



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:26 PM UTC

PDB ID : 5T9M / pdb_00005t9m
EMDB ID : EMD-8372
Title : Structure of rabbit RyR1 (Ca²⁺-only dataset, class 1)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on : 2016-09-09
Resolution : 4.00 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

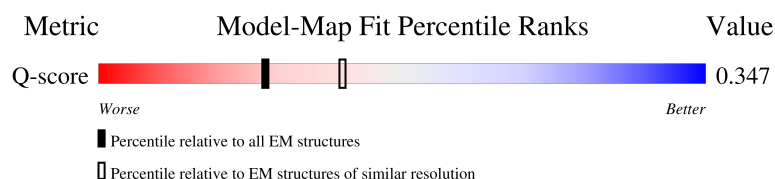
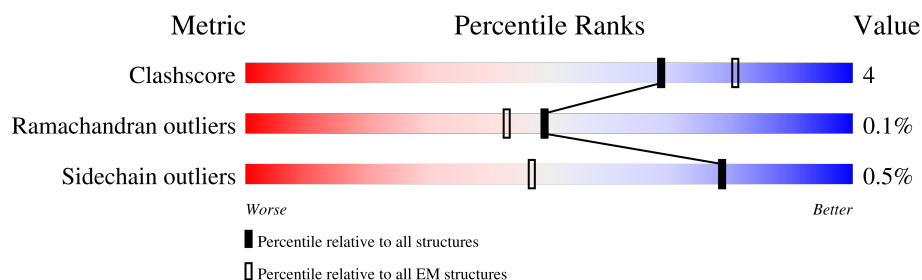
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.00 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	7587 (3.50 - 4.50)

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	13% 88% 11%
1	F	108	14% 87% 12%
1	H	108	14% 87% 12%
1	J	108	13% 87% 12%

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Mol	Chain	Length	Quality of chain
2	B	4676	19% 81% 8% 11%
2	E	4676	19% 81% 8% 11%
2	G	4676	19% 81% 8% 11%
2	I	4676	19% 81% 8% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 120756 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	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	E	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	I	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	G	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		

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

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

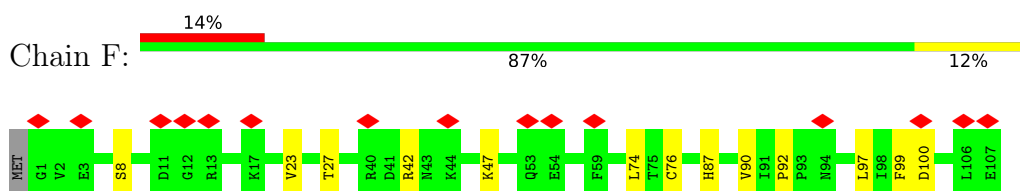
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

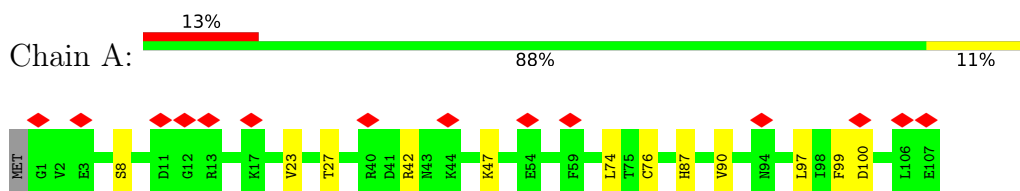
3 Residue-property plots [i](#)

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

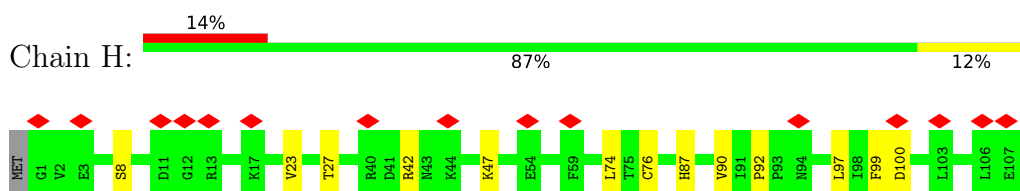
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



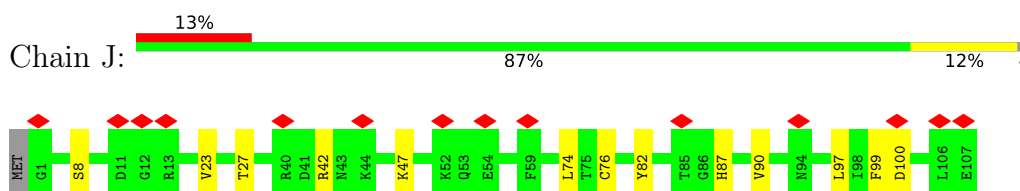
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



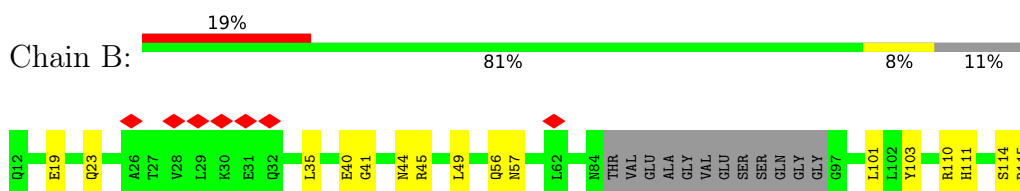
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

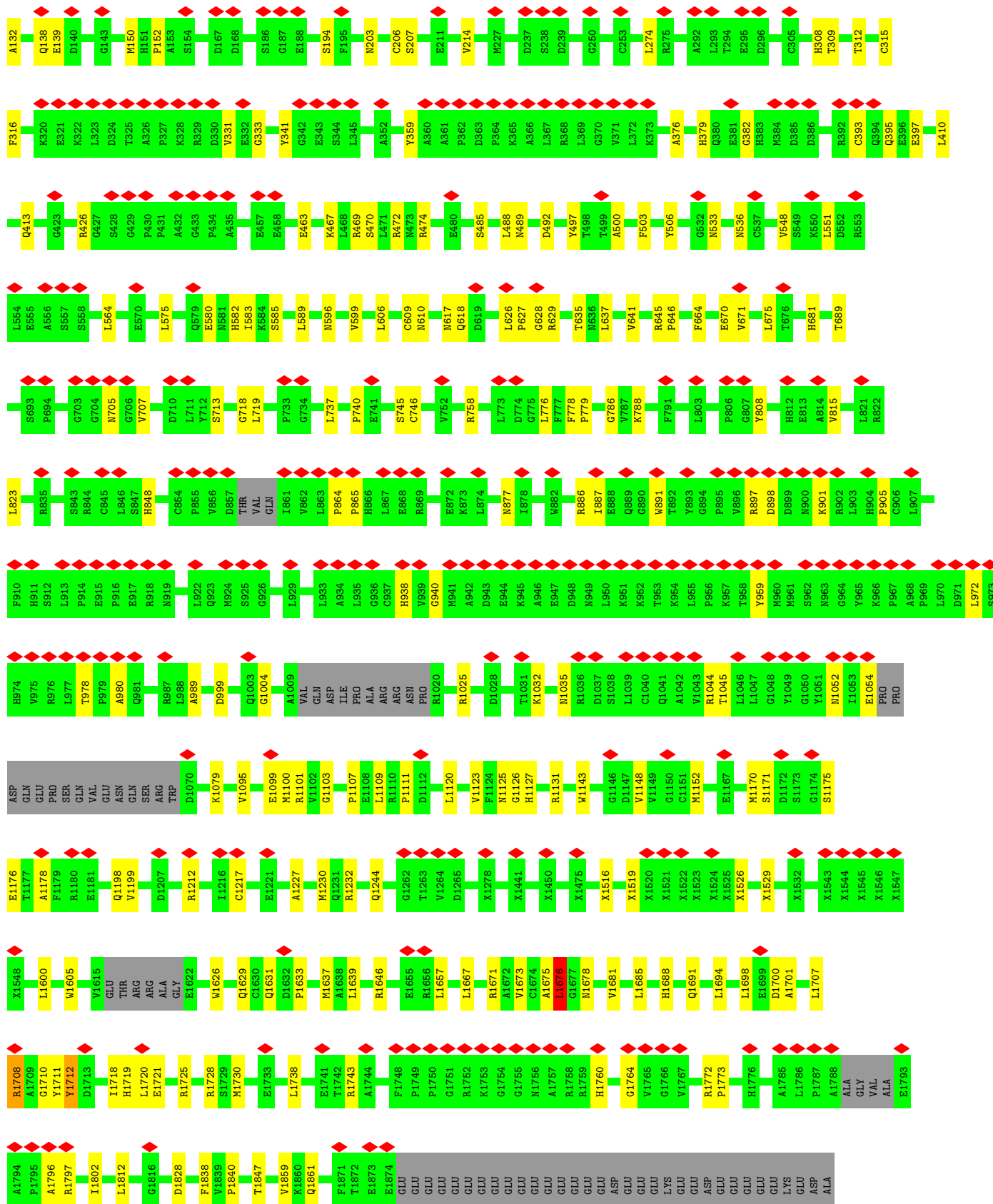


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

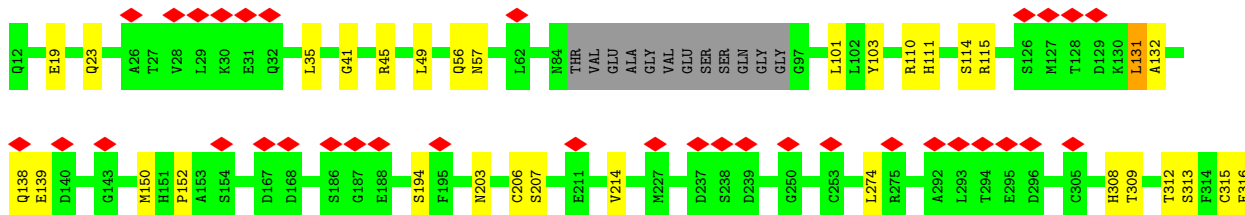


- Molecule 2: Ryanodine receptor 1

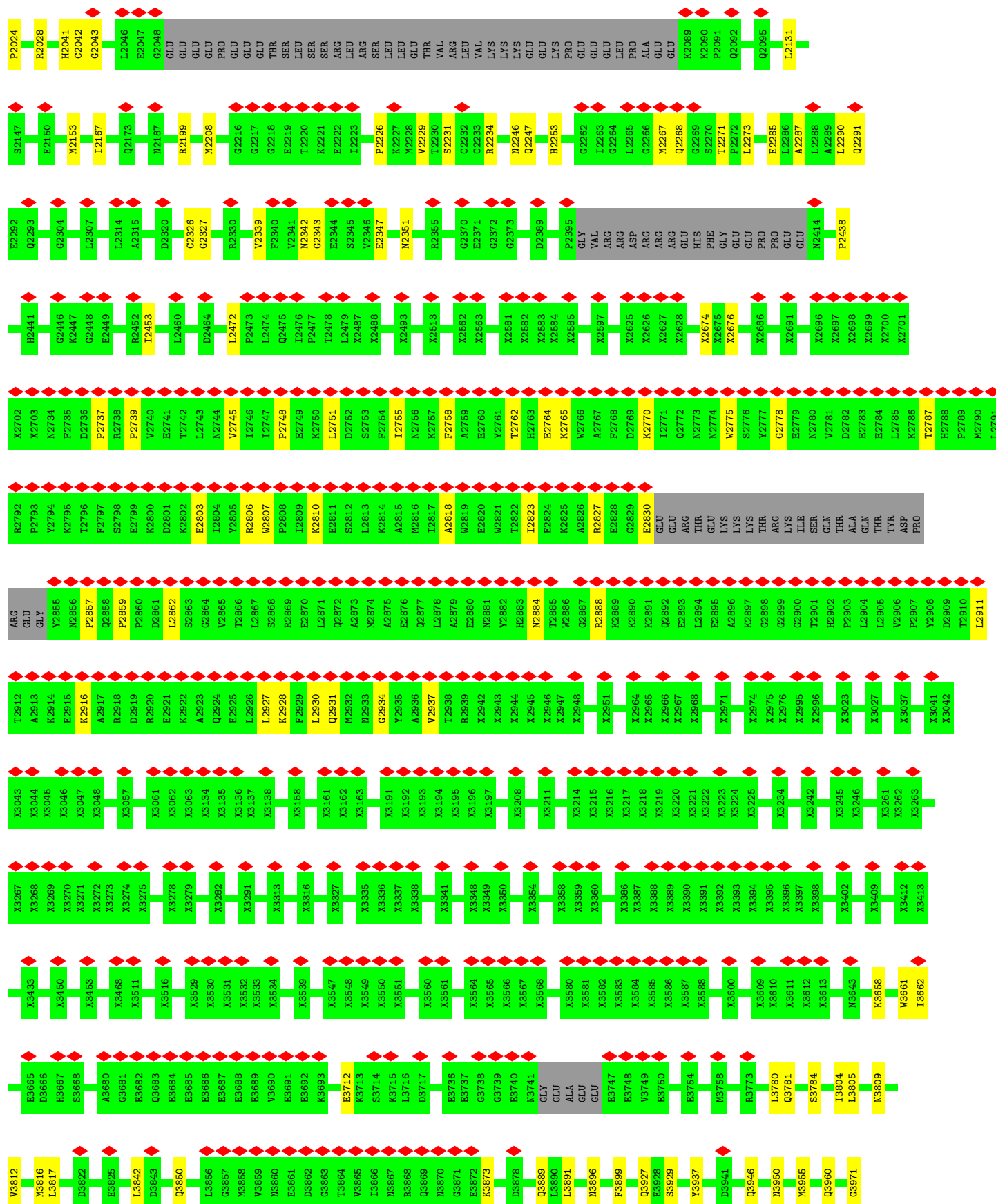


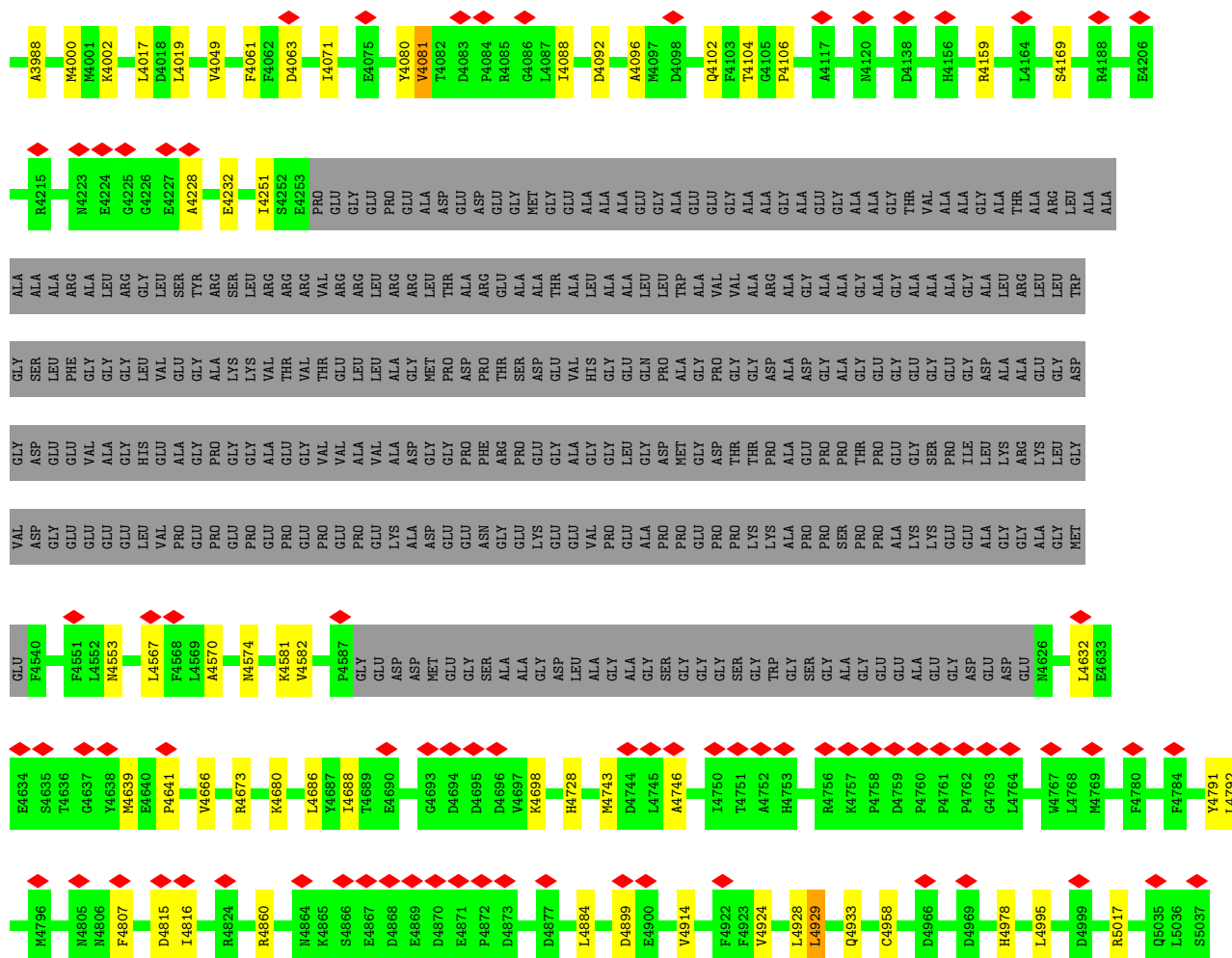




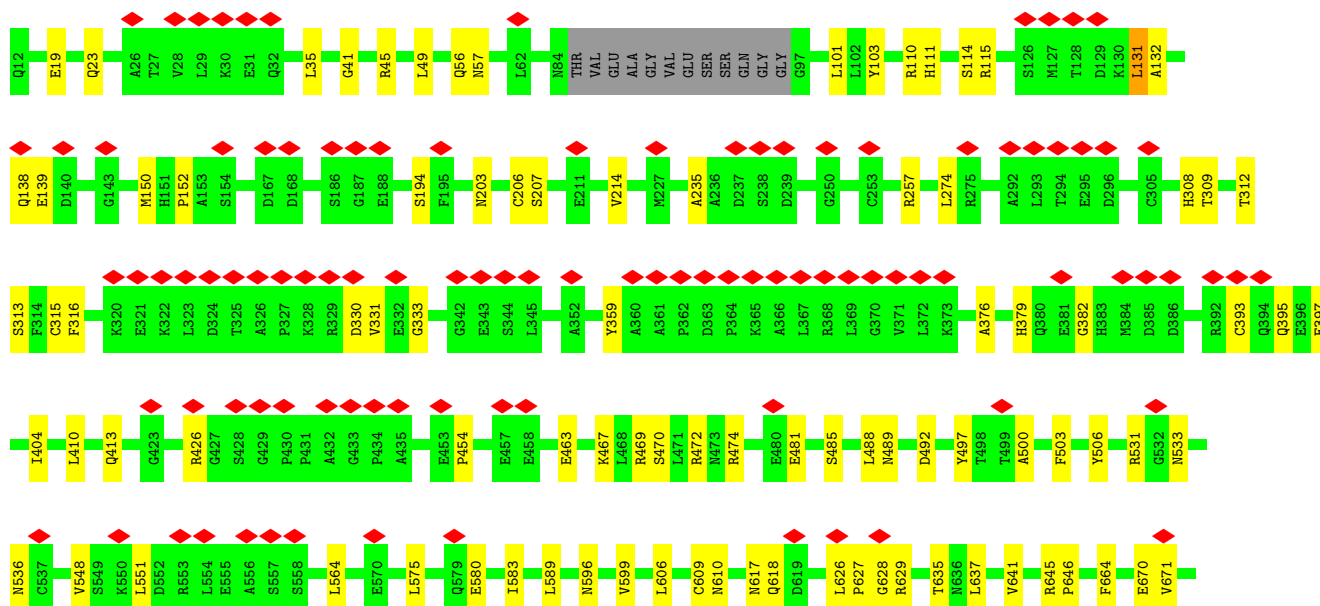
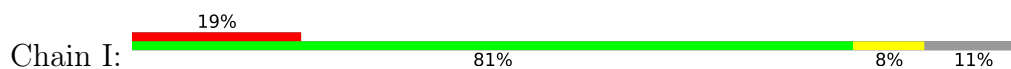








• Molecule 2: Ryanodine receptor 1





ALA	ALA	M4120	S9929	M3758	X3395	X3246	X3027	V2906	ALA	K2786	X2696	PHE
GLY	GLY	D4138	Y3937	R3773	X3396	X3251	X3037	P2907	GLN	T2787	X2697	GLY
ALA	ALA	L4147	D3941	R3773	X3397	X3251	X3037	Y2908	THR	H2788	X2698	GLU
GLY	GLY	L3780	Q3946	L3780	X3398	X3263	X3041	D2909	TVR	P2789	X2699	GLU
ALA	ALA	S4151	Q3946	Q3781	X3398	X3263	X3042	D2910	ASP	M2790	X2700	PRO
ALA	ALA	R4159	N3950	S3784	X3409	X3267	X3043	L2911	PRO	L2791	X2701	GLU
THR	THR	L3804	N3955	S3784	X3412	X3268	X3044	T2912	ARG	L2792	X2702	GLU
VAL	VAL	L3805	N3960	S3784	X3413	X3269	X3045	A2913	GLY	P2793	X2703	
ALA	ALA	L3805	Q3960	S3784	X3413	X3270	X3046	K2914	THR	Y2794	N2734	
GLY	GLY	L3805	Q3960	S3784	X3413	X3271	X3047	E2915	THR	K2795	F2735	
ALA	ALA	L3805	Q3960	S3784	X3413	X3272	X3048	K2916	THR	T2796	D2736	
ALA	ALA	L3805	Q3960	S3784	X3413	X3273	X3048	A2917	THR	P2797	P2737	
THR	THR	L3805	Q3960	S3784	X3413	X3274	X3048	D2918	THR	S2798	R2738	
ALA	ALA	L3805	Q3960	S3784	X3413	X3275	X3048	D2919	THR	E2799	P2739	
ARG	ARG	L3805	Q3960	S3784	X3413	X3276	X3048	R2920	THR	K2800	V2740	
LEU	LEU	L3805	Q3960	S3784	X3413	X3277	X3048	E2921	THR	E2741	T2742	
ALA	ALA	L3805	Q3960	S3784	X3413	X3278	X3048	A2922	THR	D2801	T2743	
ALA	ALA	L3805	Q3960	S3784	X3413	X3279	X3048	K2923	THR	E2802	L2744	
ALA	ALA	L3805	Q3960	S3784	X3413	X3282	X3048	Q2924	THR	K2803	N2745	
ALA	ALA	L3805	Q3960	S3784	X3413	X3290	X3048	E2925	THR	L2804	L2460	
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	D2926	THR	R2805	V2464	
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	L2927	THR	K2806	L2746	
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	K2928	THR	W2807	L2747	
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	L2930	THR	P2808	P2748	
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	Q2931	THR	L2809	L2474	
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	M2932	THR	K2810	Q2475	
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	N2933	THR	E2811	L2476	
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	N2934	THR	S2812	T2478	
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	K2935	THR	L2813	L2479	
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	A2936	THR	F2754	X2487	
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	T2937	THR	L2755	X2488	
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	N2938	THR	N2756		
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	R2939	THR	K2757	X2493	
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	X2942	THR	A2759	X2513	
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	X2943	THR	E2760	X2562	
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	X2944	THR	W2761	X2563	
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	X2945	THR	T2762		
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	X2946	THR	H2763	X2581	
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	X2947	THR	E2764	X2582	
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	X2948	THR	K2765	X2583	
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	X2949	THR	W2766	X2584	
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	X2950	THR	A2826	X2585	
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	X2951	THR	R2827		
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	X2952	THR	E2828	X2597	
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	X2953	THR	D2829	X2597	
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	X2954	THR	E2830		
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	X2955	THR	GLU	X2625	
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	X2956	THR	ARG	X2626	
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	X2957	THR	ARG	X2627	
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	X2958	THR	THR	X2628	
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	X2959	THR	GLU		
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	X2960	THR	LYS	X2686	
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	X2961	THR	LYS		
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	X2962	THR	LYS	X2691	
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	X2963	THR	THR		
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	X2964	THR	ARG	X2776	
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	X2965	THR	ARG	Y2777	
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	X2966	THR	LYS	G2778	
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	X2967	THR	LYS	E2779	
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	X2968	THR	ILE	N2780	
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	X2969	THR	GLN	V2781	
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	X2970	THR	THR	D2782	
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	X2971	THR	THR	E2783	
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	X2972	THR	THR	E2784	
ALA	ALA	L3805	Q3960	S3784	X3413	X3291	X3048	X2973	THR	THR	L2785	









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	0.175	Depositor
Minimum map value	-0.083	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.04	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: ZN, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.20	0/834	0.48	0/1123
1	F	0.20	0/834	0.48	0/1123
1	H	0.19	0/834	0.48	0/1123
1	J	0.20	0/834	0.48	0/1123
2	B	0.23	0/25428	0.52	5/34534 (0.0%)
2	E	0.23	0/25428	0.52	5/34534 (0.0%)
2	G	0.23	0/25428	0.52	5/34534 (0.0%)
2	I	0.23	0/25428	0.52	5/34534 (0.0%)
All	All	0.22	0/105048	0.52	20/142628 (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	1
1	F	0	1
1	H	0	1
1	J	0	1
2	B	0	14
2	E	0	14
2	G	0	14
2	I	0	14
All	All	0	60

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4639	MET	CA-C-N	5.37	134.91	121.80
2	B	4639	MET	C-N-CA	5.37	134.91	121.80
2	I	4639	MET	CA-C-N	5.37	134.89	121.80
2	I	4639	MET	C-N-CA	5.37	134.89	121.80
2	E	4639	MET	CA-C-N	5.35	134.87	121.80
2	E	4639	MET	C-N-CA	5.35	134.87	121.80
2	G	4639	MET	CA-C-N	5.34	134.83	121.80
2	G	4639	MET	C-N-CA	5.34	134.83	121.80
2	G	131	LEU	CA-CB-CG	5.28	134.78	116.30
2	E	131	LEU	CA-CB-CG	5.28	134.76	116.30
2	B	131	LEU	CA-CB-CG	5.27	134.76	116.30
2	I	131	LEU	CA-CB-CG	5.27	134.75	116.30
2	G	1838	PHE	CA-C-N	5.05	131.48	122.13
2	G	1838	PHE	C-N-CA	5.05	131.48	122.13
2	I	1838	PHE	CA-C-N	5.05	131.47	122.13
2	I	1838	PHE	C-N-CA	5.05	131.47	122.13
2	E	1838	PHE	CA-C-N	5.05	131.47	122.13
2	E	1838	PHE	C-N-CA	5.05	131.47	122.13
2	B	1838	PHE	CA-C-N	5.04	131.46	122.13
2	B	1838	PHE	C-N-CA	5.04	131.46	122.13

There are no chirality outliers.

All (60) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1712	TYR	Peptide
2	B	1828	ASP	Peptide
2	B	2291	GLN	Peptide
2	B	2342	ASN	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	4666	VAL	Peptide
2	B	4807	PHE	Peptide
2	B	808	TYR	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1712	TYR	Peptide

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Mol	Chain	Res	Type	Group
2	E	1828	ASP	Peptide
2	E	2291	GLN	Peptide
2	E	2342	ASN	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	4666	VAL	Peptide
2	E	4807	PHE	Peptide
2	E	808	TYR	Peptide
1	F	8	SER	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1712	TYR	Peptide
2	G	1828	ASP	Peptide
2	G	2291	GLN	Peptide
2	G	2342	ASN	Peptide
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	4666	VAL	Peptide
2	G	4807	PHE	Peptide
2	G	808	TYR	Peptide
1	H	8	SER	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1712	TYR	Peptide
2	I	1828	ASP	Peptide
2	I	2291	GLN	Peptide
2	I	2342	ASN	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	4666	VAL	Peptide
2	I	4807	PHE	Peptide
2	I	808	TYR	Peptide
1	J	8	SER	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	6	0
1	F	818	0	824	7	0
1	H	818	0	824	7	0
1	J	818	0	824	7	0
2	B	29369	0	24721	202	0
2	E	29369	0	24721	202	0
2	G	29369	0	24721	207	0
2	I	29369	0	24721	204	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
All	All	120756	0	102180	821	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 4.

All (821) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4958:CYS:SG	2:E:4978:HIS:CD2	2.72	0.83
2:G:4958:CYS:SG	2:G:4978:HIS:CD2	2.72	0.83
2:I:4958:CYS:SG	2:I:4978:HIS:CD2	2.72	0.82
2:B:4958:CYS:SG	2:B:4978:HIS:CD2	2.72	0.82
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.72	0.70
2:E:379:HIS:HD2	2:E:382:GLY:H	1.42	0.68
2:B:379:HIS:HD2	2:B:382:GLY:H	1.42	0.68
2:G:379:HIS:HD2	2:G:382:GLY:H	1.42	0.67
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.77	0.67
2:I:379:HIS:HD2	2:I:382:GLY:H	1.42	0.66
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.77	0.66
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.29	0.65
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.77	0.65
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.29	0.64
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.79	0.64
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.80	0.64
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.79	0.64
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.80	0.64
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.80	0.64
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.79	0.64
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.80	0.63
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.29	0.63
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.79	0.62
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.82	0.62
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.81	0.62
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.29	0.62
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.81	0.61
2:E:331:VAL:HG12	2:E:333:GLY:H	1.65	0.61
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.82	0.60
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.83	0.60
2:G:331:VAL:HG12	2:G:333:GLY:H	1.65	0.60
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.83	0.60
2:B:331:VAL:HG12	2:B:333:GLY:H	1.65	0.60
2:I:331:VAL:HG12	2:I:333:GLY:H	1.65	0.60
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.83	0.59
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.36	0.59
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.85	0.59
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.68	0.59
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.36	0.59
2:E:4924:VAL:HA	2:E:4928:LEU:HB2	1.85	0.59
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.85	0.59
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.36	0.59
2:B:1100:MET:HE2	2:B:1198:GLN:HB3	1.85	0.59
2:B:4924:VAL:HA	2:B:4928:LEU:HB2	1.85	0.59
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.83	0.59
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.68	0.59
2:E:1100:MET:HE2	2:E:1198:GLN:HB3	1.85	0.59
2:G:1100:MET:HE2	2:G:1198:GLN:HB3	1.85	0.59
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.68	0.58
2:I:1100:MET:HE2	2:I:1198:GLN:HB3	1.85	0.58
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.68	0.58
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.85	0.58
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.85	0.58
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.68	0.58
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.36	0.58
2:G:4924:VAL:HA	2:G:4928:LEU:HB2	1.85	0.58
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.37	0.58
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.68	0.58
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.36	0.58
2:G:609:CYS:SG	2:G:610:ASN:N	2.77	0.58
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.36	0.58
2:I:4924:VAL:HA	2:I:4928:LEU:HB2	1.85	0.58
2:B:609:CYS:SG	2:B:610:ASN:N	2.77	0.58
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.87	0.57
2:E:2764:GLU:HG3	2:E:2857:PRO:HB2	1.86	0.57
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.37	0.57
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.87	0.57
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.37	0.57
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.68	0.57
2:B:2764:GLU:HG3	2:B:2857:PRO:HB2	1.86	0.57
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.37	0.57
2:I:609:CYS:SG	2:I:610:ASN:N	2.77	0.57
2:E:609:CYS:SG	2:E:610:ASN:N	2.77	0.57
2:I:4933:GLN:NE2	2:G:4933:GLN:OE1	2.38	0.57
2:G:2287:ALA:HA	2:G:2290:LEU:HD13	1.87	0.57
2:B:2131:LEU:HB3	2:B:3662:ILE:HD13	1.87	0.57
2:I:2131:LEU:HB3	2:I:3662:ILE:HD13	1.87	0.56
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.70	0.56
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.86	0.56
2:I:2287:ALA:HA	2:I:2290:LEU:HD13	1.87	0.56
2:I:2764:GLU:HG3	2:I:2857:PRO:HB2	1.86	0.56
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.37	0.56
2:G:2764:GLU:HG3	2:G:2857:PRO:HB2	1.86	0.56
2:B:4933:GLN:NE2	2:I:4933:GLN:OE1	2.39	0.56
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.87	0.56
2:G:1730:MET:O	2:G:1772:ARG:NH1	2.39	0.56
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.70	0.56
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.88	0.56
2:E:4933:GLN:OE1	2:G:4933:GLN:NE2	2.38	0.56
2:I:618:GLN:OE1	2:I:1678:ASN:ND2	2.39	0.56
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.87	0.56
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.68	0.56
2:B:2287:ALA:HA	2:B:2290:LEU:HD13	1.87	0.56
2:E:4049:VAL:HG21	2:E:4159:ARG:HD2	1.88	0.56
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.87	0.56
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.70	0.56
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.88	0.56
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.88	0.56
2:B:4049:VAL:HG21	2:B:4159:ARG:HD2	1.88	0.56
2:G:2131:LEU:HB3	2:G:3662:ILE:HD13	1.87	0.56
2:G:4049:VAL:HG21	2:G:4159:ARG:HD2	1.88	0.56
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.88	0.55
2:E:2131:LEU:HB3	2:E:3662:ILE:HD13	1.87	0.55
2:G:101:LEU:HB3	2:G:150:MET:HE1	1.89	0.55
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.89	0.55
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.89	0.55
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.89	0.55
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.39	0.55
2:E:618:GLN:OE1	2:E:1678:ASN:ND2	2.39	0.55
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.87	0.55
2:I:4049:VAL:HG21	2:I:4159:ARG:HD2	1.88	0.55
2:E:2287:ALA:HA	2:E:2290:LEU:HD13	1.87	0.55
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.70	0.55
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.40	0.55
2:B:618:GLN:OE1	2:B:1678:ASN:ND2	2.39	0.55
2:E:1730:MET:O	2:E:1772:ARG:NH1	2.39	0.55
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.39	0.55
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.89	0.55
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.89	0.55
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.89	0.55
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.79	0.55
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.38	0.55
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.40	0.55
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.40	0.55
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.89	0.55
2:G:618:GLN:OE1	2:G:1678:ASN:ND2	2.39	0.55
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.87	0.55
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.38	0.55
2:I:670:GLU:HG3	2:I:788:LYS:H	1.72	0.55
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.90	0.54
2:I:1730:MET:O	2:I:1772:ARG:NH1	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.79	0.54
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.89	0.54
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.39	0.54
2:E:111:HIS:HD2	2:E:114:SER:H	1.55	0.54
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.89	0.54
2:G:575:LEU:HD22	2:G:609:CYS:HB3	1.89	0.54
2:E:101:LEU:HB3	2:E:150:MET:HE1	1.89	0.54
2:E:670:GLU:HG3	2:E:788:LYS:H	1.72	0.54
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.90	0.54
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.40	0.54
2:B:101:LEU:HB3	2:B:150:MET:HE1	1.88	0.54
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.90	0.54
2:B:1730:MET:O	2:B:1772:ARG:NH1	2.39	0.54
2:I:575:LEU:HD22	2:I:609:CYS:HB3	1.89	0.54
2:G:111:HIS:HD2	2:G:114:SER:H	1.55	0.54
2:G:1152:MET:HE1	2:G:1217:CYS:HB3	1.90	0.54
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.38	0.54
2:B:500:ALA:H	2:B:503:PHE:HB3	1.73	0.54
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.89	0.54
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.89	0.54
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.90	0.54
2:E:627:PRO:O	2:E:629:ARG:NH1	2.41	0.54
2:E:1152:MET:HE1	2:E:1217:CYS:HB3	1.90	0.54
2:G:23:GLN:OE1	2:G:203:ASN:ND2	2.41	0.54
2:G:500:ALA:H	2:G:503:PHE:HB3	1.73	0.54
2:B:23:GLN:OE1	2:B:203:ASN:ND2	2.41	0.54
2:B:111:HIS:HD2	2:B:114:SER:H	1.55	0.54
2:I:1152:MET:HE1	2:I:1217:CYS:HB3	1.90	0.54
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.90	0.54
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.90	0.54
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.79	0.54
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.90	0.54
2:I:500:ALA:H	2:I:503:PHE:HB3	1.73	0.54
2:G:670:GLU:HG3	2:G:788:LYS:H	1.72	0.54
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.89	0.53
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.81	0.53
2:E:469:ARG:HH21	2:E:3712:GLU:HB3	1.73	0.53
2:E:4581:LYS:HD2	2:E:4632:LEU:HD22	1.90	0.53
2:I:4581:LYS:HD2	2:I:4632:LEU:HD22	1.90	0.53
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.81	0.53
2:I:627:PRO:O	2:I:629:ARG:NH1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:627:PRO:O	2:B:629:ARG:NH1	2.41	0.53
2:B:1152:MET:HE1	2:B:1217:CYS:HB3	1.90	0.53
2:E:500:ALA:H	2:E:503:PHE:HB3	1.73	0.53
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.81	0.53
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.90	0.53
2:B:469:ARG:HH21	2:B:3712:GLU:HB3	1.74	0.53
2:E:23:GLN:OE1	2:E:203:ASN:ND2	2.41	0.53
2:E:575:LEU:HD22	2:E:609:CYS:HB3	1.89	0.53
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.90	0.53
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.81	0.53
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.42	0.53
2:I:101:LEU:HB3	2:I:150:MET:HE1	1.88	0.53
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.90	0.53
2:B:670:GLU:HG3	2:B:788:LYS:H	1.72	0.53
2:I:469:ARG:HH21	2:I:3712:GLU:HB3	1.74	0.53
2:G:627:PRO:O	2:G:629:ARG:NH1	2.41	0.53
2:I:23:GLN:OE1	2:I:203:ASN:ND2	2.41	0.53
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.39	0.53
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.90	0.53
2:B:575:LEU:HD22	2:B:609:CYS:HB3	1.89	0.53
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.42	0.53
2:I:111:HIS:HD2	2:I:114:SER:H	1.55	0.53
2:I:359:TYR:HA	2:I:376:ALA:HA	1.91	0.53
2:G:469:ARG:HH21	2:G:3712:GLU:HB3	1.74	0.53
2:G:132:ALA:HA	2:G:194:SER:HB2	1.91	0.53
2:B:359:TYR:HA	2:B:376:ALA:HA	1.91	0.52
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.92	0.52
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.90	0.52
2:B:4581:LYS:HD2	2:B:4632:LEU:HD22	1.90	0.52
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.92	0.52
2:I:132:ALA:HA	2:I:194:SER:HB2	1.91	0.52
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.92	0.52
2:B:2758:PHE:O	2:B:2762:THR:N	2.42	0.52
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.92	0.52
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.91	0.52
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.43	0.52
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.91	0.52
2:G:359:TYR:HA	2:G:376:ALA:HA	1.91	0.52
2:G:938:HIS:HB2	2:G:1054:GLU:HB2	1.92	0.52
2:G:4581:LYS:HD2	2:G:4632:LEU:HD22	1.91	0.52
2:B:2347:GLU:O	2:B:2351:ASN:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:551:LEU:HD21	2:E:589:LEU:HD13	1.91	0.52
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.91	0.52
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.42	0.52
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.92	0.51
2:B:4791:TYR:OH	2:B:4815:ASP:O	2.28	0.51
2:E:359:TYR:HA	2:E:376:ALA:HA	1.91	0.51
2:B:626:LEU:HG	2:B:628:GLY:H	1.75	0.51
2:E:132:ALA:HA	2:E:194:SER:HB2	1.91	0.51
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.43	0.51
2:I:2347:GLU:O	2:I:2351:ASN:N	2.43	0.51
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.42	0.51
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.43	0.51
2:E:2347:GLU:O	2:E:2351:ASN:N	2.43	0.51
2:I:938:HIS:HB2	2:I:1054:GLU:HB2	1.92	0.51
2:E:626:LEU:HG	2:E:628:GLY:H	1.75	0.51
2:I:551:LEU:HD21	2:I:589:LEU:HD13	1.92	0.51
2:G:626:LEU:HG	2:G:628:GLY:H	1.76	0.51
2:B:45:ARG:HE	2:B:138:GLN:HG3	1.76	0.51
2:E:938:HIS:HB2	2:E:1054:GLU:HB2	1.92	0.51
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.91	0.51
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.92	0.51
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.43	0.51
2:G:2347:GLU:O	2:G:2351:ASN:N	2.43	0.51
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.92	0.51
2:B:132:ALA:HA	2:B:194:SER:HB2	1.91	0.51
2:B:393:CYS:SG	2:B:395:GLN:NE2	2.84	0.51
2:I:4063:ASP:OD1	2:I:4169:SER:OG	2.26	0.51
2:I:4791:TYR:OH	2:I:4815:ASP:O	2.28	0.51
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.79	0.51
2:G:4791:TYR:OH	2:G:4815:ASP:O	2.28	0.51
2:B:4933:GLN:OE1	2:E:4933:GLN:NE2	2.42	0.51
2:E:45:ARG:HE	2:E:138:GLN:HG3	1.76	0.51
2:I:626:LEU:HG	2:I:628:GLY:H	1.76	0.51
2:I:2758:PHE:O	2:I:2762:THR:N	2.42	0.51
2:G:393:CYS:SG	2:G:395:GLN:NE2	2.84	0.51
2:B:551:LEU:HD21	2:B:589:LEU:HD13	1.92	0.51
2:G:551:LEU:HD21	2:G:589:LEU:HD13	1.91	0.51
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.93	0.51
2:B:111:HIS:CD2	2:B:114:SER:H	2.29	0.51
2:B:938:HIS:HB2	2:B:1054:GLU:HB2	1.92	0.51
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:45:ARG:HE	2:I:138:GLN:HG3	1.76	0.51
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.91	0.51
2:I:111:HIS:CD2	2:I:114:SER:H	2.29	0.51
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.44	0.51
2:G:45:ARG:HE	2:G:138:GLN:HG3	1.76	0.51
2:E:4791:TYR:OH	2:E:4815:ASP:O	2.28	0.50
2:I:393:CYS:SG	2:I:395:GLN:NE2	2.84	0.50
2:I:395:GLN:NE2	2:I:397:GLU:OE1	2.43	0.50
2:G:606:LEU:O	2:G:617:ASN:ND2	2.45	0.50
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.92	0.50
2:I:395:GLN:HG3	2:I:397:GLU:H	1.77	0.50
2:I:606:LEU:O	2:I:617:ASN:ND2	2.45	0.50
2:G:2758:PHE:O	2:G:2762:THR:N	2.42	0.50
2:G:2911:LEU:HB2	2:G:2916:LYS:HE3	1.93	0.50
1:J:76:CYS:HB2	1:J:97:LEU:HB2	1.94	0.50
2:B:606:LEU:O	2:B:617:ASN:ND2	2.44	0.50
2:E:393:CYS:SG	2:E:395:GLN:NE2	2.84	0.50
2:E:606:LEU:O	2:E:617:ASN:ND2	2.44	0.50
2:E:2911:LEU:HB2	2:E:2916:LYS:HE3	1.93	0.50
2:E:4914:VAL:HG21	2:G:4884:LEU:HD11	1.93	0.50
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.93	0.50
2:I:776:LEU:HG	2:I:848:HIS:HA	1.94	0.50
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.92	0.50
2:G:111:HIS:CD2	2:G:114:SER:H	2.29	0.50
2:G:1025:ARG:O	2:G:1032:LYS:NZ	2.40	0.50
2:B:395:GLN:HG3	2:B:397:GLU:H	1.77	0.50
2:B:4567:LEU:HD12	2:B:4816:ILE:HD12	1.94	0.50
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.92	0.50
1:H:76:CYS:HB2	1:H:97:LEU:HB2	1.94	0.50
2:B:4884:LEU:HD11	2:I:4914:VAL:HG21	1.92	0.50
2:I:2823:ILE:HG12	2:I:2937:VAL:HG22	1.94	0.50
2:G:776:LEU:HG	2:G:848:HIS:HA	1.94	0.50
2:E:2823:ILE:HG12	2:E:2937:VAL:HG22	1.94	0.50
2:I:4884:LEU:HD11	2:G:4914:VAL:HG21	1.93	0.50
2:G:395:GLN:NE2	2:G:397:GLU:OE1	2.42	0.50
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.77	0.50
2:E:111:HIS:CD2	2:E:114:SER:H	2.29	0.50
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.77	0.50
2:G:4232:GLU:OE2	2:G:5017:ARG:NH1	2.44	0.50
2:E:395:GLN:HG3	2:E:397:GLU:H	1.77	0.50
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.45	0.50
2:I:580:GLU:HG2	2:I:583:ILE:HD11	1.94	0.50
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.45	0.50
2:I:4570:ALA:O	2:I:4574:ASN:ND2	2.45	0.50
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	1.94	0.50
2:G:395:GLN:HG3	2:G:397:GLU:H	1.77	0.50
2:G:2823:ILE:HG12	2:G:2937:VAL:HG22	1.94	0.50
1:A:76:CYS:HB2	1:A:97:LEU:HB2	1.94	0.49
2:B:35:LEU:HD13	2:B:49:LEU:HD13	1.94	0.49
2:B:4232:GLU:OE2	2:B:5017:ARG:NH1	2.44	0.49
2:E:470:SER:O	2:E:474:ARG:NE	2.38	0.49
2:E:4570:ALA:O	2:E:4574:ASN:ND2	2.45	0.49
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.77	0.49
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.77	0.49
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.45	0.49
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.77	0.49
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	1.93	0.49
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.94	0.49
2:I:4147:LEU:O	2:I:4151:SER:OG	2.29	0.49
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.93	0.49
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.45	0.49
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.94	0.49
2:B:776:LEU:HG	2:B:848:HIS:HA	1.93	0.49
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.94	0.49
2:E:580:GLU:HG2	2:E:583:ILE:HD11	1.94	0.49
2:I:4567:LEU:HD12	2:I:4816:ILE:HD12	1.94	0.49
1:F:76:CYS:HB2	1:F:97:LEU:HB2	1.94	0.49
2:B:2823:ILE:HG12	2:B:2937:VAL:HG22	1.94	0.49
2:G:4570:ALA:O	2:G:4574:ASN:ND2	2.45	0.49
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.77	0.49
2:I:1025:ARG:O	2:I:1032:LYS:NZ	2.40	0.49
2:B:4570:ALA:O	2:B:4574:ASN:ND2	2.45	0.49
2:E:776:LEU:HG	2:E:848:HIS:HA	1.93	0.49
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.95	0.49
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.44	0.49
2:E:2758:PHE:O	2:E:2762:THR:N	2.42	0.49
2:G:580:GLU:HG2	2:G:583:ILE:HD11	1.94	0.49
2:B:463:GLU:OE2	2:B:467:LYS:NZ	2.46	0.49
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	1.94	0.49
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	1.95	0.49
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.44	0.49
2:E:35:LEU:HD13	2:E:49:LEU:HD13	1.94	0.48
2:E:56:GLN:O	2:E:309:THR:OG1	2.26	0.48
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.95	0.48
2:I:463:GLU:OE2	2:I:467:LYS:NZ	2.46	0.48
2:I:2911:LEU:HB2	2:I:2916:LYS:HE3	1.93	0.48
2:G:463:GLU:OE2	2:G:467:LYS:NZ	2.46	0.48
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.95	0.48
2:B:2911:LEU:HB2	2:B:2916:LYS:HE3	1.93	0.48
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	1.95	0.48
2:E:877:ASN:HD22	2:E:1045:THR:HG23	1.78	0.48
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.94	0.48
2:I:35:LEU:HD13	2:I:49:LEU:HD13	1.94	0.48
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.44	0.48
2:B:2862:LEU:HB3	2:B:2928:LYS:HB3	1.95	0.48
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	1.96	0.48
2:I:2199:ARG:NH2	2:I:2246:ASN:OD1	2.47	0.48
2:G:2765:LYS:HA	2:G:2859:PRO:HG3	1.96	0.48
2:G:4567:LEU:HD12	2:G:4816:ILE:HD12	1.94	0.48
2:B:315:CYS:SG	2:B:316:PHE:N	2.87	0.48
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.96	0.48
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.95	0.48
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.94	0.48
2:B:4914:VAL:HG21	2:E:4884:LEU:HD11	1.95	0.48
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	1.94	0.48
2:G:35:LEU:HD13	2:G:49:LEU:HD13	1.94	0.48
2:G:315:CYS:SG	2:G:316:PHE:N	2.87	0.48
2:G:2199:ARG:NH2	2:G:2246:ASN:OD1	2.47	0.48
2:B:1025:ARG:O	2:B:1032:LYS:NZ	2.40	0.48
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	1.95	0.48
2:E:315:CYS:SG	2:E:316:PHE:N	2.87	0.48
2:E:463:GLU:OE2	2:E:467:LYS:NZ	2.46	0.48
2:G:877:ASN:HD22	2:G:1045:THR:HG23	1.78	0.48
2:B:395:GLN:NE2	2:B:397:GLU:OE1	2.43	0.48
2:I:877:ASN:HD22	2:I:1045:THR:HG23	1.78	0.48
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.95	0.48
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	1.96	0.48
2:E:2765:LYS:HA	2:E:2859:PRO:HG3	1.96	0.48
2:E:2778:GLY:HA3	2:E:2787:THR:HB	1.96	0.48
2:E:2862:LEU:HB3	2:E:2928:LYS:HB3	1.95	0.48
2:E:4567:LEU:HD12	2:E:4816:ILE:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:315:CYS:SG	2:I:316:PHE:N	2.87	0.48
2:I:2231:SER:HA	2:I:2234:ARG:HG2	1.95	0.48
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.96	0.48
2:B:580:GLU:HG2	2:B:583:ILE:HD11	1.94	0.48
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	1.95	0.48
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.77	0.48
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.47	0.48
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.47	0.48
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.49	0.48
2:G:2862:LEU:HB3	2:G:2928:LYS:HB3	1.95	0.48
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.95	0.47
2:B:877:ASN:HD22	2:B:1045:THR:HG23	1.78	0.47
2:B:2199:ARG:NH2	2:B:2246:ASN:OD1	2.47	0.47
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.47	0.47
2:I:1675:ALA:HB1	2:I:1676:LEU:HD13	1.96	0.47
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.79	0.47
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.49	0.47
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.48	0.47
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.49	0.47
2:E:395:GLN:NE2	2:E:397:GLU:OE1	2.42	0.47
2:G:470:SER:O	2:G:474:ARG:NE	2.38	0.47
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.47	0.47
2:G:2778:GLY:HA3	2:G:2787:THR:HB	1.96	0.47
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.47	0.47
2:B:1675:ALA:HB1	2:B:1676:LEU:HD13	1.96	0.47
2:B:2231:SER:HA	2:B:2234:ARG:HG2	1.95	0.47
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.96	0.47
2:I:3809:ASN:HB3	2:I:3812:VAL:HG22	1.97	0.47
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	1.96	0.47
1:J:27:THR:HB	1:J:100:ASP:HB3	1.97	0.47
2:B:2778:GLY:HA3	2:B:2787:THR:HB	1.96	0.47
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.96	0.47
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.96	0.47
2:I:2765:LYS:HA	2:I:2859:PRO:HG3	1.96	0.47
2:I:2862:LEU:HB3	2:I:2928:LYS:HB3	1.95	0.47
1:H:27:THR:HB	1:H:100:ASP:HB3	1.96	0.47
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.97	0.47
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.47	0.47
2:B:2765:LYS:HA	2:B:2859:PRO:HG3	1.96	0.47
2:E:2199:ARG:NH2	2:E:2246:ASN:OD1	2.47	0.47
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.97	0.47
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	1.96	0.47
2:G:999:ASP:O	2:G:1004:GLY:N	2.48	0.47
2:G:1760:HIS:HE1	2:G:2041:HIS:HA	1.79	0.47
2:G:2231:SER:HA	2:G:2234:ARG:HG2	1.95	0.47
2:G:3809:ASN:HB3	2:G:3812:VAL:HG22	1.97	0.47
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.48	0.47
1:F:27:THR:HB	1:F:100:ASP:HB3	1.96	0.47
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.79	0.47
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.79	0.47
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.47	0.47
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.48	0.47
2:G:56:GLN:O	2:G:309:THR:OG1	2.26	0.47
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.79	0.47
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.96	0.47
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.97	0.47
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.47	0.47
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.97	0.47
2:E:1025:ARG:O	2:E:1032:LYS:NZ	2.40	0.47
2:I:2778:GLY:HA3	2:I:2787:THR:HB	1.96	0.47
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.80	0.47
2:B:1973:GLN:O	2:B:1977:TYR:N	2.48	0.46
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.80	0.46
2:B:4063:ASP:OD1	2:B:4169:SER:OG	2.26	0.46
2:E:1099:GLU:OE2	2:E:1127:HIS:ND1	2.40	0.46
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.49	0.46
2:E:2231:SER:HA	2:E:2234:ARG:HG2	1.95	0.46
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.80	0.46
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.49	0.46
2:E:1760:HIS:HE1	2:E:2041:HIS:HA	1.79	0.46
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.47	0.46
2:B:470:SER:O	2:B:474:ARG:NE	2.38	0.46
2:B:1244:GLN:OE1	2:B:1646:ARG:NH1	2.49	0.46
2:B:3809:ASN:HB3	2:B:3812:VAL:HG22	1.97	0.46
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.96	0.46
2:I:999:ASP:O	2:I:1004:GLY:N	2.48	0.46
2:I:1244:GLN:OE1	2:I:1646:ARG:NH1	2.49	0.46
2:G:4071:ILE:HD11	2:G:4102:GLN:HE21	1.81	0.46
2:B:898:ASP:HB3	2:B:901:LYS:HB2	1.97	0.46
2:E:1973:GLN:O	2:E:1977:TYR:N	2.48	0.46
2:E:3809:ASN:HB3	2:E:3812:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3850:GLN:HB3	2:E:3873:LYS:HD3	1.98	0.46
2:G:1244:GLN:OE1	2:G:1646:ARG:NH1	2.49	0.46
2:G:1675:ALA:HB1	2:G:1676:LEU:HD13	1.96	0.46
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.49	0.46
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.49	0.46
2:B:1760:HIS:HE1	2:B:2041:HIS:HA	1.79	0.46
2:B:3850:GLN:HB3	2:B:3873:LYS:HD3	1.97	0.46
2:E:1675:ALA:HB1	2:E:1676:LEU:HD13	1.96	0.46
2:I:898:ASP:HB3	2:I:901:LYS:HB2	1.97	0.46
2:I:4071:ILE:HD11	2:I:4102:GLN:HE21	1.81	0.46
2:B:999:ASP:O	2:B:1004:GLY:N	2.48	0.46
2:E:999:ASP:O	2:E:1004:GLY:N	2.48	0.46
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.42	0.46
2:G:1973:GLN:O	2:G:1977:TYR:N	2.48	0.46
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.41	0.46
2:G:3850:GLN:HB3	2:G:3873:LYS:HD3	1.97	0.46
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.49	0.46
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.98	0.46
2:I:4232:GLU:OE2	2:I:5017:ARG:NH1	2.44	0.46
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.98	0.46
2:G:645:ARG:HH11	2:G:778:PHE:HE1	1.63	0.46
1:A:27:THR:HB	1:A:100:ASP:HB3	1.96	0.46
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.97	0.46
2:I:645:ARG:HH11	2:I:778:PHE:HE1	1.63	0.46
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.49	0.46
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.49	0.46
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.97	0.46
2:E:214:VAL:HG12	2:E:274:LEU:HD12	1.98	0.46
2:E:4232:GLU:OE2	2:E:5017:ARG:NH1	2.44	0.46
2:I:1760:HIS:HE1	2:I:2041:HIS:HA	1.79	0.46
2:G:823:LEU:HD23	2:G:1626:TRP:HB3	1.98	0.46
2:B:645:ARG:HH11	2:B:778:PHE:HE1	1.63	0.46
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.49	0.46
2:E:1244:GLN:OE1	2:E:1646:ARG:NH1	2.49	0.46
2:B:214:VAL:HG12	2:B:274:LEU:HD12	1.98	0.45
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.80	0.45
2:I:3891:LEU:HB3	2:I:3899:PHE:HE2	1.81	0.45
2:G:898:ASP:HB3	2:G:901:LYS:HB2	1.97	0.45
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.49	0.45
2:E:788:LYS:HG2	2:E:1629:GLN:HA	1.98	0.45
2:E:1708:ARG:HG2	2:E:1711:TYR:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1708:ARG:HG2	2:I:1711:TYR:CE2	2.51	0.45
2:I:3850:GLN:HB3	2:I:3873:LYS:HD3	1.97	0.45
2:E:3804:ILE:O	2:E:3809:ASN:ND2	2.50	0.45
2:I:823:LEU:HD23	2:I:1626:TRP:HB3	1.98	0.45
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.52	0.45
2:E:645:ARG:HH11	2:E:778:PHE:HE1	1.63	0.45
2:I:470:SER:O	2:I:474:ARG:NE	2.38	0.45
2:I:3804:ILE:O	2:I:3809:ASN:ND2	2.50	0.45
2:G:788:LYS:HG2	2:G:1629:GLN:HA	1.98	0.45
2:B:823:LEU:HD23	2:B:1626:TRP:HB3	1.98	0.45
2:E:898:ASP:HB3	2:E:901:LYS:HB2	1.97	0.45
2:E:4071:ILE:HD11	2:E:4102:GLN:HE21	1.81	0.45
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.41	0.45
2:I:3927:GLN:NE2	2:I:3988:ALA:O	2.47	0.45
2:G:1099:GLU:OE2	2:G:1127:HIS:ND1	2.40	0.45
2:G:2267:MET:HE3	2:G:2268:GLN:HG2	1.99	0.45
2:G:3804:ILE:O	2:G:3809:ASN:ND2	2.50	0.45
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.82	0.45
2:I:1170:MET:HE1	2:I:1176:GLU:HG3	1.99	0.45
2:I:1973:GLN:O	2:I:1977:TYR:N	2.48	0.45
2:G:1773:PRO:HA	2:G:2153:MET:HE1	1.99	0.45
2:G:3891:LEU:HB3	2:G:3899:PHE:HE2	1.82	0.45
2:B:56:GLN:O	2:B:309:THR:OG1	2.26	0.45
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.99	0.45
2:B:3891:LEU:HB3	2:B:3899:PHE:HE2	1.81	0.45
2:E:823:LEU:HD23	2:E:1626:TRP:HB3	1.98	0.45
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.99	0.45
2:B:533:ASN:ND2	2:B:536:ASN:OD1	2.42	0.45
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.52	0.45
2:E:1170:MET:HE1	2:E:1176:GLU:HG3	1.99	0.45
2:E:1773:PRO:HA	2:E:2153:MET:HE1	1.99	0.45
2:I:596:ASN:HB3	2:I:599:VAL:HG22	1.99	0.45
2:I:4080:TYR:CZ	2:I:4096:ALA:HB3	2.52	0.45
2:G:214:VAL:HG12	2:G:274:LEU:HD12	1.98	0.45
1:F:92:PRO:HD3	2:E:627:PRO:HB2	1.99	0.45
2:B:485:SER:HA	2:B:488:LEU:HB2	1.98	0.45
2:B:1708:ARG:HG2	2:B:1711:TYR:CE2	2.52	0.45
2:B:2342:ASN:OD1	2:B:2342:ASN:N	2.44	0.45
2:B:3804:ILE:O	2:B:3809:ASN:ND2	2.50	0.45
2:B:4080:TYR:CZ	2:B:4096:ALA:HB3	2.52	0.45
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2267:MET:HE3	2:E:2268:GLN:HG2	1.99	0.45
2:G:1170:MET:HE1	2:G:1176:GLU:HG3	1.99	0.45
2:E:309:THR:O	2:E:313:SER:OG	2.29	0.45
2:I:1099:GLU:OE2	2:I:1127:HIS:ND1	2.40	0.45
2:I:2247:GLN:NE2	2:I:2285:GLU:OE2	2.50	0.45
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.99	0.45
1:J:82:TYR:OH	2:I:1784:ALA:O	2.36	0.44
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	2.00	0.44
2:E:4080:TYR:CZ	2:E:4096:ALA:HB3	2.52	0.44
2:I:214:VAL:HG12	2:I:274:LEU:HD12	1.98	0.44
2:E:1148:VAL:HG21	2:E:1212:ARG:HG2	2.00	0.44
2:G:1708:ARG:HG2	2:G:1711:TYR:CE2	2.52	0.44
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.52	0.44
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.99	0.44
2:B:788:LYS:HG2	2:B:1629:GLN:HA	1.98	0.44
2:B:1773:PRO:HA	2:B:2153:MET:HE1	1.99	0.44
2:I:788:LYS:HG2	2:I:1629:GLN:HA	1.98	0.44
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.82	0.44
2:G:1131:ARG:HH12	2:G:1178:ALA:HB3	1.83	0.44
2:B:596:ASN:HB3	2:B:599:VAL:HG22	1.99	0.44
2:B:1148:VAL:HG21	2:B:1212:ARG:HG2	2.00	0.44
2:B:2247:GLN:NE2	2:B:2285:GLU:OE2	2.50	0.44
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.52	0.44
2:I:786:GLY:HA2	2:I:1631:GLN:HA	2.00	0.44
2:I:2745:VAL:HG21	2:I:2818:ALA:HB2	1.99	0.44
2:G:485:SER:HA	2:G:488:LEU:HB2	1.98	0.44
2:G:4080:TYR:CZ	2:G:4096:ALA:HB3	2.52	0.44
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.82	0.44
2:B:4071:ILE:HD11	2:B:4102:GLN:HE21	1.81	0.44
2:E:3891:LEU:HB3	2:E:3899:PHE:HE2	1.81	0.44
2:I:2267:MET:HE3	2:I:2268:GLN:HG2	1.99	0.44
2:G:1227:ALA:HB1	2:G:1230:MET:HG3	2.00	0.44
2:G:2247:GLN:NE2	2:G:2285:GLU:OE2	2.50	0.44
2:G:3927:GLN:NE2	2:G:3988:ALA:O	2.47	0.44
2:B:2745:VAL:HG21	2:B:2818:ALA:HB2	1.99	0.44
2:G:596:ASN:HB3	2:G:599:VAL:HG22	1.99	0.44
2:G:689:THR:H	2:G:778:PHE:HE2	1.65	0.44
2:G:1148:VAL:HG21	2:G:1212:ARG:HG2	2.00	0.44
2:G:2745:VAL:HG21	2:G:2818:ALA:HB2	1.99	0.44
2:B:786:GLY:HA2	2:B:1631:GLN:HA	2.00	0.44
2:B:1170:MET:HE1	2:B:1176:GLU:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:485:SER:HA	2:E:488:LEU:HB2	1.98	0.44
2:E:2247:GLN:NE2	2:E:2285:GLU:OE2	2.50	0.44
2:I:485:SER:HA	2:I:488:LEU:HB2	1.98	0.44
2:I:1773:PRO:HA	2:I:2153:MET:HE1	1.99	0.44
2:B:2267:MET:HE3	2:B:2268:GLN:HG2	1.99	0.44
2:E:41:GLY:O	2:E:45:ARG:NH1	2.51	0.44
2:I:1131:ARG:HH12	2:I:1178:ALA:HB3	1.83	0.44
2:B:2884:ASN:O	2:B:2888:ARG:N	2.47	0.43
2:B:3781:GLN:HA	2:B:3784:SER:HB3	2.01	0.43
2:E:1227:ALA:HB1	2:E:1230:MET:HG3	2.00	0.43
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.41	0.43
2:E:2745:VAL:HG21	2:E:2818:ALA:HB2	1.99	0.43
2:I:41:GLY:O	2:I:45:ARG:NH1	2.51	0.43
2:G:786:GLY:HA2	2:G:1631:GLN:HA	2.00	0.43
2:G:1093:GLU:OE1	2:G:1201:HIS:NE2	2.46	0.43
2:G:1101:ARG:HG2	2:G:1125:ASN:HA	2.00	0.43
2:G:2297:LYS:O	2:G:2300:SER:OG	2.35	0.43
2:E:786:GLY:HA2	2:E:1631:GLN:HA	2.00	0.43
2:E:887:ILE:HG21	2:E:959:TYR:HA	2.00	0.43
2:E:1101:ARG:HG2	2:E:1125:ASN:HA	2.00	0.43
2:E:3927:GLN:NE2	2:E:3988:ALA:O	2.47	0.43
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.82	0.43
2:G:2830:GLU:OE2	2:G:2931:GLN:NE2	2.52	0.43
2:B:1227:ALA:HB1	2:B:1230:MET:HG3	2.00	0.43
2:I:887:ILE:HG21	2:I:959:TYR:HA	2.00	0.43
2:I:1148:VAL:HG21	2:I:1212:ARG:HG2	2.00	0.43
2:I:1227:ALA:HB1	2:I:1230:MET:HG3	2.00	0.43
2:I:4688:ILE:HG21	2:I:4728:HIS:HB3	1.99	0.43
2:G:41:GLY:O	2:G:45:ARG:NH1	2.51	0.43
2:B:206:CYS:SG	2:B:207:SER:N	2.91	0.43
2:B:2830:GLU:OE2	2:B:2931:GLN:NE2	2.52	0.43
2:E:596:ASN:HB3	2:E:599:VAL:HG22	1.99	0.43
2:E:4688:ILE:HG21	2:E:4728:HIS:HB3	1.99	0.43
2:I:309:THR:O	2:I:313:SER:OG	2.29	0.43
2:I:1812:LEU:HD21	2:I:1861:GLN:HG2	2.00	0.43
2:G:1232:ARG:HH21	2:G:1701:ALA:HB1	1.83	0.43
2:B:41:GLY:O	2:B:45:ARG:NH1	2.51	0.43
2:B:887:ILE:HG21	2:B:959:TYR:HA	2.00	0.43
2:B:1812:LEU:HD21	2:B:1861:GLN:HG2	2.00	0.43
2:E:1131:ARG:HH12	2:E:1178:ALA:HB3	1.83	0.43
2:I:2830:GLU:OE2	2:I:2931:GLN:NE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4688:ILE:HG21	2:B:4728:HIS:HB3	1.99	0.43
2:G:887:ILE:HG21	2:G:959:TYR:HA	2.00	0.43
2:B:689:THR:H	2:B:778:PHE:HE2	1.65	0.43
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.84	0.43
2:E:206:CYS:SG	2:E:207:SER:N	2.91	0.43
2:E:689:THR:H	2:E:778:PHE:HE2	1.65	0.43
2:I:1232:ARG:HH21	2:I:1701:ALA:HB1	1.83	0.43
2:I:4092:ASP:OD1	2:I:4092:ASP:N	2.52	0.43
2:G:4688:ILE:HG21	2:G:4728:HIS:HB3	1.99	0.43
2:B:4081:VAL:HB	2:B:4088:ILE:HD12	2.00	0.43
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.84	0.43
2:I:206:CYS:SG	2:I:207:SER:N	2.91	0.43
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	2.00	0.43
2:I:3781:GLN:HA	2:I:3784:SER:HB3	2.01	0.43
2:B:1126:GLY:HA3	2:B:1143:TRP:CE2	2.54	0.43
2:B:1232:ARG:HH21	2:B:1701:ALA:HB1	1.83	0.43
2:G:206:CYS:SG	2:G:207:SER:N	2.91	0.43
2:G:548:VAL:HG12	2:G:564:LEU:HD22	2.00	0.43
2:G:1516:UNK:N	2:G:1529:UNK:O	2.52	0.43
2:G:4081:VAL:HB	2:G:4088:ILE:HD12	2.00	0.43
2:B:2024:PRO:O	2:B:2028:ARG:NE	2.45	0.43
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	2.01	0.43
2:E:3781:GLN:HA	2:E:3784:SER:HB3	2.00	0.43
2:E:4899:ASP:OD1	2:G:4892:ARG:NH2	2.52	0.43
2:I:3842:LEU:O	2:I:3929:SER:OG	2.37	0.43
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.84	0.43
2:G:4092:ASP:OD1	2:G:4092:ASP:N	2.52	0.43
2:B:1131:ARG:HH12	2:B:1178:ALA:HB3	1.83	0.42
2:B:4092:ASP:OD1	2:B:4092:ASP:N	2.52	0.42
2:E:1126:GLY:HA3	2:E:1143:TRP:CE2	2.54	0.42
2:I:940:GLY:O	2:I:1052:ASN:N	2.52	0.42
2:I:1101:ARG:HG2	2:I:1125:ASN:HA	2.00	0.42
2:G:533:ASN:ND2	2:G:536:ASN:OD1	2.42	0.42
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	2.01	0.42
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	2.00	0.42
2:E:548:VAL:HG12	2:E:564:LEU:HD22	2.00	0.42
2:E:4063:ASP:OD1	2:E:4169:SER:OG	2.26	0.42
2:I:548:VAL:HG12	2:I:564:LEU:HD22	2.00	0.42
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	2.01	0.42
2:G:940:GLY:O	2:G:1052:ASN:N	2.52	0.42
2:B:940:GLY:O	2:B:1052:ASN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1232:ARG:HH21	2:E:1701:ALA:HB1	1.83	0.42
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	2.01	0.42
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	2.01	0.42
2:G:870:ILE:O	2:G:874:LEU:N	2.42	0.42
2:G:978:THR:HB	2:G:980:ALA:H	1.84	0.42
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	2.01	0.42
2:G:1126:GLY:HA3	2:G:1143:TRP:CE2	2.54	0.42
2:G:1812:LEU:HD21	2:G:1861:GLN:HG2	2.00	0.42
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	2.01	0.42
2:B:489:ASN:HA	2:B:492:ASP:HB2	2.02	0.42
2:E:940:GLY:O	2:E:1052:ASN:N	2.52	0.42
2:E:4092:ASP:N	2:E:4092:ASP:OD1	2.52	0.42
2:I:637:LEU:HD23	2:I:1637:MET:HB3	2.01	0.42
2:I:1676:LEU:HD23	2:I:2167:ILE:HG23	2.01	0.42
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.84	0.42
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	2.00	0.42
2:B:864:PRO:HA	2:B:865:PRO:HD3	1.92	0.42
2:B:978:THR:HB	2:B:980:ALA:H	1.84	0.42
2:B:1099:GLU:OE2	2:B:1127:HIS:ND1	2.40	0.42
2:B:1101:ARG:HG2	2:B:1125:ASN:HA	2.00	0.42
2:B:2022:PRO:HB2	2:B:2024:PRO:HD2	2.01	0.42
2:E:489:ASN:HA	2:E:492:ASP:HB2	2.02	0.42
2:E:1676:LEU:HD23	2:E:2167:ILE:HG23	2.01	0.42
2:I:1126:GLY:HA3	2:I:1143:TRP:CE2	2.54	0.42
2:G:330:ASP:OD1	2:G:330:ASP:N	2.53	0.42
2:G:637:LEU:HD23	2:G:1637:MET:HB3	2.01	0.42
2:G:1694:LEU:O	2:G:1712:TYR:OH	2.29	0.42
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	2.00	0.42
2:B:548:VAL:HG12	2:B:564:LEU:HD22	2.00	0.42
2:E:978:THR:HB	2:E:980:ALA:H	1.84	0.42
2:B:3842:LEU:O	2:B:3929:SER:OG	2.37	0.42
2:E:2022:PRO:HB2	2:E:2024:PRO:HD2	2.01	0.42
2:I:689:THR:H	2:I:778:PHE:HE2	1.65	0.42
2:G:3842:LEU:O	2:G:3929:SER:OG	2.37	0.42
2:B:1707:LEU:HG	2:B:1708:ARG:HG3	2.02	0.42
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	2.01	0.42
2:E:1516:UNK:N	2:E:1529:UNK:O	2.52	0.42
2:E:1707:LEU:HG	2:E:1708:ARG:HG3	2.02	0.42
2:I:4081:VAL:HB	2:I:4088:ILE:HD12	2.00	0.42
2:B:1676:LEU:HD23	2:B:2167:ILE:HG23	2.01	0.42
2:B:1694:LEU:O	2:B:1712:TYR:OH	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:637:LEU:HD23	2:E:1637:MET:HB3	2.01	0.42
2:E:4251:ILE:HG22	2:E:4553:ASN:HD22	1.85	0.42
2:G:1676:LEU:HD23	2:G:2167:ILE:HG23	2.01	0.42
2:G:2884:ASN:O	2:G:2888:ARG:N	2.47	0.42
2:G:3781:GLN:HA	2:G:3784:SER:HB3	2.01	0.42
2:G:4680:LYS:HD3	2:G:4686:LEU:HD22	2.02	0.42
2:B:582:HIS:O	2:B:585:SER:OG	2.29	0.42
2:E:2830:GLU:OE2	2:E:2931:GLN:NE2	2.52	0.42
2:G:1171:SER:OG	2:G:1175:SER:N	2.45	0.42
2:G:1673:VAL:HG12	2:G:1681:VAL:HG11	2.02	0.42
2:B:637:LEU:HD23	2:B:1637:MET:HB3	2.01	0.41
2:B:3927:GLN:NE2	2:B:3988:ALA:O	2.47	0.41
2:E:4680:LYS:HD3	2:E:4686:LEU:HD22	2.02	0.41
2:G:3780:LEU:HD11	2:G:3816:MET:HG3	2.01	0.41
2:B:1673:VAL:HG12	2:B:1681:VAL:HG11	2.02	0.41
2:E:1812:LEU:HD21	2:E:1861:GLN:HG2	2.00	0.41
2:E:3780:LEU:HD11	2:E:3816:MET:HG3	2.01	0.41
2:E:3842:LEU:O	2:E:3929:SER:OG	2.37	0.41
2:E:4929:LEU:HD13	2:E:4929:LEU:HA	1.90	0.41
2:I:876:GLU:O	2:I:880:GLU:N	2.53	0.41
2:I:1673:VAL:HG12	2:I:1681:VAL:HG11	2.02	0.41
2:I:2022:PRO:HB2	2:I:2024:PRO:HD2	2.01	0.41
2:I:4251:ILE:HG22	2:I:4553:ASN:HD22	1.85	0.41
2:G:410:LEU:HD12	2:G:413:GLN:HE21	1.85	0.41
2:G:582:HIS:O	2:G:585:SER:OG	2.29	0.41
2:G:2208:MET:HE1	2:G:2253:HIS:HB3	2.02	0.41
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	2.01	0.41
2:E:410:LEU:HD12	2:E:413:GLN:HE21	1.85	0.41
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	2.01	0.41
2:E:4000:MET:HE2	2:E:4061:PHE:CD2	2.56	0.41
2:I:56:GLN:O	2:I:309:THR:OG1	2.26	0.41
2:I:454:PRO:HG2	2:I:531:ARG:HH12	1.85	0.41
2:I:1516:UNK:N	2:I:1529:UNK:O	2.53	0.41
2:B:641:VAL:HG11	2:B:681:HIS:HD1	1.86	0.41
2:B:1516:UNK:N	2:B:1529:UNK:O	2.52	0.41
2:B:3780:LEU:HD11	2:B:3816:MET:HG3	2.01	0.41
2:B:4000:MET:HE2	2:B:4061:PHE:CD2	2.56	0.41
2:E:1796:ALA:HB1	2:E:1797:ARG:HH21	1.86	0.41
2:I:897:ARG:HB2	2:I:905:PRO:HG3	2.03	0.41
2:G:4251:ILE:HG22	2:G:4553:ASN:HD22	1.85	0.41
2:B:2208:MET:HE1	2:B:2253:HIS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4680:LYS:HD3	2:B:4686:LEU:HD22	2.02	0.41
2:E:1673:VAL:HG12	2:E:1681:VAL:HG11	2.02	0.41
2:B:897:ARG:HB2	2:B:905:PRO:HG3	2.03	0.41
2:B:1796:ALA:HB1	2:B:1797:ARG:HH21	1.86	0.41
2:I:4000:MET:HE2	2:I:4061:PHE:CD2	2.56	0.41
2:G:235:ALA:HA	2:G:257:ARG:HD3	2.03	0.41
2:G:489:ASN:HA	2:G:492:ASP:HB2	2.01	0.41
2:G:1707:LEU:HG	2:G:1708:ARG:HG3	2.02	0.41
2:G:2022:PRO:HB2	2:G:2024:PRO:HD2	2.01	0.41
2:B:1738:LEU:HB3	2:B:2146:PRO:HD3	2.03	0.41
2:E:330:ASP:OD1	2:E:330:ASP:N	2.53	0.41
2:E:4081:VAL:HB	2:E:4088:ILE:HD12	2.00	0.41
2:I:235:ALA:HA	2:I:257:ARG:HD3	2.03	0.41
2:I:1707:LEU:HG	2:I:1708:ARG:HG3	2.02	0.41
2:I:3780:LEU:HD11	2:I:3816:MET:HG3	2.01	0.41
2:I:4680:LYS:HD3	2:I:4686:LEU:HD22	2.02	0.41
2:G:454:PRO:HG2	2:G:531:ARG:HH12	1.86	0.41
2:G:897:ARG:HB2	2:G:905:PRO:HG3	2.03	0.41
2:B:2827:ARG:H	2:B:2934:GLY:HA3	1.86	0.41
2:I:641:VAL:HG11	2:I:681:HIS:HD1	1.86	0.41
2:I:864:PRO:HA	2:I:865:PRO:HD3	1.92	0.41
2:I:978:THR:HB	2:I:980:ALA:H	1.84	0.41
2:I:1796:ALA:HB1	2:I:1797:ARG:HH21	1.86	0.41
2:B:410:LEU:HD12	2:B:413:GLN:HE21	1.85	0.41
2:E:1152:MET:HB2	2:E:1161:ILE:HB	2.03	0.41
2:E:2208:MET:HE1	2:E:2253:HIS:HB3	2.02	0.41
2:E:2827:ARG:H	2:E:2934:GLY:HA3	1.86	0.41
2:I:410:LEU:HD12	2:I:413:GLN:HE21	1.85	0.41
2:I:489:ASN:HA	2:I:492:ASP:HB2	2.02	0.41
2:I:1152:MET:HB2	2:I:1161:ILE:HB	2.03	0.41
2:I:2208:MET:HE1	2:I:2253:HIS:HB3	2.02	0.41
2:I:4929:LEU:HD13	2:I:4929:LEU:HA	1.90	0.41
2:G:278:GLN:N	2:G:315:CYS:SG	2.83	0.41
2:G:309:THR:O	2:G:313:SER:OG	2.29	0.41
2:E:675:LEU:HD11	2:E:1633:PRO:HB3	2.03	0.41
2:G:4000:MET:HE2	2:G:4061:PHE:CD2	2.56	0.41
1:H:92:PRO:HD3	2:G:627:PRO:HB2	2.02	0.40
2:B:1720:LEU:HD12	2:B:1847:THR:HG23	2.03	0.40
2:B:4956:THR:O	2:B:4965:SER:N	2.55	0.40
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.42	0.40
2:E:897:ARG:HB2	2:E:905:PRO:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4181:ILE:HG22	2:I:4193:ILE:HB	2.03	0.40
2:I:4892:ARG:NH2	2:G:4899:ASP:OD1	2.54	0.40
2:G:4763:GLY:O	2:G:4766:THR:OG1	2.33	0.40
2:E:641:VAL:HG11	2:E:681:HIS:HD1	1.86	0.40
2:I:404:ILE:HG21	2:I:481:GLU:HG3	2.04	0.40
2:I:1667:LEU:HD23	2:I:1671:ARG:HH12	1.87	0.40
2:G:641:VAL:HG11	2:G:681:HIS:HD1	1.86	0.40
2:G:1796:ALA:HB1	2:G:1797:ARG:HH21	1.86	0.40
2:G:4147:LEU:O	2:G:4151:SER:OG	2.29	0.40
2:G:4956:THR:O	2:G:4965:SER:N	2.55	0.40
2:B:40:GLU:HB3	2:B:44:ASN:HB3	2.04	0.40
2:B:1171:SER:OG	2:B:1175:SER:N	2.44	0.40
2:B:1667:LEU:HD23	2:B:1671:ARG:HH12	1.87	0.40
2:E:214:VAL:HG22	2:E:341:TYR:CE1	2.57	0.40
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	2.03	0.40
2:E:1622:GLU:N	2:E:1627:ALA:O	2.55	0.40
2:E:1667:LEU:HD23	2:E:1671:ARG:HH12	1.87	0.40
2:E:2674:UNK:O	2:E:2676:UNK:N	2.54	0.40
2:I:330:ASP:OD1	2:I:330:ASP:N	2.53	0.40
2:I:4956:THR:O	2:I:4965:SER:N	2.55	0.40
2:G:1622:GLU:N	2:G:1627:ALA:O	2.55	0.40
2:G:2827:ARG:H	2:G:2934:GLY:HA3	1.86	0.40
2:B:214:VAL:HG22	2:B:341:TYR:CE1	2.57	0.40
2:B:675:LEU:HD11	2:B:1633:PRO:HB3	2.03	0.40
2:B:2674:UNK:O	2:B:2676:UNK:N	2.55	0.40
2:B:4251:ILE:HG22	2:B:4553:ASN:HD22	1.85	0.40
2:E:4000:MET:HE3	2:E:4017:LEU:HD21	2.04	0.40
2:E:4567:LEU:HA	2:E:4816:ILE:HD12	2.03	0.40
2:I:675:LEU:HD11	2:I:1633:PRO:HB3	2.03	0.40
2:I:4000:MET:HE3	2:I:4017:LEU:HD21	2.04	0.40
2:G:3364:UNK:O	2:G:3368:UNK:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
1	F	105/108 (97%)	98 (93%)	7 (7%)	0	100	100
1	H	105/108 (97%)	98 (93%)	7 (7%)	0	100	100
1	J	105/108 (97%)	97 (92%)	8 (8%)	0	100	100
2	B	3235/4676 (69%)	2881 (89%)	349 (11%)	5 (0%)	43	75
2	E	3235/4676 (69%)	2883 (89%)	347 (11%)	5 (0%)	43	75
2	G	3235/4676 (69%)	2879 (89%)	351 (11%)	5 (0%)	43	75
2	I	3235/4676 (69%)	2880 (89%)	350 (11%)	5 (0%)	43	75
All	All	13360/19136 (70%)	11913 (89%)	1427 (11%)	20 (0%)	49	81

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	E	1708	ARG
2	I	1708	ARG
2	G	1708	ARG
2	B	1932	PRO
2	E	1932	PRO
2	I	1932	PRO
2	G	1932	PRO
2	B	1840	PRO
2	B	4641	PRO
2	E	1840	PRO
2	E	4641	PRO
2	I	1840	PRO
2	I	4641	PRO
2	G	1840	PRO
2	G	4641	PRO
2	B	4228	ALA
2	E	4228	ALA
2	I	4228	ALA
2	G	4228	ALA

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	2493/3202 (78%)	2481 (100%)	12 (0%)	81	82
2	E	2493/3202 (78%)	2480 (100%)	13 (0%)	81	82
2	G	2493/3202 (78%)	2480 (100%)	13 (0%)	81	82
2	I	2493/3202 (78%)	2480 (100%)	13 (0%)	81	82
All	All	10324/13164 (78%)	10273 (100%)	51 (0%)	78	82

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	719	LEU
2	B	815	VAL
2	B	1600	LEU
2	B	1657	LEU
2	B	1676	LEU
2	B	2339	VAL
2	B	3805	LEU
2	B	3896	ASN
2	B	4081	VAL
2	B	4929	LEU
2	B	4995	LEU
2	E	131	LEU
2	E	719	LEU
2	E	815	VAL
2	E	1600	LEU
2	E	1657	LEU
2	E	1676	LEU
2	E	2339	VAL

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Mol	Chain	Res	Type
2	E	3805	LEU
2	E	3896	ASN
2	E	4081	VAL
2	E	4792	LEU
2	E	4929	LEU
2	E	4995	LEU
2	I	131	LEU
2	I	719	LEU
2	I	815	VAL
2	I	1600	LEU
2	I	1657	LEU
2	I	1676	LEU
2	I	2339	VAL
2	I	3805	LEU
2	I	3896	ASN
2	I	4081	VAL
2	I	4792	LEU
2	I	4929	LEU
2	I	4995	LEU
2	G	131	LEU
2	G	719	LEU
2	G	815	VAL
2	G	1600	LEU
2	G	1657	LEU
2	G	1676	LEU
2	G	2339	VAL
2	G	3805	LEU
2	G	3896	ASN
2	G	4081	VAL
2	G	4792	LEU
2	G	4929	LEU
2	G	4995	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (221) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	25	HIS
1	F	87	HIS
1	A	25	HIS
1	A	87	HIS
1	H	25	HIS
1	H	87	HIS

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Mol	Chain	Res	Type
1	J	25	HIS
1	J	87	HIS
2	B	32	GLN
2	B	57	ASN
2	B	105	HIS
2	B	111	HIS
2	B	113	HIS
2	B	201	ASN
2	B	203	ASN
2	B	379	HIS
2	B	383	HIS
2	B	395	GLN
2	B	413	GLN
2	B	465	GLN
2	B	479	GLN
2	B	520	ASN
2	B	765	GLN
2	B	797	HIS
2	B	866	HIS
2	B	877	ASN
2	B	1133	HIS
2	B	1220	GLN
2	B	1688	HIS
2	B	1691	GLN
2	B	1693	GLN
2	B	1719	HIS
2	B	1760	HIS
2	B	1775	HIS
2	B	1861	GLN
2	B	1949	GLN
2	B	2005	GLN
2	B	2127	GLN
2	B	2260	ASN
2	B	3761	GLN
2	B	3766	GLN
2	B	3771	HIS
2	B	3850	GLN
2	B	3895	HIS
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	3960	GLN

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Mol	Chain	Res	Type
2	B	4034	ASN
2	B	4102	GLN
2	B	4156	HIS
2	B	4246	GLN
2	B	4553	ASN
2	B	4691	GLN
2	B	4728	HIS
2	B	4806	ASN
2	B	4864	ASN
2	B	4949	GLN
2	B	4984	ASN
2	E	32	GLN
2	E	57	ASN
2	E	105	HIS
2	E	111	HIS
2	E	201	ASN
2	E	203	ASN
2	E	379	HIS
2	E	383	HIS
2	E	395	GLN
2	E	413	GLN
2	E	465	GLN
2	E	479	GLN
2	E	520	ASN
2	E	582	HIS
2	E	765	GLN
2	E	797	HIS
2	E	866	HIS
2	E	877	ASN
2	E	1220	GLN
2	E	1691	GLN
2	E	1693	GLN
2	E	1719	HIS
2	E	1760	HIS
2	E	1775	HIS
2	E	1861	GLN
2	E	1949	GLN
2	E	2005	GLN
2	E	2127	GLN
2	E	2260	ASN
2	E	2773	ASN
2	E	3704	HIS

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Mol	Chain	Res	Type
2	E	3761	GLN
2	E	3766	GLN
2	E	3771	HIS
2	E	3814	GLN
2	E	3850	GLN
2	E	3895	HIS
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	3960	GLN
2	E	4102	GLN
2	E	4156	HIS
2	E	4246	GLN
2	E	4553	ASN
2	E	4691	GLN
2	E	4728	HIS
2	E	4776	GLN
2	E	4806	ASN
2	E	4864	ASN
2	E	4949	GLN
2	E	4984	ASN
2	E	5015	GLN
2	I	23	GLN
2	I	32	GLN
2	I	57	ASN
2	I	105	HIS
2	I	111	HIS
2	I	201	ASN
2	I	203	ASN
2	I	379	HIS
2	I	383	HIS
2	I	395	GLN
2	I	413	GLN
2	I	479	GLN
2	I	520	ASN
2	I	582	HIS
2	I	765	GLN
2	I	797	HIS
2	I	866	HIS
2	I	877	ASN
2	I	1220	GLN
2	I	1688	HIS

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Mol	Chain	Res	Type
2	I	1691	GLN
2	I	1693	GLN
2	I	1719	HIS
2	I	1760	HIS
2	I	1775	HIS
2	I	1861	GLN
2	I	1949	GLN
2	I	2005	GLN
2	I	2127	GLN
2	I	2260	ASN
2	I	2773	ASN
2	I	2931	GLN
2	I	3704	HIS
2	I	3761	GLN
2	I	3766	GLN
2	I	3771	HIS
2	I	3814	GLN
2	I	3850	GLN
2	I	3895	HIS
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	4034	ASN
2	I	4102	GLN
2	I	4156	HIS
2	I	4246	GLN
2	I	4553	ASN
2	I	4691	GLN
2	I	4728	HIS
2	I	4806	ASN
2	I	4864	ASN
2	I	4949	GLN
2	I	4984	ASN
2	I	5015	GLN
2	G	23	GLN
2	G	32	GLN
2	G	57	ASN
2	G	105	HIS
2	G	111	HIS
2	G	201	ASN
2	G	203	ASN
2	G	379	HIS

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Mol	Chain	Res	Type
2	G	383	HIS
2	G	395	GLN
2	G	413	GLN
2	G	479	GLN
2	G	520	ASN
2	G	582	HIS
2	G	765	GLN
2	G	797	HIS
2	G	866	HIS
2	G	877	ASN
2	G	1133	HIS
2	G	1220	GLN
2	G	1691	GLN
2	G	1693	GLN
2	G	1719	HIS
2	G	1760	HIS
2	G	1775	HIS
2	G	1861	GLN
2	G	1949	GLN
2	G	2005	GLN
2	G	2127	GLN
2	G	2260	ASN
2	G	2773	ASN
2	G	2931	GLN
2	G	3704	HIS
2	G	3761	GLN
2	G	3766	GLN
2	G	3771	HIS
2	G	3814	GLN
2	G	3850	GLN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	4034	ASN
2	G	4102	GLN
2	G	4156	HIS
2	G	4246	GLN
2	G	4553	ASN
2	G	4691	GLN
2	G	4728	HIS
2	G	4776	GLN

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Mol	Chain	Res	Type
2	G	4806	ASN
2	G	4864	ASN
2	G	4949	GLN
2	G	4984	ASN
2	G	5015	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	I	12
2	B	12
2	G	12
2	E	12

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	3613:UNK	C	3639:THR	N	42.97
1	B	3613:UNK	C	3639:THR	N	42.95
1	G	3613:UNK	C	3639:THR	N	42.95
1	E	3613:UNK	C	3639:THR	N	42.94
1	B	3163:UNK	C	3170:UNK	N	16.52
1	E	3163:UNK	C	3170:UNK	N	16.52
1	I	3163:UNK	C	3170:UNK	N	16.52
1	G	3163:UNK	C	3170:UNK	N	16.52
1	E	3468:UNK	C	3511:UNK	N	14.99
1	G	3468:UNK	C	3511:UNK	N	14.99
1	B	3468:UNK	C	3511:UNK	N	14.98
1	I	3468:UNK	C	3511:UNK	N	14.98
1	B	3063:UNK	C	3134:UNK	N	14.61
1	E	3063:UNK	C	3134:UNK	N	14.61
1	I	3063:UNK	C	3134:UNK	N	14.61
1	G	3063:UNK	C	3134:UNK	N	14.61
1	B	2703:UNK	C	2734:ASN	N	14.43
1	I	2703:UNK	C	2734:ASN	N	14.43
1	G	2703:UNK	C	2734:ASN	N	14.43
1	E	2703:UNK	C	2734:ASN	N	14.42
1	B	3236:UNK	C	3241:UNK	N	13.59
1	E	3236:UNK	C	3241:UNK	N	13.59
1	I	3236:UNK	C	3241:UNK	N	13.59
1	G	3236:UNK	C	3241:UNK	N	13.59
1	I	1564:UNK	C	1573:MET	N	12.75
1	B	1564:UNK	C	1573:MET	N	12.73
1	G	1564:UNK	C	1573:MET	N	12.73
1	E	1564:UNK	C	1573:MET	N	12.71
1	B	2976:UNK	C	2995:UNK	N	12.12
1	E	2976:UNK	C	2995:UNK	N	12.12
1	I	2976:UNK	C	2995:UNK	N	12.12
1	G	2976:UNK	C	2995:UNK	N	12.12
1	B	3254:UNK	C	3261:UNK	N	8.52
1	E	3254:UNK	C	3261:UNK	N	8.52
1	I	3254:UNK	C	3261:UNK	N	8.52
1	G	3254:UNK	C	3261:UNK	N	8.52

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1297:UNK	C	1430:UNK	N	5.67
1	E	1297:UNK	C	1430:UNK	N	5.67
1	G	1297:UNK	C	1430:UNK	N	5.67
1	I	1297:UNK	C	1430:UNK	N	5.66
1	I	2939:ARG	C	2942:UNK	N	3.56
1	G	2939:ARG	C	2942:UNK	N	3.55
1	B	2939:ARG	C	2942:UNK	N	3.54
1	E	2479:LEU	C	2487:UNK	N	3.53
1	E	2939:ARG	C	2942:UNK	N	3.53
1	B	2479:LEU	C	2487:UNK	N	3.51
1	G	2479:LEU	C	2487:UNK	N	3.51
1	I	2479:LEU	C	2487:UNK	N	3.49

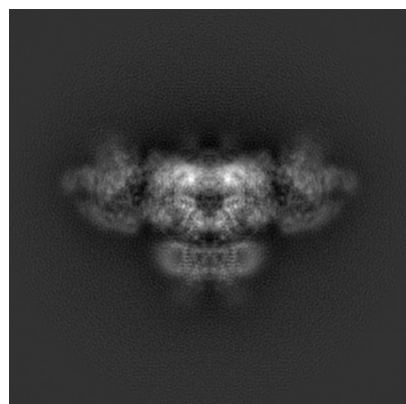
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8372. These allow visual inspection of the internal detail of the map and identification of artifacts.

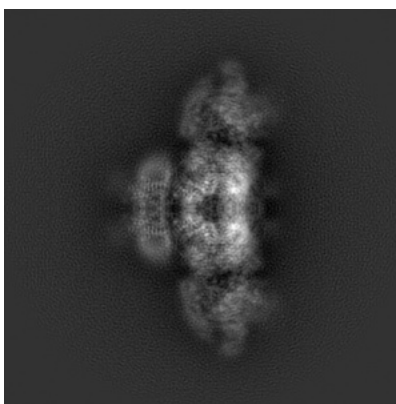
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

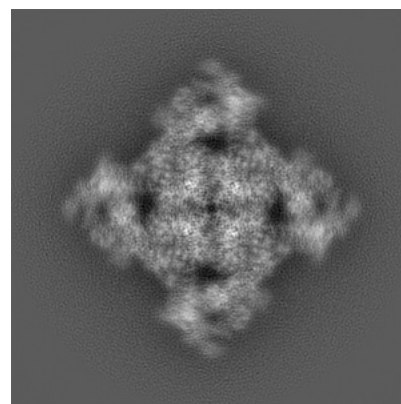
6.1.1 Primary map



X

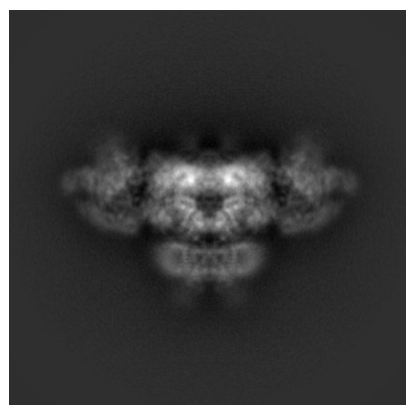


Y

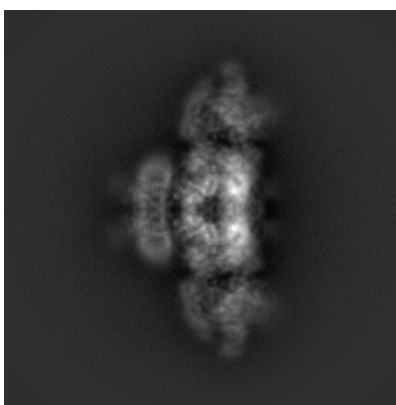


Z

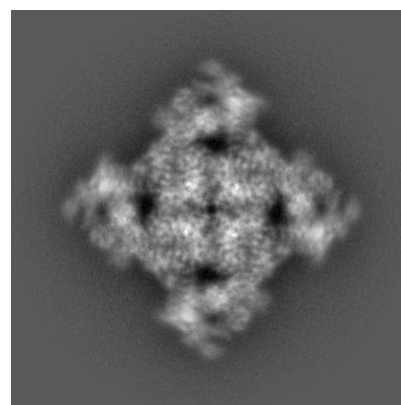
6.1.2 Raw map



X



Y

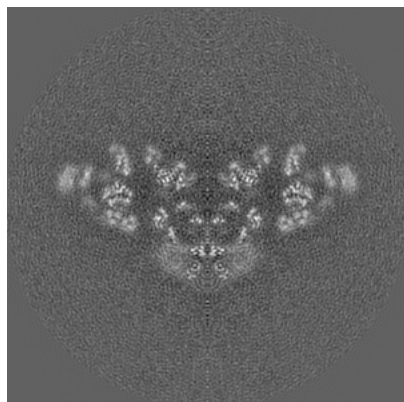


Z

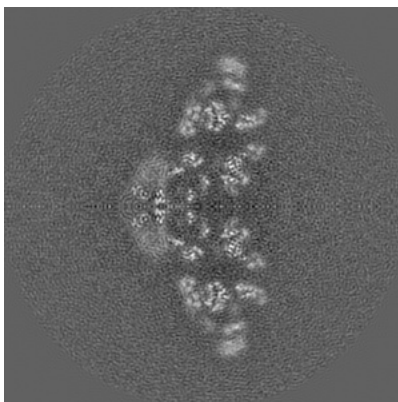
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

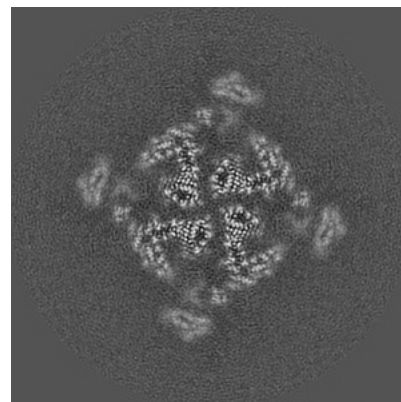
6.2.1 Primary map



X Index: 200

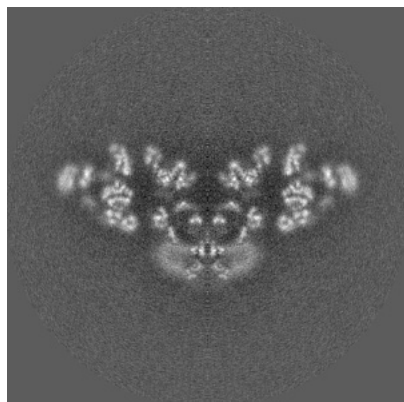


Y Index: 200

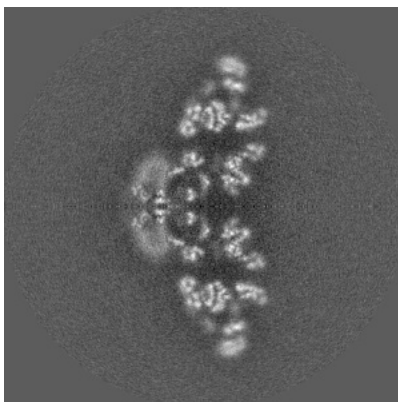


Z Index: 200

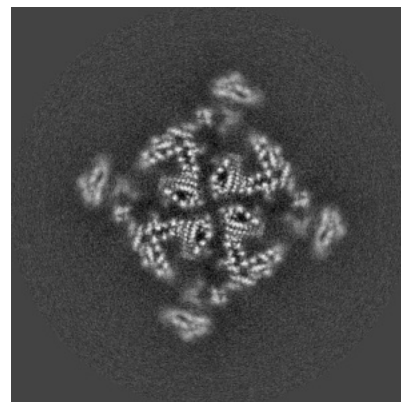
6.2.2 Raw map



X Index: 200



Y Index: 200

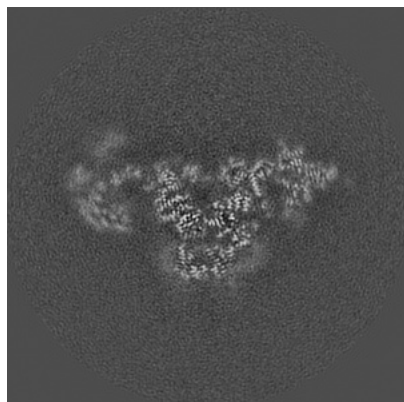


Z Index: 200

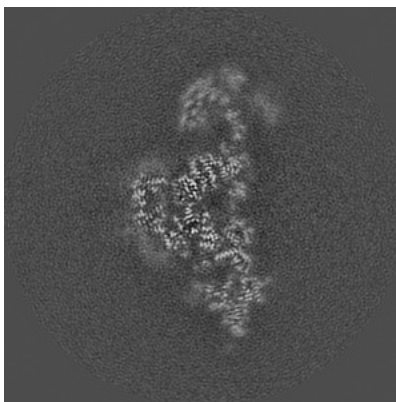
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

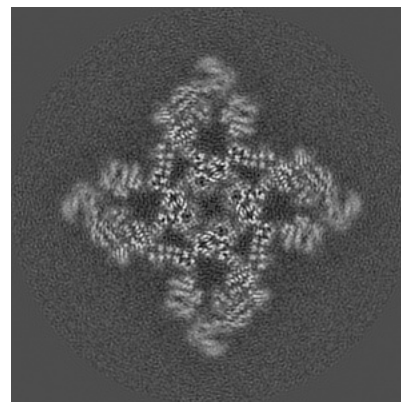
6.3.1 Primary map



X Index: 184

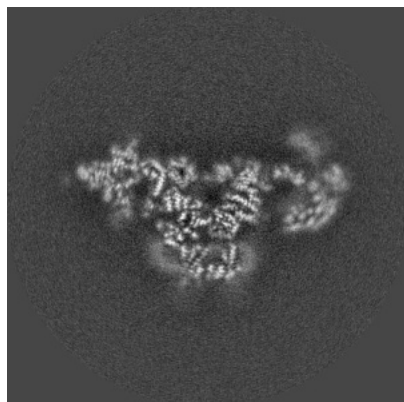


Y Index: 184

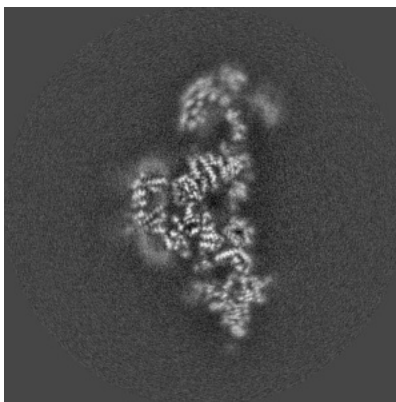


Z Index: 227

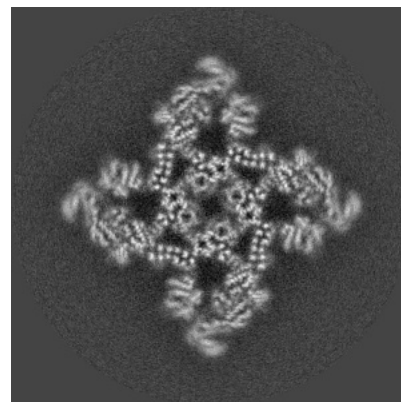
6.3.2 Raw map



X Index: 216



Y Index: 184

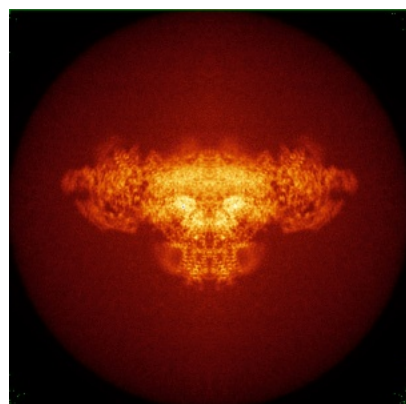


Z Index: 227

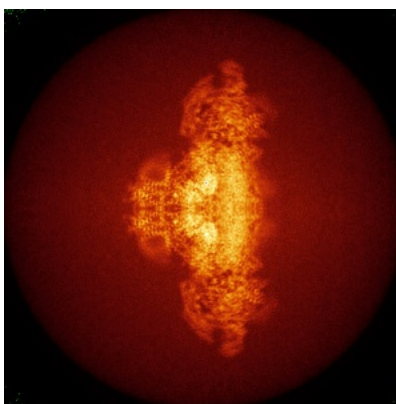
The images above show the largest variance slices of the map in three orthogonal directions.

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

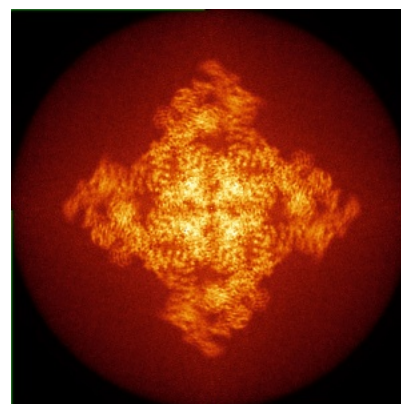
6.4.1 Primary map



X

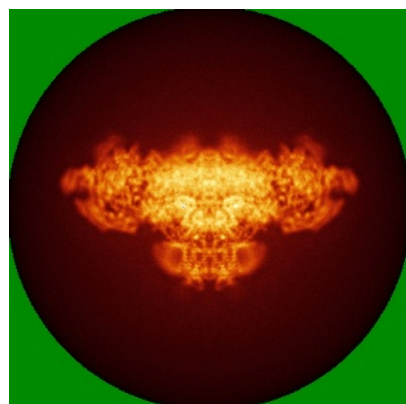


Y

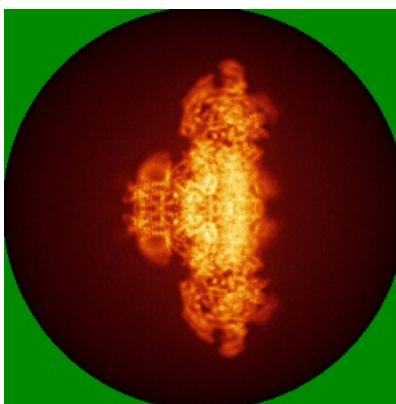


Z

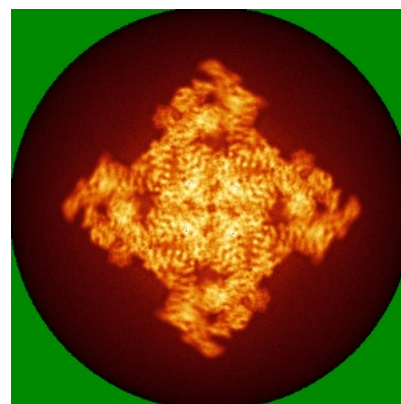
6.4.2 Raw map



X



Y

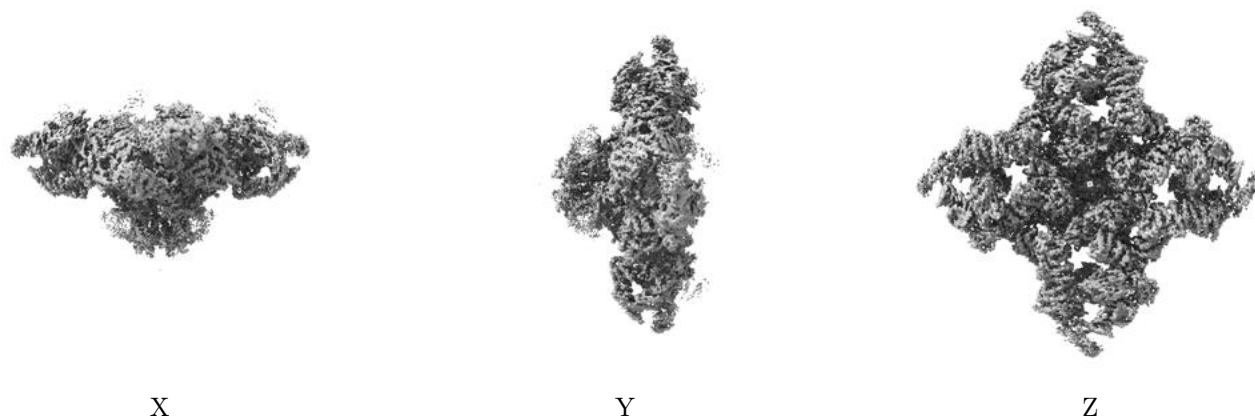


Z

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 0.04. 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.

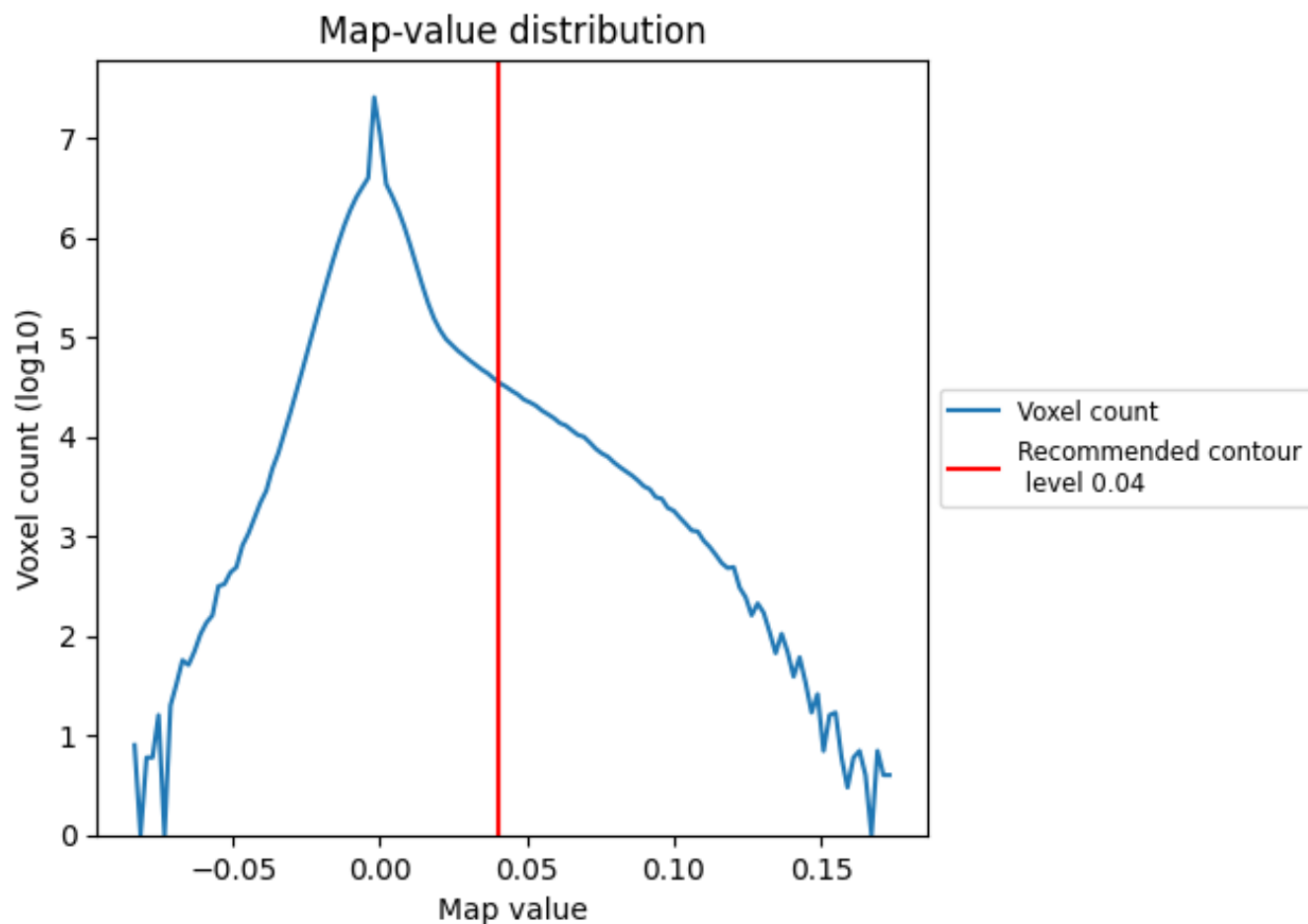
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

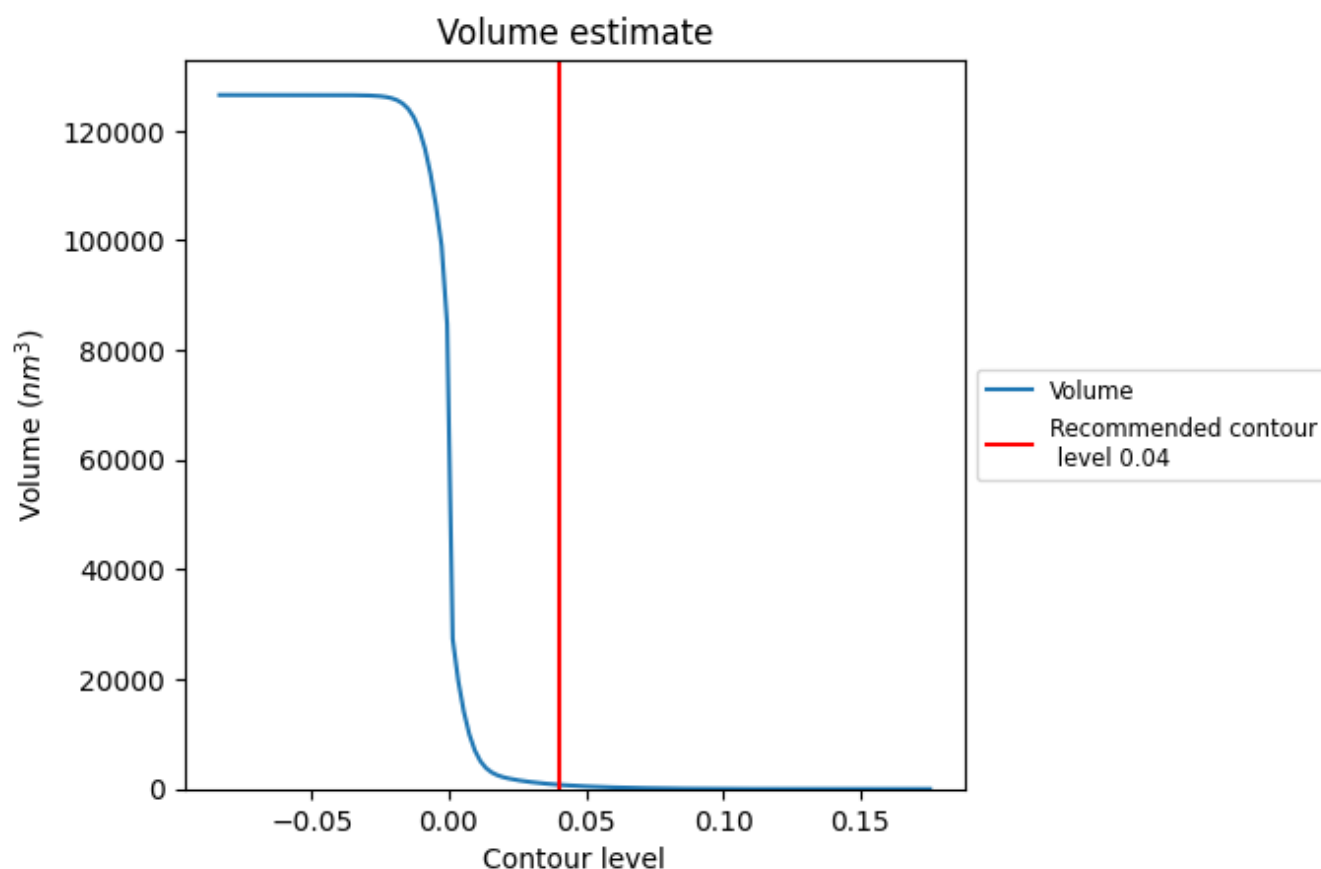
This section contains the results of statistical analysis of the map.

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.

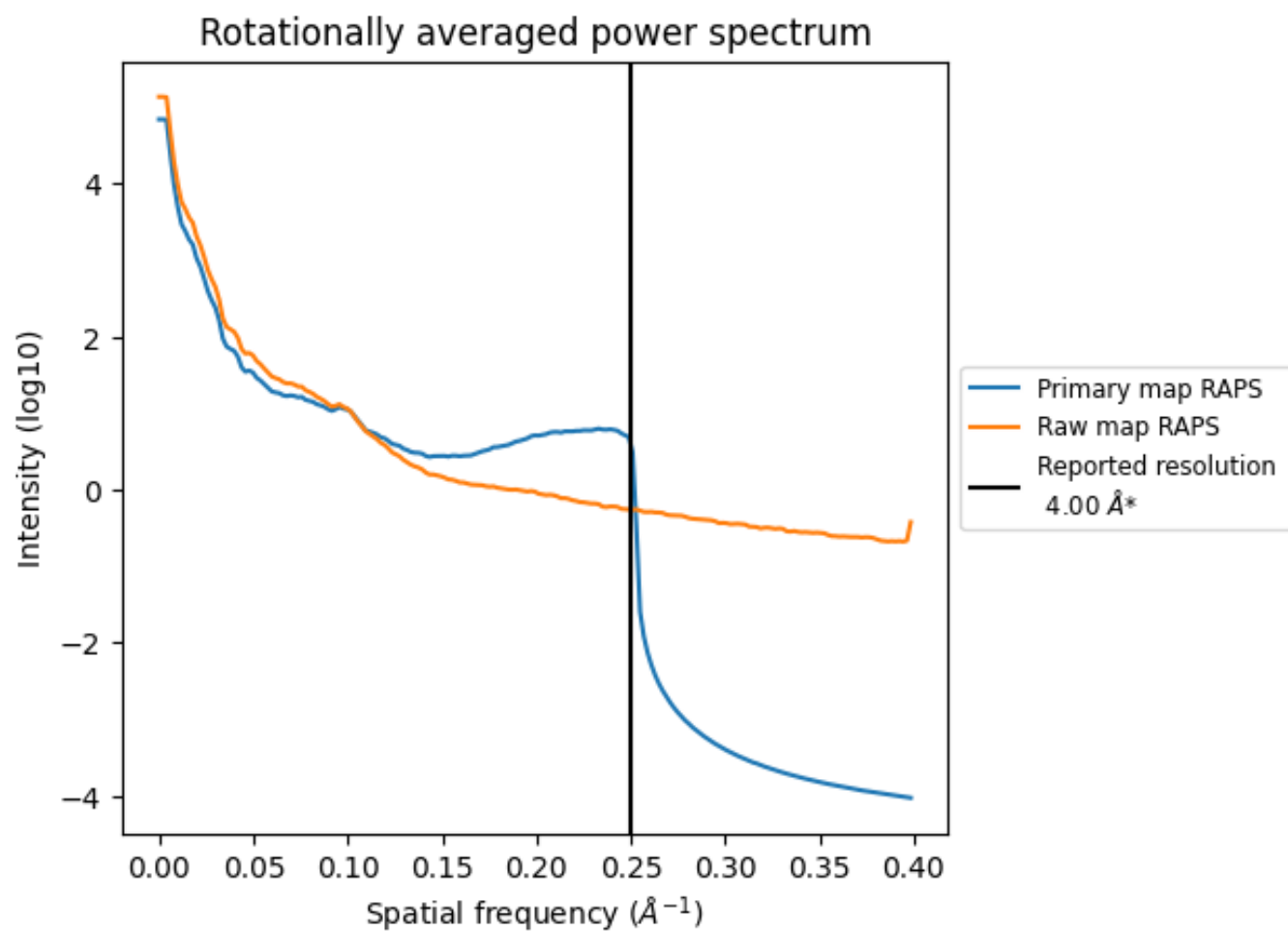
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 771 nm³; this corresponds to an approximate mass of 696 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 ⓘ

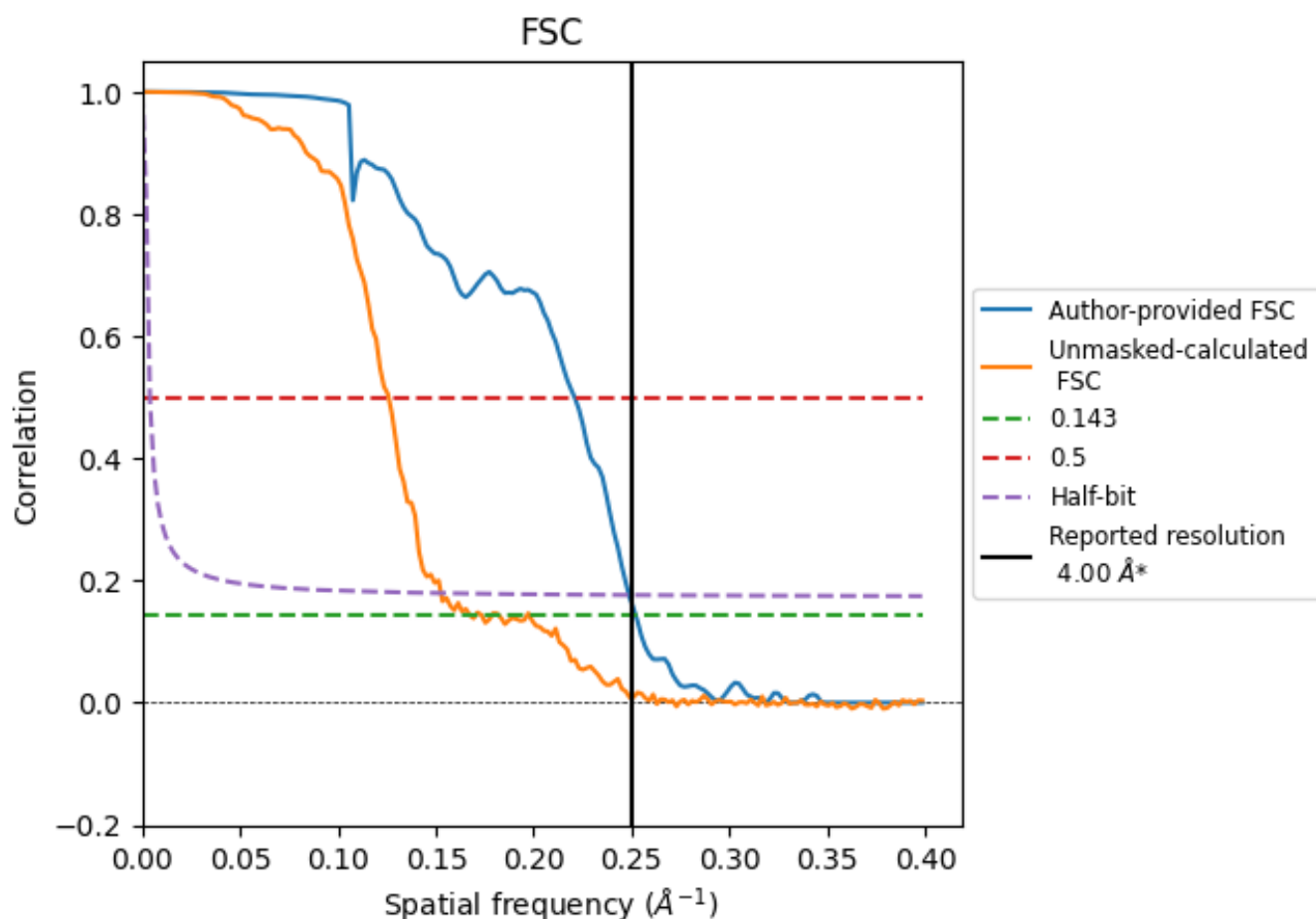


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

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 0.250 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

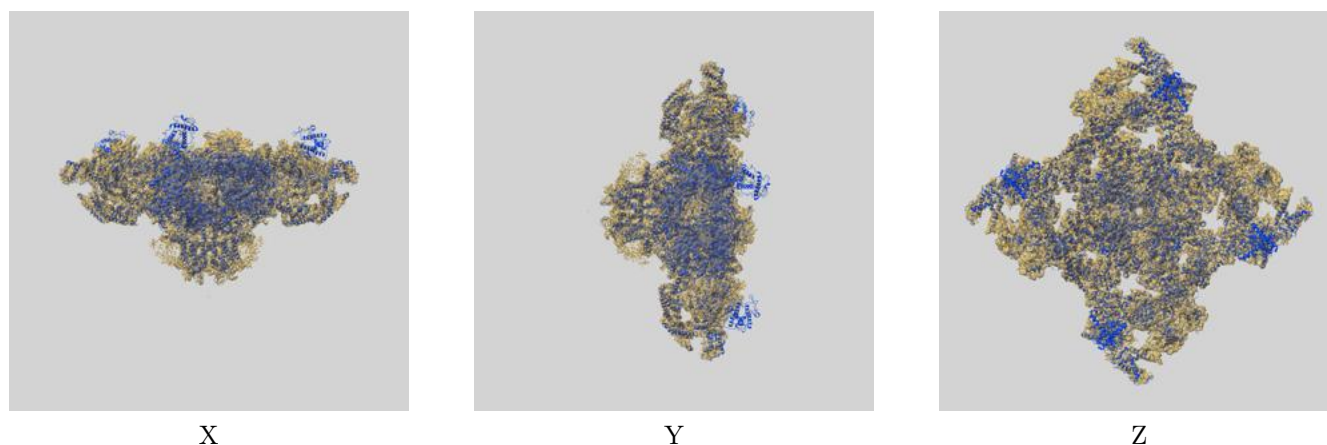
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.97	4.53	4.02
Unmasked-calculated*	5.97	7.95	6.55

*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 5.97 differs from the reported value 4.0 by more than 10 %

9 Map-model fit [i](#)

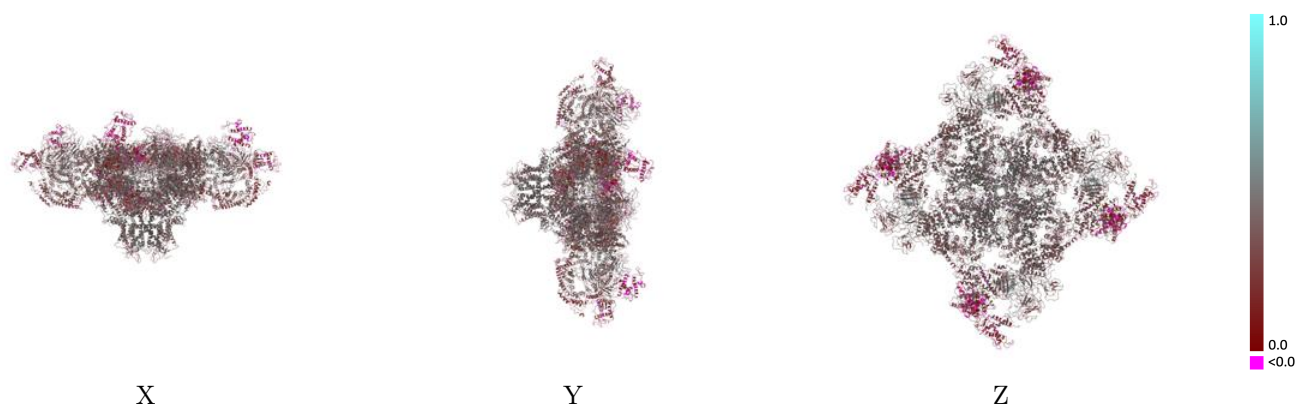
This section contains information regarding the fit between EMDB map EMD-8372 and PDB model 5T9M. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



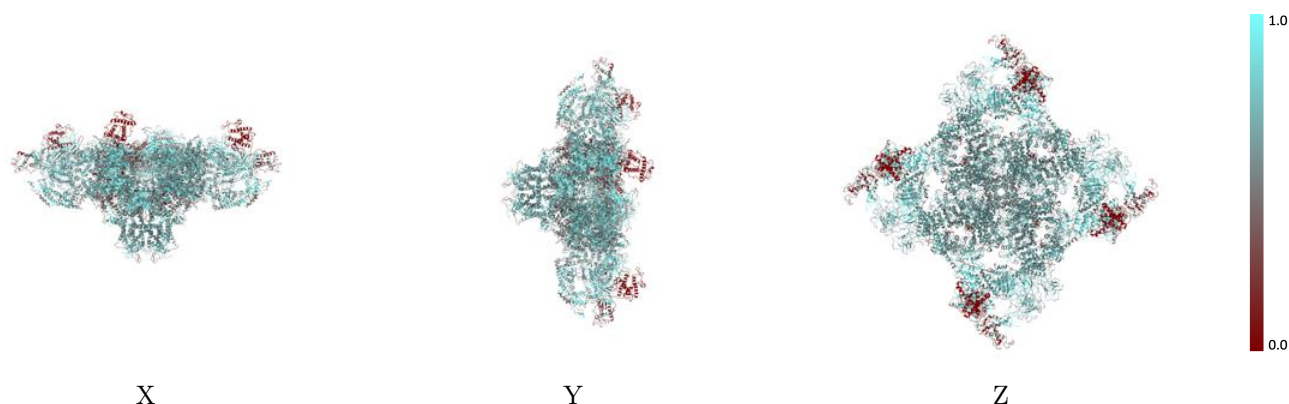
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



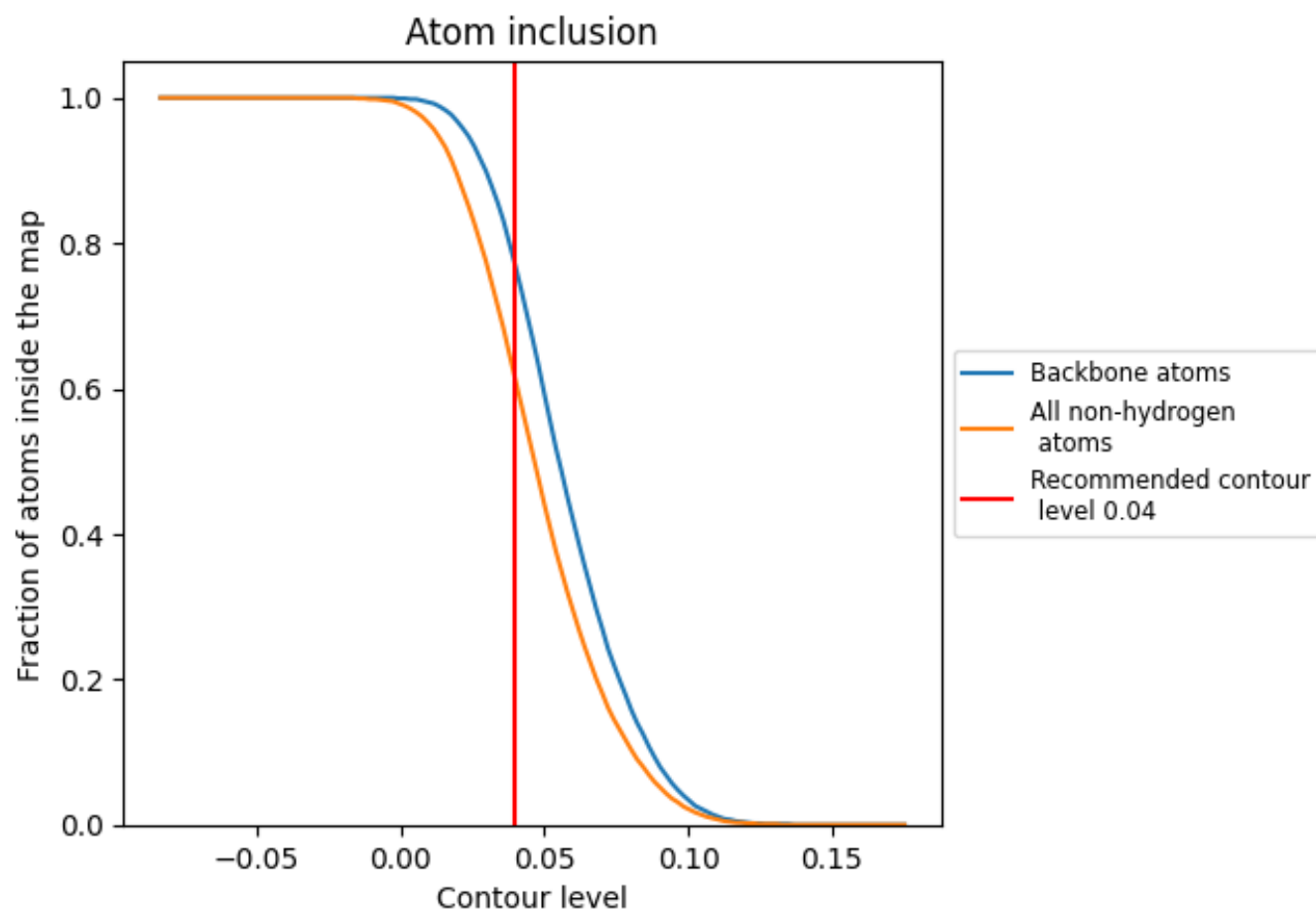
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 61% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6120	0.3470
A	0.6190	0.3590
B	0.6120	0.3470
E	0.6120	0.3470
F	0.6120	0.3630
G	0.6120	0.3470
H	0.6100	0.3650
I	0.6120	0.3470
J	0.6130	0.3660

1.0

0.0

<0.0