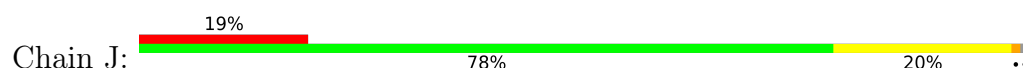
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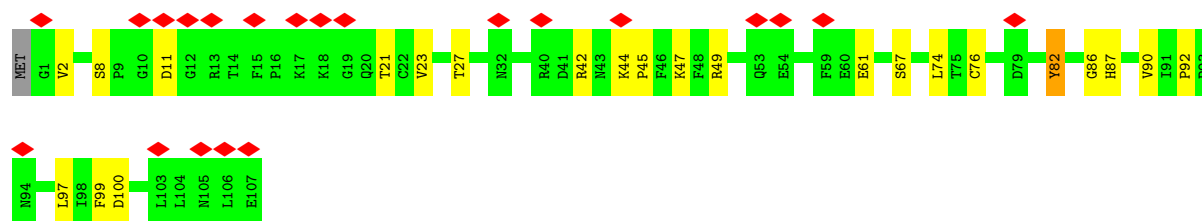


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

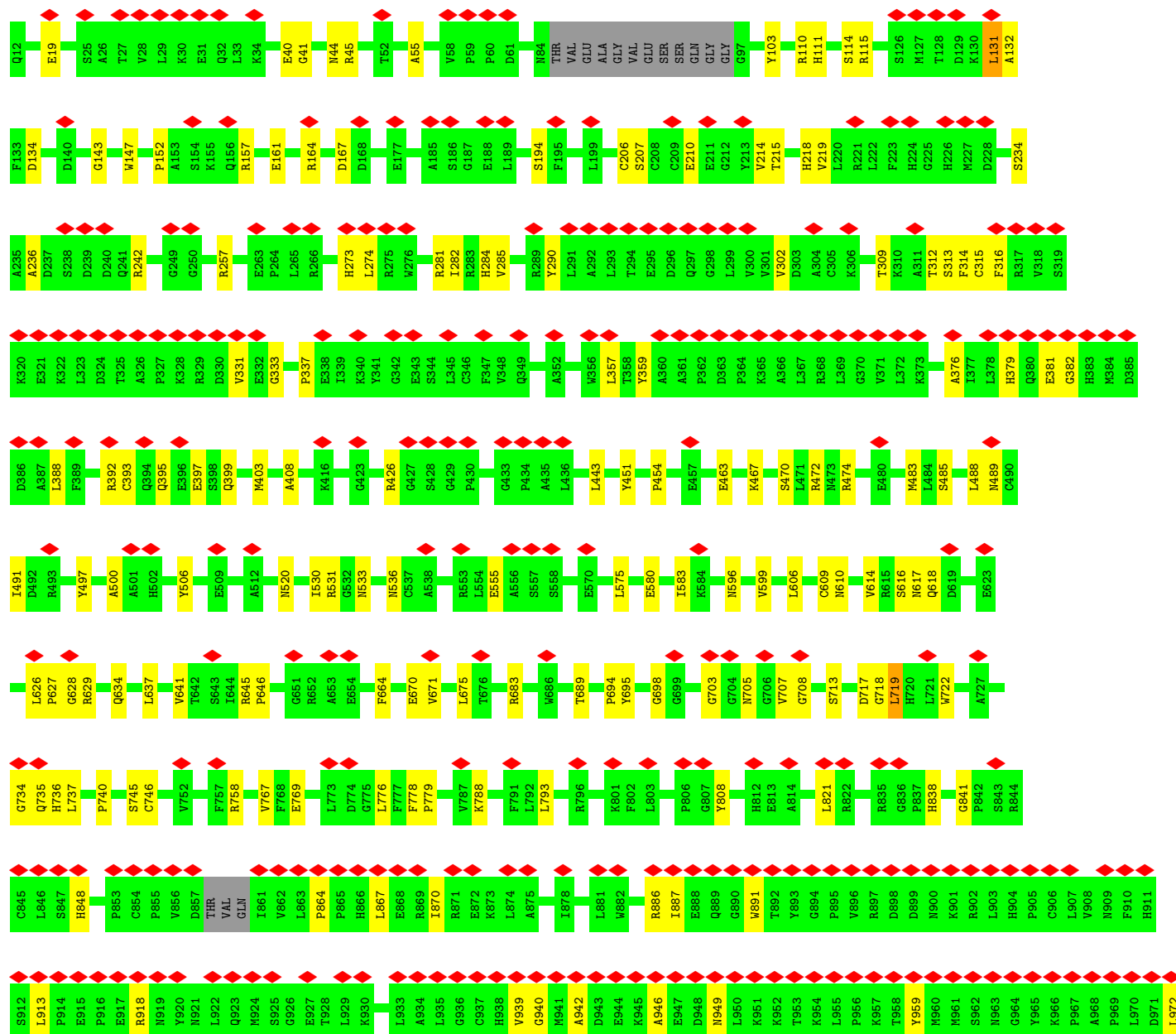
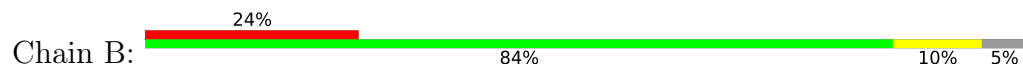


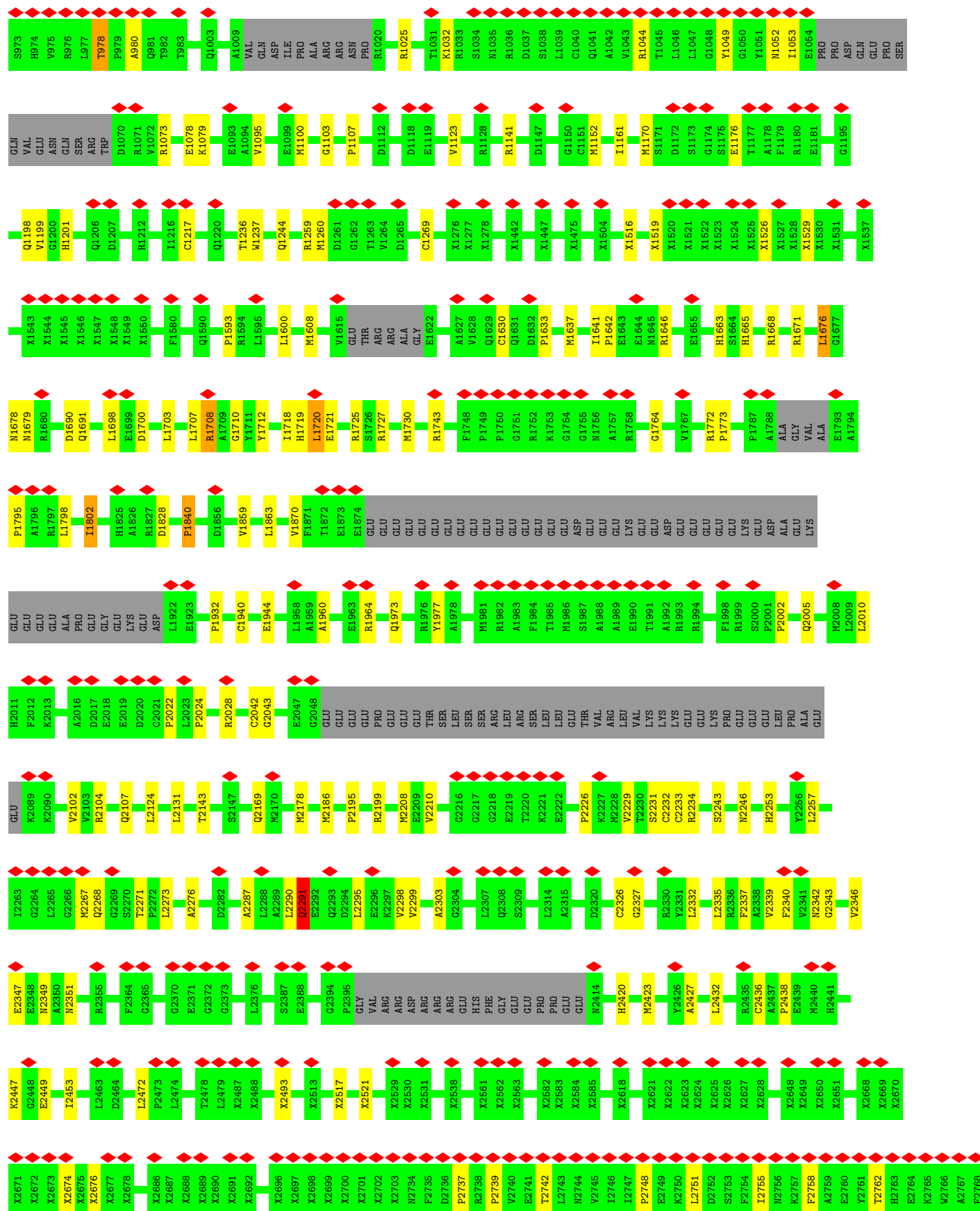
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



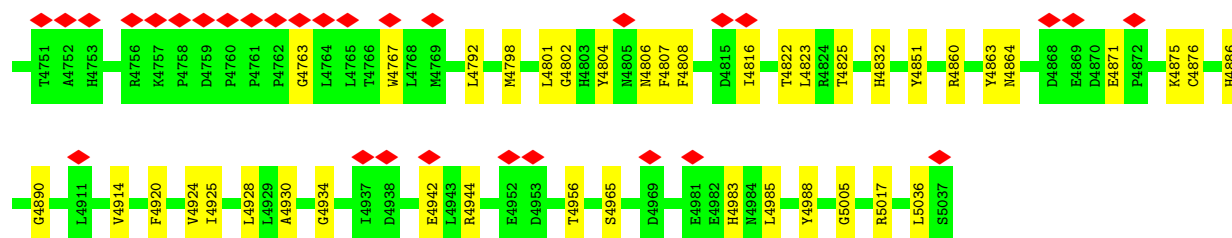


• Molecule 2: Ryanodine receptor 1

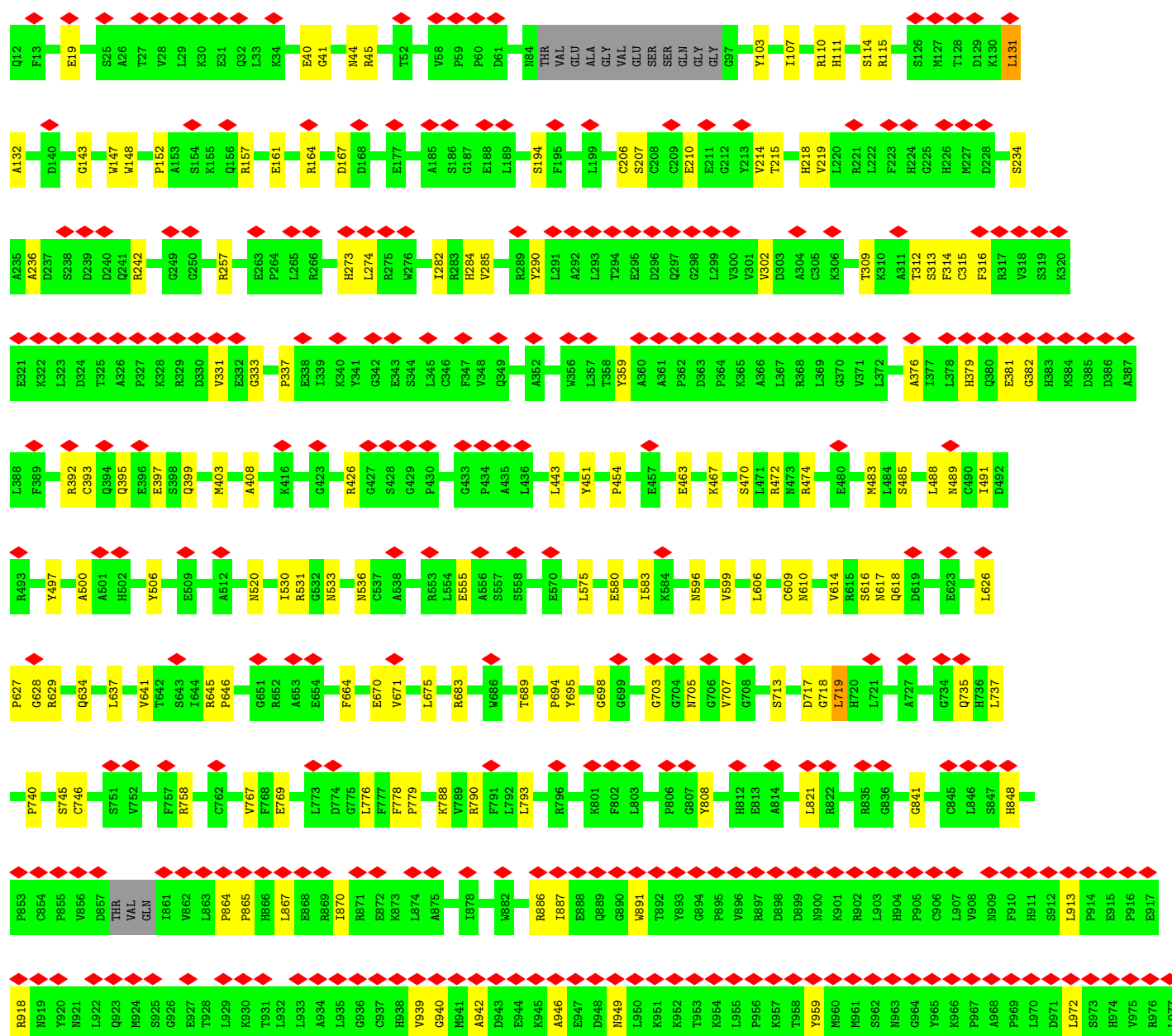
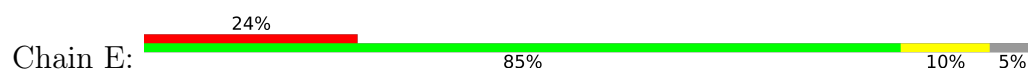




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TRP	R4188	M3955	ALA	X3436	X3341	X3243	X3137	K2890	E2830
GLY	E4206	Q3960	GLU	X3441	X3348	X3244	X3138	K2891	K2770
ALA	Q4209	Q3961	E3747	X3452	X3349	X3245	X3142	Q2892	I2771
GLY	R4215	G3971	E3748	X3453	X3350	X3246	X3143	R2893	Q2772
GLU	R4219	R3984	V3749	X3454	X3351	X3247	X3144	E2894	R2773
ALA	F4219	M4000	E3750	X3455	X3352	X3248	X3153	L2895	R2774
GLU	F4219	M4001	T3772	X3456	X3358	X3249	X3156	E2896	W2775
GLY	G4226	K4002	R3773	X3464	X3359	X3250	X3157	A2897	S2776
ASP	E4227	L4017	V3779	X3467	X3360	X3251	X3158	K2897	T2777
GLU	E4228	D4018	L3780	X3468	X3361	X3252	X3159	Q2898	Q2778
ASP	A4228	L4019	Q3781	X3511	X3362	X3253	X3160	G2899	E2779
GLU	E4232	L4019	S3784	X3512	X3365	X3254	X3161	Q2900	W2780
ALA	L4233	D4046	I3804	X3514	X3366	X3255	X3162	T2901	V2781
GLU	S4236	M4047	L3805	X3515	X3369	X3256	X3163	H2902	D2782
GLY	X4321	D4083	M3809	X3520	X3370	X3257	X3170	P2903	E2783
ASP	X4322	L4066	K3815	X3530	X3378	X3258	X3171	L2904	E2784
GLU	F4540	D4070	L3842	X3533	X3385	X3259	X3172	L2905	L2785
ALA	R4548	D4079	D3843	X3534	X3386	X3260	X3173	V2906	K2786
GLY	Y4560	V4081	Q3850	X3540	X3387	X3261	X3174	P2907	T2787
GLY	L4567	T4082	G3857	X3543	X3388	X3262	X3177	Y2908	H2788
GLY	A4570	D4083	M3858	X3544	X3389	X3263	X3178	T2909	P2789
GLY	M4574	G4086	V3859	X3545	X3390	X3264	X3190	L2910	W2790
GLY	V4582	K4091	E3861	X3546	X3391	X3265	X3191	L2911	L2791
GLY	P4587	K4095	G3862	X3547	X3392	X3266	X3192	T2912	R2792
GLU	GLY	D4097	T3864	X3548	X3393	X3267	X3193	A2913	P2793
ASP	ASP	D4098	V3865	X3550	X3394	X3268	X3194	E2915	Y2794
ASP	ASP	T4104	I3866	X3553	X3395	X3269	X3195	K2916	K2795
MET	GLY	G4105	R3867	X3554	X3396	X3270	X3196	A2917	T2796
GLY	GLY	P4106	Q3869	X3558	X3397	X3271	X3197	S2863	F2797
SER	ALA	M4142	N3870	X3559	X3398	X3272	X3200	G2864	S2798
ALA	ALA	V4145	G3871	X3560	X3399	X3273	X3207	E2865	E2799
ASP	ASP	E4152	E3872	X3561	X3400	X3274	X3211	T2866	K2800
LEU	ALA	P4155	K3873	X3562	X3401	X3275	X3212	L2867	D2801
ALA	GLY	H4156	D3878	X3563	X3402	X3276	X3213	S2868	E2802
GLY	GLY	Y4173	Q3889	X3564	X3403	X3277	X3214	E2869	E2803
SER	GLY	R4180	I3915	X3565	X3404	X3278	X3215	Q2870	T2804
GLY	GLY	A4186	T3919	X3566	X3405	X3279	X3216	E2871	T2805
SER	SER		S3929	X3567	X3409	X3280	X3217	Q2872	R2806
			D3932	X3568	X3410	X3281	X3218	L2873	W2807
				X3576	X3411	X3282	X3219	M2874	T2808
				X3580	X3412	X3283	X3220	A2875	L2809
				X3581	X3413	X3284	X3221	E2876	K2810
				X3582	X3414	X3285	X3222	Q2877	E2811
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						X3289	X3226	Y2881	A2815
						X3290	X3227	Y2882	M2816
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						X3298	X3235		E2824
						X3299	X3236		K2825
						X3300	X3237		A2826
						X3301	X3238		R2827
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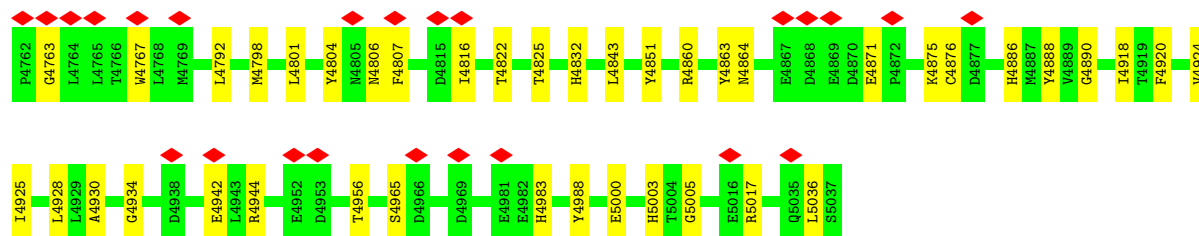


• Molecule 2: Ryanodine receptor 1

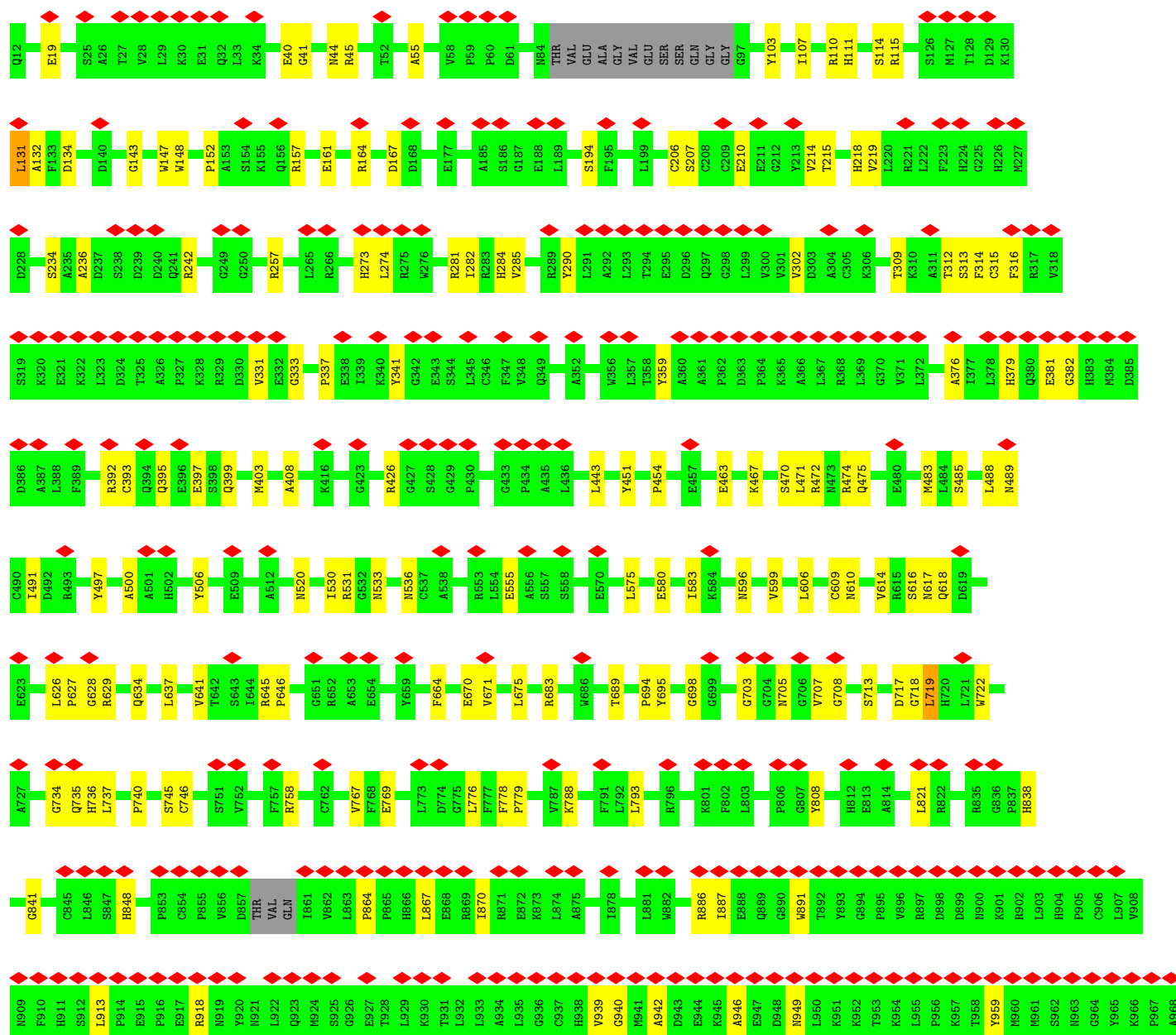
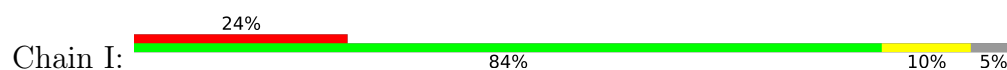






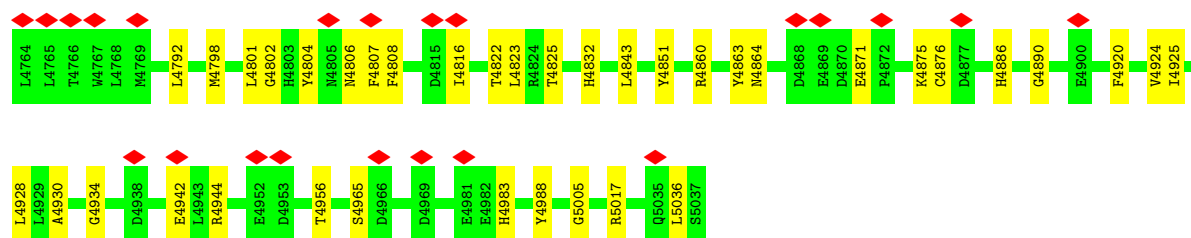


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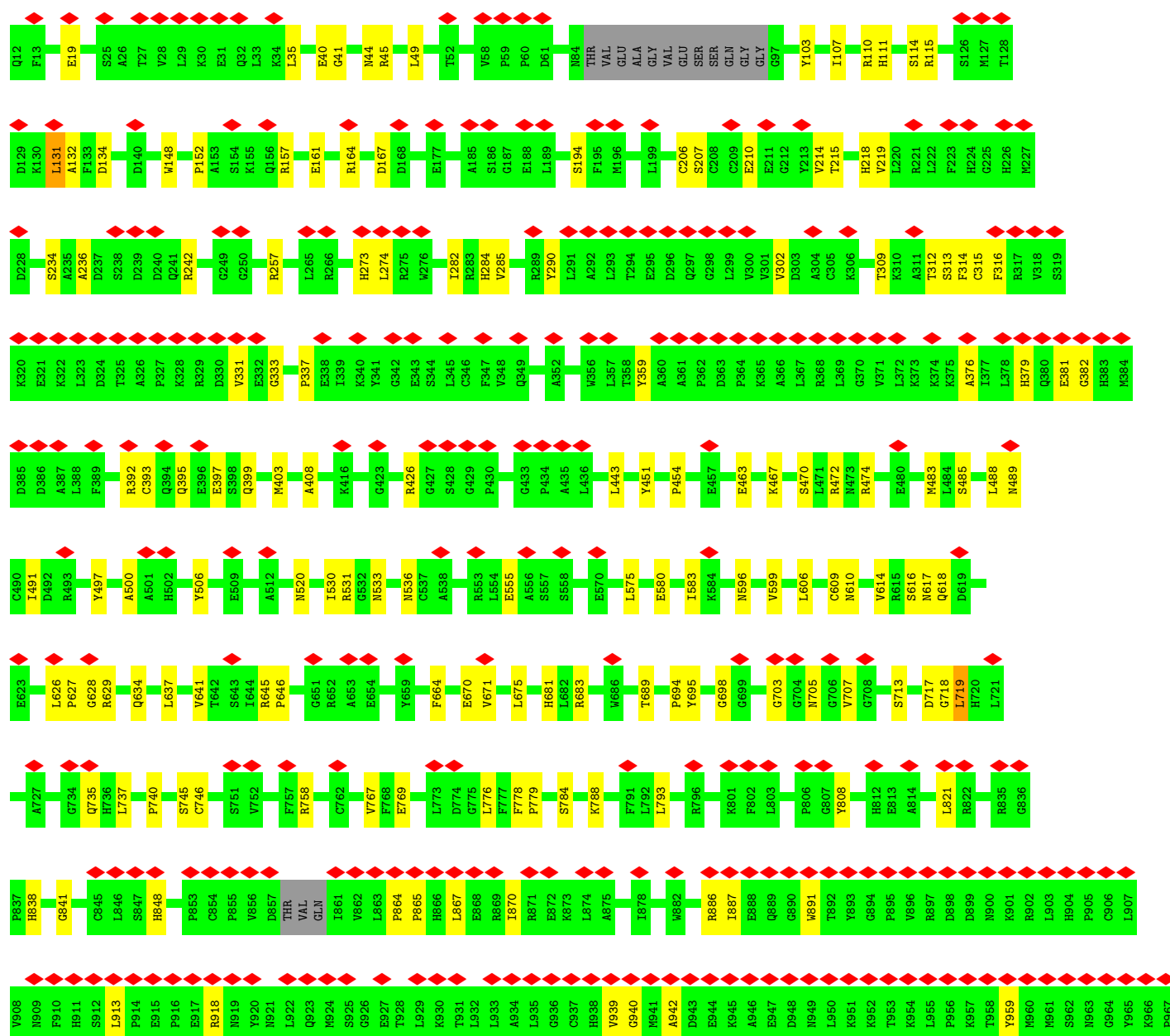
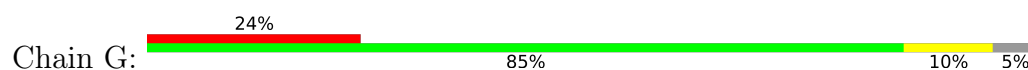






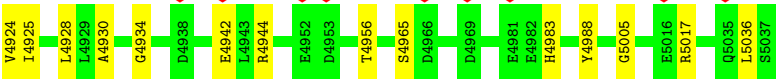
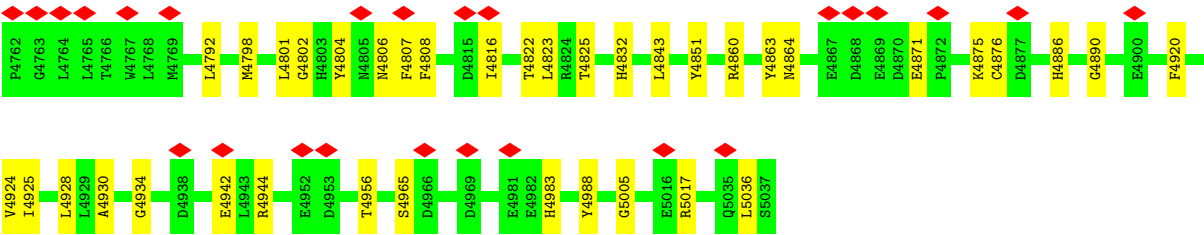


• Molecule 2: Ryanodine receptor 1









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	0.114	Depositor
Minimum map value	-0.070	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.025	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, CFF, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.22	0/834	0.51	0/1123
1	F	0.22	0/834	0.51	0/1123
1	H	0.22	0/834	0.51	0/1123
1	J	0.22	0/834	0.51	0/1123
2	B	0.26	0/25428	0.57	9/34534 (0.0%)
2	E	0.26	0/25428	0.57	8/34534 (0.0%)
2	G	0.26	0/25428	0.57	8/34534 (0.0%)
2	I	0.25	0/25428	0.57	8/34534 (0.0%)
All	All	0.25	0/105048	0.57	33/142628 (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
1	A	0	2
1	F	0	2
1	H	0	2
1	J	0	2
2	B	0	18
2	E	0	18
2	G	0	18
2	I	0	18
All	All	0	80

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	4666	VAL	CA-C-N	-9.47	109.58	121.04
2	G	4666	VAL	C-N-CA	-9.47	109.58	121.04
2	B	4666	VAL	CA-C-N	-9.46	109.59	121.04
2	B	4666	VAL	C-N-CA	-9.46	109.59	121.04
2	E	4666	VAL	CA-C-N	-9.46	109.60	121.04
2	E	4666	VAL	C-N-CA	-9.46	109.60	121.04
2	I	4666	VAL	CA-C-N	-9.46	109.60	121.04
2	I	4666	VAL	C-N-CA	-9.46	109.60	121.04
2	E	4639	MET	CA-C-N	6.96	138.79	121.80
2	E	4639	MET	C-N-CA	6.96	138.79	121.80
2	B	4639	MET	CA-C-N	6.95	138.75	121.80
2	B	4639	MET	C-N-CA	6.95	138.75	121.80
2	I	4639	MET	CA-C-N	6.94	138.73	121.80
2	I	4639	MET	C-N-CA	6.94	138.73	121.80
2	G	4639	MET	CA-C-N	6.93	138.72	121.80
2	G	4639	MET	C-N-CA	6.93	138.72	121.80
2	E	4667	PRO	N-CA-C	-5.25	107.32	114.98
2	B	4667	PRO	N-CA-C	-5.22	107.36	114.98
2	I	4667	PRO	N-CA-C	-5.21	107.37	114.98
2	B	2291	GLN	CA-C-N	5.21	135.38	126.32
2	B	2291	GLN	C-N-CA	5.21	135.38	126.32
2	E	2291	GLN	CA-C-N	5.18	135.34	126.32
2	E	2291	GLN	C-N-CA	5.18	135.34	126.32
2	G	4667	PRO	N-CA-C	-5.18	107.42	114.98
2	G	2291	GLN	CA-C-N	5.16	135.29	126.32
2	G	2291	GLN	C-N-CA	5.16	135.29	126.32
2	I	2291	GLN	CA-C-N	5.13	135.25	126.32
2	I	2291	GLN	C-N-CA	5.13	135.25	126.32
2	B	1802	ILE	N-CA-C	-5.13	104.98	109.19
2	G	131	LEU	CA-CB-CG	5.07	134.03	116.30
2	B	131	LEU	CA-CB-CG	5.06	134.00	116.30
2	E	131	LEU	CA-CB-CG	5.06	134.00	116.30
2	I	131	LEU	CA-CB-CG	5.06	134.00	116.30

There are no chirality outliers.

All (80) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
1	A	82	TYR	Peptide
2	B	1676	LEU	Peptide
2	B	1690	ASP	Peptide
2	B	1720	LEU	Peptide

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Mol	Chain	Res	Type	Group
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	1840	PRO	Peptide
2	B	2291	GLN	Peptide
2	B	2343	GLY	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	312	THR	Peptide
2	B	3971	GLY	Peptide
2	B	4096	ALA	Peptide
2	B	4641	PRO	Peptide
2	B	4666	VAL	Peptide
2	B	4807	PHE	Peptide
2	B	694	PRO	Peptide
2	B	808	TYR	Peptide
2	E	1676	LEU	Peptide
2	E	1690	ASP	Peptide
2	E	1720	LEU	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide
2	E	1840	PRO	Peptide
2	E	2291	GLN	Peptide
2	E	2343	GLY	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	312	THR	Peptide
2	E	3971	GLY	Peptide
2	E	4096	ALA	Peptide
2	E	4641	PRO	Peptide
2	E	4666	VAL	Peptide
2	E	4807	PHE	Peptide
2	E	694	PRO	Peptide
2	E	808	TYR	Peptide
1	F	8	SER	Peptide
1	F	82	TYR	Peptide
2	G	1676	LEU	Peptide
2	G	1690	ASP	Peptide
2	G	1720	LEU	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	Peptide
2	G	1840	PRO	Peptide
2	G	2291	GLN	Peptide

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Mol	Chain	Res	Type	Group
2	G	2343	GLY	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	312	THR	Peptide
2	G	3971	GLY	Peptide
2	G	4096	ALA	Peptide
2	G	4641	PRO	Peptide
2	G	4666	VAL	Peptide
2	G	4807	PHE	Peptide
2	G	694	PRO	Peptide
2	G	808	TYR	Peptide
1	H	8	SER	Peptide
1	H	82	TYR	Peptide
2	I	1676	LEU	Peptide
2	I	1690	ASP	Peptide
2	I	1720	LEU	Peptide
2	I	1795	PRO	Peptide
2	I	1828	ASP	Peptide
2	I	1840	PRO	Peptide
2	I	2291	GLN	Peptide
2	I	2343	GLY	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	312	THR	Peptide
2	I	3971	GLY	Peptide
2	I	4096	ALA	Peptide
2	I	4641	PRO	Peptide
2	I	4666	VAL	Peptide
2	I	4807	PHE	Peptide
2	I	694	PRO	Peptide
2	I	808	TYR	Peptide
1	J	8	SER	Peptide
1	J	82	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	11	0
1	F	818	0	824	11	0
1	H	818	0	824	11	0
1	J	818	0	824	12	0
2	B	29499	0	24752	256	0
2	E	29499	0	24752	251	0
2	G	29499	0	24752	251	0
2	I	29499	0	24752	255	0
3	B	31	0	12	1	0
3	E	31	0	12	0	0
3	G	31	0	12	0	0
3	I	31	0	12	0	0
4	B	14	0	10	0	0
4	E	14	0	10	0	0
4	G	14	0	10	0	0
4	I	14	0	10	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
6	B	1	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
All	All	121456	0	102392	1034	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 (1034) 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:G:646:PRO:HD2	2:G:779:PRO:HB2	1.73	0.70
2:I:379:HIS:HD2	2:I:382:GLY:H	1.40	0.69
2:G:379:HIS:HD2	2:G:382:GLY:H	1.40	0.69
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.73	0.69
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.75	0.69
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.75	0.69
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.74	0.68
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.73	0.68
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.76	0.67
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.76	0.67
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.75	0.67
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.76	0.67
2:B:379:HIS:HD2	2:B:382:GLY:H	1.40	0.67
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.75	0.67
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.60	0.67
2:E:379:HIS:HD2	2:E:382:GLY:H	1.40	0.66
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.78	0.66
2:B:3984:ARG:HH22	2:I:161:GLU:HA	1.59	0.66
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.78	0.66
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.61	0.65
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.60	0.65
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.60	0.64
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.78	0.64
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.78	0.64
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.31	0.64
2:B:2178:MET:HE1	2:B:2210:VAL:HG11	1.81	0.63
2:G:2178:MET:HE1	2:G:2210:VAL:HG11	1.81	0.63
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.31	0.63
2:E:2178:MET:HE1	2:E:2210:VAL:HG11	1.81	0.63
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.31	0.63
2:I:2178:MET:HE1	2:I:2210:VAL:HG11	1.81	0.63
2:E:683:ARG:HG2	2:E:717:ASP:HB3	1.81	0.62
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.31	0.62
2:I:683:ARG:HG2	2:I:717:ASP:HB3	1.81	0.62
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.64	0.62
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.64	0.62
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.64	0.61
2:B:1703:LEU:HD12	2:B:1708:ARG:HB2	1.83	0.61
2:I:1703:LEU:HD12	2:I:1708:ARG:HB2	1.83	0.61
2:B:683:ARG:HG2	2:B:717:ASP:HB3	1.81	0.61
2:E:1703:LEU:HD12	2:E:1708:ARG:HB2	1.83	0.61
2:G:683:ARG:HG2	2:G:717:ASP:HB3	1.81	0.61
2:G:1703:LEU:HD12	2:G:1708:ARG:HB2	1.82	0.60
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.64	0.60
2:B:2347:GLU:O	2:B:2351:ASN:N	2.31	0.60
2:I:331:VAL:HG12	2:I:333:GLY:H	1.66	0.60
2:G:331:VAL:HG12	2:G:333:GLY:H	1.66	0.60
2:B:331:VAL:HG12	2:B:333:GLY:H	1.67	0.60
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.84	0.59
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.84	0.59
2:E:331:VAL:HG12	2:E:333:GLY:H	1.67	0.59
2:E:609:CYS:SG	2:E:610:ASN:N	2.76	0.59
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.85	0.59
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.68	0.59
2:G:2347:GLU:O	2:G:2351:ASN:N	2.31	0.59
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.36	0.59
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.68	0.58
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.85	0.58
2:G:609:CYS:SG	2:G:610:ASN:N	2.76	0.58
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.84	0.58
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.85	0.58
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.85	0.58
2:G:309:THR:O	2:G:313:SER:OG	2.22	0.58
2:B:626:LEU:HG	2:B:628:GLY:H	1.68	0.58
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.37	0.58
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.85	0.58
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.85	0.58
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.86	0.58
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.85	0.58
2:E:309:THR:O	2:E:313:SER:OG	2.22	0.58
2:I:609:CYS:SG	2:I:610:ASN:N	2.76	0.58
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.84	0.58
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.86	0.58
2:B:609:CYS:SG	2:B:610:ASN:N	2.76	0.58
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.37	0.58
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.37	0.58
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.86	0.58
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.85	0.58
2:I:3850:GLN:HB3	2:I:3873:LYS:HD3	1.86	0.58
2:B:3850:GLN:HB3	2:B:3873:LYS:HD3	1.86	0.58
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.36	0.58
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.37	0.58
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.85	0.58
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.86	0.57
2:I:626:LEU:HG	2:I:628:GLY:H	1.69	0.57
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.86	0.57
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.36	0.57
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.84	0.57
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.36	0.57
2:B:2287:ALA:HA	2:B:2290:LEU:HD13	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.85	0.57
2:I:2347:GLU:O	2:I:2351:ASN:N	2.31	0.57
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.68	0.57
2:E:408:ALA:HB2	2:E:483:MET:HE1	1.87	0.57
2:B:309:THR:O	2:B:313:SER:OG	2.22	0.57
2:E:2347:GLU:O	2:E:2351:ASN:N	2.31	0.57
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.38	0.57
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.38	0.57
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.86	0.57
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.38	0.57
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.38	0.57
2:G:2287:ALA:HA	2:G:2290:LEU:HD13	1.87	0.57
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.86	0.57
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.38	0.57
2:I:309:THR:O	2:I:313:SER:OG	2.22	0.57
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.38	0.57
2:G:257:ARG:O	2:G:284:HIS:NE2	2.38	0.57
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.38	0.57
2:G:3850:GLN:HB3	2:G:3873:LYS:HD3	1.86	0.57
2:B:257:ARG:O	2:B:284:HIS:NE2	2.37	0.56
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.38	0.56
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.85	0.56
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.38	0.56
2:G:626:LEU:HG	2:G:628:GLY:H	1.68	0.56
2:B:408:ALA:HB2	2:B:483:MET:HE1	1.87	0.56
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.38	0.56
2:E:626:LEU:HG	2:E:628:GLY:H	1.69	0.56
2:E:3850:GLN:HB3	2:E:3873:LYS:HD3	1.86	0.56
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.38	0.56
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.38	0.56
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.39	0.56
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.88	0.56
2:I:257:ARG:O	2:I:284:HIS:NE2	2.38	0.56
2:I:315:CYS:SG	2:I:316:PHE:N	2.79	0.56
2:I:675:LEU:HD11	2:I:1633:PRO:HB3	1.88	0.56
2:G:614:VAL:HG22	2:G:616:SER:H	1.70	0.56
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.38	0.56
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.79	0.56
2:I:408:ALA:HB2	2:I:483:MET:HE1	1.87	0.56
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	1.88	0.56
2:G:315:CYS:SG	2:G:316:PHE:N	2.79	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1170:MET:HE1	2:E:1176:GLU:HG3	1.88	0.56
2:I:1170:MET:HE1	2:I:1176:GLU:HG3	1.88	0.56
2:I:2287:ALA:HA	2:I:2290:LEU:HD13	1.87	0.56
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.79	0.56
1:H:27:THR:HB	1:H:100:ASP:HB3	1.88	0.56
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.86	0.56
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.86	0.56
2:G:675:LEU:HD11	2:G:1633:PRO:HB3	1.88	0.56
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.88	0.56
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	1.88	0.56
2:E:2287:ALA:HA	2:E:2290:LEU:HD13	1.87	0.56
2:I:614:VAL:HG22	2:I:616:SER:H	1.70	0.56
2:G:132:ALA:HA	2:G:194:SER:HB2	1.88	0.56
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.38	0.56
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.71	0.56
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.38	0.56
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.71	0.56
2:G:1170:MET:HE1	2:G:1176:GLU:HG3	1.88	0.56
1:A:27:THR:HB	1:A:100:ASP:HB3	1.88	0.55
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.79	0.55
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.38	0.55
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.38	0.55
2:E:315:CYS:SG	2:E:316:PHE:N	2.79	0.55
2:E:3971:GLY:H	2:E:5005:GLY:HA3	1.71	0.55
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.38	0.55
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.79	0.55
2:B:2827:ARG:HH21	2:B:2931:GLN:HG3	1.72	0.55
2:I:3984:ARG:HH22	2:G:161:GLU:HA	1.71	0.55
2:B:675:LEU:HD11	2:B:1633:PRO:HB3	1.88	0.55
2:E:161:GLU:HA	2:G:3984:ARG:HH22	1.72	0.55
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.38	0.55
2:I:132:ALA:HA	2:I:194:SER:HB2	1.88	0.55
2:B:488:LEU:HD23	2:B:491:ILE:HD12	1.89	0.55
2:B:3971:GLY:H	2:B:5005:GLY:HA3	1.71	0.55
2:E:257:ARG:O	2:E:284:HIS:NE2	2.38	0.55
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.89	0.55
2:B:315:CYS:SG	2:B:316:PHE:N	2.79	0.55
2:E:2827:ARG:HH21	2:E:2931:GLN:HG3	1.72	0.55
2:I:2827:ARG:HH21	2:I:2931:GLN:HG3	1.72	0.55
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.38	0.55
2:G:2827:ARG:HH21	2:G:2931:GLN:HG3	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:488:LEU:HD23	2:I:491:ILE:HD12	1.89	0.55
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.89	0.55
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.71	0.55
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	1.88	0.55
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.89	0.55
2:I:4232:GLU:OE2	2:I:5017:ARG:NH1	2.40	0.55
2:G:488:LEU:HD23	2:G:491:ILE:HD12	1.89	0.55
2:B:614:VAL:HG22	2:B:616:SER:H	1.71	0.55
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	1.88	0.55
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.88	0.55
2:G:408:ALA:HB2	2:G:483:MET:HE1	1.87	0.55
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.88	0.55
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.89	0.55
1:F:27:THR:HB	1:F:100:ASP:HB3	1.88	0.54
2:B:1170:MET:HE1	2:B:1176:GLU:HG3	1.88	0.54
2:E:132:ALA:HA	2:E:194:SER:HB2	1.88	0.54
2:I:3971:GLY:H	2:I:5005:GLY:HA3	1.71	0.54
2:G:4232:GLU:OE2	2:G:5017:ARG:NH1	2.40	0.54
2:B:161:GLU:HA	2:E:3984:ARG:HH22	1.73	0.54
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.88	0.54
2:E:4232:GLU:OE2	2:E:5017:ARG:NH1	2.40	0.54
2:B:4232:GLU:OE2	2:B:5017:ARG:NH1	2.40	0.54
2:E:675:LEU:HD11	2:E:1633:PRO:HB3	1.88	0.54
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.88	0.54
2:B:111:HIS:CD2	2:B:114:SER:H	2.26	0.54
2:E:488:LEU:HD23	2:E:491:ILE:HD12	1.89	0.54
2:I:111:HIS:CD2	2:I:114:SER:H	2.26	0.54
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.89	0.54
2:G:3971:GLY:H	2:G:5005:GLY:HA3	1.71	0.54
1:J:27:THR:HB	1:J:100:ASP:HB3	1.88	0.54
1:J:76:CYS:HB2	1:J:97:LEU:HB2	1.90	0.54
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.89	0.54
2:E:614:VAL:HG22	2:E:616:SER:H	1.71	0.54
2:E:4924:VAL:HG23	2:E:4925:ILE:HG12	1.90	0.54
2:B:132:ALA:HA	2:B:194:SER:HB2	1.88	0.54
2:E:111:HIS:HD2	2:E:114:SER:H	1.56	0.54
2:E:111:HIS:CD2	2:E:114:SER:H	2.26	0.54
2:G:4924:VAL:HG23	2:G:4925:ILE:HG12	1.90	0.54
2:B:111:HIS:HD2	2:B:114:SER:H	1.56	0.54
2:I:2143:THR:O	2:I:3651:ASN:ND2	2.38	0.54
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.71	0.54
1:H:76:CYS:HB2	1:H:97:LEU:HB2	1.90	0.53
2:E:359:TYR:HA	2:E:376:ALA:HA	1.90	0.53
1:A:76:CYS:HB2	1:A:97:LEU:HB2	1.90	0.53
2:B:4924:VAL:HG23	2:B:4925:ILE:HG12	1.90	0.53
2:I:111:HIS:HD2	2:I:114:SER:H	1.56	0.53
2:I:4924:VAL:HG23	2:I:4925:ILE:HG12	1.90	0.53
2:G:111:HIS:CD2	2:G:114:SER:H	2.26	0.53
2:G:359:TYR:HA	2:G:376:ALA:HA	1.90	0.53
2:G:533:ASN:ND2	2:G:536:ASN:OD1	2.38	0.53
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.91	0.53
2:B:1663:HIS:HD2	2:B:1707:LEU:HD11	1.74	0.53
2:G:111:HIS:HD2	2:G:114:SER:H	1.56	0.53
2:G:3781:GLN:HA	2:G:3784:SER:HB3	1.91	0.53
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.42	0.53
2:E:776:LEU:HG	2:E:848:HIS:HA	1.91	0.53
2:I:470:SER:O	2:I:474:ARG:NE	2.38	0.53
2:B:2267:MET:HE3	2:B:2268:GLN:HG2	1.91	0.53
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.91	0.53
2:B:533:ASN:ND2	2:B:536:ASN:OD1	2.38	0.53
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.89	0.53
2:E:3781:GLN:HA	2:E:3784:SER:HB3	1.91	0.53
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.91	0.53
2:I:2267:MET:HE3	2:I:2268:GLN:HG2	1.91	0.53
2:B:4944:ARG:HH12	2:I:4942:GLU:HB2	1.74	0.53
2:E:1663:HIS:HD2	2:E:1707:LEU:HD11	1.74	0.53
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.89	0.53
1:F:76:CYS:HB2	1:F:97:LEU:HB2	1.90	0.53
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.42	0.53
2:I:1663:HIS:HD2	2:I:1707:LEU:HD11	1.74	0.53
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.42	0.53
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.74	0.52
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.42	0.52
2:G:4924:VAL:HA	2:G:4928:LEU:HB2	1.91	0.52
2:B:776:LEU:HG	2:B:848:HIS:HA	1.91	0.52
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.38	0.52
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.91	0.52
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.91	0.52
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.74	0.52
2:B:359:TYR:HA	2:B:376:ALA:HA	1.90	0.52
2:B:1100:MET:HE2	2:B:1198:GLN:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1100:MET:HE2	2:E:1198:GLN:HB3	1.92	0.52
2:G:1663:HIS:HD2	2:G:1707:LEU:HD11	1.74	0.52
2:B:2420:HIS:ND1	2:B:2493:UNK:O	2.42	0.52
2:E:4924:VAL:HA	2:E:4928:LEU:HB2	1.91	0.52
2:I:359:TYR:HA	2:I:376:ALA:HA	1.90	0.52
2:B:4924:VAL:HA	2:B:4928:LEU:HB2	1.91	0.52
2:E:2267:MET:HE3	2:E:2268:GLN:HG2	1.91	0.52
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.91	0.52
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.91	0.52
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.91	0.52
2:I:4924:VAL:HA	2:I:4928:LEU:HB2	1.91	0.52
2:B:3781:GLN:HA	2:B:3784:SER:HB3	1.91	0.52
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.92	0.52
2:E:2420:HIS:ND1	2:E:2493:UNK:O	2.43	0.52
2:I:776:LEU:HG	2:I:848:HIS:HA	1.91	0.52
2:I:1100:MET:HE2	2:I:1198:GLN:HB3	1.91	0.52
2:G:1100:MET:HE2	2:G:1198:GLN:HB3	1.92	0.52
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.93	0.51
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.92	0.51
2:I:1707:LEU:HG	2:I:1708:ARG:HG3	1.92	0.51
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.93	0.51
2:I:282:ILE:HD12	2:I:314:PHE:HD2	1.76	0.51
2:G:1707:LEU:HG	2:G:1708:ARG:HG3	1.92	0.51
2:G:282:ILE:HD12	2:G:314:PHE:HD2	1.76	0.51
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.92	0.51
2:G:776:LEU:HG	2:G:848:HIS:HA	1.91	0.51
2:E:282:ILE:HD12	2:E:314:PHE:HD2	1.76	0.51
2:E:4843:LEU:HD12	2:G:4823:LEU:HD23	1.92	0.51
2:I:1078:GLU:HG3	2:I:1237:TRP:HE1	1.76	0.51
2:I:1259:ARG:HH12	2:I:1593:PRO:HA	1.76	0.51
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	1.93	0.51
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.91	0.51
2:G:2267:MET:HE3	2:G:2268:GLN:HG2	1.91	0.51
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	1.93	0.51
2:G:1259:ARG:HH12	2:G:1593:PRO:HA	1.76	0.51
2:B:1259:ARG:HH12	2:B:1593:PRO:HA	1.76	0.51
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	1.93	0.51
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.93	0.51
2:I:2420:HIS:ND1	2:I:2493:UNK:O	2.43	0.51
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.93	0.51
2:E:1259:ARG:HH12	2:E:1593:PRO:HA	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.93	0.51
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.74	0.51
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.92	0.51
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.91	0.51
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.74	0.51
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.76	0.51
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.92	0.51
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	1.93	0.51
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.93	0.51
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.92	0.50
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	1.92	0.50
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	1.92	0.50
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.93	0.50
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.84	0.50
2:B:282:ILE:HD12	2:B:314:PHE:HD2	1.76	0.50
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.94	0.50
2:B:1078:GLU:HG3	2:B:1237:TRP:HE1	1.76	0.50
2:E:2131:LEU:HB3	2:E:3662:ILE:HD13	1.93	0.50
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.93	0.50
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.94	0.50
2:B:1707:LEU:HG	2:B:1708:ARG:HG3	1.92	0.50
2:I:2131:LEU:HB3	2:I:3662:ILE:HD13	1.93	0.50
2:B:470:SER:O	2:B:474:ARG:NE	2.38	0.50
2:B:520:ASN:ND2	2:B:555:GLU:OE2	2.45	0.50
2:E:520:ASN:ND2	2:E:555:GLU:OE2	2.45	0.50
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.92	0.50
2:G:520:ASN:ND2	2:G:555:GLU:OE2	2.45	0.50
1:F:2:VAL:HG21	1:F:61:GLU:HB2	1.94	0.50
2:E:1078:GLU:HG3	2:E:1237:TRP:HE1	1.76	0.50
2:E:1707:LEU:HG	2:E:1708:ARG:HG3	1.92	0.50
2:I:942:ALA:HB2	2:I:1052:ASN:HB2	1.94	0.50
2:I:4228:ALA:O	2:I:4232:GLU:N	2.43	0.50
2:G:1078:GLU:HG3	2:G:1237:TRP:HE1	1.76	0.50
2:G:2131:LEU:HB3	2:G:3662:ILE:HD13	1.93	0.50
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	1.93	0.50
2:G:2420:HIS:ND1	2:G:2493:UNK:O	2.43	0.50
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.46	0.50
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.94	0.50
2:I:451:TYR:O	2:I:474:ARG:NH1	2.39	0.50
2:I:520:ASN:ND2	2:I:555:GLU:OE2	2.45	0.50
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.36	0.50
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.46	0.50
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.93	0.50
2:B:485:SER:O	2:B:489:ASN:N	2.37	0.50
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.84	0.50
2:B:2131:LEU:HB3	2:B:3662:ILE:HD13	1.93	0.50
2:E:698:GLY:HA2	2:E:703:GLY:HA2	1.94	0.50
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.46	0.50
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.76	0.50
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.94	0.50
2:E:3772:THR:HG1	2:E:3815:LYS:HZ2	1.57	0.50
2:I:4886:HIS:O	2:I:4890:GLY:N	2.45	0.50
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	1.92	0.50
2:B:698:GLY:HA2	2:B:703:GLY:HA2	1.94	0.49
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.36	0.49
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.84	0.49
2:I:2231:SER:HA	2:I:2234:ARG:HG2	1.94	0.49
2:G:2199:ARG:NH2	2:G:2246:ASN:OD1	2.45	0.49
1:H:2:VAL:HG21	1:H:61:GLU:HB2	1.94	0.49
2:B:2231:SER:HA	2:B:2234:ARG:HG2	1.94	0.49
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.93	0.49
2:E:219:VAL:O	2:E:392:ARG:NH1	2.45	0.49
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.46	0.49
2:I:219:VAL:O	2:I:392:ARG:NH1	2.45	0.49
2:G:2143:THR:O	2:G:3651:ASN:ND2	2.38	0.49
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.76	0.49
2:E:4798:MET:HA	2:E:4801:LEU:HB2	1.95	0.49
2:I:2199:ARG:NH2	2:I:2246:ASN:OD1	2.45	0.49
2:B:942:ALA:HB2	2:B:1052:ASN:HB2	1.94	0.49
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.76	0.49
1:J:21:THR:HA	1:J:49:ARG:HA	1.94	0.49
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.93	0.49
2:B:2199:ARG:NH2	2:B:2246:ASN:OD1	2.45	0.49
2:B:2758:PHE:O	2:B:2762:THR:N	2.44	0.49
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.95	0.49
2:E:2231:SER:HA	2:E:2234:ARG:HG2	1.94	0.49
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.93	0.49
2:I:210:GLU:HG3	2:I:337:PRO:HG3	1.94	0.49
2:I:596:ASN:HB3	2:I:599:VAL:HG22	1.95	0.49
2:I:4823:LEU:HD23	2:G:4843:LEU:HD12	1.95	0.49
2:G:1516:UNK:N	2:G:1529:UNK:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2231:SER:HA	2:G:2234:ARG:HG2	1.94	0.49
2:B:978:THR:HB	2:B:980:ALA:H	1.77	0.49
2:I:2104:ARG:HA	2:I:2107:GLN:HB3	1.95	0.49
2:G:219:VAL:O	2:G:392:ARG:NH1	2.45	0.49
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.95	0.49
1:A:2:VAL:HG21	1:A:61:GLU:HB2	1.94	0.49
2:G:1727:ARG:NH2	2:G:1773:PRO:O	2.43	0.49
2:G:4228:ALA:O	2:G:4232:GLU:N	2.43	0.49
2:B:1516:UNK:N	2:B:1529:UNK:O	2.46	0.49
2:E:3842:LEU:O	2:E:3929:SER:OG	2.30	0.49
1:F:21:THR:HA	1:F:49:ARG:HA	1.94	0.49
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.95	0.49
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.95	0.49
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.95	0.49
2:E:1516:UNK:N	2:E:1529:UNK:O	2.46	0.49
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.93	0.49
2:G:4798:MET:HA	2:G:4801:LEU:HB2	1.95	0.49
1:H:21:THR:HA	1:H:49:ARG:HA	1.94	0.49
2:B:596:ASN:HB3	2:B:599:VAL:HG22	1.95	0.49
2:E:2199:ARG:NH2	2:E:2246:ASN:OD1	2.45	0.49
2:E:3773:ARG:HG3	2:E:3815:LYS:HZ3	1.78	0.49
2:I:1516:UNK:N	2:I:1529:UNK:O	2.46	0.49
2:G:210:GLU:HG3	2:G:337:PRO:HG3	1.94	0.49
2:B:210:GLU:HG3	2:B:337:PRO:HG3	1.94	0.48
2:B:219:VAL:O	2:B:392:ARG:NH1	2.45	0.48
2:B:2143:THR:O	2:B:3651:ASN:ND2	2.38	0.48
2:E:210:GLU:HG3	2:E:337:PRO:HG3	1.94	0.48
2:E:2337:PHE:HA	2:E:2340:PHE:HB2	1.95	0.48
2:G:942:ALA:HB2	2:G:1052:ASN:HB2	1.94	0.48
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.95	0.48
1:J:2:VAL:HG21	1:J:61:GLU:HB2	1.94	0.48
2:I:4152:GLU:OE2	2:I:4180:ARG:NH1	2.46	0.48
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.95	0.48
2:G:2104:ARG:HA	2:G:2107:GLN:HB3	1.95	0.48
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.93	0.48
2:B:4228:ALA:O	2:B:4232:GLU:N	2.43	0.48
2:E:942:ALA:HB2	2:E:1052:ASN:HB2	1.94	0.48
2:I:4738:ALA:HA	2:I:4743:MET:HE3	1.95	0.48
1:A:21:THR:HA	1:A:49:ARG:HA	1.94	0.48
2:B:1973:GLN:O	2:B:1977:TYR:N	2.44	0.48
2:B:4738:ALA:HA	2:B:4743:MET:HE3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4798:MET:HA	2:B:4801:LEU:HB2	1.95	0.48
2:I:698:GLY:HA2	2:I:703:GLY:HA2	1.94	0.48
2:G:395:GLN:HG3	2:G:397:GLU:H	1.79	0.48
2:G:596:ASN:HB3	2:G:599:VAL:HG22	1.95	0.48
2:G:2337:PHE:HA	2:G:2340:PHE:HB2	1.95	0.48
2:B:645:ARG:HH11	2:B:778:PHE:HE1	1.62	0.48
2:B:1727:ARG:NH2	2:B:1773:PRO:O	2.43	0.48
2:B:3842:LEU:O	2:B:3929:SER:OG	2.30	0.48
2:B:4152:GLU:OE2	2:B:4180:ARG:NH1	2.46	0.48
2:E:1727:ARG:NH2	2:E:1773:PRO:O	2.43	0.48
2:I:645:ARG:HH11	2:I:778:PHE:HE1	1.62	0.48
2:G:164:ARG:N	2:G:167:ASP:OD2	2.42	0.48
2:G:698:GLY:HA2	2:G:703:GLY:HA2	1.94	0.48
2:G:1973:GLN:O	2:G:1977:TYR:N	2.44	0.48
2:G:4822:THR:O	2:G:4825:THR:OG1	2.31	0.48
2:B:3365:UNK:O	2:B:3369:UNK:N	2.47	0.48
2:E:596:ASN:HB3	2:E:599:VAL:HG22	1.95	0.48
2:E:2104:ARG:HA	2:E:2107:GLN:HB3	1.95	0.48
2:I:2337:PHE:HA	2:I:2340:PHE:HB2	1.95	0.48
2:I:3365:UNK:O	2:I:3369:UNK:N	2.47	0.48
2:E:3365:UNK:O	2:E:3369:UNK:N	2.47	0.48
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.95	0.48
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.47	0.48
2:B:395:GLN:HG3	2:B:397:GLU:H	1.78	0.48
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.46	0.48
2:E:451:TYR:O	2:E:474:ARG:NH1	2.39	0.48
2:E:978:THR:HB	2:E:980:ALA:H	1.77	0.48
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.46	0.48
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.46	0.48
2:I:978:THR:HB	2:I:980:ALA:H	1.77	0.48
2:I:4798:MET:HA	2:I:4801:LEU:HB2	1.95	0.48
2:I:4822:THR:O	2:I:4825:THR:OG1	2.31	0.48
2:G:2862:LEU:HB3	2:G:2928:LYS:HB3	1.96	0.48
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.46	0.48
2:G:978:THR:HB	2:G:980:ALA:H	1.77	0.48
2:B:2862:LEU:HB3	2:B:2928:LYS:HB3	1.96	0.47
2:G:1730:MET:O	2:G:1772:ARG:NH1	2.46	0.47
2:B:451:TYR:O	2:B:474:ARG:NH1	2.39	0.47
2:E:395:GLN:HG3	2:E:397:GLU:H	1.78	0.47
2:E:645:ARG:HH11	2:E:778:PHE:HE1	1.62	0.47
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.46	0.47
2:E:1973:GLN:O	2:E:1977:TYR:N	2.44	0.47
2:E:4930:ALA:O	2:E:4934:GLY:N	2.47	0.47
2:G:4886:HIS:O	2:G:4890:GLY:N	2.45	0.47
2:B:2104:ARG:HA	2:B:2107:GLN:HB3	1.95	0.47
2:E:463:GLU:OE2	2:E:467:LYS:NZ	2.47	0.47
2:I:1973:GLN:O	2:I:1977:TYR:N	2.44	0.47
2:G:645:ARG:HH11	2:G:778:PHE:HE1	1.62	0.47
2:G:3365:UNK:O	2:G:3369:UNK:N	2.47	0.47
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.46	0.47
1:J:82:TYR:O	1:J:86:GLY:N	2.45	0.47
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.97	0.47
2:I:606:LEU:O	2:I:617:ASN:ND2	2.48	0.47
2:G:606:LEU:O	2:G:617:ASN:ND2	2.48	0.47
2:G:4930:ALA:O	2:G:4934:GLY:N	2.47	0.47
2:B:2337:PHE:HA	2:B:2340:PHE:HB2	1.95	0.47
2:B:4930:ALA:O	2:B:4934:GLY:N	2.47	0.47
2:E:3362:UNK:O	2:E:3366:UNK:N	2.48	0.47
2:E:3804:ILE:O	2:E:3809:ASN:ND2	2.48	0.47
2:I:2862:LEU:HB3	2:I:2928:LYS:HB3	1.96	0.47
2:I:4155:PRO:HD2	2:I:5036:LEU:HD23	1.96	0.47
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.46	0.47
2:G:3842:LEU:O	2:G:3929:SER:OG	2.30	0.47
2:G:4152:GLU:OE2	2:G:4180:ARG:NH1	2.47	0.47
2:G:4738:ALA:HA	2:G:4743:MET:HE3	1.95	0.47
2:B:4822:THR:O	2:B:4825:THR:OG1	2.31	0.47
2:E:606:LEU:O	2:E:617:ASN:ND2	2.48	0.47
2:E:2143:THR:O	2:E:3651:ASN:ND2	2.38	0.47
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.50	0.47
2:E:4738:ALA:HA	2:E:4743:MET:HE3	1.96	0.47
2:I:395:GLN:HG3	2:I:397:GLU:H	1.78	0.47
2:I:3842:LEU:O	2:I:3929:SER:OG	2.30	0.47
2:I:4930:ALA:O	2:I:4934:GLY:N	2.47	0.47
1:J:92:PRO:HD3	2:I:627:PRO:HB2	1.96	0.47
2:B:606:LEU:O	2:B:617:ASN:ND2	2.48	0.47
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.96	0.47
2:E:4063:ASP:OD1	2:E:4169:SER:OG	2.30	0.47
2:G:3362:UNK:O	2:G:3366:UNK:N	2.48	0.47
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.50	0.47
2:B:290:TYR:O	2:B:302:VAL:N	2.48	0.47
2:E:4152:GLU:OE2	2:E:4180:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4236:SER:HG	2:E:4675:LYS:HZ1	1.58	0.47
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.97	0.47
2:G:157:ARG:HH21	2:G:164:ARG:HD2	1.80	0.47
2:G:913:LEU:O	2:G:918:ARG:NH2	2.48	0.47
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.96	0.47
2:G:4155:PRO:HD2	2:G:5036:LEU:HD23	1.96	0.47
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.47	0.47
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.97	0.47
2:B:4155:PRO:HD2	2:B:5036:LEU:HD23	1.96	0.47
2:E:470:SER:O	2:E:474:ARG:NE	2.39	0.47
2:E:913:LEU:O	2:E:918:ARG:NH2	2.48	0.47
2:E:2862:LEU:HB3	2:E:2928:LYS:HB3	1.96	0.47
2:I:157:ARG:HH21	2:I:164:ARG:HD2	1.80	0.47
2:I:463:GLU:OE2	2:I:467:LYS:NZ	2.47	0.47
2:I:695:TYR:OH	2:I:1073:ARG:NH1	2.45	0.47
2:I:3362:UNK:O	2:I:3366:UNK:N	2.48	0.47
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.48	0.47
2:B:3773:ARG:HG3	2:B:3815:LYS:HZ3	1.80	0.47
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.97	0.47
2:E:290:TYR:O	2:E:302:VAL:N	2.48	0.46
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.97	0.46
2:E:4209:GLN:HE22	2:E:4560:TYR:HE2	1.63	0.46
2:E:4860:ARG:HG3	2:E:4876:CYS:HB3	1.98	0.46
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.46	0.46
2:G:463:GLU:OE2	2:G:467:LYS:NZ	2.47	0.46
2:G:4209:GLN:HE22	2:G:4560:TYR:HE2	1.63	0.46
2:B:164:ARG:N	2:B:167:ASP:OD2	2.42	0.46
2:B:463:GLU:OE2	2:B:467:LYS:NZ	2.47	0.46
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.50	0.46
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.97	0.46
2:E:4228:ALA:O	2:E:4232:GLU:N	2.43	0.46
2:I:290:TYR:O	2:I:302:VAL:N	2.48	0.46
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.97	0.46
1:H:82:TYR:O	1:H:86:GLY:N	2.45	0.46
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.97	0.46
2:E:164:ARG:N	2:E:167:ASP:OD2	2.42	0.46
2:E:236:ALA:HA	2:E:242:ARG:HD2	1.98	0.46
2:E:695:TYR:OH	2:E:1073:ARG:NH1	2.45	0.46
2:E:2299:VAL:O	2:E:2303:ALA:N	2.48	0.46
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.97	0.46
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1727:ARG:NH2	2:I:1773:PRO:O	2.42	0.46
2:G:3804:ILE:O	2:G:3809:ASN:ND2	2.48	0.46
2:B:3362:UNK:O	2:B:3366:UNK:N	2.48	0.46
2:B:3804:ILE:O	2:B:3809:ASN:ND2	2.48	0.46
2:E:4886:HIS:O	2:E:4890:GLY:N	2.45	0.46
2:I:913:LEU:O	2:I:918:ARG:NH2	2.48	0.46
2:I:1730:MET:O	2:I:1772:ARG:NH1	2.46	0.46
2:I:3804:ILE:O	2:I:3809:ASN:ND2	2.48	0.46
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.33	0.46
2:B:157:ARG:HH21	2:B:164:ARG:HD2	1.80	0.46
2:B:2295:LEU:HA	2:B:2298:VAL:HG22	1.97	0.46
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.48	0.46
2:E:1730:MET:O	2:E:1772:ARG:NH1	2.46	0.46
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.33	0.46
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.48	0.46
2:G:4860:ARG:HG3	2:G:4876:CYS:HB3	1.98	0.46
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.97	0.46
2:B:913:LEU:O	2:B:918:ARG:NH2	2.48	0.46
2:B:4832:HIS:NE2	2:B:4942:GLU:OE2	2.48	0.46
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.48	0.46
2:B:2022:PRO:HB2	2:B:2024:PRO:HD2	1.97	0.46
2:B:4860:ARG:HG3	2:B:4876:CYS:HB3	1.98	0.46
2:E:157:ARG:HH21	2:E:164:ARG:HD2	1.80	0.46
2:E:4155:PRO:HD2	2:E:5036:LEU:HD23	1.96	0.46
2:I:2758:PHE:O	2:I:2762:THR:N	2.44	0.46
2:G:3773:ARG:HG3	2:G:3815:LYS:HZ3	1.81	0.46
2:G:4832:HIS:NE2	2:G:4942:GLU:OE2	2.48	0.46
2:B:236:ALA:HA	2:B:242:ARG:HD2	1.98	0.46
2:B:1152:MET:HE1	2:B:1217:CYS:HB3	1.98	0.46
2:B:2432:LEU:O	2:B:2436:CYS:N	2.49	0.46
2:E:689:THR:H	2:E:778:PHE:HE2	1.64	0.46
2:E:4822:THR:O	2:E:4825:THR:OG1	2.31	0.46
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.96	0.46
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.50	0.46
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.97	0.46
2:B:1025:ARG:O	2:B:1032:LYS:NZ	2.46	0.46
2:B:4080:TYR:CZ	2:B:4096:ALA:HB3	2.51	0.46
2:E:4832:HIS:NE2	2:E:4942:GLU:OE2	2.48	0.46
2:I:485:SER:O	2:I:489:ASN:N	2.37	0.46
2:I:670:GLU:HG3	2:I:788:LYS:H	1.81	0.46
2:I:2432:LEU:O	2:I:2436:CYS:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:689:THR:H	2:B:778:PHE:HE2	1.64	0.46
2:B:2299:VAL:O	2:B:2303:ALA:N	2.49	0.46
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.49	0.46
2:E:2758:PHE:O	2:E:2762:THR:N	2.44	0.46
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.97	0.46
2:G:290:TYR:O	2:G:302:VAL:N	2.48	0.46
2:G:399:GLN:HG2	2:G:403:MET:HE3	1.98	0.46
2:G:1152:MET:HE1	2:G:1217:CYS:HB3	1.98	0.46
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.99	0.45
2:B:4209:GLN:HE22	2:B:4560:TYR:HE2	1.63	0.45
2:E:2295:LEU:HA	2:E:2298:VAL:HG22	1.97	0.45
2:I:236:ALA:HA	2:I:242:ARG:HD2	1.98	0.45
2:I:4209:GLN:HE22	2:I:4560:TYR:HE2	1.63	0.45
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.49	0.45
2:G:695:TYR:OH	2:G:1073:ARG:NH1	2.45	0.45
2:G:841:GLY:HA2	2:G:1073:ARG:HD2	1.98	0.45
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.97	0.45
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.36	0.45
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.97	0.45
2:I:1152:MET:HE1	2:I:1217:CYS:HB3	1.97	0.45
2:G:2022:PRO:HB2	2:G:2024:PRO:HD2	1.97	0.45
2:B:399:GLN:HG2	2:B:403:MET:HE3	1.98	0.45
2:B:670:GLU:HG3	2:B:788:LYS:H	1.81	0.45
2:E:670:GLU:HG3	2:E:788:LYS:H	1.81	0.45
2:I:841:GLY:HA2	2:I:1073:ARG:HD2	1.98	0.45
2:I:4860:ARG:HG3	2:I:4876:CYS:HB3	1.98	0.45
1:H:92:PRO:HD3	2:G:627:PRO:HB2	1.97	0.45
2:B:841:GLY:HA2	2:B:1073:ARG:HD2	1.98	0.45
2:E:1152:MET:HE1	2:E:1217:CYS:HB3	1.97	0.45
2:G:215:THR:HG22	2:G:273:HIS:HA	1.98	0.45
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.97	0.45
2:G:2447:LYS:HG3	2:G:2449:GLU:H	1.82	0.45
2:G:4863:TYR:HD2	2:G:4875:LYS:HB2	1.82	0.45
2:B:695:TYR:OH	2:B:1073:ARG:NH1	2.45	0.45
2:B:4642:ALA:HA	2:B:4645:CYS:HB2	1.98	0.45
2:E:2022:PRO:HB2	2:E:2024:PRO:HD2	1.97	0.45
2:G:670:GLU:HG3	2:G:788:LYS:H	1.81	0.45
2:B:4886:HIS:O	2:B:4890:GLY:N	2.45	0.45
2:E:399:GLN:HG2	2:E:403:MET:HE3	1.98	0.45
2:E:841:GLY:HA2	2:E:1073:ARG:HD2	1.98	0.45
2:I:399:GLN:HG2	2:I:403:MET:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2022:PRO:HB2	2:I:2024:PRO:HD2	1.97	0.45
2:I:2447:LYS:HG3	2:I:2449:GLU:H	1.82	0.45
2:I:4863:TYR:HD2	2:I:4875:LYS:HB2	1.82	0.45
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.99	0.45
2:G:2295:LEU:HA	2:G:2298:VAL:HG22	1.97	0.45
2:B:215:THR:HG22	2:B:273:HIS:HA	1.98	0.45
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.50	0.45
2:B:4863:TYR:HD2	2:B:4875:LYS:HB2	1.82	0.45
2:I:2295:LEU:HA	2:I:2298:VAL:HG22	1.97	0.45
2:I:2299:VAL:O	2:I:2303:ALA:N	2.49	0.45
2:I:4642:ALA:HA	2:I:4645:CYS:HB2	1.98	0.45
2:G:2290:LEU:HG	2:G:2291:GLN:H	1.82	0.45
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.33	0.45
2:B:2290:LEU:HG	2:B:2291:GLN:H	1.82	0.45
2:E:4863:TYR:HD2	2:E:4875:LYS:HB2	1.82	0.45
2:I:2290:LEU:HG	2:I:2291:GLN:H	1.82	0.45
2:G:236:ALA:HA	2:G:242:ARG:HD2	1.98	0.45
2:I:939:VAL:HG22	2:I:1053:ILE:HG23	1.99	0.45
2:I:4688:ILE:HG21	2:I:4728:HIS:HB3	1.99	0.45
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.97	0.45
2:B:4942:GLU:HB2	2:E:4944:ARG:HH12	1.81	0.45
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.97	0.45
2:I:689:THR:H	2:I:778:PHE:HE2	1.64	0.45
2:I:4851:TYR:HD2	2:I:4920:PHE:HD1	1.65	0.45
2:G:2758:PHE:O	2:G:2762:THR:N	2.44	0.45
2:G:4642:ALA:HA	2:G:4645:CYS:HB2	1.98	0.45
1:A:82:TYR:O	1:A:86:GLY:N	2.45	0.44
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.84	0.44
2:E:2290:LEU:HG	2:E:2291:GLN:H	1.82	0.44
2:E:2342:ASN:OD1	2:E:2342:ASN:N	2.50	0.44
2:E:4080:TYR:CZ	2:E:4096:ALA:HB3	2.51	0.44
2:I:210:GLU:H	2:I:273:HIS:HE1	1.66	0.44
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.99	0.44
2:G:470:SER:O	2:G:474:ARG:NE	2.38	0.44
2:G:4688:ILE:HG21	2:G:4728:HIS:HB3	1.99	0.44
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.49	0.44
2:I:618:GLN:OE1	2:I:1678:ASN:ND2	2.51	0.44
2:I:4080:TYR:CZ	2:I:4096:ALA:HB3	2.51	0.44
2:G:45:ARG:HG2	2:G:443:LEU:HD21	2.00	0.44
2:G:1244:GLN:OE1	2:G:1646:ARG:NH1	2.51	0.44
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4642:ALA:HA	2:E:4645:CYS:HB2	1.98	0.44
2:G:485:SER:O	2:G:489:ASN:N	2.37	0.44
2:G:618:GLN:OE1	2:G:1678:ASN:ND2	2.51	0.44
2:G:2102:VAL:HB	2:G:2124:LEU:HD12	1.99	0.44
2:G:4080:TYR:CZ	2:G:4096:ALA:HB3	2.51	0.44
1:F:11:ASP:OD1	1:F:67:SER:OG	2.34	0.44
2:B:1244:GLN:OE1	2:B:1646:ARG:NH1	2.50	0.44
2:B:2894:LEU:HD11	2:B:2902:HIS:HB2	2.00	0.44
2:B:4666:VAL:HG23	2:B:4669:VAL:HB	2.00	0.44
2:B:4851:TYR:HD2	2:B:4920:PHE:HD1	1.65	0.44
2:E:210:GLU:H	2:E:273:HIS:HE1	1.66	0.44
2:E:215:THR:HG22	2:E:273:HIS:HA	1.98	0.44
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.99	0.44
2:G:451:TYR:O	2:G:474:ARG:NH1	2.39	0.44
1:A:92:PRO:HD3	2:B:627:PRO:HB2	1.99	0.44
2:I:2243:SER:HB3	2:I:2246:ASN:H	1.82	0.44
2:B:210:GLU:H	2:B:273:HIS:HE1	1.66	0.44
2:B:939:VAL:HG22	2:B:1053:ILE:HG23	1.99	0.44
2:B:4680:LYS:HD3	2:B:4686:LEU:HD22	2.00	0.44
2:E:41:GLY:O	2:E:45:ARG:NH1	2.51	0.44
2:E:1025:ARG:O	2:E:1032:LYS:NZ	2.46	0.44
2:E:4666:VAL:HG23	2:E:4669:VAL:HB	2.00	0.44
2:E:4942:GLU:HB2	2:G:4944:ARG:HH12	1.82	0.44
2:I:41:GLY:O	2:I:45:ARG:NH1	2.51	0.44
2:G:4666:VAL:HG23	2:G:4669:VAL:HB	2.00	0.44
2:B:1730:MET:O	2:B:1772:ARG:NH1	2.46	0.44
2:E:580:GLU:HG2	2:E:583:ILE:HD11	2.00	0.44
2:E:1244:GLN:OE1	2:E:1646:ARG:NH1	2.50	0.44
2:I:45:ARG:HG2	2:I:443:LEU:HD21	2.00	0.44
2:I:2102:VAL:HB	2:I:2124:LEU:HD12	1.99	0.44
2:G:1025:ARG:O	2:G:1032:LYS:NZ	2.46	0.44
2:B:2815:ALA:HB3	2:B:2881:ASN:HD21	1.83	0.44
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	2.00	0.44
2:B:4914:VAL:HG23	2:E:4888:TYR:HD1	1.83	0.44
2:E:2815:ALA:HB3	2:E:2881:ASN:HD21	1.83	0.44
2:I:4666:VAL:HG23	2:I:4669:VAL:HB	2.00	0.44
2:G:2342:ASN:OD1	2:G:2342:ASN:N	2.50	0.44
1:F:82:TYR:O	1:F:86:GLY:N	2.45	0.44
2:E:2102:VAL:HB	2:E:2124:LEU:HD12	1.99	0.44
2:E:2894:LEU:HD11	2:E:2902:HIS:HB2	2.00	0.44
2:I:215:THR:HG22	2:I:273:HIS:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1244:GLN:OE1	2:I:1646:ARG:NH1	2.50	0.44
2:I:4680:LYS:HD3	2:I:4686:LEU:HD22	2.00	0.44
2:G:210:GLU:H	2:G:273:HIS:HE1	1.66	0.44
2:B:41:GLY:O	2:B:45:ARG:NH1	2.51	0.43
2:E:2447:LYS:HG3	2:E:2449:GLU:H	1.82	0.43
2:G:689:THR:H	2:G:778:PHE:HE2	1.64	0.43
2:G:4851:TYR:HD2	2:G:4920:PHE:HD1	1.65	0.43
2:I:575:LEU:HD22	2:I:609:CYS:HB3	2.01	0.43
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.51	0.43
2:I:3779:VAL:HG23	2:I:3780:LEU:HD12	2.00	0.43
2:G:41:GLY:O	2:G:45:ARG:NH1	2.51	0.43
2:B:4985:LEU:HB2	3:B:5101:ATP:HN61	1.83	0.43
2:E:618:GLN:OE1	2:E:1678:ASN:ND2	2.51	0.43
2:E:1236:THR:OG1	2:E:1608:MET:SD	2.76	0.43
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.36	0.43
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	1.99	0.43
2:E:4688:ILE:HG21	2:E:4728:HIS:HB3	1.99	0.43
2:I:4832:HIS:NE2	2:I:4942:GLU:OE2	2.48	0.43
2:G:4066:LEU:HD11	2:G:4173:TYR:HB2	2.00	0.43
2:B:2102:VAL:HB	2:B:2124:LEU:HD12	1.99	0.43
2:B:2208:MET:HE1	2:B:2253:HIS:HB3	2.00	0.43
2:I:2815:ALA:HB3	2:I:2881:ASN:HD21	1.83	0.43
2:G:214:VAL:HG12	2:G:274:LEU:HD12	2.00	0.43
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.51	0.43
2:G:2243:SER:HB3	2:G:2246:ASN:H	1.83	0.43
1:A:74:LEU:HB2	1:A:99:PHE:HB2	2.00	0.43
2:E:218:HIS:HB3	2:E:392:ARG:HD3	2.01	0.43
2:E:939:VAL:HG22	2:E:1053:ILE:HG23	1.99	0.43
2:I:2894:LEU:HD11	2:I:2902:HIS:HB2	2.00	0.43
2:G:206:CYS:SG	2:G:207:SER:N	2.92	0.43
2:G:575:LEU:HD22	2:G:609:CYS:HB3	2.01	0.43
2:G:939:VAL:HG22	2:G:1053:ILE:HG23	1.99	0.43
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	2.00	0.43
2:B:580:GLU:HG2	2:B:583:ILE:HD11	2.00	0.43
2:B:618:GLN:OE1	2:B:1678:ASN:ND2	2.51	0.43
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.52	0.43
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	2.00	0.43
2:E:4680:LYS:HD3	2:E:4686:LEU:HD22	2.00	0.43
2:E:4851:TYR:HD2	2:E:4920:PHE:HD1	1.65	0.43
2:I:214:VAL:HG12	2:I:274:LEU:HD12	2.00	0.43
2:I:4944:ARG:HH12	2:G:4942:GLU:HB2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1236:THR:OG1	2:G:1608:MET:SD	2.76	0.43
2:G:2208:MET:HE1	2:G:2253:HIS:HB3	2.00	0.43
2:G:2815:ALA:HB3	2:G:2881:ASN:HD21	1.83	0.43
1:F:74:LEU:HB2	1:F:99:PHE:HB2	2.00	0.43
2:B:45:ARG:HG2	2:B:443:LEU:HD21	2.00	0.43
2:B:2243:SER:HB3	2:B:2246:ASN:H	1.83	0.43
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.84	0.43
2:B:2447:LYS:HG3	2:B:2449:GLU:H	1.82	0.43
2:E:1641:ILE:HA	2:E:1642:PRO:HD3	1.89	0.43
2:I:1665:HIS:HA	2:I:1668:ARG:HG2	2.00	0.43
2:I:4066:LEU:HD11	2:I:4173:TYR:HB2	2.00	0.43
2:G:864:PRO:HD2	2:G:867:LEU:HD12	2.01	0.43
2:G:2332:LEU:HD13	2:G:2335:LEU:HD12	2.01	0.43
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.52	0.43
2:I:767:VAL:HG12	2:I:769:GLU:HG3	2.01	0.43
2:I:1025:ARG:O	2:I:1032:LYS:NZ	2.46	0.43
2:G:767:VAL:HG12	2:G:769:GLU:HG3	2.01	0.43
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.84	0.43
2:B:793:LEU:HD22	2:B:821:LEU:HD13	2.00	0.43
2:B:864:PRO:HD2	2:B:867:LEU:HD12	2.01	0.43
2:B:1665:HIS:HA	2:B:1668:ARG:HG2	2.00	0.43
2:B:2342:ASN:OD1	2:B:2342:ASN:N	2.50	0.43
2:E:1665:HIS:HA	2:E:1668:ARG:HG2	2.00	0.43
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.51	0.43
2:E:2243:SER:HB3	2:E:2246:ASN:H	1.83	0.43
2:I:454:PRO:HG2	2:I:531:ARG:HH12	1.84	0.43
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.52	0.43
2:G:4047:MET:HE3	2:G:4047:MET:HB2	1.94	0.43
1:J:11:ASP:OD1	1:J:67:SER:OG	2.34	0.43
2:B:206:CYS:SG	2:B:207:SER:N	2.92	0.43
2:B:2742:THR:OG1	2:B:2811:GLU:OE1	2.33	0.43
2:B:4066:LEU:HD11	2:B:4173:TYR:HB2	2.00	0.43
2:B:4570:ALA:O	2:B:4574:ASN:ND2	2.52	0.43
2:E:4066:LEU:HD11	2:E:4173:TYR:HB2	2.00	0.43
2:I:2342:ASN:OD1	2:I:2342:ASN:N	2.50	0.43
2:G:580:GLU:HG2	2:G:583:ILE:HD11	2.00	0.43
2:B:214:VAL:HG12	2:B:274:LEU:HD12	2.00	0.42
2:I:164:ARG:N	2:I:167:ASP:OD2	2.41	0.42
2:I:580:GLU:HG2	2:I:583:ILE:HD11	2.00	0.42
2:G:1141:ARG:H	2:G:1141:ARG:HD2	1.84	0.42
2:G:2894:LEU:HD11	2:G:2902:HIS:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:74:LEU:HB2	1:J:99:PHE:HB2	2.00	0.42
2:B:575:LEU:HD22	2:B:609:CYS:HB3	2.01	0.42
2:B:767:VAL:HG12	2:B:769:GLU:HG3	2.01	0.42
2:B:2332:LEU:HD13	2:B:2335:LEU:HD12	2.01	0.42
2:B:4688:ILE:HG21	2:B:4728:HIS:HB3	1.99	0.42
2:E:575:LEU:HD22	2:E:609:CYS:HB3	2.01	0.42
2:E:4956:THR:O	2:E:4965:SER:N	2.52	0.42
2:I:206:CYS:SG	2:I:207:SER:N	2.92	0.42
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.84	0.42
2:G:1665:HIS:HA	2:G:1668:ARG:HG2	2.00	0.42
2:G:4680:LYS:HD3	2:G:4686:LEU:HD22	2.00	0.42
2:E:485:SER:O	2:E:489:ASN:N	2.37	0.42
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.84	0.42
2:I:1641:ILE:HA	2:I:1642:PRO:HD3	1.89	0.42
2:I:4570:ALA:O	2:I:4574:ASN:ND2	2.52	0.42
2:I:4956:THR:O	2:I:4965:SER:N	2.52	0.42
1:H:74:LEU:HB2	1:H:99:PHE:HB2	2.00	0.42
2:B:218:HIS:HB3	2:B:392:ARG:HD3	2.01	0.42
2:B:454:PRO:HG2	2:B:531:ARG:HH12	1.84	0.42
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.51	0.42
2:E:454:PRO:HG2	2:E:531:ARG:HH12	1.84	0.42
2:E:629:ARG:HD3	2:E:634:GLN:HG2	2.01	0.42
2:E:767:VAL:HG12	2:E:769:GLU:HG3	2.01	0.42
2:I:1236:THR:OG1	2:I:1608:MET:SD	2.76	0.42
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.52	0.42
2:G:218:HIS:HB3	2:G:392:ARG:HD3	2.01	0.42
2:G:2432:LEU:O	2:G:2436:CYS:N	2.49	0.42
2:B:734:GLY:O	2:B:736:HIS:ND1	2.53	0.42
2:B:940:GLY:O	2:B:1052:ASN:N	2.53	0.42
2:B:1720:LEU:HD23	2:B:1721:GLU:HA	2.02	0.42
2:E:1141:ARG:H	2:E:1141:ARG:HD2	1.84	0.42
2:I:870:ILE:HD11	2:I:1049:TYR:CG	2.55	0.42
2:I:1141:ARG:H	2:I:1141:ARG:HD2	1.84	0.42
2:G:530:ILE:HD13	2:G:536:ASN:HB3	2.02	0.42
2:B:379:HIS:CD2	2:B:381:GLU:H	2.37	0.42
2:B:2423:MET:O	2:B:2427:ALA:N	2.48	0.42
2:E:45:ARG:HG2	2:E:443:LEU:HD21	2.00	0.42
2:E:530:ILE:HD13	2:E:536:ASN:HB3	2.02	0.42
2:E:793:LEU:HD22	2:E:821:LEU:HD13	2.00	0.42
2:I:218:HIS:HB3	2:I:392:ARG:HD3	2.01	0.42
2:I:793:LEU:HD22	2:I:821:LEU:HD13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1720:LEU:HD23	2:I:1721:GLU:HA	2.02	0.42
2:G:2299:VAL:O	2:G:2303:ALA:N	2.48	0.42
2:G:4570:ALA:O	2:G:4574:ASN:ND2	2.52	0.42
2:B:134:ASP:OD1	2:B:134:ASP:N	2.53	0.42
2:B:4956:THR:O	2:B:4965:SER:N	2.52	0.42
2:E:4570:ALA:O	2:E:4574:ASN:ND2	2.52	0.42
2:I:2208:MET:HE1	2:I:2253:HIS:HB3	2.00	0.42
2:G:793:LEU:HD22	2:G:821:LEU:HD13	2.00	0.42
2:B:629:ARG:HD3	2:B:634:GLN:HG2	2.01	0.42
2:B:1141:ARG:H	2:B:1141:ARG:HD2	1.84	0.42
2:B:2195:PRO:HB3	2:B:2246:ASN:HD21	1.84	0.42
2:B:2517:UNK:O	2:B:2521:UNK:N	2.53	0.42
2:E:2195:PRO:HB3	2:E:2246:ASN:HD21	1.84	0.42
2:E:2517:UNK:O	2:E:2521:UNK:N	2.53	0.42
2:I:629:ARG:HB3	2:I:634:GLN:NE2	2.35	0.42
2:I:2823:ILE:HG12	2:I:2937:VAL:HG22	2.01	0.42
2:I:3773:ARG:HG3	2:I:3815:LYS:HZ3	1.84	0.42
2:G:940:GLY:O	2:G:1052:ASN:N	2.53	0.42
2:G:1641:ILE:HA	2:G:1642:PRO:HD3	1.89	0.42
2:B:4083:ASP:HB3	2:B:4086:GLY:H	1.85	0.42
2:I:103:TYR:HB3	2:I:152:PRO:HD3	2.02	0.42
2:I:379:HIS:CD2	2:I:381:GLU:H	2.37	0.42
2:I:4083:ASP:HB3	2:I:4086:GLY:H	1.85	0.42
2:G:629:ARG:HD3	2:G:634:GLN:HG2	2.01	0.42
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	2.02	0.42
2:B:4641:PRO:O	2:B:4645:CYS:N	2.52	0.42
2:E:206:CYS:SG	2:E:207:SER:N	2.92	0.42
2:E:214:VAL:HG12	2:E:274:LEU:HD12	2.00	0.42
2:E:2823:ILE:HG12	2:E:2937:VAL:HG22	2.01	0.42
2:I:864:PRO:HD2	2:I:867:LEU:HD12	2.01	0.42
2:I:1940:CYS:O	2:I:1944:GLU:N	2.53	0.42
2:I:2517:UNK:O	2:I:2521:UNK:N	2.53	0.42
2:G:870:ILE:HD11	2:G:1049:TYR:CG	2.55	0.42
2:B:2257:LEU:HD11	2:B:2276:ALA:HB2	2.02	0.41
2:B:2823:ILE:HG12	2:B:2937:VAL:HG22	2.01	0.41
2:B:3915:ILE:O	2:B:3919:THR:N	2.52	0.41
2:E:393:CYS:SG	2:E:395:GLN:NE2	2.93	0.41
2:E:870:ILE:HD11	2:E:1049:TYR:CG	2.55	0.41
2:E:2208:MET:HE1	2:E:2253:HIS:HB3	2.00	0.41
2:E:2332:LEU:HD13	2:E:2335:LEU:HD12	2.01	0.41
2:E:2432:LEU:O	2:E:2436:CYS:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:40:GLU:HB3	2:I:44:ASN:HB3	2.02	0.41
2:G:234:SER:O	2:G:242:ARG:NE	2.52	0.41
2:G:454:PRO:HG2	2:G:531:ARG:HH12	1.84	0.41
2:B:4673:ARG:HH12	2:B:4698:LYS:HE3	1.85	0.41
2:E:103:TYR:HB3	2:E:152:PRO:HD3	2.02	0.41
2:I:234:SER:O	2:I:242:ARG:NE	2.52	0.41
2:I:530:ILE:HD13	2:I:536:ASN:HB3	2.02	0.41
2:I:2257:LEU:HD11	2:I:2276:ALA:HB2	2.02	0.41
2:G:4956:THR:O	2:G:4965:SER:N	2.52	0.41
1:H:44:LYS:HA	1:H:45:PRO:HD3	1.88	0.41
2:E:40:GLU:HB3	2:E:44:ASN:HB3	2.03	0.41
2:E:234:SER:O	2:E:242:ARG:NE	2.52	0.41
2:E:379:HIS:CD2	2:E:381:GLU:H	2.37	0.41
2:E:940:GLY:O	2:E:1052:ASN:N	2.53	0.41
2:E:1720:LEU:HD23	2:E:1721:GLU:HA	2.02	0.41
2:I:734:GLY:O	2:I:736:HIS:ND1	2.53	0.41
2:G:107:ILE:HG22	2:G:148:TRP:HB2	2.03	0.41
2:G:379:HIS:CD2	2:G:381:GLU:H	2.37	0.41
2:G:2517:UNK:O	2:G:2521:UNK:N	2.53	0.41
1:A:11:ASP:OD1	1:A:67:SER:OG	2.34	0.41
2:B:393:CYS:SG	2:B:395:GLN:NE2	2.93	0.41
2:B:870:ILE:HD11	2:B:1049:TYR:CG	2.55	0.41
2:E:107:ILE:HG22	2:E:148:TRP:HB2	2.03	0.41
2:E:2257:LEU:HD11	2:E:2276:ALA:HB2	2.02	0.41
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	2.02	0.41
2:E:4233:LEU:HA	2:E:4236:SER:HB3	2.03	0.41
2:I:395:GLN:NE2	2:I:397:GLU:OE1	2.54	0.41
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	2.03	0.41
2:I:4673:ARG:HH12	2:I:4698:LYS:HE3	1.85	0.41
2:G:134:ASP:OD1	2:G:134:ASP:N	2.53	0.41
2:G:393:CYS:SG	2:G:395:GLN:NE2	2.93	0.41
2:G:629:ARG:HB3	2:G:634:GLN:NE2	2.35	0.41
2:G:1720:LEU:HD23	2:G:1721:GLU:HA	2.02	0.41
2:G:2823:ILE:HG12	2:G:2937:VAL:HG22	2.01	0.41
2:B:530:ILE:HD13	2:B:536:ASN:HB3	2.02	0.41
2:B:4233:LEU:HA	2:B:4236:SER:HB3	2.03	0.41
2:E:864:PRO:HD2	2:E:867:LEU:HD12	2.01	0.41
2:E:946:ALA:HA	2:E:949:ASN:HB2	2.03	0.41
2:I:629:ARG:HD3	2:I:634:GLN:HG2	2.01	0.41
2:I:940:GLY:O	2:I:1052:ASN:N	2.53	0.41
2:G:395:GLN:NE2	2:G:397:GLU:OE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2195:PRO:HB3	2:G:2246:ASN:HD21	1.85	0.41
2:G:2423:MET:O	2:G:2427:ALA:N	2.48	0.41
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	2.02	0.41
2:G:4673:ARG:HH12	2:G:4698:LYS:HE3	1.85	0.41
2:B:40:GLU:HB3	2:B:44:ASN:HB3	2.02	0.41
2:B:629:ARG:HB3	2:B:634:GLN:NE2	2.35	0.41
2:B:4804:TYR:HB3	2:B:4806:ASN:HD22	1.85	0.41
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.86	0.41
2:I:4063:ASP:OD1	2:I:4169:SER:OG	2.30	0.41
2:I:4804:TYR:HB3	2:I:4806:ASN:HD22	1.85	0.41
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.39	0.41
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	2.03	0.41
2:B:357:LEU:HD12	2:B:388:LEU:HD11	2.03	0.41
2:B:606:LEU:HG	2:B:617:ASN:HD22	1.86	0.41
2:B:4142:ASN:HA	2:B:4145:VAL:HG12	2.02	0.41
2:E:629:ARG:HB3	2:E:634:GLN:NE2	2.35	0.41
2:E:864:PRO:HA	2:E:865:PRO:HD3	1.94	0.41
2:E:1940:CYS:O	2:E:1944:GLU:N	2.53	0.41
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	2.03	0.41
2:I:393:CYS:SG	2:I:395:GLN:NE2	2.93	0.41
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	2.02	0.41
2:I:2674:UNK:O	2:I:2676:UNK:N	2.54	0.41
2:G:2674:UNK:O	2:G:2676:UNK:N	2.54	0.41
2:G:4804:TYR:HB3	2:G:4806:ASN:HD22	1.85	0.41
2:B:103:TYR:HB3	2:B:152:PRO:HD3	2.02	0.41
2:B:143:GLY:HA3	2:B:147:TRP:HE1	1.86	0.41
2:B:2232:CYS:SG	2:B:2233:CYS:N	2.94	0.41
2:B:4567:LEU:HA	2:B:4816:ILE:HD12	2.03	0.41
2:E:395:GLN:NE2	2:E:397:GLU:OE1	2.54	0.41
2:E:2143:THR:N	2:E:3651:ASN:OD1	2.54	0.41
2:I:946:ALA:HA	2:I:949:ASN:HB2	2.03	0.41
2:I:2332:LEU:HD13	2:I:2335:LEU:HD12	2.01	0.41
2:I:3513:UNK:O	2:I:3515:UNK:N	2.54	0.41
2:I:3889:GLN:HG3	2:I:3967:GLU:HG3	2.03	0.41
2:I:4567:LEU:HA	2:I:4816:ILE:HD12	2.03	0.41
2:I:4802:GLY:HA2	2:I:4808:PHE:HB2	2.03	0.41
2:G:2257:LEU:HD11	2:G:2276:ALA:HB2	2.02	0.41
2:G:2327:GLY:HA2	2:G:2330:ARG:HD3	2.03	0.41
2:G:4802:GLY:HA2	2:G:4808:PHE:HB2	2.03	0.41
1:F:92:PRO:HD3	2:E:627:PRO:HB2	2.02	0.41
2:B:55:ALA:O	2:B:281:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2674:UNK:O	2:B:2676:UNK:N	2.54	0.41
2:B:4047:MET:HE3	2:B:4047:MET:HB2	1.94	0.41
2:E:2674:UNK:O	2:E:2676:UNK:N	2.54	0.41
2:E:4083:ASP:HB3	2:E:4086:GLY:H	1.85	0.41
2:E:4142:ASN:HA	2:E:4145:VAL:HG12	2.02	0.41
2:E:4641:PRO:O	2:E:4645:CYS:N	2.52	0.41
2:I:134:ASP:OD1	2:I:134:ASP:N	2.53	0.41
2:I:2143:THR:N	2:I:3651:ASN:OD1	2.54	0.41
2:I:2186:MET:HE3	2:I:2186:MET:HB3	1.97	0.41
2:I:2195:PRO:HB3	2:I:2246:ASN:HD21	1.84	0.41
2:I:2232:CYS:SG	2:I:2233:CYS:N	2.94	0.41
2:I:2327:GLY:HA2	2:I:2330:ARG:HD3	2.03	0.41
2:I:4047:MET:HE3	2:I:4047:MET:HB2	1.94	0.41
2:G:40:GLU:HB3	2:G:44:ASN:HB3	2.03	0.41
2:G:103:TYR:HB3	2:G:152:PRO:HD3	2.02	0.41
2:G:4083:ASP:HB3	2:G:4086:GLY:H	1.85	0.41
2:B:1863:LEU:HB3	2:B:1870:VAL:HG21	2.02	0.41
2:B:4823:LEU:HD23	2:I:4843:LEU:HD12	2.03	0.41
2:E:1863:LEU:HB3	2:E:1870:VAL:HG21	2.03	0.41
2:E:4567:LEU:HA	2:E:4816:ILE:HD12	2.03	0.41
2:E:4918:ILE:HD13	2:E:4918:ILE:HA	1.93	0.41
2:I:2346:VAL:HG13	2:I:2349:ASN:H	1.86	0.41
2:G:3513:UNK:O	2:G:3515:UNK:N	2.54	0.41
2:G:4233:LEU:HA	2:G:4236:SER:HB3	2.02	0.41
1:J:44:LYS:HA	1:J:45:PRO:HD3	1.88	0.40
2:B:2186:MET:HE3	2:B:2186:MET:HB3	1.97	0.40
2:B:2346:VAL:HG13	2:B:2349:ASN:H	1.86	0.40
2:B:3513:UNK:O	2:B:3515:UNK:N	2.54	0.40
2:I:214:VAL:HG22	2:I:341:TYR:CE1	2.56	0.40
2:I:4983:HIS:HB2	2:I:4988:TYR:HE2	1.86	0.40
2:G:35:LEU:HD13	2:G:49:LEU:HD13	2.03	0.40
2:G:3915:ILE:O	2:G:3919:THR:N	2.52	0.40
2:G:3971:GLY:N	2:G:4032:GLU:OE2	2.53	0.40
2:G:4567:LEU:HA	2:G:4816:ILE:HD12	2.03	0.40
2:G:4983:HIS:HB2	2:G:4988:TYR:HE2	1.86	0.40
2:B:234:SER:O	2:B:242:ARG:NE	2.52	0.40
2:B:1641:ILE:HA	2:B:1642:PRO:HD3	1.89	0.40
2:B:1940:CYS:O	2:B:1944:GLU:N	2.53	0.40
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	2.03	0.40
2:B:4802:GLY:HA2	2:B:4808:PHE:HB2	2.03	0.40
2:E:790:ARG:HG2	2:E:1627:ALA:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4673:ARG:HH12	2:E:4698:LYS:HE3	1.85	0.40
2:I:143:GLY:HA3	2:I:147:TRP:HE1	1.86	0.40
2:I:1863:LEU:HB3	2:I:1870:VAL:HG21	2.03	0.40
2:G:681:HIS:HB3	2:G:784:SER:HB3	2.03	0.40
2:G:838:HIS:HA	2:G:1201:HIS:HB3	2.04	0.40
2:G:2143:THR:N	2:G:3651:ASN:OD1	2.54	0.40
2:G:2742:THR:OG1	2:G:2811:GLU:OE1	2.33	0.40
2:B:4000:MET:HE3	2:B:4017:LEU:HD21	2.03	0.40
2:E:143:GLY:HA3	2:E:147:TRP:HE1	1.86	0.40
2:E:3513:UNK:O	2:E:3515:UNK:N	2.54	0.40
2:E:4763:GLY:H	2:E:4767:TRP:HE1	1.69	0.40
2:E:4804:TYR:HB3	2:E:4806:ASN:HD22	1.85	0.40
2:I:4233:LEU:HA	2:I:4236:SER:HB3	2.03	0.40
2:G:1096:THR:HG23	2:G:1199:VAL:HG22	2.03	0.40
2:B:614:VAL:HA	2:B:2169:GLN:HB3	2.03	0.40
2:B:708:GLY:HA3	2:B:722:TRP:HB3	2.03	0.40
2:B:1236:THR:OG1	2:B:1608:MET:SD	2.76	0.40
2:B:4763:GLY:H	2:B:4767:TRP:HE1	1.69	0.40
2:B:4983:HIS:HB2	2:B:4988:TYR:HE2	1.86	0.40
2:E:1096:THR:HG23	2:E:1199:VAL:HG22	2.03	0.40
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.39	0.40
2:E:4983:HIS:HB2	2:E:4988:TYR:HE2	1.86	0.40
2:E:5000:GLU:HA	2:E:5003:HIS:CD2	2.57	0.40
2:I:55:ALA:O	2:I:281:ARG:NH2	2.54	0.40
2:I:107:ILE:HG22	2:I:148:TRP:HB2	2.03	0.40
2:I:838:HIS:HA	2:I:1201:HIS:HB3	2.03	0.40
2:I:2021:CYS:HA	2:I:2022:PRO:HD3	1.96	0.40
2:G:606:LEU:HG	2:G:617:ASN:HD22	1.86	0.40
2:B:395:GLN:NE2	2:B:397:GLU:OE1	2.54	0.40
2:B:838:HIS:HA	2:B:1201:HIS:HB3	2.04	0.40
2:B:946:ALA:HA	2:B:949:ASN:HB2	2.03	0.40
2:E:2034:PHE:O	2:E:2038:LEU:N	2.55	0.40
2:E:3971:GLY:N	2:E:4032:GLU:OE2	2.53	0.40
2:I:471:LEU:O	2:I:475:GLN:N	2.53	0.40
2:I:708:GLY:HA3	2:I:722:TRP:HB3	2.03	0.40
2:I:3971:GLY:N	2:I:4032:GLU:OE2	2.53	0.40
2:G:864:PRO:HA	2:G:865:PRO:HD3	1.94	0.40
2:G:1940:CYS:O	2:G:1944:GLU:N	2.53	0.40
2:G:2437:ALA:HA	2:G:2438:PRO:HD3	1.96	0.40
2:G:3804:ILE:HG22	2:G:3812:VAL:HG21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	94 (90%)	11 (10%)	0	100	100
1	F	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	H	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	J	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
2	B	3235/4416 (73%)	2877 (89%)	352 (11%)	6 (0%)	43	76
2	E	3235/4416 (73%)	2878 (89%)	351 (11%)	6 (0%)	43	76
2	G	3235/4416 (73%)	2877 (89%)	352 (11%)	6 (0%)	43	76
2	I	3235/4416 (73%)	2878 (89%)	351 (11%)	6 (0%)	43	76
All	All	13360/18096 (74%)	11884 (89%)	1452 (11%)	24 (0%)	44	76

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	B	1840	PRO
2	B	1932	PRO
2	B	4641	PRO
2	E	1708	ARG
2	E	1840	PRO
2	E	1932	PRO
2	E	4641	PRO
2	I	1708	ARG
2	I	1840	PRO
2	I	1932	PRO
2	I	4641	PRO
2	G	1708	ARG
2	G	1840	PRO
2	G	1932	PRO
2	G	4641	PRO
2	B	2291	GLN

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Mol	Chain	Res	Type
2	B	4640	GLU
2	E	2291	GLN
2	E	4640	GLU
2	I	2291	GLN
2	I	4640	GLU
2	G	2291	GLN
2	G	4640	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	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%)	2482 (100%)	11 (0%)	84	83
2	E	2493/3022 (82%)	2482 (100%)	11 (0%)	84	83
2	G	2493/3022 (82%)	2482 (100%)	11 (0%)	84	83
2	I	2493/3022 (82%)	2482 (100%)	11 (0%)	84	83
All	All	10324/12444 (83%)	10280 (100%)	44 (0%)	81	83

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	719	LEU
2	B	978	THR
2	B	1600	LEU
2	B	1676	LEU
2	B	2010	LEU
2	B	2339	VAL
2	B	3663	LEU

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Mol	Chain	Res	Type
2	B	3805	LEU
2	B	4081	VAL
2	B	4792	LEU
2	E	131	LEU
2	E	719	LEU
2	E	978	THR
2	E	1600	LEU
2	E	1676	LEU
2	E	2010	LEU
2	E	2339	VAL
2	E	3663	LEU
2	E	3805	LEU
2	E	4081	VAL
2	E	4792	LEU
2	I	131	LEU
2	I	719	LEU
2	I	978	THR
2	I	1600	LEU
2	I	1676	LEU
2	I	2010	LEU
2	I	2339	VAL
2	I	3663	LEU
2	I	3805	LEU
2	I	4081	VAL
2	I	4792	LEU
2	G	131	LEU
2	G	719	LEU
2	G	978	THR
2	G	1600	LEU
2	G	1676	LEU
2	G	2010	LEU
2	G	2339	VAL
2	G	3663	LEU
2	G	3805	LEU
2	G	4081	VAL
2	G	4792	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (224) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	87	HIS
1	A	87	HIS

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Mol	Chain	Res	Type
1	H	87	HIS
1	J	25	HIS
1	J	87	HIS
2	B	57	ASN
2	B	113	HIS
2	B	151	HIS
2	B	224	HIS
2	B	273	HIS
2	B	379	HIS
2	B	383	HIS
2	B	395	GLN
2	B	399	GLN
2	B	405	HIS
2	B	413	GLN
2	B	479	GLN
2	B	520	ASN
2	B	725	HIS
2	B	866	HIS
2	B	949	ASN
2	B	1220	GLN
2	B	1598	GLN
2	B	1663	HIS
2	B	1679	ASN
2	B	1691	GLN
2	B	1693	GLN
2	B	1702	HIS
2	B	1719	HIS
2	B	1775	HIS
2	B	1861	GLN
2	B	1972	ASN
2	B	2005	GLN
2	B	2035	HIS
2	B	2127	GLN
2	B	2260	ASN
2	B	2772	GLN
2	B	2773	ASN
2	B	3761	GLN
2	B	3771	HIS
2	B	3814	GLN
2	B	3882	GLN
2	B	3896	ASN
2	B	3946	GLN

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Mol	Chain	Res	Type
2	B	3950	ASN
2	B	3960	GLN
2	B	4034	ASN
2	B	4054	ASN
2	B	4078	GLN
2	B	4142	ASN
2	B	4153	HIS
2	B	4209	GLN
2	B	4246	GLN
2	B	4691	GLN
2	B	4700	GLN
2	B	4776	GLN
2	B	4806	ASN
2	B	4933	GLN
2	B	4947	GLN
2	B	5003	HIS
2	E	57	ASN
2	E	113	HIS
2	E	151	HIS
2	E	224	HIS
2	E	273	HIS
2	E	379	HIS
2	E	383	HIS
2	E	395	GLN
2	E	399	GLN
2	E	405	HIS
2	E	413	GLN
2	E	479	GLN
2	E	520	ASN
2	E	725	HIS
2	E	866	HIS
2	E	1220	GLN
2	E	1598	GLN
2	E	1663	HIS
2	E	1679	ASN
2	E	1691	GLN
2	E	1693	GLN
2	E	1702	HIS
2	E	1719	HIS
2	E	1775	HIS
2	E	1861	GLN
2	E	1972	ASN

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Mol	Chain	Res	Type
2	E	2005	GLN
2	E	2035	HIS
2	E	2127	GLN
2	E	2260	ASN
2	E	2772	GLN
2	E	2773	ASN
2	E	3761	GLN
2	E	3771	HIS
2	E	3814	GLN
2	E	3882	GLN
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	3960	GLN
2	E	3982	HIS
2	E	4034	ASN
2	E	4054	ASN
2	E	4078	GLN
2	E	4142	ASN
2	E	4209	GLN
2	E	4246	GLN
2	E	4691	GLN
2	E	4700	GLN
2	E	4776	GLN
2	E	4806	ASN
2	E	4833	ASN
2	E	4933	GLN
2	E	4947	GLN
2	E	5003	HIS
2	I	57	ASN
2	I	105	HIS
2	I	113	HIS
2	I	151	HIS
2	I	156	GLN
2	I	224	HIS
2	I	273	HIS
2	I	379	HIS
2	I	383	HIS
2	I	395	GLN
2	I	399	GLN
2	I	405	HIS
2	I	413	GLN

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Mol	Chain	Res	Type
2	I	479	GLN
2	I	520	ASN
2	I	725	HIS
2	I	866	HIS
2	I	1220	GLN
2	I	1598	GLN
2	I	1663	HIS
2	I	1679	ASN
2	I	1691	GLN
2	I	1693	GLN
2	I	1702	HIS
2	I	1719	HIS
2	I	1775	HIS
2	I	1861	GLN
2	I	1972	ASN
2	I	2005	GLN
2	I	2035	HIS
2	I	2127	GLN
2	I	2260	ASN
2	I	2772	GLN
2	I	3761	GLN
2	I	3771	HIS
2	I	3814	GLN
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	3982	HIS
2	I	4034	ASN
2	I	4054	ASN
2	I	4078	GLN
2	I	4142	ASN
2	I	4209	GLN
2	I	4246	GLN
2	I	4691	GLN
2	I	4700	GLN
2	I	4776	GLN
2	I	4806	ASN
2	I	4933	GLN
2	I	4947	GLN
2	I	5003	HIS
2	G	57	ASN

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Mol	Chain	Res	Type
2	G	113	HIS
2	G	151	HIS
2	G	224	HIS
2	G	273	HIS
2	G	379	HIS
2	G	383	HIS
2	G	395	GLN
2	G	399	GLN
2	G	405	HIS
2	G	413	GLN
2	G	479	GLN
2	G	520	ASN
2	G	725	HIS
2	G	866	HIS
2	G	949	ASN
2	G	1220	GLN
2	G	1598	GLN
2	G	1663	HIS
2	G	1679	ASN
2	G	1691	GLN
2	G	1693	GLN
2	G	1702	HIS
2	G	1719	HIS
2	G	1775	HIS
2	G	1861	GLN
2	G	1972	ASN
2	G	2005	GLN
2	G	2035	HIS
2	G	2127	GLN
2	G	2260	ASN
2	G	2772	GLN
2	G	2788	HIS
2	G	2856	ASN
2	G	3761	GLN
2	G	3771	HIS
2	G	3781	GLN
2	G	3814	GLN
2	G	3882	GLN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	3982	HIS

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Mol	Chain	Res	Type
2	G	4034	ASN
2	G	4054	ASN
2	G	4142	ASN
2	G	4209	GLN
2	G	4246	GLN
2	G	4691	GLN
2	G	4700	GLN
2	G	4776	GLN
2	G	4806	ASN
2	G	4933	GLN
2	G	4947	GLN
2	G	5003	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ATP	B	5101	-	32,33,33	1.34	5 (15%)	48,52,52	1.70	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CFF	E	5102	-	15,15,15	1.99	6 (40%)	23,23,23	2.74	10 (43%)
4	CFF	B	5102	-	15,15,15	1.98	6 (40%)	23,23,23	2.74	10 (43%)
4	CFF	I	5102	-	15,15,15	1.98	6 (40%)	23,23,23	2.74	10 (43%)
3	ATP	I	5101	-	32,33,33	1.34	5 (15%)	48,52,52	1.71	9 (18%)
3	ATP	E	5101	-	32,33,33	1.33	5 (15%)	48,52,52	1.71	9 (18%)
3	ATP	G	5101	-	32,33,33	1.33	5 (15%)	48,52,52	1.71	9 (18%)
4	CFF	G	5102	-	15,15,15	1.98	7 (46%)	23,23,23	2.74	10 (43%)

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	ATP	B	5101	-	-	3/22/38/38	0/3/3/3
4	CFF	E	5102	-	-	-	0/2/2/2
4	CFF	B	5102	-	-	-	0/2/2/2
4	CFF	I	5102	-	-	-	0/2/2/2
3	ATP	I	5101	-	-	3/22/38/38	0/3/3/3
3	ATP	E	5101	-	-	3/22/38/38	0/3/3/3
3	ATP	G	5101	-	-	3/22/38/38	0/3/3/3
4	CFF	G	5102	-	-	-	0/2/2/2

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	5101	ATP	C5-C4	4.30	1.46	1.39
3	E	5101	ATP	C5-C4	4.29	1.46	1.39
3	G	5101	ATP	C5-C4	4.28	1.46	1.39
3	B	5101	ATP	C5-C4	4.28	1.46	1.39
4	E	5102	CFF	C6-N1	-4.14	1.31	1.40
4	I	5102	CFF	C6-N1	-4.14	1.31	1.40
4	G	5102	CFF	C6-N1	-4.12	1.31	1.40
4	B	5102	CFF	C6-N1	-4.12	1.31	1.40
4	E	5102	CFF	C4-N3	-2.93	1.33	1.38
4	B	5102	CFF	C4-N3	-2.93	1.33	1.38
4	I	5102	CFF	C4-N3	-2.86	1.33	1.38
4	G	5102	CFF	C4-N3	-2.84	1.33	1.38
3	E	5101	ATP	C5-N7	-2.60	1.34	1.39
3	I	5101	ATP	C5-N7	-2.60	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5101	ATP	C5-N7	-2.58	1.34	1.39
3	G	5101	ATP	C5-N7	-2.56	1.34	1.39
4	G	5102	CFF	C5-N7	-2.54	1.34	1.38
4	I	5102	CFF	C5-N7	-2.52	1.34	1.38
4	B	5102	CFF	C5-N7	-2.51	1.34	1.38
4	E	5102	CFF	C5-N7	-2.49	1.34	1.38
3	B	5101	ATP	C4-N9	-2.41	1.32	1.37
3	E	5101	ATP	C4-N9	-2.34	1.32	1.37
3	I	5101	ATP	C4-N9	-2.34	1.32	1.37
3	B	5101	ATP	C8-N7	2.31	1.36	1.31
3	I	5101	ATP	C8-N7	2.30	1.36	1.31
3	G	5101	ATP	C4-N9	-2.27	1.33	1.37
3	G	5101	ATP	C8-N7	2.26	1.36	1.31
3	B	5101	ATP	C5-C6	2.26	1.47	1.41
3	I	5101	ATP	C5-C6	2.25	1.47	1.41
3	E	5101	ATP	C8-N7	2.25	1.36	1.31
3	G	5101	ATP	C5-C6	2.25	1.47	1.41
3	E	5101	ATP	C5-C6	2.22	1.47	1.41
4	E	5102	CFF	O11-C2	-2.14	1.18	1.22
4	G	5102	CFF	O11-C2	-2.13	1.18	1.22
4	B	5102	CFF	O11-C2	-2.12	1.18	1.22
4	I	5102	CFF	O11-C2	-2.11	1.18	1.22
4	E	5102	CFF	O13-C6	-2.10	1.18	1.23
4	G	5102	CFF	O13-C6	-2.09	1.18	1.23
4	I	5102	CFF	O13-C6	-2.08	1.18	1.23
4	B	5102	CFF	C2-N3	-2.07	1.35	1.39
4	B	5102	CFF	O13-C6	-2.06	1.18	1.23
4	I	5102	CFF	C2-N3	-2.03	1.35	1.39
4	E	5102	CFF	C2-N3	-2.03	1.35	1.39
4	G	5102	CFF	C2-N3	-2.03	1.35	1.39
4	G	5102	CFF	C5-C6	-2.02	1.37	1.43

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	5102	CFF	C14-N7-C8	-7.69	111.89	126.28
4	G	5102	CFF	C14-N7-C8	-7.68	111.91	126.28
4	E	5102	CFF	C14-N7-C8	-7.67	111.93	126.28
4	I	5102	CFF	C14-N7-C8	-7.66	111.94	126.28
3	E	5101	ATP	C5-C4-N3	-5.31	119.41	126.72
3	G	5101	ATP	C5-C4-N3	-5.29	119.43	126.72
3	I	5101	ATP	C5-C4-N3	-5.28	119.44	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5101	ATP	C5-C4-N3	-5.16	119.61	126.72
4	B	5102	CFF	C14-N7-C5	5.10	139.91	127.77
4	E	5102	CFF	C14-N7-C5	5.10	139.90	127.77
4	I	5102	CFF	C14-N7-C5	5.09	139.89	127.77
4	G	5102	CFF	C14-N7-C5	5.08	139.87	127.77
4	E	5102	CFF	C5-C6-N1	4.05	119.47	112.06
4	I	5102	CFF	C5-C6-N1	4.02	119.42	112.06
3	G	5101	ATP	N3-C4-N9	4.01	133.99	127.17
4	G	5102	CFF	C5-C6-N1	4.01	119.41	112.06
3	I	5101	ATP	N3-C4-N9	3.99	133.96	127.17
4	B	5102	CFF	C5-C6-N1	3.99	119.36	112.06
3	E	5101	ATP	N3-C4-N9	3.99	133.95	127.17
3	B	5101	ATP	N3-C4-N9	3.84	133.69	127.17
3	B	5101	ATP	C4-C5-N7	-3.54	106.53	110.58
3	E	5101	ATP	C4-C5-N7	-3.53	106.55	110.58
3	G	5101	ATP	C4-C5-N7	-3.51	106.57	110.58
3	I	5101	ATP	C4-C5-N7	-3.50	106.58	110.58
3	G	5101	ATP	C2-N3-C4	3.43	120.20	111.83
3	E	5101	ATP	C2-N3-C4	3.42	120.18	111.83
3	I	5101	ATP	C2-N3-C4	3.40	120.14	111.83
3	B	5101	ATP	C2-N3-C4	3.40	120.13	111.83
4	E	5102	CFF	C6-N1-C2	-3.34	120.23	125.66
4	B	5102	CFF	C6-N1-C2	-3.33	120.25	125.66
4	I	5102	CFF	C6-N1-C2	-3.32	120.27	125.66
4	G	5102	CFF	C6-N1-C2	-3.29	120.31	125.66
3	B	5101	ATP	N3-C2-N1	-3.27	123.64	128.58
3	G	5101	ATP	N3-C2-N1	-3.18	123.77	128.58
3	E	5101	ATP	N3-C2-N1	-3.16	123.80	128.58
3	I	5101	ATP	N3-C2-N1	-3.14	123.83	128.58
4	E	5102	CFF	N3-C4-N9	2.91	130.84	126.27
4	G	5102	CFF	N3-C4-N9	2.89	130.81	126.27
4	I	5102	CFF	N3-C4-N9	2.88	130.80	126.27
4	E	5102	CFF	N7-C8-N9	-2.88	108.25	113.48
4	B	5102	CFF	N7-C8-N9	-2.87	108.28	113.48
4	B	5102	CFF	N3-C4-N9	2.86	130.77	126.27
4	G	5102	CFF	N7-C8-N9	-2.86	108.29	113.48
4	I	5102	CFF	N7-C8-N9	-2.85	108.32	113.48
3	I	5101	ATP	C4-N9-C8	2.68	108.55	105.74
3	B	5101	ATP	C4-N9-C8	2.66	108.53	105.74
3	G	5101	ATP	C4-N9-C8	2.65	108.52	105.74
3	E	5101	ATP	C4-N9-C8	2.62	108.49	105.74
4	I	5102	CFF	N3-C2-N1	2.59	120.37	117.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	5102	CFF	N3-C2-N1	2.58	120.36	117.14
3	E	5101	ATP	C5-N7-C8	2.58	107.50	103.45
4	G	5102	CFF	N3-C2-N1	2.55	120.33	117.14
3	B	5101	ATP	C6-C5-N7	2.55	137.00	132.09
3	G	5101	ATP	C5-N7-C8	2.55	107.45	103.45
3	I	5101	ATP	C5-N7-C8	2.55	107.45	103.45
4	B	5102	CFF	O13-C6-C5	-2.53	121.19	126.38
3	B	5101	ATP	C5-N7-C8	2.53	107.43	103.45
4	E	5102	CFF	N3-C2-N1	2.53	120.29	117.14
4	E	5102	CFF	O13-C6-C5	-2.52	121.21	126.38
4	I	5102	CFF	O13-C6-C5	-2.52	121.21	126.38
4	G	5102	CFF	O13-C6-C5	-2.51	121.24	126.38
4	B	5102	CFF	C12-N3-C2	2.50	121.69	117.33
4	I	5102	CFF	C12-N3-C2	2.49	121.67	117.33
4	G	5102	CFF	C12-N3-C2	2.49	121.67	117.33
4	E	5102	CFF	C12-N3-C2	2.47	121.63	117.33
3	E	5101	ATP	C6-C5-N7	2.46	136.83	132.09
3	G	5101	ATP	C6-C5-N7	2.46	136.83	132.09
3	I	5101	ATP	C6-C5-N7	2.44	136.80	132.09
4	E	5102	CFF	C6-C5-C4	-2.40	119.89	122.92
4	I	5102	CFF	C6-C5-C4	-2.39	119.91	122.92
4	G	5102	CFF	C6-C5-C4	-2.38	119.92	122.92
4	B	5102	CFF	C6-C5-C4	-2.36	119.95	122.92
3	E	5101	ATP	N9-C8-N7	-2.19	110.82	113.94
3	I	5101	ATP	N9-C8-N7	-2.19	110.82	113.94
3	B	5101	ATP	N9-C8-N7	-2.19	110.83	113.94
3	G	5101	ATP	N9-C8-N7	-2.15	110.88	113.94
3	B	5101	ATP	C2-N1-C6	2.09	122.16	118.73

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	C5'-O5'-PA-O1A
3	E	5101	ATP	C5'-O5'-PA-O1A
3	I	5101	ATP	C5'-O5'-PA-O1A
3	G	5101	ATP	C5'-O5'-PA-O1A
3	B	5101	ATP	PA-O3A-PB-O1B
3	E	5101	ATP	PA-O3A-PB-O1B
3	I	5101	ATP	PA-O3A-PB-O1B
3	G	5101	ATP	PA-O3A-PB-O1B
3	E	5101	ATP	PA-O3A-PB-O2B

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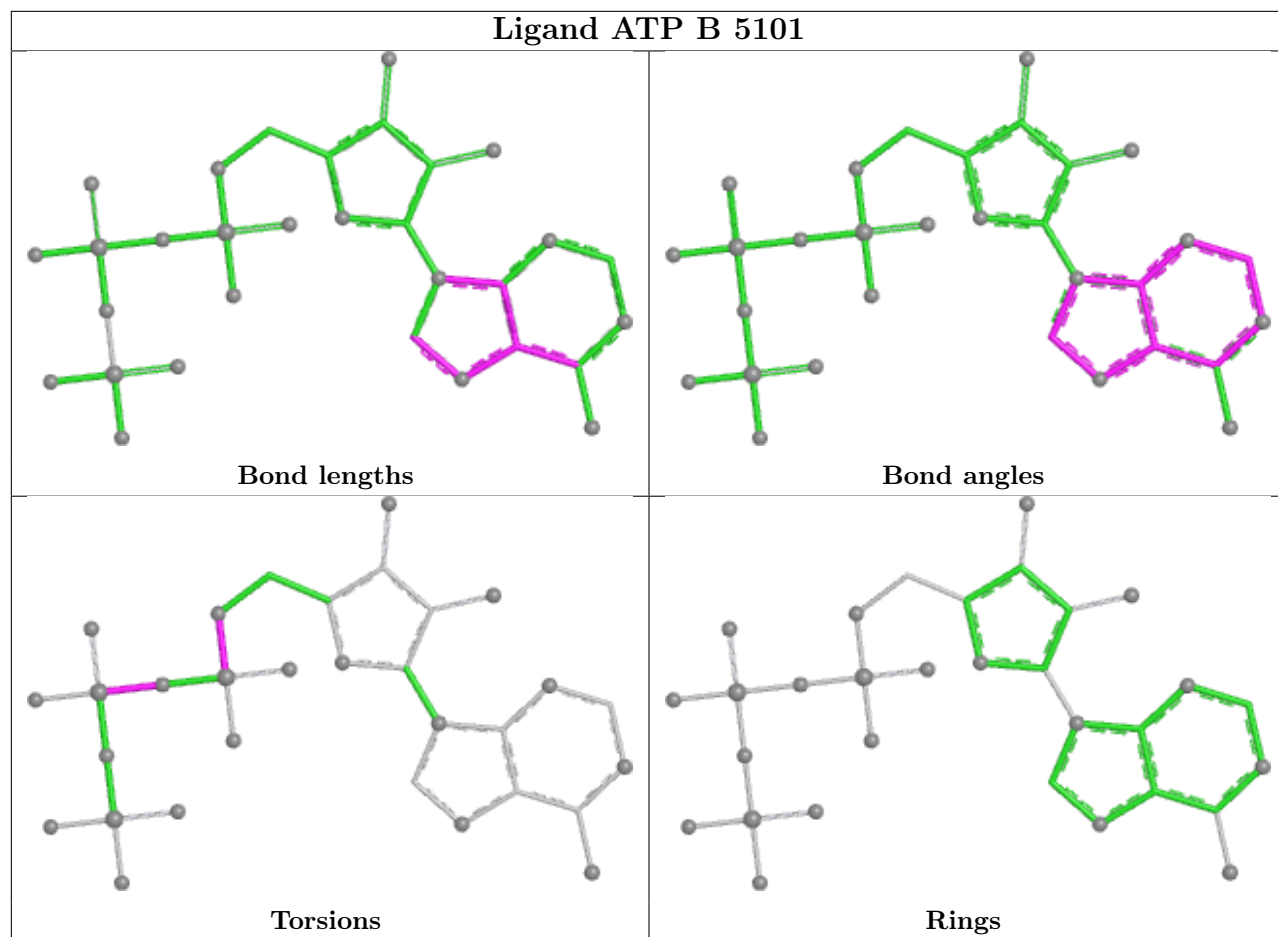
Mol	Chain	Res	Type	Atoms
3	I	5101	ATP	PA-O3A-PB-O2B
3	G	5101	ATP	PA-O3A-PB-O2B
3	B	5101	ATP	PA-O3A-PB-O2B

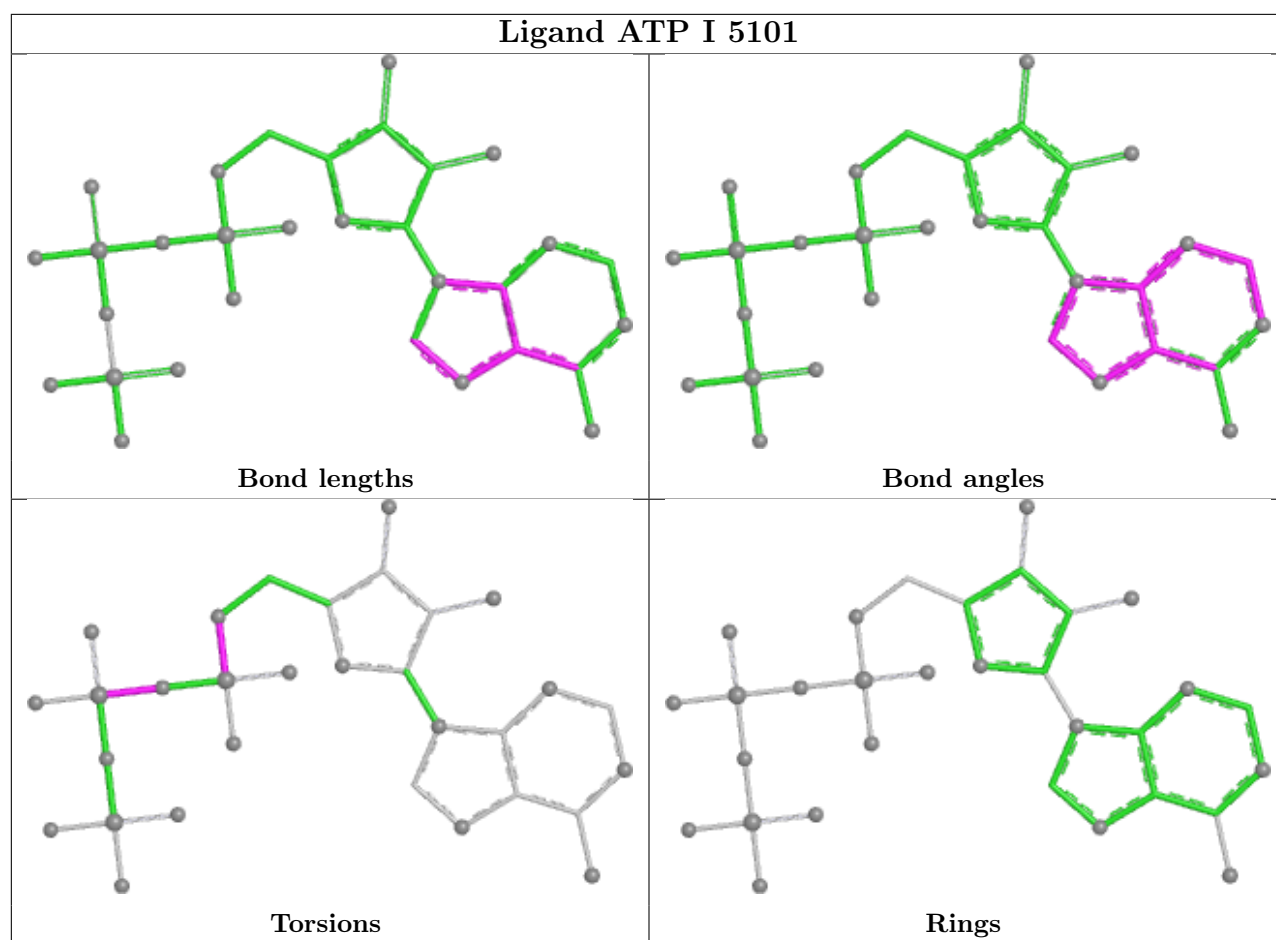
There are no ring outliers.

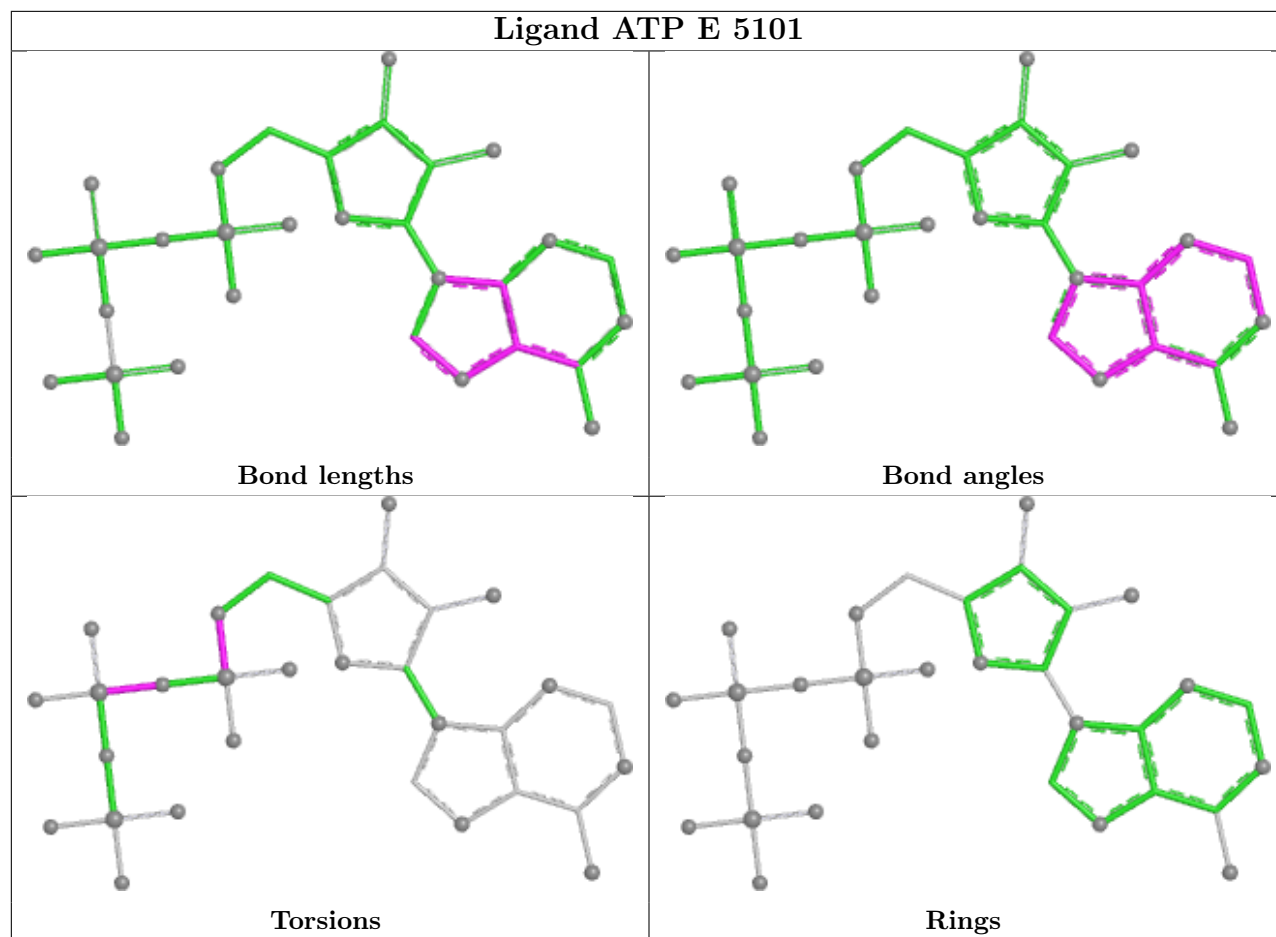
1 monomer is involved in 1 short contact:

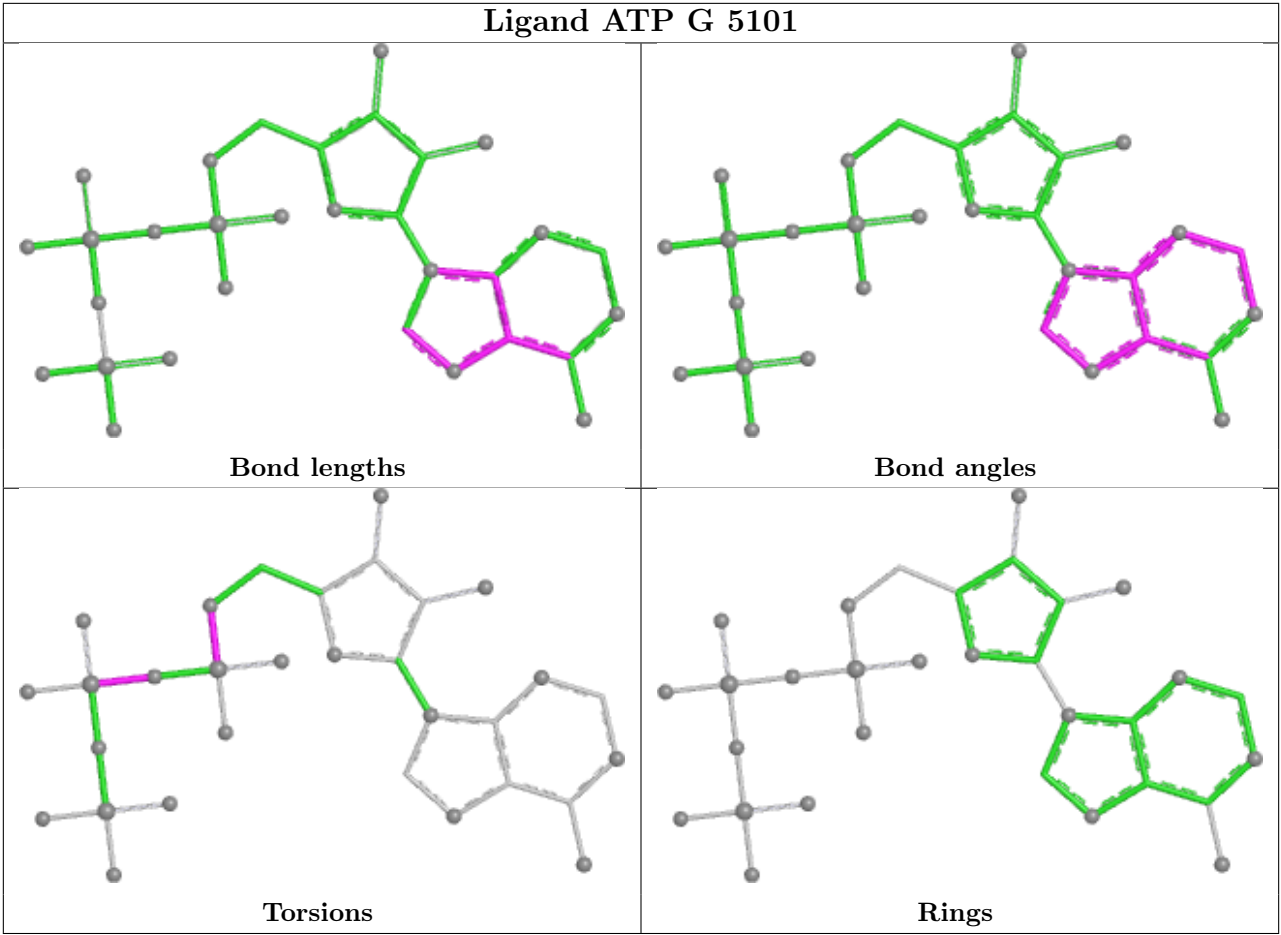
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5101	ATP	1	0

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









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

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

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	4345:UNK	C	4540:PHE	N	72.62
1	B	4345:UNK	C	4540:PHE	N	72.61

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	4345:UNK	C	4540:PHE	N	72.60
1	G	4345:UNK	C	4540:PHE	N	72.60
1	E	3613:UNK	C	3639:THR	N	43.07
1	B	3613:UNK	C	3639:THR	N	43.04
1	I	3613:UNK	C	3639:THR	N	43.03
1	G	3613:UNK	C	3639:THR	N	43.03
1	B	4253:GLU	C	4320:UNK	N	27.32
1	E	4253:GLU	C	4320:UNK	N	27.31
1	I	4253:GLU	C	4320:UNK	N	27.29
1	G	4253:GLU	C	4320:UNK	N	27.28
1	B	3163:UNK	C	3170:UNK	N	16.19
1	E	3163:UNK	C	3170:UNK	N	16.19
1	I	3163:UNK	C	3170:UNK	N	16.19
1	G	3163:UNK	C	3170:UNK	N	16.19
1	B	3063:UNK	C	3134:UNK	N	14.97
1	E	3063:UNK	C	3134:UNK	N	14.96
1	I	3063:UNK	C	3134:UNK	N	14.96
1	G	3063:UNK	C	3134:UNK	N	14.96
1	E	3468:UNK	C	3511:UNK	N	14.60
1	G	3468:UNK	C	3511:UNK	N	14.60
1	B	3468:UNK	C	3511:UNK	N	14.59
1	I	3468:UNK	C	3511:UNK	N	14.59
1	B	2703:UNK	C	2734:ASN	N	14.53
1	G	2703:UNK	C	2734:ASN	N	14.49
1	E	2703:UNK	C	2734:ASN	N	14.48
1	I	2703:UNK	C	2734:ASN	N	14.48
1	E	3236:UNK	C	3241:UNK	N	13.44
1	B	3236:UNK	C	3241:UNK	N	13.43
1	I	3236:UNK	C	3241:UNK	N	13.43
1	G	3236:UNK	C	3241:UNK	N	13.43
1	E	2976:UNK	C	2995:UNK	N	12.55
1	B	2976:UNK	C	2995:UNK	N	12.54
1	I	2976:UNK	C	2995:UNK	N	12.54
1	G	2976:UNK	C	2995:UNK	N	12.54
1	B	1564:UNK	C	1573:MET	N	12.29
1	E	1564:UNK	C	1573:MET	N	12.29
1	I	1564:UNK	C	1573:MET	N	12.27
1	G	1564:UNK	C	1573:MET	N	12.27
1	B	3254:UNK	C	3261:UNK	N	8.31
1	E	3254:UNK	C	3261:UNK	N	8.31
1	I	3254:UNK	C	3261:UNK	N	8.31
1	G	3254:UNK	C	3261:UNK	N	8.31

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	1297:UNK	C	1430:UNK	N	6.25
1	I	1297:UNK	C	1430:UNK	N	6.25
1	G	1297:UNK	C	1430:UNK	N	6.25
1	B	1297:UNK	C	1430:UNK	N	6.24
1	B	2939:ARG	C	2942:UNK	N	3.30
1	E	2939:ARG	C	2942:UNK	N	3.27
1	G	2939:ARG	C	2942:UNK	N	3.27
1	I	2939:ARG	C	2942:UNK	N	3.26
1	I	2479:LEU	C	2487:UNK	N	3.25
1	E	2479:LEU	C	2487:UNK	N	3.24
1	G	2479:LEU	C	2487:UNK	N	3.24
1	B	2479:LEU	C	2487:UNK	N	3.23

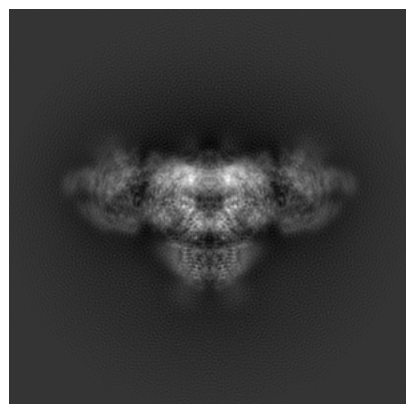
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8382. These allow visual inspection of the internal detail of the map and identification of artifacts.

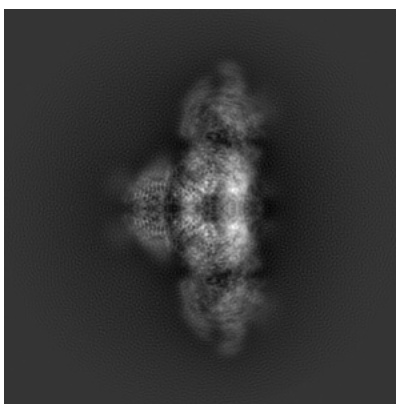
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

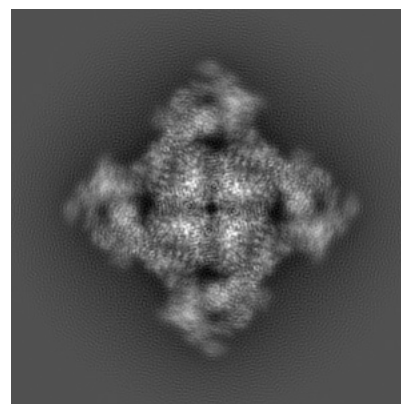
6.1.1 Primary map



X

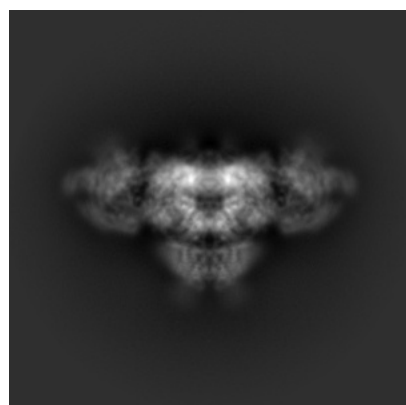


Y

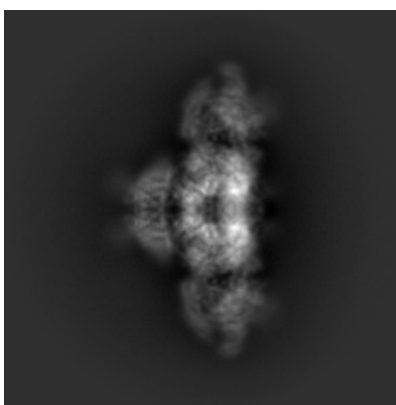


Z

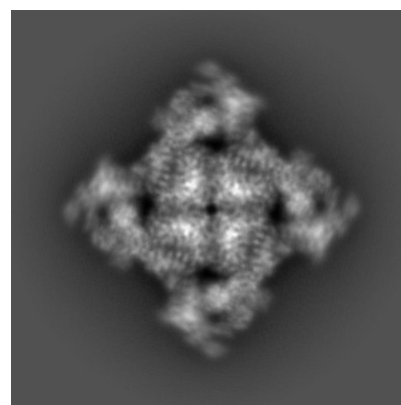
6.1.2 Raw map



X



Y

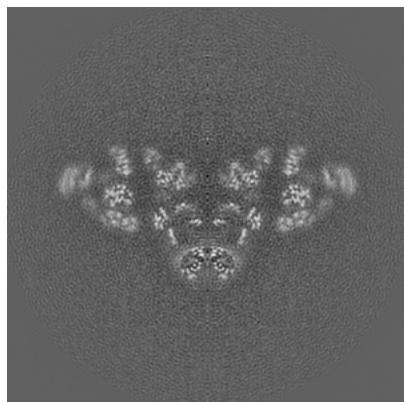


Z

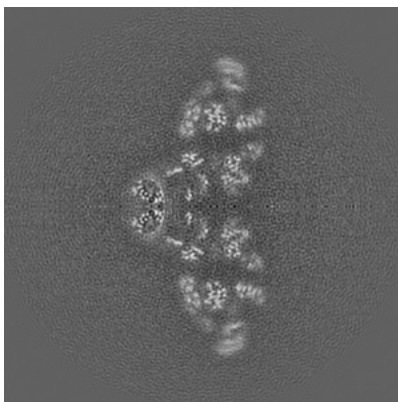
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

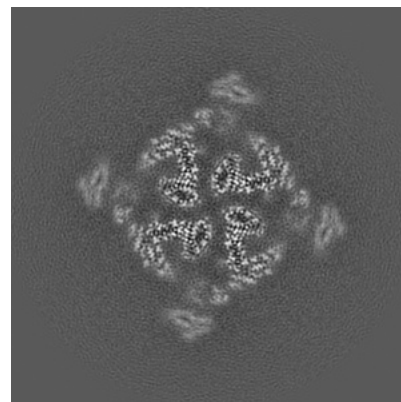
6.2.1 Primary map



X Index: 200

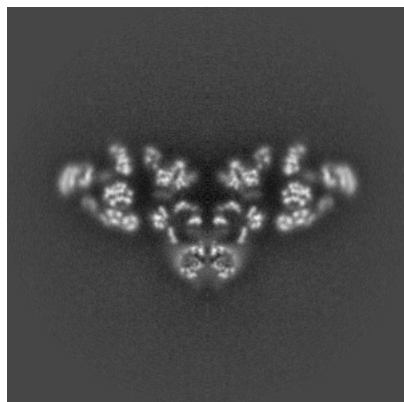


Y Index: 200

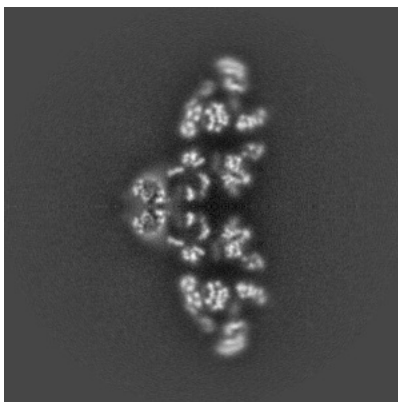


Z Index: 200

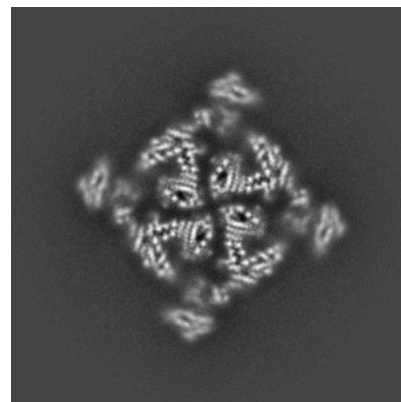
6.2.2 Raw map



X Index: 200



Y Index: 200

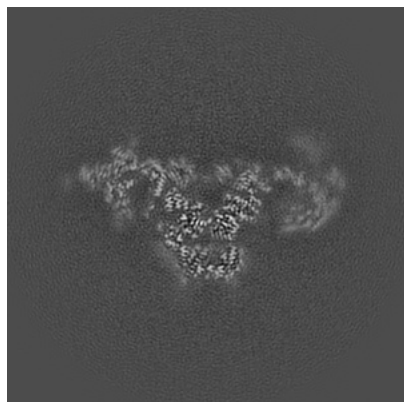


Z Index: 200

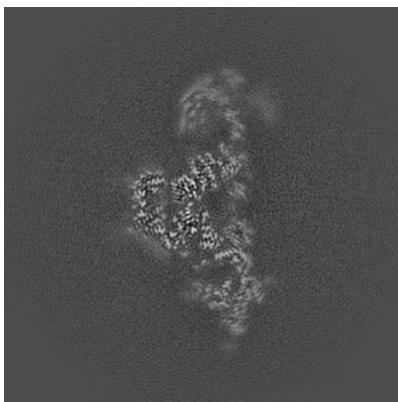
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

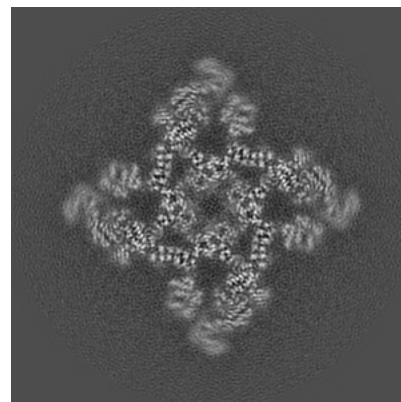
6.3.1 Primary map



X Index: 216

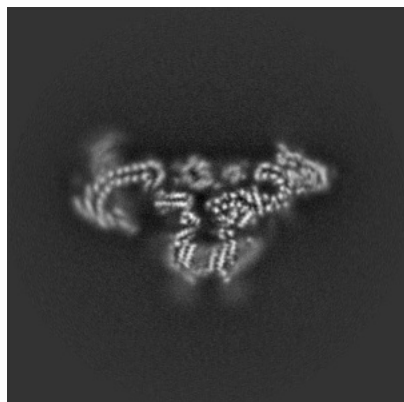


Y Index: 184

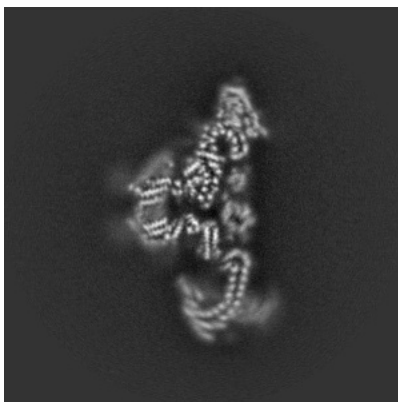


Z Index: 226

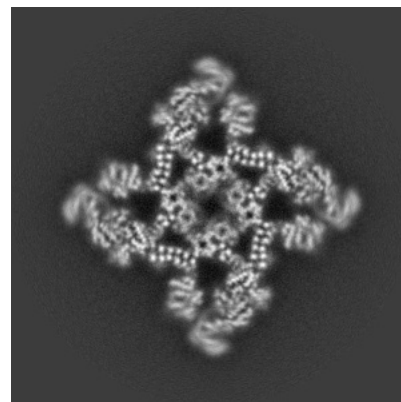
6.3.2 Raw map



X Index: 176



Y Index: 224

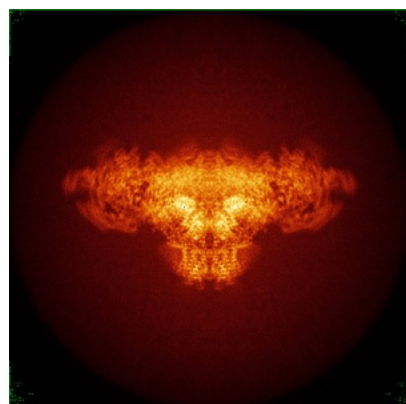


Z Index: 227

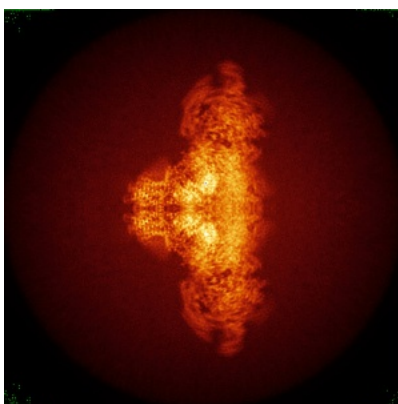
The images above show the largest variance slices of the map in three orthogonal directions.

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

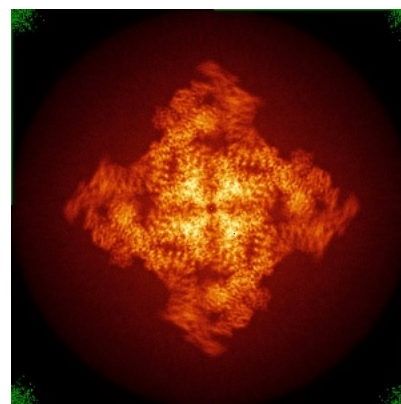
6.4.1 Primary map



X

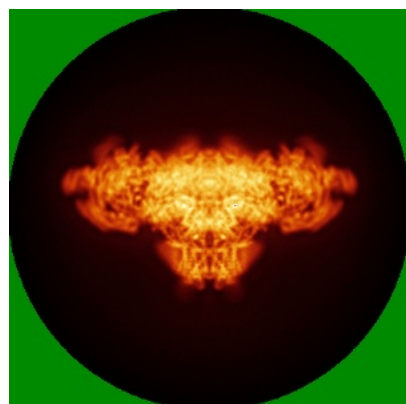


Y

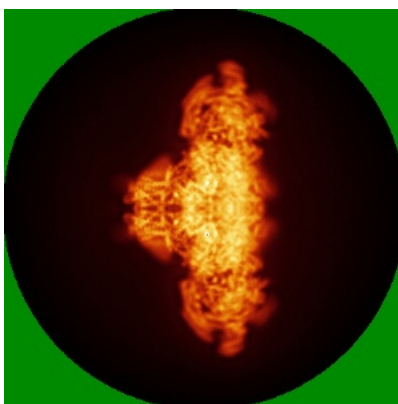


Z

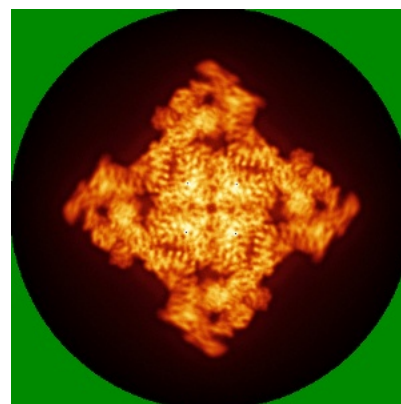
6.4.2 Raw map



X



Y

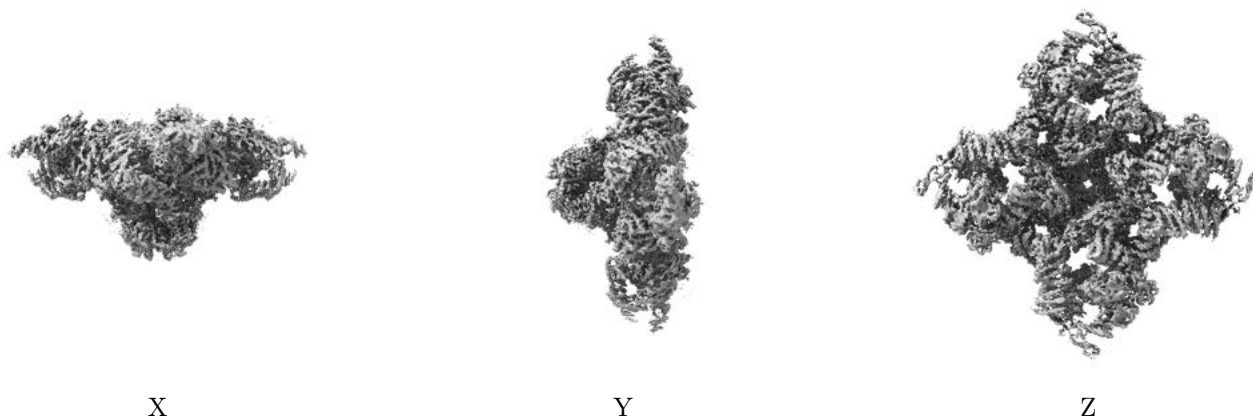


Z

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.

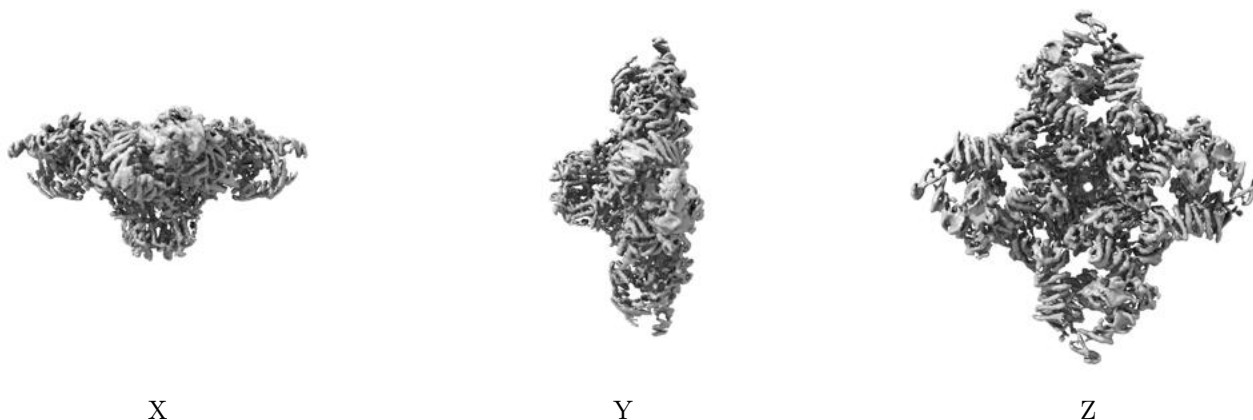
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. 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.

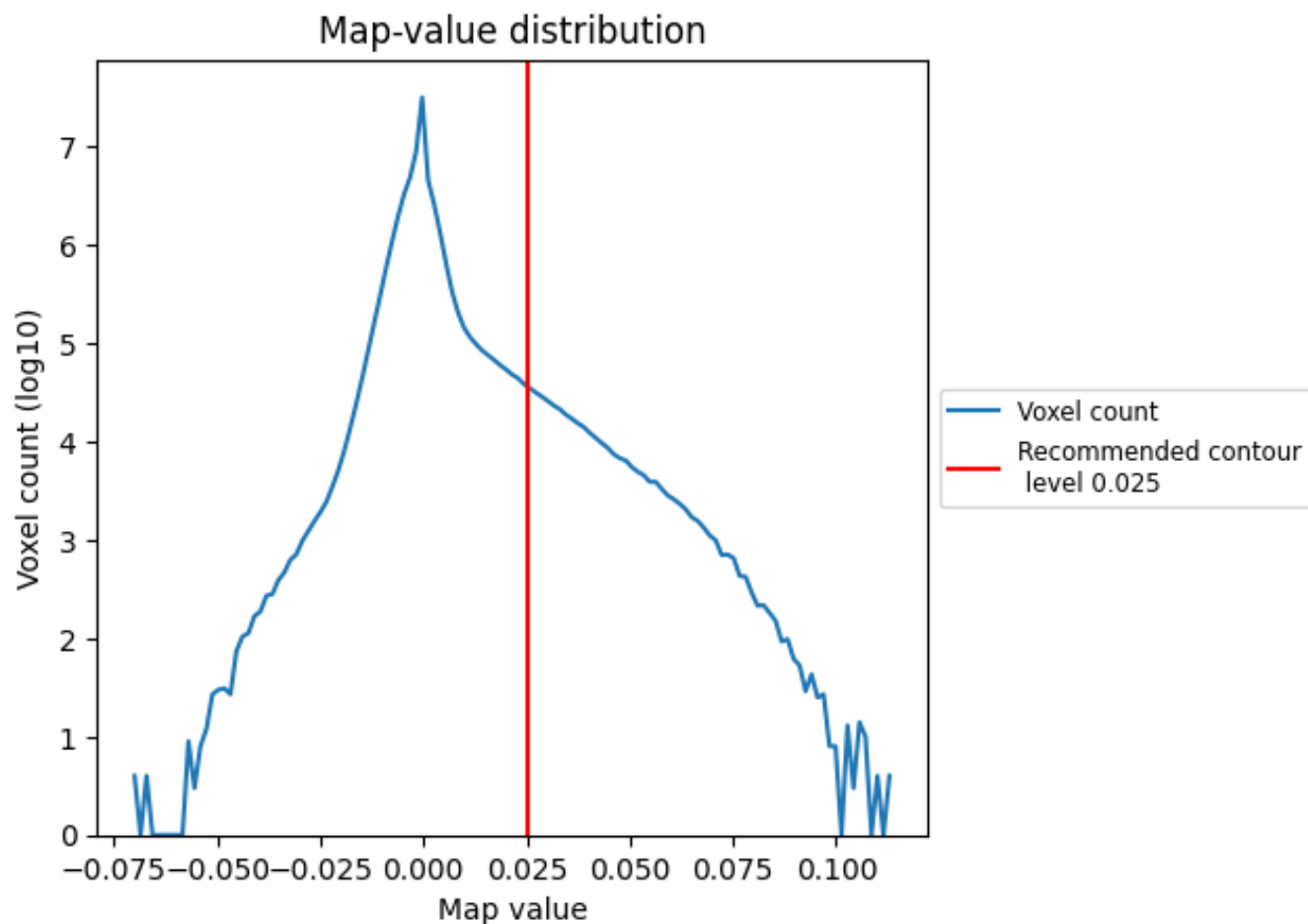
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

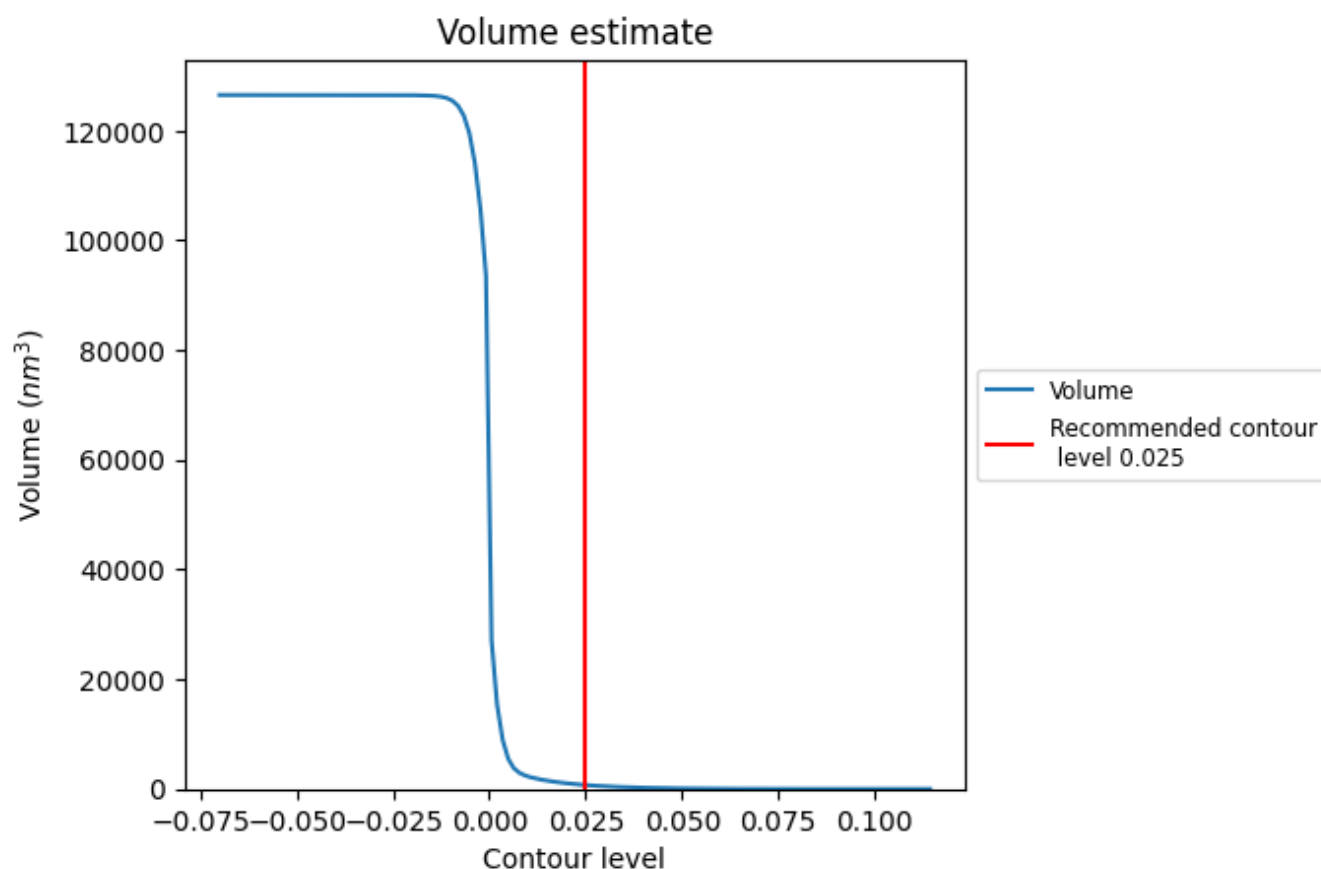
This section contains the results of statistical analysis of the map.

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.

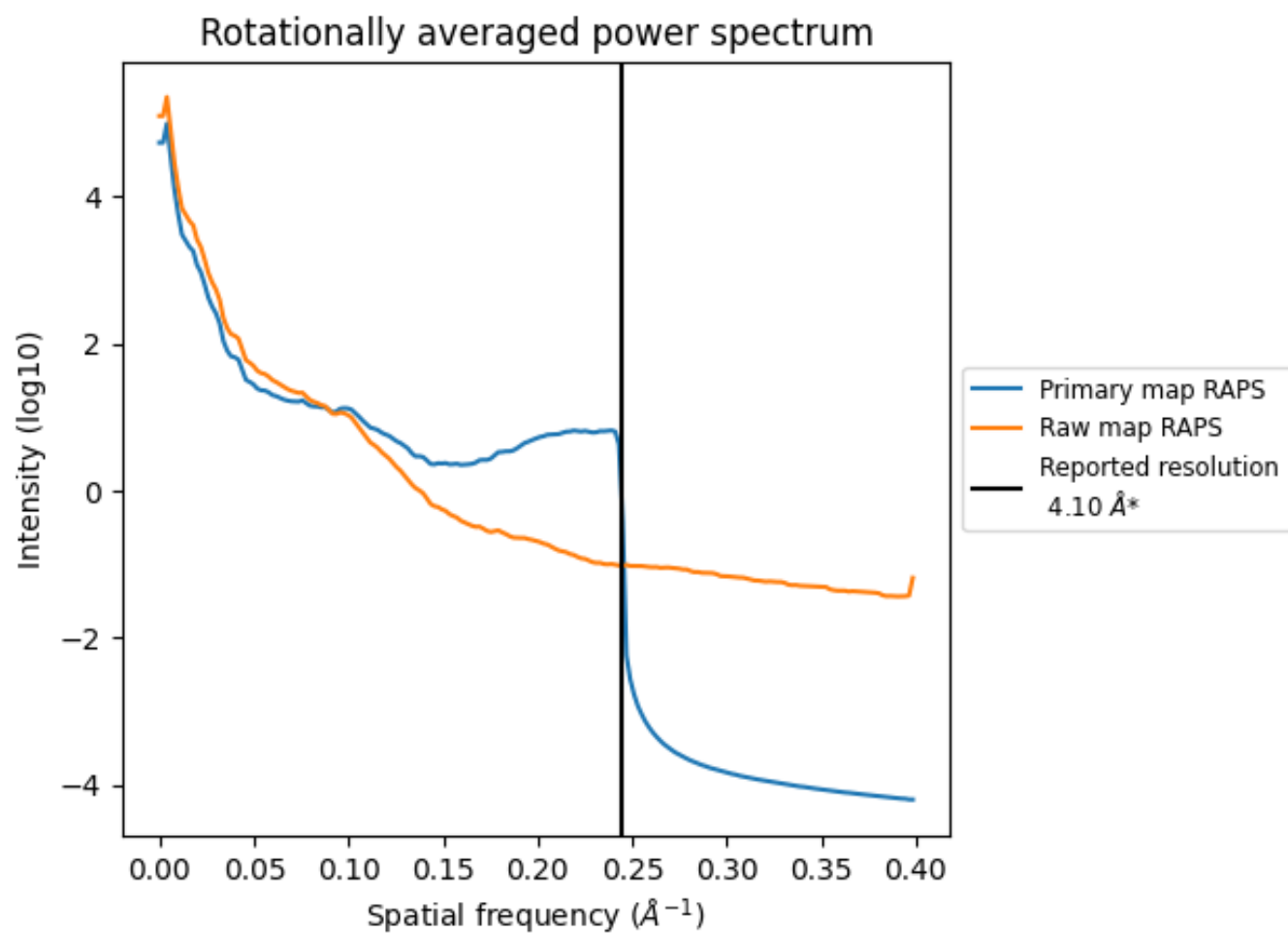
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 713 nm³; this corresponds to an approximate mass of 644 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 ⓘ

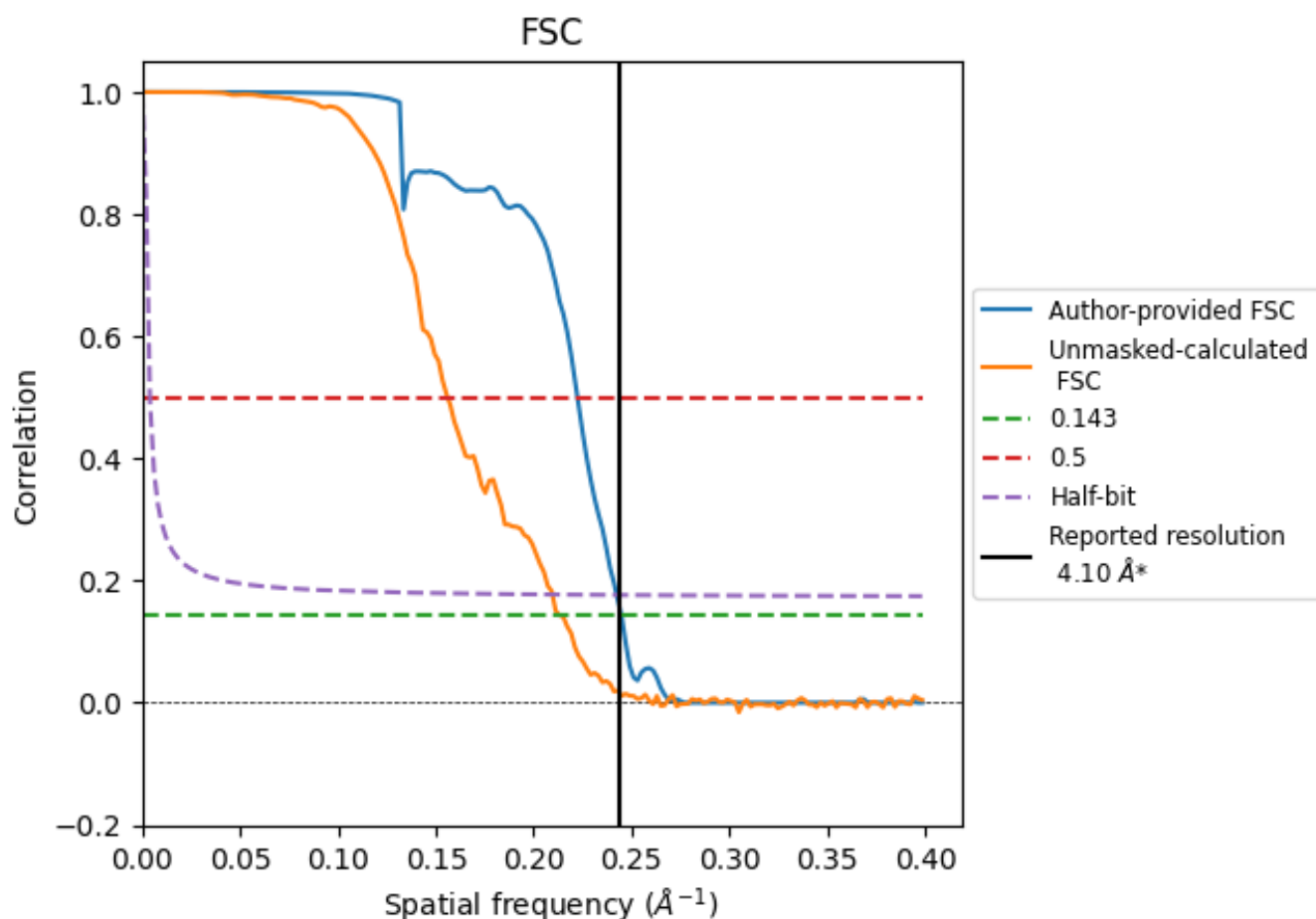


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

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 0.244 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.08	4.50	4.13
Unmasked-calculated*	4.69	6.41	4.77

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.69 differs from the reported value 4.1 by more than 10 %

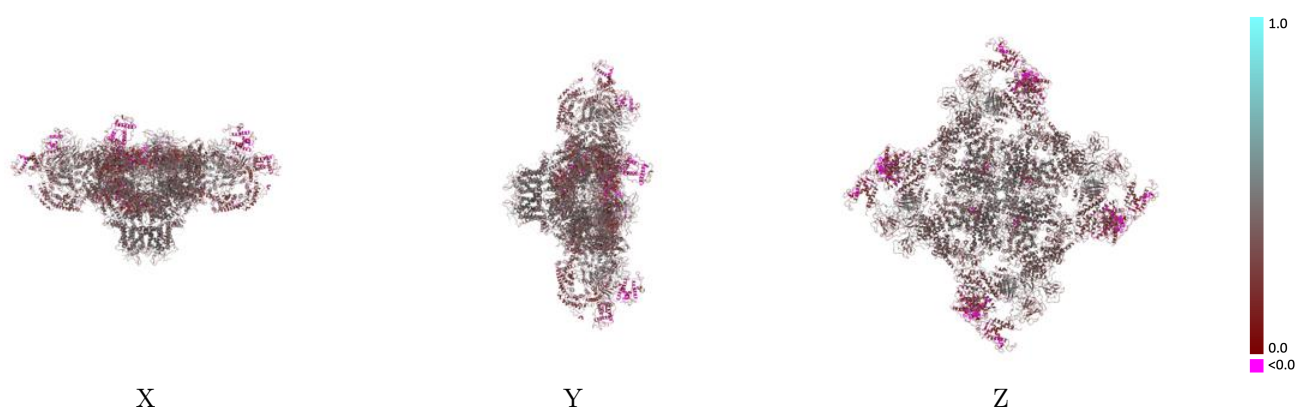
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8382 and PDB model 5TAQ. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

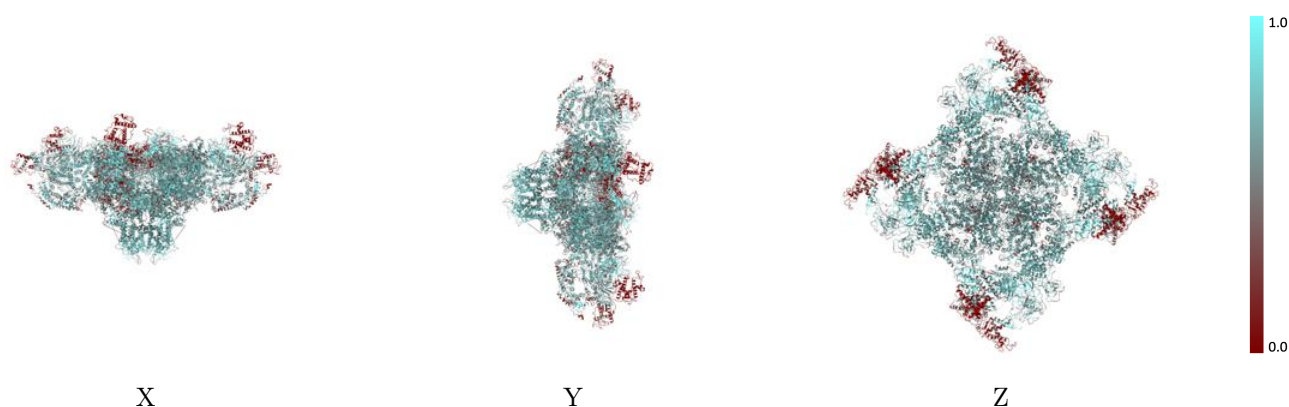
This section was not generated.

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



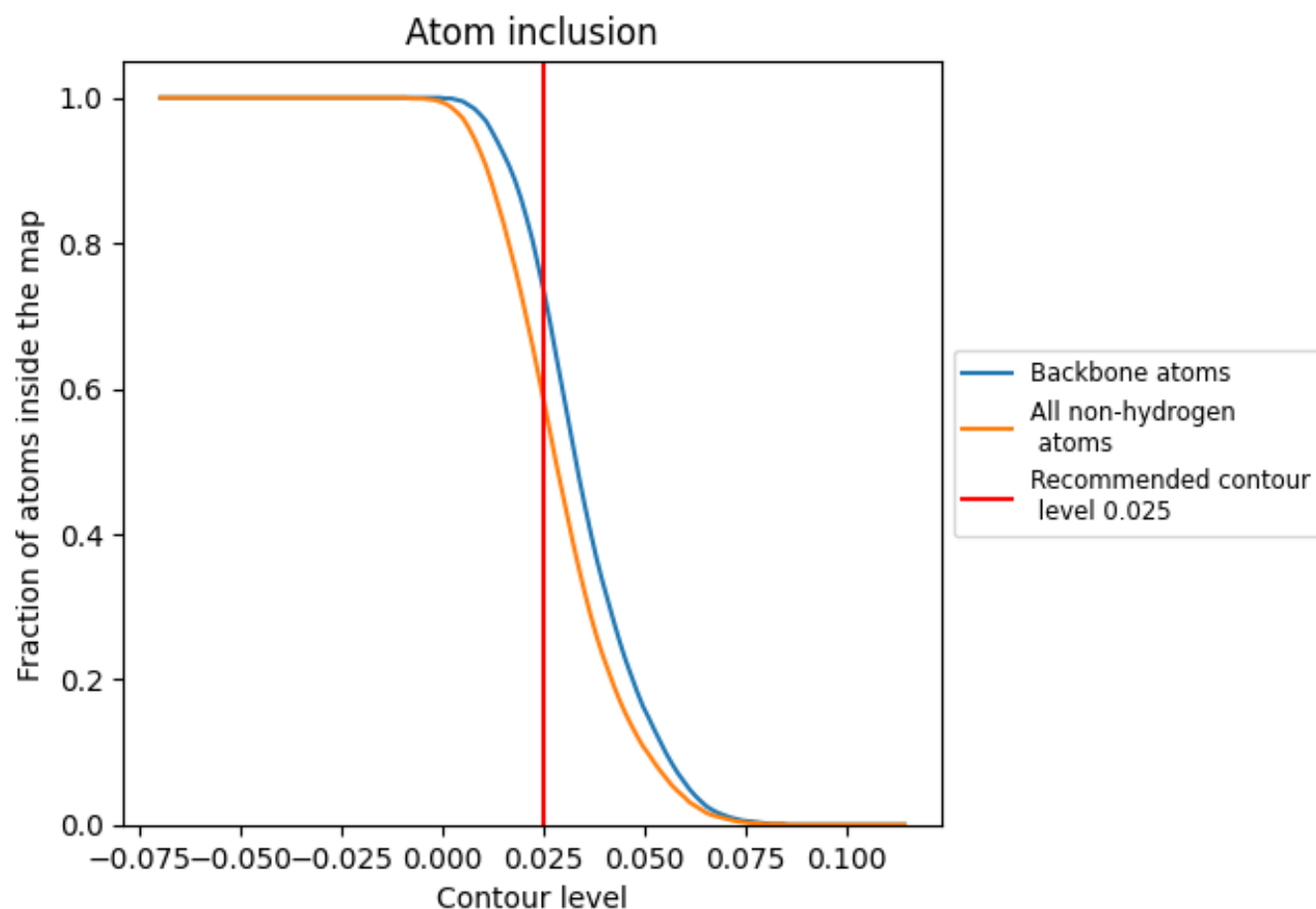
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 58% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5830	0.3350
A	0.5570	0.3500
B	0.5830	0.3340
E	0.5840	0.3340
F	0.5600	0.3560
G	0.5840	0.3350
H	0.5560	0.3530
I	0.5840	0.3350
J	0.5620	0.3490

1.0

0.0

<0.0