



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 06:55 AM UTC

PDB ID : 5T15 / pdb_00005t15
EMDB ID : EMD-8342
Title : Structural basis for gating and activation of RyR1 (30 uM Ca²⁺ dataset, all particles)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on : 2016-08-17
Resolution : 3.60 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:

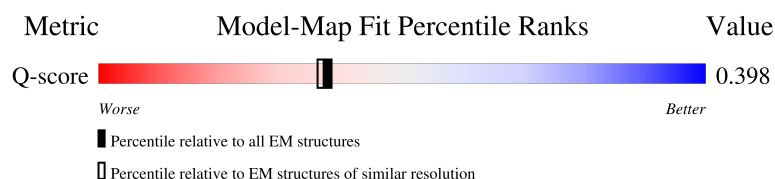
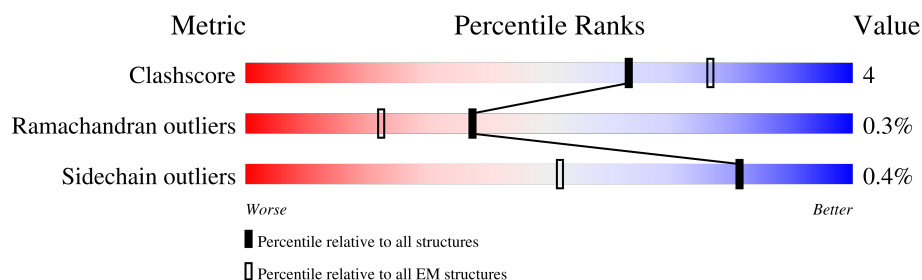
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.60 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.



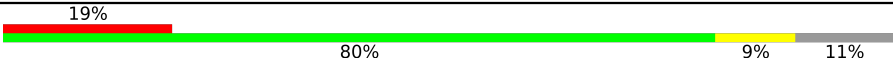
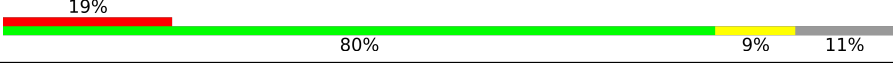
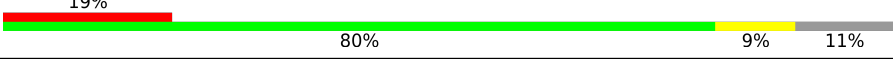
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	7% 87% 12% .
1	F	108	7% 89% 10% .
1	H	108	8% 88% 11% .
1	J	108	8% 89% 10% .

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Mol	Chain	Length	Quality of chain
2	B	4676	
2	E	4676	
2	G	4676	
2	I	4676	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 120796 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,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4170	Total	C	N	O	S	0	0
			29379	18614	5204	5404	157		
2	E	4170	Total	C	N	O	S	0	0
			29379	18614	5204	5404	157		
2	I	4170	Total	C	N	O	S	0	0
			29379	18614	5204	5404	157		
2	G	4170	Total	C	N	O	S	0	0
			29379	18614	5204	5404	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	

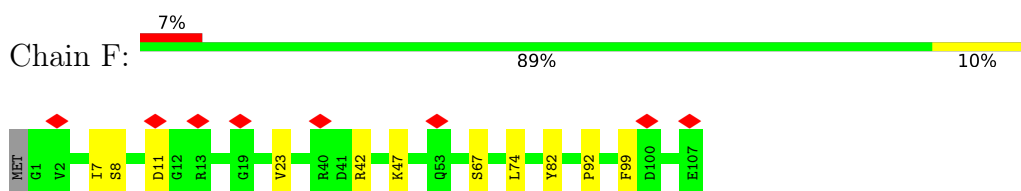
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

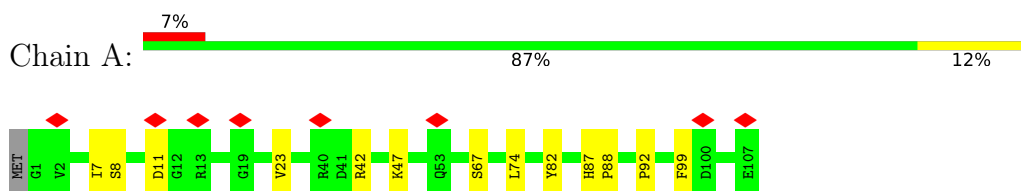
3 Residue-property plots [i](#)

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.

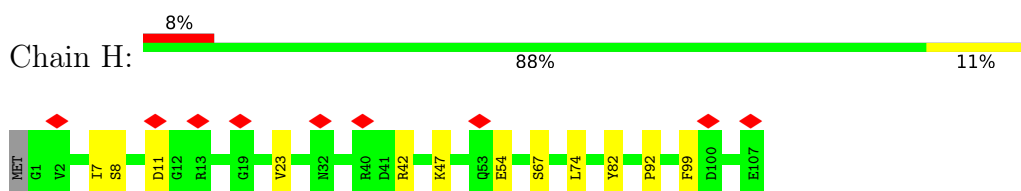
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



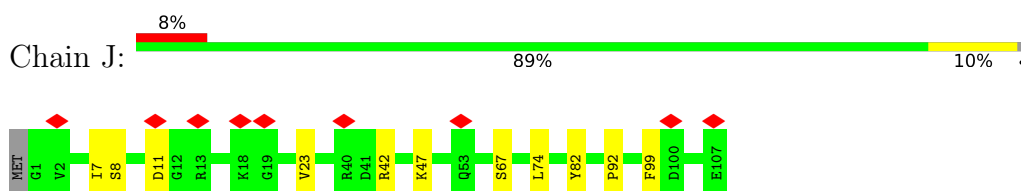
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



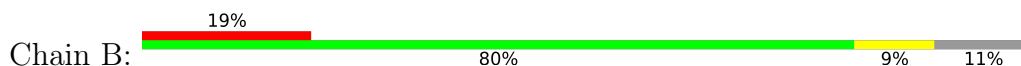
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

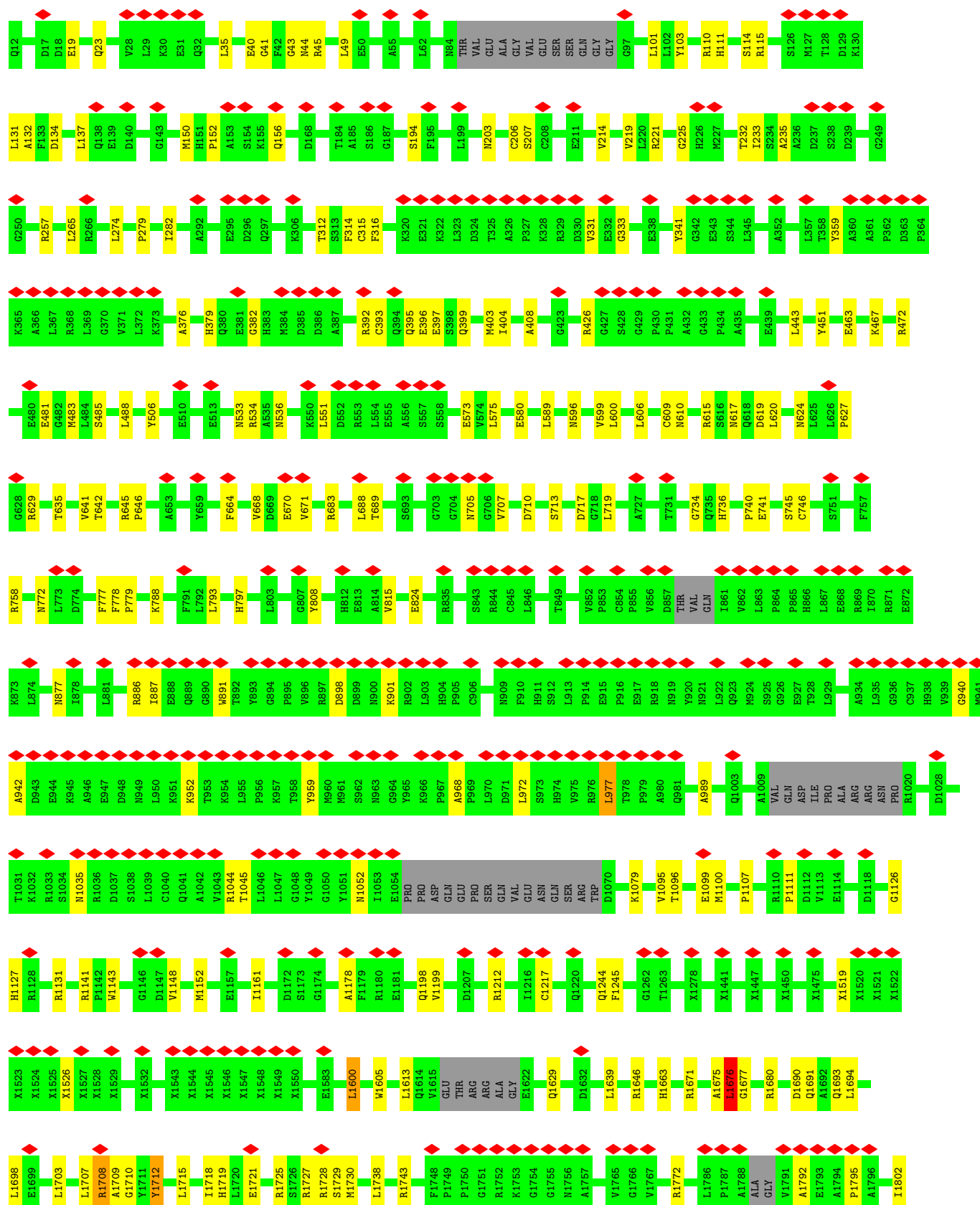


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



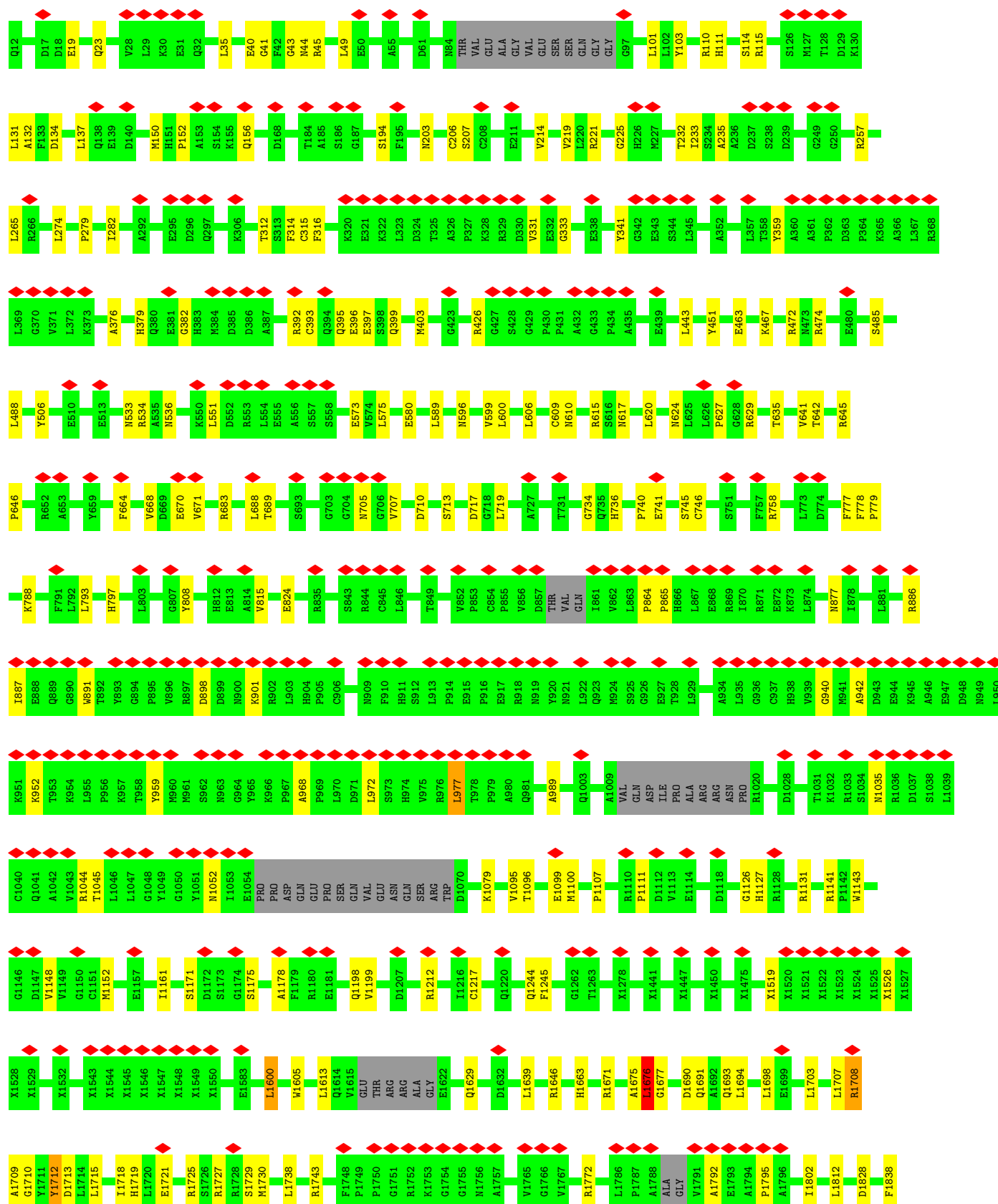
- Molecule 2: Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1





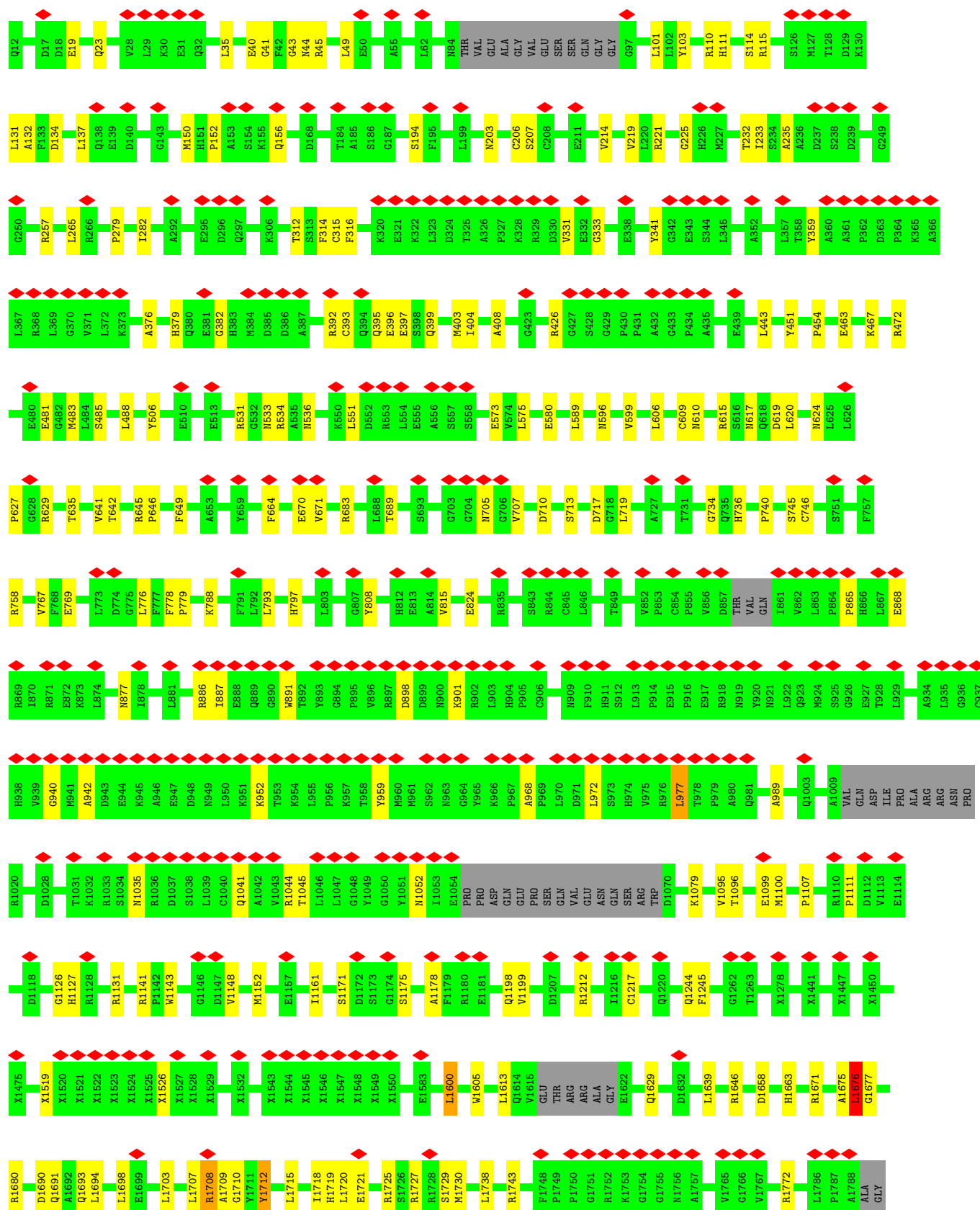




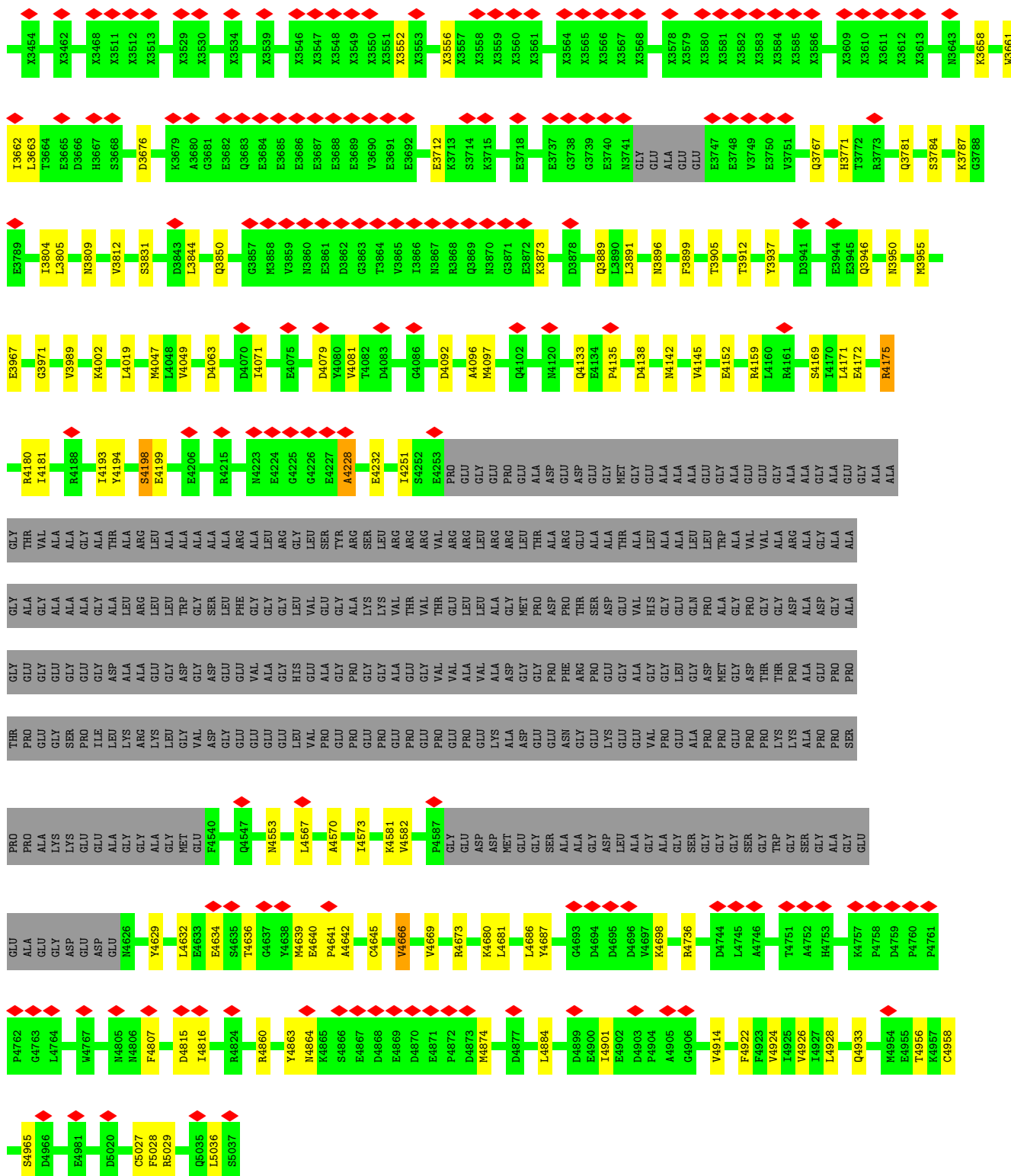




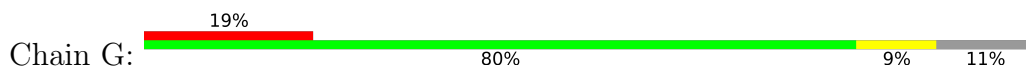


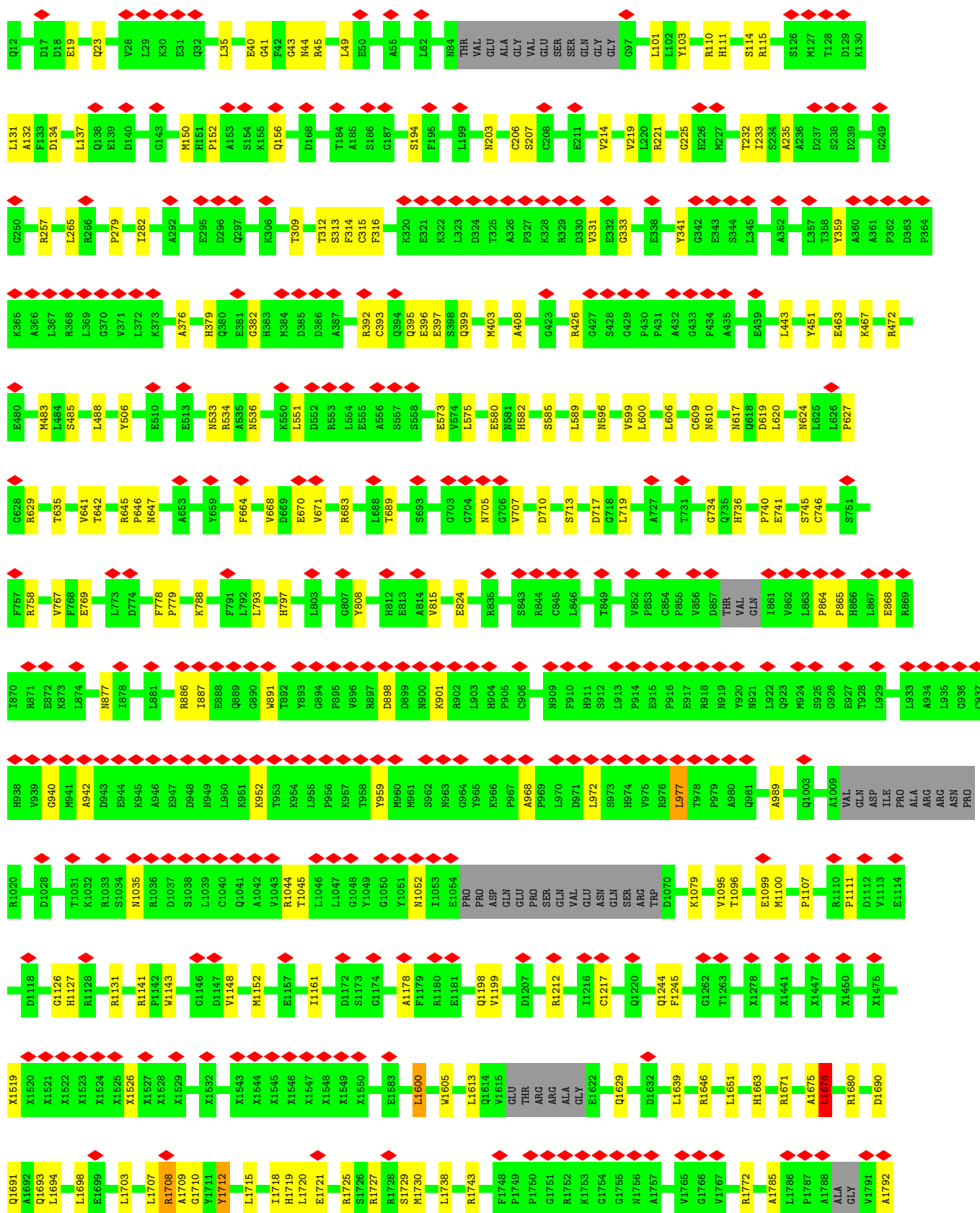






● Molecule 2: Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1,Ryanodine receptor 1









4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
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	0.185	Depositor
Minimum map value	-0.085	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	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: CA, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.27	0/834	0.53	0/1123
1	F	0.27	0/834	0.53	0/1123
1	H	0.27	0/834	0.53	0/1123
1	J	0.27	0/834	0.53	0/1123
2	B	0.35	0/25438	0.60	13/34548 (0.0%)
2	E	0.35	0/25438	0.60	13/34548 (0.0%)
2	G	0.35	0/25438	0.60	13/34548 (0.0%)
2	I	0.35	0/25438	0.60	13/34548 (0.0%)
All	All	0.34	0/105088	0.60	52/142684 (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	3
1	F	0	3
1	H	0	3
1	J	0	3
2	B	0	22
2	E	0	22
2	G	0	22
2	I	0	22
All	All	0	100

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1712	TYR	CA-CB-CG	-6.60	102.02	113.90
2	I	1712	TYR	CA-CB-CG	-6.59	102.03	113.90
2	B	1712	TYR	CA-CB-CG	-6.58	102.06	113.90
2	E	1712	TYR	CA-CB-CG	-6.57	102.07	113.90
2	E	4639	MET	CA-C-N	6.32	137.21	121.80
2	E	4639	MET	C-N-CA	6.32	137.21	121.80
2	B	4639	MET	CA-C-N	6.31	137.20	121.80
2	B	4639	MET	C-N-CA	6.31	137.20	121.80
2	G	4639	MET	CA-C-N	6.30	137.18	121.80
2	G	4639	MET	C-N-CA	6.30	137.18	121.80
2	I	4639	MET	CA-C-N	6.29	137.15	121.80
2	I	4639	MET	C-N-CA	6.29	137.15	121.80
2	G	1872	THR	CA-C-N	5.86	129.61	120.82
2	G	1872	THR	C-N-CA	5.86	129.61	120.82
2	B	1872	THR	CA-C-N	5.85	129.59	120.82
2	B	1872	THR	C-N-CA	5.85	129.59	120.82
2	I	1872	THR	CA-C-N	5.85	129.59	120.82
2	I	1872	THR	C-N-CA	5.85	129.59	120.82
2	E	1872	THR	CA-C-N	5.84	129.58	120.82
2	E	1872	THR	C-N-CA	5.84	129.58	120.82
2	I	1838	PHE	CA-C-N	5.71	132.69	122.13
2	I	1838	PHE	C-N-CA	5.71	132.69	122.13
2	G	1838	PHE	CA-C-N	5.70	132.67	122.13
2	G	1838	PHE	C-N-CA	5.70	132.67	122.13
2	B	1838	PHE	CA-C-N	5.68	132.63	122.13
2	B	1838	PHE	C-N-CA	5.68	132.63	122.13
2	E	1838	PHE	CA-C-N	5.66	132.60	122.13
2	E	1838	PHE	C-N-CA	5.66	132.60	122.13
2	B	1866	ILE	CA-C-N	5.19	129.77	121.62
2	B	1866	ILE	C-N-CA	5.19	129.77	121.62
2	I	1866	ILE	CA-C-N	5.18	129.76	121.62
2	I	1866	ILE	C-N-CA	5.18	129.76	121.62
2	E	1866	ILE	CA-C-N	5.17	129.74	121.62
2	E	1866	ILE	C-N-CA	5.17	129.74	121.62
2	G	1866	ILE	CA-C-N	5.17	129.73	121.62
2	G	1866	ILE	C-N-CA	5.17	129.73	121.62
2	E	4133	GLN	CA-C-N	5.16	134.39	121.80
2	E	4133	GLN	C-N-CA	5.16	134.39	121.80
2	B	4133	GLN	CA-C-N	5.15	134.35	121.80
2	B	4133	GLN	C-N-CA	5.15	134.35	121.80
2	I	4133	GLN	CA-C-N	5.13	134.31	121.80
2	I	4133	GLN	C-N-CA	5.13	134.31	121.80
2	G	4133	GLN	CA-C-N	5.13	134.31	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	4133	GLN	C-N-CA	5.13	134.31	121.80
2	I	977	LEU	CA-C-N	5.07	134.16	121.80
2	I	977	LEU	C-N-CA	5.07	134.16	121.80
2	E	977	LEU	CA-C-N	5.06	134.15	121.80
2	E	977	LEU	C-N-CA	5.06	134.15	121.80
2	G	977	LEU	CA-C-N	5.05	134.13	121.80
2	G	977	LEU	C-N-CA	5.05	134.13	121.80
2	B	977	LEU	CA-C-N	5.05	134.12	121.80
2	B	977	LEU	C-N-CA	5.05	134.12	121.80

There are no chirality outliers.

All (100) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	7	ILE	Peptide
1	A	8	SER	Peptide
1	A	82	TYR	Peptide
2	B	137	LEU	Peptide
2	B	1676	LEU	Peptide
2	B	1690	ASP	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	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	3771	HIS	Peptide
2	B	3971	GLY	Peptide
2	B	4096	ALA	Peptide
2	B	4175	ARG	Peptide
2	B	4198	SER	Peptide
2	B	4228	ALA	Peptide
2	B	4666	VAL	Peptide
2	B	4807	PHE	Peptide
2	B	4958	CYS	Peptide
2	B	624	ASN	Peptide
2	B	808	TYR	Peptide
2	B	977	LEU	Peptide
2	E	137	LEU	Peptide
2	E	1676	LEU	Peptide
2	E	1690	ASP	Peptide

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Mol	Chain	Res	Type	Group
2	E	1795	PRO	Peptide
2	E	1828	ASP	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	3771	HIS	Peptide
2	E	3971	GLY	Peptide
2	E	4096	ALA	Peptide
2	E	4175	ARG	Peptide
2	E	4198	SER	Peptide
2	E	4228	ALA	Peptide
2	E	4666	VAL	Peptide
2	E	4807	PHE	Peptide
2	E	4958	CYS	Peptide
2	E	624	ASN	Peptide
2	E	808	TYR	Peptide
2	E	977	LEU	Peptide
1	F	7	ILE	Peptide
1	F	8	SER	Peptide
1	F	82	TYR	Peptide
2	G	137	LEU	Peptide
2	G	1676	LEU	Peptide
2	G	1690	ASP	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	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	3771	HIS	Peptide
2	G	3971	GLY	Peptide
2	G	4096	ALA	Peptide
2	G	4175	ARG	Peptide
2	G	4198	SER	Peptide
2	G	4228	ALA	Peptide
2	G	4666	VAL	Peptide
2	G	4807	PHE	Peptide
2	G	4958	CYS	Peptide
2	G	624	ASN	Peptide

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Mol	Chain	Res	Type	Group
2	G	808	TYR	Peptide
2	G	977	LEU	Peptide
1	H	7	ILE	Peptide
1	H	8	SER	Peptide
1	H	82	TYR	Peptide
2	I	137	LEU	Peptide
2	I	1676	LEU	Peptide
2	I	1690	ASP	Peptide
2	I	1795	PRO	Peptide
2	I	1828	ASP	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	3771	HIS	Peptide
2	I	3971	GLY	Peptide
2	I	4096	ALA	Peptide
2	I	4175	ARG	Peptide
2	I	4198	SER	Peptide
2	I	4228	ALA	Peptide
2	I	4666	VAL	Peptide
2	I	4807	PHE	Peptide
2	I	4958	CYS	Peptide
2	I	624	ASN	Peptide
2	I	808	TYR	Peptide
2	I	977	LEU	Peptide
1	J	7	ILE	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	6	0
1	F	818	0	824	5	0
1	H	818	0	824	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	818	0	824	5	0
2	B	29379	0	24731	233	0
2	E	29379	0	24730	232	0
2	G	29379	0	24731	235	0
2	I	29379	0	24730	235	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	120796	0	102218	926	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 (926) 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:I:379:HIS:HD2	2:I:382:GLY:H	1.40	0.70
2:G:379:HIS:HD2	2:G:382:GLY:H	1.40	0.70
2:G:2287:ALA:HA	2:G:2290:LEU:HD13	1.75	0.69
2:B:2287:ALA:HA	2:B:2290:LEU:HD13	1.75	0.69
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.74	0.69
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.74	0.69
2:B:379:HIS:HD2	2:B:382:GLY:H	1.40	0.67
2:I:2287:ALA:HA	2:I:2290:LEU:HD13	1.75	0.67
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.74	0.67
2:E:2287:ALA:HA	2:E:2290:LEU:HD13	1.75	0.67
2:E:379:HIS:HD2	2:E:382:GLY:H	1.40	0.67
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.74	0.67
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.77	0.67
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.77	0.66
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.78	0.66
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.78	0.66
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.78	0.66
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.77	0.66
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.78	0.65
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:393:CYS:SG	2:G:395:GLN:NE2	2.71	0.64
2:E:393:CYS:SG	2:E:395:GLN:NE2	2.71	0.64
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.79	0.64
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.79	0.64
2:I:393:CYS:SG	2:I:395:GLN:NE2	2.71	0.64
2:B:393:CYS:SG	2:B:395:GLN:NE2	2.71	0.64
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.81	0.63
2:I:670:GLU:HG3	2:I:788:LYS:H	1.64	0.63
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.79	0.63
2:G:670:GLU:HG3	2:G:788:LYS:H	1.64	0.63
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.81	0.63
2:B:670:GLU:HG3	2:B:788:LYS:H	1.64	0.63
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.79	0.62
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.81	0.62
2:E:670:GLU:HG3	2:E:788:LYS:H	1.64	0.62
1:H:92:PRO:HD3	2:G:627:PRO:HB2	1.81	0.62
2:B:3767:GLN:OE1	2:B:3809:ASN:ND2	2.33	0.62
2:E:3767:GLN:OE1	2:E:3809:ASN:ND2	2.33	0.62
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.81	0.62
2:I:463:GLU:OE2	2:I:467:LYS:NZ	2.33	0.61
2:B:463:GLU:OE2	2:B:467:LYS:NZ	2.33	0.61
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.34	0.61
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.34	0.61
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.34	0.61
2:G:3767:GLN:OE1	2:G:3809:ASN:ND2	2.33	0.61
2:I:4567:LEU:HA	2:I:4816:ILE:HD12	1.83	0.61
2:E:463:GLU:OE2	2:E:467:LYS:NZ	2.33	0.60
2:G:463:GLU:OE2	2:G:467:LYS:NZ	2.33	0.60
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.34	0.60
2:E:4567:LEU:HA	2:E:4816:ILE:HD12	1.83	0.60
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.66	0.60
2:I:645:ARG:HH11	2:I:778:PHE:HE1	1.49	0.60
2:G:4567:LEU:HA	2:G:4816:ILE:HD12	1.83	0.60
2:B:41:GLY:O	2:B:45:ARG:NH1	2.35	0.60
2:B:1148:VAL:HG21	2:B:1212:ARG:HG2	1.84	0.59
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.66	0.59
2:I:3767:GLN:OE1	2:I:3809:ASN:ND2	2.33	0.59
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.85	0.59
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.66	0.59
2:B:4567:LEU:HA	2:B:4816:ILE:HD12	1.83	0.59
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:645:ARG:HH11	2:B:778:PHE:HE1	1.49	0.59
2:I:41:GLY:O	2:I:45:ARG:NH1	2.35	0.59
2:G:1148:VAL:HG21	2:G:1212:ARG:HG2	1.84	0.59
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.35	0.59
2:B:2764:GLU:HG3	2:B:2857:PRO:HB2	1.84	0.59
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.85	0.59
2:I:2764:GLU:HG3	2:I:2857:PRO:HB2	1.84	0.59
2:E:41:GLY:O	2:E:45:ARG:NH1	2.35	0.59
2:E:2764:GLU:HG3	2:E:2857:PRO:HB2	1.84	0.59
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.85	0.59
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.66	0.59
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.67	0.59
2:E:1148:VAL:HG21	2:E:1212:ARG:HG2	1.84	0.58
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.67	0.58
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.85	0.58
2:E:645:ARG:HH11	2:E:778:PHE:HE1	1.49	0.58
2:I:1148:VAL:HG21	2:I:1212:ARG:HG2	1.84	0.58
2:G:41:GLY:O	2:G:45:ARG:NH1	2.35	0.58
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.35	0.58
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.36	0.58
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.85	0.58
2:G:645:ARG:HH11	2:G:778:PHE:HE1	1.49	0.58
2:G:2764:GLU:HG3	2:G:2857:PRO:HB2	1.84	0.58
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.67	0.58
2:B:2758:PHE:O	2:B:2762:THR:N	2.36	0.58
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.86	0.58
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.85	0.58
2:E:359:TYR:HA	2:E:376:ALA:HA	1.85	0.58
2:I:359:TYR:HA	2:I:376:ALA:HA	1.85	0.58
2:B:359:TYR:HA	2:B:376:ALA:HA	1.85	0.58
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.67	0.58
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.85	0.58
2:G:1100:MET:HE2	2:G:1198:GLN:HB3	1.86	0.57
2:G:359:TYR:HA	2:G:376:ALA:HA	1.85	0.57
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.85	0.57
2:I:1100:MET:HE2	2:I:1198:GLN:HB3	1.87	0.57
2:I:2758:PHE:O	2:I:2762:THR:N	2.36	0.57
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.86	0.57
2:B:3809:ASN:HB3	2:B:3812:VAL:HG22	1.86	0.57
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.37	0.57
2:B:1703:LEU:HD12	2:B:1708:ARG:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.37	0.57
2:G:1244:GLN:OE1	2:G:1646:ARG:NH1	2.38	0.57
2:B:35:LEU:HD13	2:B:49:LEU:HD13	1.86	0.57
2:B:1100:MET:HE2	2:B:1198:GLN:HB3	1.87	0.57
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.85	0.57
2:E:1244:GLN:OE1	2:E:1646:ARG:NH1	2.38	0.57
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.85	0.57
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.35	0.57
2:G:1703:LEU:HD12	2:G:1708:ARG:HB2	1.87	0.57
2:B:4933:GLN:OE1	2:E:4933:GLN:NE2	2.37	0.57
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.85	0.57
2:I:4933:GLN:NE2	2:G:4933:GLN:OE1	2.38	0.57
2:B:4914:VAL:HG21	2:E:4884:LEU:HD11	1.87	0.57
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.38	0.57
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.78	0.57
2:I:1244:GLN:OE1	2:I:1646:ARG:NH1	2.38	0.57
2:E:1100:MET:HE2	2:E:1198:GLN:HB3	1.86	0.57
2:I:627:PRO:O	2:I:629:ARG:NH1	2.38	0.57
2:I:1703:LEU:HD12	2:I:1708:ARG:HB2	1.87	0.57
2:G:35:LEU:HD13	2:G:49:LEU:HD13	1.86	0.57
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.78	0.57
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.38	0.56
2:G:533:ASN:ND2	2:G:536:ASN:OD1	2.38	0.56
2:G:627:PRO:O	2:G:629:ARG:NH1	2.38	0.56
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.37	0.56
2:G:2758:PHE:O	2:G:2762:THR:N	2.36	0.56
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.85	0.56
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.38	0.56
2:E:627:PRO:O	2:E:629:ARG:NH1	2.38	0.56
2:B:23:GLN:OE1	2:B:203:ASN:ND2	2.38	0.56
2:E:23:GLN:OE1	2:E:203:ASN:ND2	2.38	0.56
2:I:35:LEU:HD13	2:I:49:LEU:HD13	1.86	0.56
2:I:3809:ASN:HB3	2:I:3812:VAL:HG22	1.86	0.56
2:I:3850:GLN:HB3	2:I:3873:LYS:HD3	1.87	0.56
2:G:23:GLN:OE1	2:G:203:ASN:ND2	2.38	0.56
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.38	0.56
2:G:3809:ASN:HB3	2:G:3812:VAL:HG22	1.86	0.56
2:B:132:ALA:HA	2:B:194:SER:HB2	1.87	0.56
2:B:4933:GLN:NE2	2:I:4933:GLN:OE1	2.38	0.56
2:E:1703:LEU:HD12	2:E:1708:ARG:HB2	1.87	0.56
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:35:LEU:HD13	2:E:49:LEU:HD13	1.86	0.56
2:E:132:ALA:HA	2:E:194:SER:HB2	1.88	0.56
2:E:3809:ASN:HB3	2:E:3812:VAL:HG22	1.86	0.56
2:E:4049:VAL:HG21	2:E:4159:ARG:HD2	1.88	0.56
2:E:4933:GLN:OE1	2:G:4933:GLN:NE2	2.37	0.56
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.86	0.56
2:B:4049:VAL:HG21	2:B:4159:ARG:HD2	1.88	0.56
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.86	0.56
2:B:1244:GLN:OE1	2:B:1646:ARG:NH1	2.38	0.56
2:B:3850:GLN:HB3	2:B:3873:LYS:HD3	1.87	0.56
2:I:793:LEU:HD12	2:I:797:HIS:H	1.71	0.56
2:B:533:ASN:ND2	2:B:536:ASN:OD1	2.38	0.56
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.38	0.56
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.38	0.56
2:B:627:PRO:O	2:B:629:ARG:NH1	2.38	0.56
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	1.88	0.56
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	1.88	0.56
2:I:609:CYS:SG	2:I:610:ASN:N	2.80	0.55
2:I:4049:VAL:HG21	2:I:4159:ARG:HD2	1.88	0.55
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.78	0.55
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.38	0.55
2:E:331:VAL:HG12	2:E:333:GLY:H	1.72	0.55
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	1.88	0.55
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.80	0.55
2:E:3850:GLN:HB3	2:E:3873:LYS:HD3	1.87	0.55
2:I:23:GLN:OE1	2:I:203:ASN:ND2	2.38	0.55
2:G:4049:VAL:HG21	2:G:4159:ARG:HD2	1.88	0.55
2:B:4581:LYS:HD2	2:B:4632:LEU:HD22	1.89	0.55
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.38	0.55
2:G:609:CYS:SG	2:G:610:ASN:N	2.79	0.55
2:B:609:CYS:SG	2:B:610:ASN:N	2.79	0.55
2:E:2758:PHE:O	2:E:2762:THR:N	2.36	0.55
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.80	0.55
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.80	0.55
2:E:4914:VAL:HG21	2:G:4884:LEU:HD11	1.89	0.55
2:G:793:LEU:HD12	2:G:797:HIS:H	1.71	0.55
2:G:3850:GLN:HB3	2:G:3873:LYS:HD3	1.87	0.55
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.80	0.55
2:I:132:ALA:HA	2:I:194:SER:HB2	1.88	0.55
2:G:331:VAL:HG12	2:G:333:GLY:H	1.72	0.55
2:B:4079:ASP:OD2	2:I:4736:ARG:NH1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:101:LEU:HB3	2:I:150:MET:HE1	1.89	0.55
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	1.88	0.55
2:I:4171:LEU:O	2:I:4175:ARG:NH2	2.41	0.54
2:B:101:LEU:HB3	2:B:150:MET:HE1	1.89	0.54
2:E:101:LEU:HB3	2:E:150:MET:HE1	1.89	0.54
2:E:609:CYS:SG	2:E:610:ASN:N	2.79	0.54
2:G:101:LEU:HB3	2:G:150:MET:HE1	1.89	0.54
2:G:132:ALA:HA	2:G:194:SER:HB2	1.88	0.54
2:G:4171:LEU:O	2:G:4175:ARG:NH2	2.41	0.54
2:I:4581:LYS:HD2	2:I:4632:LEU:HD22	1.89	0.54
2:I:4884:LEU:HD11	2:G:4914:VAL:HG21	1.88	0.54
2:B:793:LEU:HD12	2:B:797:HIS:H	1.71	0.54
2:B:1812:LEU:HD21	2:B:1861:GLN:HG2	1.90	0.54
2:I:1694:LEU:O	2:I:1712:TYR:OH	2.23	0.54
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.78	0.54
2:B:331:VAL:HG12	2:B:333:GLY:H	1.72	0.54
2:I:331:VAL:HG12	2:I:333:GLY:H	1.72	0.54
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.38	0.54
2:B:4171:LEU:O	2:B:4175:ARG:NH2	2.41	0.54
2:E:793:LEU:HD12	2:E:797:HIS:H	1.71	0.54
2:I:4198:SER:OG	2:I:4199:GLU:N	2.41	0.54
2:B:2347:GLU:O	2:B:2351:ASN:N	2.41	0.54
2:B:4198:SER:OG	2:B:4199:GLU:N	2.41	0.53
2:I:1812:LEU:HD21	2:I:1861:GLN:HG2	1.90	0.53
2:E:1812:LEU:HD21	2:E:1861:GLN:HG2	1.90	0.53
2:G:2347:GLU:O	2:G:2351:ASN:N	2.41	0.53
2:B:4884:LEU:HD11	2:I:4914:VAL:HG21	1.90	0.53
2:E:1152:MET:HE1	2:E:1217:CYS:HB3	1.90	0.53
2:I:2347:GLU:O	2:I:2351:ASN:N	2.41	0.53
2:G:1152:MET:HE1	2:G:1217:CYS:HB3	1.90	0.53
2:G:4581:LYS:HD2	2:G:4632:LEU:HD22	1.89	0.53
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.90	0.53
2:B:4736:ARG:NH1	2:E:4079:ASP:OD2	2.41	0.53
2:I:1663:HIS:HD2	2:I:1707:LEU:HD11	1.73	0.53
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.90	0.53
2:B:1152:MET:HE1	2:B:1217:CYS:HB3	1.90	0.53
2:E:683:ARG:HG2	2:E:717:ASP:HB3	1.91	0.53
2:E:4171:LEU:O	2:E:4175:ARG:NH2	2.41	0.53
2:E:4581:LYS:HD2	2:E:4632:LEU:HD22	1.89	0.53
2:I:1152:MET:HE1	2:I:1217:CYS:HB3	1.90	0.53
2:G:399:GLN:HG2	2:G:403:MET:HE3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1812:LEU:HD21	2:G:1861:GLN:HG2	1.90	0.53
2:B:399:GLN:HG2	2:B:403:MET:HE3	1.91	0.53
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.42	0.53
2:E:2342:ASN:OD1	2:E:2342:ASN:N	2.34	0.53
2:E:2347:GLU:O	2:E:2351:ASN:N	2.41	0.53
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.38	0.53
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.42	0.53
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.42	0.53
2:I:606:LEU:O	2:I:617:ASN:ND2	2.42	0.53
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.90	0.52
2:B:1663:HIS:HD2	2:B:1707:LEU:HD11	1.74	0.52
2:E:606:LEU:O	2:E:617:ASN:ND2	2.42	0.52
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.42	0.52
2:I:4956:THR:O	2:I:4965:SER:N	2.43	0.52
2:B:156:GLN:HE22	2:E:225:GLY:HA2	1.75	0.52
2:E:4198:SER:OG	2:E:4199:GLU:N	2.41	0.52
2:I:1973:GLN:O	2:I:1977:TYR:N	2.43	0.52
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.43	0.52
2:G:606:LEU:O	2:G:617:ASN:ND2	2.42	0.52
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.90	0.52
2:B:683:ARG:HG2	2:B:717:ASP:HB3	1.91	0.52
2:G:1663:HIS:HD2	2:G:1707:LEU:HD11	1.74	0.52
2:G:1131:ARG:HH12	2:G:1178:ALA:HB3	1.75	0.52
2:B:4956:THR:O	2:B:4965:SER:N	2.43	0.52
2:E:1131:ARG:HH12	2:E:1178:ALA:HB3	1.75	0.52
2:B:606:LEU:O	2:B:617:ASN:ND2	2.42	0.52
2:I:225:GLY:HA2	2:G:156:GLN:HE22	1.74	0.52
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.43	0.52
2:G:2862:LEU:HB3	2:G:2928:LYS:HB3	1.92	0.52
2:I:399:GLN:HG2	2:I:403:MET:HE3	1.91	0.52
2:G:1973:GLN:O	2:G:1977:TYR:N	2.43	0.52
2:G:4956:THR:O	2:G:4965:SER:N	2.43	0.52
2:I:683:ARG:HG2	2:I:717:ASP:HB3	1.91	0.51
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.91	0.51
2:G:2815:ALA:HB3	2:G:2881:ASN:HD21	1.75	0.51
2:B:1131:ARG:HH12	2:B:1178:ALA:HB3	1.75	0.51
2:I:1738:LEU:HB3	2:I:2146:PRO:HD3	1.93	0.51
2:I:2342:ASN:OD1	2:I:2342:ASN:N	2.34	0.51
2:G:4198:SER:OG	2:G:4199:GLU:N	2.41	0.51
2:B:2862:LEU:HB3	2:B:2928:LYS:HB3	1.91	0.51
2:E:399:GLN:HG2	2:E:403:MET:HE3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1663:HIS:HD2	2:E:1707:LEU:HD11	1.74	0.51
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.43	0.51
2:I:4666:VAL:HG23	2:I:4669:VAL:HB	1.93	0.51
2:G:683:ARG:HG2	2:G:717:ASP:HB3	1.91	0.51
2:B:225:GLY:HA2	2:I:156:GLN:HE22	1.74	0.51
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.92	0.51
2:E:1738:LEU:HB3	2:E:2146:PRO:HD3	1.93	0.51
2:I:2862:LEU:HB3	2:I:2928:LYS:HB3	1.91	0.51
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.91	0.51
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.92	0.51
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.92	0.51
2:B:1973:GLN:O	2:B:1977:TYR:N	2.43	0.51
2:B:2131:LEU:HB3	2:B:3662:ILE:HD13	1.93	0.51
2:B:2290:LEU:HG	2:B:2291:GLN:H	1.76	0.51
2:B:4666:VAL:HG23	2:B:4669:VAL:HB	1.93	0.51
2:E:1973:GLN:O	2:E:1977:TYR:N	2.43	0.51
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.91	0.51
2:E:156:GLN:HE22	2:G:225:GLY:HA2	1.76	0.51
2:E:4666:VAL:HG23	2:E:4669:VAL:HB	1.93	0.51
2:I:2131:LEU:HB3	2:I:3662:ILE:HD13	1.93	0.51
2:G:1738:LEU:HB3	2:G:2146:PRO:HD3	1.92	0.51
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.46	0.51
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.43	0.51
2:E:2290:LEU:HG	2:E:2291:GLN:H	1.76	0.51
2:G:1729:SER:HB3	2:G:2163:ARG:HH11	1.76	0.51
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.91	0.50
2:E:4956:THR:O	2:E:4965:SER:N	2.43	0.50
2:G:551:LEU:HD21	2:G:589:LEU:HD13	1.93	0.50
2:B:1738:LEU:HB3	2:B:2146:PRO:HD3	1.92	0.50
2:E:2862:LEU:HB3	2:E:2928:LYS:HB3	1.91	0.50
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.44	0.50
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.45	0.50
2:B:2815:ALA:HB3	2:B:2881:ASN:HD21	1.75	0.50
2:I:1729:SER:HB3	2:I:2163:ARG:HH11	1.76	0.50
2:G:1245:PHE:HD1	2:G:1600:LEU:HB3	1.76	0.50
2:I:4079:ASP:OD2	2:G:4736:ARG:NH1	2.41	0.50
2:E:235:ALA:HA	2:E:257:ARG:HD3	1.93	0.50
2:I:1131:ARG:HH12	2:I:1178:ALA:HB3	1.75	0.50
2:I:2236:LEU:HD23	2:I:2275:VAL:HG21	1.94	0.50
2:I:2290:LEU:HG	2:I:2291:GLN:H	1.76	0.50
2:B:4848:VAL:O	2:B:4852:THR:OG1	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:551:LEU:HD21	2:E:589:LEU:HD13	1.94	0.50
2:E:2236:LEU:HD23	2:E:2275:VAL:HG21	1.94	0.50
2:E:2815:ALA:HB3	2:E:2881:ASN:HD21	1.76	0.50
2:G:2131:LEU:HB3	2:G:3662:ILE:HD13	1.93	0.50
2:G:2236:LEU:HD23	2:G:2275:VAL:HG21	1.94	0.50
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.92	0.50
2:B:2236:LEU:HD23	2:B:2275:VAL:HG21	1.94	0.50
2:I:551:LEU:HD21	2:I:589:LEU:HD13	1.94	0.50
2:G:4666:VAL:HG23	2:G:4669:VAL:HB	1.93	0.50
2:B:235:ALA:HA	2:B:257:ARG:HD3	1.93	0.50
2:B:1729:SER:HB3	2:B:2163:ARG:HH11	1.76	0.50
2:I:235:ALA:HA	2:I:257:ARG:HD3	1.93	0.50
2:I:1245:PHE:HD1	2:I:1600:LEU:HB3	1.76	0.50
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.46	0.50
2:B:1245:PHE:HD1	2:B:1600:LEU:HB3	1.76	0.50
2:E:2131:LEU:HB3	2:E:3662:ILE:HD13	1.93	0.50
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.46	0.50
2:I:1730:MET:O	2:I:1772:ARG:NH1	2.45	0.50
2:G:1675:ALA:HB1	2:G:1676:LEU:HD13	1.94	0.50
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.94	0.49
2:B:551:LEU:HD21	2:B:589:LEU:HD13	1.94	0.49
2:E:1675:ALA:HB1	2:E:1676:LEU:HD13	1.94	0.49
2:I:1840:PRO:O	2:I:1844:LEU:N	2.45	0.49
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.45	0.49
2:G:4092:ASP:OD1	2:G:4092:ASP:N	2.45	0.49
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.45	0.49
2:G:1840:PRO:O	2:G:1844:LEU:N	2.45	0.49
2:G:2290:LEU:HG	2:G:2291:GLN:H	1.76	0.49
2:B:1840:PRO:O	2:B:1844:LEU:N	2.45	0.49
2:E:1245:PHE:HD1	2:E:1600:LEU:HB3	1.76	0.49
2:E:1729:SER:HB3	2:E:2163:ARG:HH11	1.76	0.49
2:I:2815:ALA:HB3	2:I:2881:ASN:HD21	1.75	0.49
2:I:4152:GLU:OE1	2:I:4194:TYR:OH	2.31	0.49
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.46	0.49
2:I:3889:GLN:HG3	2:I:3967:GLU:HG3	1.95	0.49
1:F:92:PRO:HD3	2:E:627:PRO:HB2	1.95	0.49
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.45	0.49
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.45	0.49
2:E:4152:GLU:OE1	2:E:4194:TYR:OH	2.31	0.49
2:B:4092:ASP:OD1	2:B:4092:ASP:N	2.45	0.49
2:E:1730:MET:O	2:E:1772:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2868:SER:O	2:I:2872:GLN:N	2.46	0.49
2:E:580:GLU:HG3	2:E:620:LEU:HD22	1.94	0.49
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.95	0.49
2:I:1096:THR:HG23	2:I:1199:VAL:HG22	1.95	0.49
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.95	0.49
2:G:1730:MET:O	2:G:1772:ARG:NH1	2.45	0.49
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.45	0.49
2:B:1096:THR:HG23	2:B:1199:VAL:HG22	1.95	0.49
2:B:1730:MET:O	2:B:1772:ARG:NH1	2.45	0.49
2:E:2159:LEU:HD22	2:E:2201:LEU:HD23	1.94	0.49
2:I:580:GLU:HG3	2:I:620:LEU:HD22	1.94	0.49
2:G:221:ARG:NH2	2:G:397:GLU:OE2	2.45	0.49
2:G:580:GLU:HG3	2:G:620:LEU:HD22	1.94	0.49
2:E:2823:ILE:HG12	2:E:2937:VAL:HG22	1.95	0.49
2:I:1675:ALA:HB1	2:I:1676:LEU:HD13	1.94	0.49
2:G:3889:GLN:HG3	2:G:3967:GLU:HG3	1.95	0.49
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.45	0.49
2:I:2823:ILE:HG12	2:I:2937:VAL:HG22	1.95	0.49
2:I:4634:GLU:HG3	2:I:4636:THR:H	1.77	0.49
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.95	0.48
2:B:1675:ALA:HB1	2:B:1676:LEU:HD13	1.94	0.48
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.95	0.48
1:F:11:ASP:OD1	1:F:67:SER:OG	2.31	0.48
1:H:11:ASP:OD1	1:H:67:SER:OG	2.31	0.48
2:B:575:LEU:HD22	2:B:609:CYS:HB3	1.95	0.48
2:B:4071:ILE:HG21	2:B:4097:MET:HE1	1.95	0.48
2:E:3889:GLN:HG3	2:E:3967:GLU:HG3	1.95	0.48
2:E:4071:ILE:HG21	2:E:4097:MET:HE1	1.95	0.48
2:G:1096:THR:HG23	2:G:1199:VAL:HG22	1.95	0.48
2:B:4634:GLU:HG3	2:B:4636:THR:H	1.77	0.48
2:I:575:LEU:HD22	2:I:609:CYS:HB3	1.95	0.48
2:G:235:ALA:HA	2:G:257:ARG:HD3	1.93	0.48
2:G:4152:GLU:OE1	2:G:4194:TYR:OH	2.31	0.48
2:B:877:ASN:HD22	2:B:1045:THR:HG23	1.78	0.48
2:E:1096:THR:HG23	2:E:1199:VAL:HG22	1.95	0.48
2:E:1840:PRO:O	2:E:1844:LEU:N	2.45	0.48
2:G:4071:ILE:HG21	2:G:4097:MET:HE1	1.95	0.48
2:G:4634:GLU:HG3	2:G:4636:THR:H	1.77	0.48
2:B:2823:ILE:HG12	2:B:2937:VAL:HG22	1.95	0.48
2:B:4152:GLU:OE1	2:B:4194:TYR:OH	2.31	0.48
2:E:4634:GLU:HG3	2:E:4636:THR:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2159:LEU:HD22	2:I:2201:LEU:HD23	1.94	0.48
2:G:2823:ILE:HG12	2:G:2937:VAL:HG22	1.95	0.48
2:E:940:GLY:O	2:E:1052:ASN:N	2.47	0.48
2:I:4680:LYS:HD3	2:I:4686:LEU:HD22	1.96	0.48
2:G:4680:LYS:HD3	2:G:4686:LEU:HD22	1.96	0.48
2:B:2159:LEU:HD22	2:B:2201:LEU:HD23	1.94	0.48
2:B:3889:GLN:HG3	2:B:3967:GLU:HG3	1.95	0.48
2:E:1694:LEU:O	2:E:1712:TYR:OH	2.23	0.48
2:B:2342:ASN:OD1	2:B:2342:ASN:N	2.34	0.48
2:E:645:ARG:O	2:E:824:GLU:N	2.47	0.48
2:I:940:GLY:O	2:I:1052:ASN:N	2.47	0.48
2:I:4071:ILE:HG21	2:I:4097:MET:HE1	1.95	0.48
2:B:940:GLY:O	2:B:1052:ASN:N	2.47	0.48
2:E:4680:LYS:HD3	2:E:4686:LEU:HD22	1.96	0.48
2:G:2159:LEU:HD22	2:G:2201:LEU:HD23	1.94	0.48
2:E:2868:SER:O	2:E:2872:GLN:N	2.46	0.48
2:G:689:THR:H	2:G:778:PHE:HE2	1.62	0.48
2:G:2868:SER:O	2:G:2872:GLN:N	2.46	0.48
2:G:3552:UNK:O	2:G:3556:UNK:N	2.47	0.48
2:B:645:ARG:O	2:B:824:GLU:N	2.47	0.47
2:B:734:GLY:O	2:B:736:HIS:ND1	2.47	0.47
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.96	0.47
2:I:4092:ASP:OD1	2:I:4092:ASP:N	2.45	0.47
2:I:4629:TYR:OH	2:G:4860:ARG:NH2	2.42	0.47
2:E:4092:ASP:N	2:E:4092:ASP:OD1	2.45	0.47
2:I:3552:UNK:O	2:I:3556:UNK:N	2.47	0.47
2:B:221:ARG:NH2	2:B:397:GLU:OE2	2.45	0.47
2:B:689:THR:H	2:B:778:PHE:HE2	1.61	0.47
2:B:2267:MET:HE3	2:B:2268:GLN:HG2	1.96	0.47
2:E:4063:ASP:OD1	2:E:4169:SER:OG	2.28	0.47
2:I:2267:MET:HE3	2:I:2268:GLN:HG2	1.96	0.47
2:G:265:LEU:HD12	2:G:279:PRO:HB2	1.97	0.47
2:G:940:GLY:O	2:G:1052:ASN:N	2.47	0.47
1:A:11:ASP:OD1	1:A:67:SER:OG	2.31	0.47
2:B:2022:PRO:HB2	2:B:2024:PRO:HD2	1.96	0.47
2:B:4680:LYS:HD3	2:B:4686:LEU:HD22	1.96	0.47
2:E:4736:ARG:NH1	2:G:4079:ASP:OD2	2.42	0.47
2:I:877:ASN:HD22	2:I:1045:THR:HG23	1.78	0.47
2:B:219:VAL:O	2:B:392:ARG:NH1	2.48	0.47
2:E:265:LEU:HD12	2:E:279:PRO:HB2	1.96	0.47
2:I:219:VAL:O	2:I:392:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:534:ARG:NH2	2:I:573:GLU:OE2	2.42	0.47
2:B:580:GLU:HG3	2:B:620:LEU:HD22	1.94	0.47
2:E:1839:VAL:O	2:E:1841:VAL:N	2.48	0.47
2:I:4228:ALA:O	2:I:4232:GLU:N	2.48	0.47
2:B:2868:SER:O	2:B:2872:GLN:N	2.46	0.47
2:E:575:LEU:HD22	2:E:609:CYS:HB3	1.95	0.47
2:E:3552:UNK:O	2:E:3556:UNK:N	2.47	0.47
2:I:734:GLY:O	2:I:736:HIS:ND1	2.47	0.47
2:G:219:VAL:O	2:G:392:ARG:NH1	2.48	0.47
2:G:645:ARG:O	2:G:824:GLU:N	2.47	0.47
2:G:877:ASN:HD22	2:G:1045:THR:HG23	1.78	0.47
2:G:4978:HIS:ND1	2:G:4982:GLU:OE1	2.32	0.47
2:E:4978:HIS:ND1	2:E:4982:GLU:OE1	2.32	0.47
2:I:1839:VAL:O	2:I:1841:VAL:N	2.48	0.47
2:G:3770:LEU:HD12	2:G:3770:LEU:HA	1.74	0.47
2:G:4228:ALA:O	2:G:4232:GLU:N	2.48	0.47
2:B:111:HIS:CD2	2:B:114:SER:H	2.33	0.47
2:B:615:ARG:NH1	2:B:1677:GLY:O	2.39	0.47
2:B:3781:GLN:HA	2:B:3784:SER:HB3	1.97	0.47
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.80	0.47
2:E:2022:PRO:HB2	2:E:2024:PRO:HD2	1.96	0.47
2:E:4181:ILE:HG22	2:E:4193:ILE:HB	1.97	0.47
2:I:265:LEU:HD12	2:I:279:PRO:HB2	1.97	0.47
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.80	0.47
2:I:1792:ALA:HB2	2:I:2173:GLN:HG3	1.97	0.47
2:I:3989:VAL:HG12	2:I:4047:MET:HE1	1.97	0.47
2:G:575:LEU:HD22	2:G:609:CYS:HB3	1.95	0.47
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.96	0.47
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.80	0.47
2:E:111:HIS:CD2	2:E:114:SER:H	2.33	0.47
2:E:3989:VAL:HG12	2:E:4047:MET:HE1	1.97	0.47
2:I:111:HIS:CD2	2:I:114:SER:H	2.33	0.47
2:I:221:ARG:NH2	2:I:397:GLU:OE2	2.45	0.47
2:I:689:THR:H	2:I:778:PHE:HE2	1.62	0.47
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.96	0.47
2:I:2022:PRO:HB2	2:I:2024:PRO:HD2	1.96	0.47
2:G:111:HIS:CD2	2:G:114:SER:H	2.33	0.47
2:B:1839:VAL:O	2:B:1841:VAL:N	2.48	0.46
2:E:877:ASN:HD22	2:E:1045:THR:HG23	1.78	0.46
2:E:1715:LEU:HD12	2:E:1719:HIS:HD2	1.80	0.46
2:G:1792:ALA:HB2	2:G:2173:GLN:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3552:UNK:O	2:B:3556:UNK:N	2.48	0.46
2:G:734:GLY:O	2:G:736:HIS:ND1	2.47	0.46
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.80	0.46
2:G:1715:LEU:HD12	2:G:1719:HIS:HD2	1.80	0.46
2:B:265:LEU:HD12	2:B:279:PRO:HB2	1.96	0.46
2:B:4228:ALA:O	2:B:4232:GLU:N	2.48	0.46
2:E:689:THR:H	2:E:778:PHE:HE2	1.62	0.46
2:E:898:ASP:HB3	2:E:901:LYS:HB2	1.98	0.46
2:E:2267:MET:HE3	2:E:2268:GLN:HG2	1.96	0.46
2:I:645:ARG:O	2:I:824:GLU:N	2.47	0.46
2:G:898:ASP:HB3	2:G:901:LYS:HB2	1.98	0.46
2:G:1839:VAL:O	2:G:1841:VAL:N	2.48	0.46
2:G:2022:PRO:HB2	2:G:2024:PRO:HD2	1.96	0.46
2:G:4181:ILE:HG22	2:G:4193:ILE:HB	1.97	0.46
1:J:92:PRO:HD3	2:I:627:PRO:HB2	1.97	0.46
2:B:396:GLU:OE2	2:B:451:TYR:OH	2.34	0.46
2:G:2267:MET:HE3	2:G:2268:GLN:HG2	1.96	0.46
2:G:4848:VAL:O	2:G:4852:THR:OG1	2.28	0.46
2:B:1715:LEU:HD12	2:B:1719:HIS:HD2	1.80	0.46
2:I:2827:ARG:HH21	2:I:2931:GLN:HG3	1.81	0.46
2:G:534:ARG:NH2	2:G:573:GLU:OE2	2.42	0.46
2:G:617:ASN:OD1	2:G:617:ASN:N	2.49	0.46
2:G:619:ASP:OD1	2:G:1680:ARG:NH1	2.40	0.46
2:B:3989:VAL:HG12	2:B:4047:MET:HE1	1.97	0.46
2:I:898:ASP:HB3	2:I:901:LYS:HB2	1.98	0.46
2:G:2827:ARG:HH21	2:G:2931:GLN:HG3	1.81	0.46
2:B:898:ASP:HB3	2:B:901:LYS:HB2	1.98	0.46
2:B:2827:ARG:HH21	2:B:2931:GLN:HG3	1.81	0.46
2:E:219:VAL:O	2:E:392:ARG:NH1	2.48	0.46
2:G:2745:VAL:HG21	2:G:2818:ALA:HB2	1.98	0.46
2:I:396:GLU:OE2	2:I:451:TYR:OH	2.34	0.46
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.98	0.46
2:I:1772:ARG:HH21	2:I:1952:GLN:NE2	2.14	0.46
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.97	0.46
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.96	0.46
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.98	0.46
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.98	0.46
2:B:1772:ARG:HH21	2:B:1952:GLN:NE2	2.14	0.46
2:G:3989:VAL:HG12	2:G:4047:MET:HE1	1.98	0.46
2:E:111:HIS:HD2	2:E:114:SER:H	1.64	0.46
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2745:VAL:HG21	2:E:2818:ALA:HB2	1.98	0.46
2:I:485:SER:HA	2:I:488:LEU:HB2	1.98	0.46
2:I:1715:LEU:HD12	2:I:1719:HIS:HD2	1.80	0.46
2:I:4181:ILE:HG22	2:I:4193:ILE:HB	1.97	0.46
2:G:3781:GLN:HA	2:G:3784:SER:HB3	1.97	0.46
1:J:11:ASP:OD1	1:J:67:SER:OG	2.31	0.45
2:B:1792:ALA:HB2	2:B:2173:GLN:HG3	1.97	0.45
2:E:1772:ARG:HH21	2:E:1952:GLN:NE2	2.14	0.45
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.81	0.45
2:G:2288:LEU:O	2:G:3873:LYS:NZ	2.41	0.45
2:B:4181:ILE:HG22	2:B:4193:ILE:HB	1.97	0.45
2:B:4629:TYR:OH	2:I:4860:ARG:NH2	2.41	0.45
2:B:4860:ARG:NH2	2:E:4629:TYR:OH	2.40	0.45
2:I:2029:GLN:O	2:I:2033:ASP:N	2.49	0.45
2:G:485:SER:HA	2:G:488:LEU:HB2	1.98	0.45
2:E:1099:GLU:OE2	2:E:1127:HIS:ND1	2.38	0.45
2:E:2827:ARG:HH21	2:E:2931:GLN:HG3	1.81	0.45
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.98	0.45
2:E:3781:GLN:HA	2:E:3784:SER:HB3	1.97	0.45
2:E:5027:CYS:O	2:E:5029:ARG:N	2.48	0.45
2:B:668:VAL:O	2:B:741:GLU:N	2.47	0.45
2:B:1694:LEU:O	2:B:1712:TYR:OH	2.23	0.45
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.82	0.45
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.50	0.45
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.82	0.45
2:I:2024:PRO:O	2:I:2028:ARG:NE	2.40	0.45
2:B:619:ASP:OD1	2:B:1680:ARG:NH1	2.40	0.45
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.81	0.45
2:E:485:SER:HA	2:E:488:LEU:HB2	1.98	0.45
2:E:1792:ALA:HB2	2:E:2173:GLN:HG3	1.97	0.45
2:I:596:ASN:HB3	2:I:599:VAL:HG22	1.99	0.45
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.82	0.45
2:G:596:ASN:HB3	2:G:599:VAL:HG22	1.99	0.45
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.98	0.45
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.50	0.45
2:E:221:ARG:NH2	2:E:397:GLU:OE2	2.45	0.45
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.98	0.45
2:B:596:ASN:HB3	2:B:599:VAL:HG22	1.99	0.45
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.82	0.45
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.98	0.45
2:E:396:GLU:OE2	2:E:451:TYR:OH	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:596:ASN:HB3	2:E:599:VAL:HG22	1.99	0.45
2:E:668:VAL:O	2:E:741:GLU:N	2.47	0.45
2:E:4228:ALA:O	2:E:4232:GLU:N	2.48	0.45
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.98	0.45
2:B:617:ASN:N	2:B:617:ASN:OD1	2.49	0.45
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.50	0.45
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	1.98	0.45
2:E:2747:ILE:HG12	2:E:2817:ILE:HD12	1.99	0.45
2:I:111:HIS:HD2	2:I:114:SER:H	1.64	0.45
2:B:485:SER:HA	2:B:488:LEU:HB2	1.98	0.45
2:B:534:ARG:NH2	2:B:573:GLU:OE2	2.42	0.45
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	1.98	0.45
2:I:4864:ASN:H	2:I:4874:MET:HE3	1.82	0.45
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.81	0.45
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.25	0.45
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.50	0.44
2:B:2765:LYS:HA	2:B:2859:PRO:HG3	1.99	0.44
2:E:40:GLU:HB3	2:E:44:ASN:HB3	1.99	0.44
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.98	0.44
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.99	0.44
2:I:232:THR:OG1	2:I:233:ILE:N	2.50	0.44
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.98	0.44
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.50	0.44
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.98	0.44
2:B:1855:GLY:H	2:B:1858:ASP:HB2	1.83	0.44
2:B:4864:ASN:H	2:B:4874:MET:HE3	1.82	0.44
2:E:615:ARG:NH1	2:E:1677:GLY:O	2.39	0.44
2:E:788:LYS:HG2	2:E:1629:GLN:HA	1.99	0.44
2:I:1099:GLU:OE2	2:I:1127:HIS:ND1	2.38	0.44
2:G:40:GLU:HB3	2:G:44:ASN:HB3	1.99	0.44
2:G:396:GLU:OE2	2:G:451:TYR:OH	2.34	0.44
2:G:788:LYS:HG2	2:G:1629:GLN:HA	1.99	0.44
2:G:1855:GLY:H	2:G:1858:ASP:HB2	1.82	0.44
2:B:2231:SER:HA	2:B:2234:ARG:HG2	2.00	0.44
2:I:1855:GLY:H	2:I:1858:ASP:HB2	1.82	0.44
2:I:2231:SER:HA	2:I:2234:ARG:HG2	2.00	0.44
2:I:2288:LEU:O	2:I:3873:LYS:NZ	2.41	0.44
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	1.98	0.44
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.99	0.44
2:G:2024:PRO:O	2:G:2028:ARG:NE	2.40	0.44
2:B:40:GLU:HB3	2:B:44:ASN:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.81	0.44
2:B:111:HIS:HD2	2:B:114:SER:H	1.64	0.44
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.99	0.44
2:B:2029:GLN:O	2:B:2033:ASP:N	2.49	0.44
2:B:2745:VAL:HG21	2:B:2818:ALA:HB2	1.98	0.44
2:I:40:GLU:HB3	2:I:44:ASN:HB3	1.99	0.44
2:I:2188:ASN:N	2:I:2188:ASN:OD1	2.49	0.44
2:I:2745:VAL:HG21	2:I:2818:ALA:HB2	1.98	0.44
2:I:2747:ILE:HG12	2:I:2817:ILE:HD12	1.99	0.44
2:G:2342:ASN:OD1	2:G:2342:ASN:N	2.34	0.44
2:B:788:LYS:HG2	2:B:1629:GLN:HA	1.99	0.44
2:E:1855:GLY:H	2:E:1858:ASP:HB2	1.82	0.44
2:E:4864:ASN:H	2:E:4874:MET:HE3	1.82	0.44
2:I:4642:ALA:HA	2:I:4645:CYS:HB2	2.00	0.44
2:G:111:HIS:HD2	2:G:114:SER:H	1.64	0.44
2:B:5027:CYS:O	2:B:5029:ARG:N	2.48	0.44
2:E:4642:ALA:HA	2:E:4645:CYS:HB2	2.00	0.44
2:G:43:GLY:HA2	2:G:443:LEU:HG	2.00	0.44
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.50	0.44
2:G:2029:GLN:O	2:G:2033:ASP:N	2.49	0.44
2:G:4864:ASN:H	2:G:4874:MET:HE3	1.82	0.44
2:B:3770:LEU:HD12	2:B:3770:LEU:HA	1.74	0.44
2:E:617:ASN:N	2:E:617:ASN:OD1	2.49	0.44
2:E:2231:SER:HA	2:E:2234:ARG:HG2	2.00	0.44
2:I:2765:LYS:HA	2:I:2859:PRO:HG3	1.99	0.44
2:G:2102:VAL:HB	2:G:2124:LEU:HD12	1.99	0.44
2:E:2102:VAL:HB	2:E:2124:LEU:HD12	1.99	0.44
2:E:2765:LYS:HA	2:E:2859:PRO:HG3	1.98	0.44
2:I:942:ALA:HB2	2:I:1052:ASN:HB2	2.00	0.44
2:G:1772:ARG:HH21	2:G:1952:GLN:NE2	2.14	0.44
2:G:2747:ILE:HG12	2:G:2817:ILE:HD12	1.99	0.44
2:G:4642:ALA:HA	2:G:4645:CYS:HB2	2.00	0.44
2:B:134:ASP:OD1	2:B:134:ASP:N	2.51	0.44
2:B:2747:ILE:HG12	2:B:2817:ILE:HD12	1.99	0.44
2:B:3365:UNK:O	2:B:3369:UNK:N	2.51	0.44
2:E:4138:ASP:OD1	2:E:4138:ASP:N	2.51	0.44
2:I:615:ARG:NH1	2:I:1677:GLY:O	2.39	0.44
2:I:788:LYS:HG2	2:I:1629:GLN:HA	1.99	0.44
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.50	0.44
2:I:2739:PRO:HD2	2:I:2888:ARG:HH21	1.83	0.44
2:G:232:THR:OG1	2:G:233:ILE:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4642:ALA:HA	2:B:4645:CYS:HB2	2.00	0.43
2:B:4924:VAL:HA	2:B:4928:LEU:HB2	2.00	0.43
2:E:43:GLY:HA2	2:E:443:LEU:HG	2.00	0.43
2:G:2231:SER:HA	2:G:2234:ARG:HG2	2.00	0.43
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.98	0.43
2:G:4815:ASP:OD1	2:G:4815:ASP:N	2.50	0.43
2:B:2447:LYS:HG3	2:B:2449:GLU:H	1.83	0.43
2:B:2739:PRO:HD2	2:B:2888:ARG:HH21	1.83	0.43
2:E:2447:LYS:HG3	2:E:2449:GLU:H	1.83	0.43
2:G:206:CYS:SG	2:G:207:SER:N	2.92	0.43
2:G:668:VAL:O	2:G:741:GLU:N	2.47	0.43
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	1.98	0.43
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	2.00	0.43
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	2.00	0.43
2:G:309:THR:O	2:G:313:SER:OG	2.29	0.43
2:G:1707:LEU:O	2:G:1709:ALA:N	2.51	0.43
2:B:942:ALA:HB2	2:B:1052:ASN:HB2	2.00	0.43
2:E:734:GLY:O	2:E:736:HIS:ND1	2.47	0.43
2:E:4681:LEU:HD21	2:E:4687:TYR:HD2	1.84	0.43
2:I:206:CYS:SG	2:I:207:SER:N	2.92	0.43
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.99	0.43
2:B:1707:LEU:O	2:B:1709:ALA:N	2.51	0.43
2:E:206:CYS:SG	2:E:207:SER:N	2.92	0.43
2:G:2188:ASN:N	2:G:2188:ASN:OD1	2.49	0.43
2:G:2765:LYS:HA	2:G:2859:PRO:HG3	1.98	0.43
1:A:92:PRO:HD3	2:B:627:PRO:HB2	2.00	0.43
2:B:206:CYS:SG	2:B:207:SER:N	2.92	0.43
2:B:2102:VAL:HB	2:B:2124:LEU:HD12	1.99	0.43
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.52	0.43
2:E:1707:LEU:O	2:E:1709:ALA:N	2.51	0.43
2:E:2739:PRO:HD2	2:E:2888:ARG:HH21	1.83	0.43
2:I:43:GLY:HA2	2:I:443:LEU:HG	2.00	0.43
2:I:2447:LYS:HG3	2:I:2449:GLU:H	1.83	0.43
2:G:4924:VAL:HA	2:G:4928:LEU:HB2	2.00	0.43
2:B:43:GLY:HA2	2:B:443:LEU:HG	2.00	0.43
2:E:232:THR:OG1	2:E:233:ILE:N	2.51	0.43
2:E:635:THR:HG23	2:E:1693:GLN:HE22	1.84	0.43
2:E:2188:ASN:N	2:E:2188:ASN:OD1	2.49	0.43
2:I:4681:LEU:HD21	2:I:4687:TYR:HD2	1.84	0.43
2:G:635:THR:HG23	2:G:1693:GLN:HE22	1.84	0.43
2:G:5027:CYS:O	2:G:5029:ARG:N	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1126:GLY:HA3	2:E:1143:TRP:CE2	2.54	0.43
2:E:4142:ASN:HA	2:E:4145:VAL:HG12	2.01	0.43
2:E:4924:VAL:HA	2:E:4928:LEU:HB2	2.00	0.43
2:I:2102:VAL:HB	2:I:2124:LEU:HD12	1.99	0.43
2:G:134:ASP:OD1	2:G:134:ASP:N	2.51	0.43
2:G:3905:THR:HA	2:G:3912:THR:HG23	2.01	0.43
2:G:4681:LEU:HD21	2:G:4687:TYR:HD2	1.84	0.43
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.54	0.43
2:E:942:ALA:HB2	2:E:1052:ASN:HB2	2.00	0.43
2:I:710:ASP:OD1	2:I:710:ASP:N	2.52	0.43
2:G:2447:LYS:HG3	2:G:2449:GLU:H	1.83	0.43
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.25	0.43
2:B:4681:LEU:HD21	2:B:4687:TYR:HD2	1.84	0.43
2:I:4063:ASP:OD1	2:I:4169:SER:OG	2.28	0.43
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.50	0.43
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	2.00	0.43
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.54	0.43
2:G:4791:TYR:OH	2:G:4815:ASP:O	2.33	0.43
2:B:232:THR:OG1	2:B:233:ILE:N	2.50	0.42
2:B:710:ASP:OD1	2:B:710:ASP:N	2.52	0.42
2:B:1126:GLY:HA3	2:B:1143:TRP:CE2	2.54	0.42
2:I:3804:ILE:HG22	2:I:3812:VAL:HG21	2.01	0.42
2:I:4138:ASP:OD1	2:I:4138:ASP:N	2.51	0.42
2:G:2739:PRO:HD2	2:G:2888:ARG:HH21	1.83	0.42
2:G:4063:ASP:OD1	2:G:4169:SER:OG	2.28	0.42
2:B:2188:ASN:OD1	2:B:2188:ASN:N	2.49	0.42
2:B:4063:ASP:OD1	2:B:4169:SER:OG	2.28	0.42
2:G:315:CYS:SG	2:G:316:PHE:N	2.92	0.42
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	2.01	0.42
2:E:534:ARG:NH2	2:E:573:GLU:OE2	2.43	0.42
2:E:2788:HIS:HE1	2:E:2790:MET:HB2	1.84	0.42
2:I:619:ASP:OD1	2:I:1680:ARG:NH1	2.40	0.42
2:I:1707:LEU:O	2:I:1709:ALA:N	2.51	0.42
2:I:2788:HIS:HE1	2:I:2790:MET:HB2	1.84	0.42
2:I:2827:ARG:H	2:I:2934:GLY:HA3	1.85	0.42
2:G:2827:ARG:H	2:G:2934:GLY:HA3	1.85	0.42
2:G:3365:UNK:O	2:G:3369:UNK:N	2.52	0.42
2:G:4138:ASP:OD1	2:G:4138:ASP:N	2.51	0.42
2:B:3676:ASP:OD1	2:B:3676:ASP:N	2.52	0.42
2:E:134:ASP:OD1	2:E:134:ASP:N	2.51	0.42
2:E:2029:GLN:O	2:E:2033:ASP:N	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2339:VAL:HG12	2:E:2345:SER:H	1.85	0.42
2:E:3365:UNK:O	2:E:3369:UNK:N	2.52	0.42
2:I:1171:SER:HG	2:I:1175:SER:H	1.63	0.42
2:I:1840:PRO:HB3	2:I:1843:LYS:HB3	2.02	0.42
2:I:3365:UNK:O	2:I:3369:UNK:N	2.52	0.42
2:I:3905:THR:HA	2:I:3912:THR:HG23	2.01	0.42
2:I:4142:ASN:HA	2:I:4145:VAL:HG12	2.01	0.42
2:I:4815:ASP:OD1	2:I:4815:ASP:N	2.50	0.42
2:I:4924:VAL:HA	2:I:4928:LEU:HB2	2.00	0.42
2:G:942:ALA:HB2	2:G:1052:ASN:HB2	2.00	0.42
1:A:87:HIS:HA	1:A:88:PRO:HD3	1.94	0.42
2:B:1840:PRO:HB3	2:B:1843:LYS:HB3	2.02	0.42
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.49	0.42
2:B:2788:HIS:HE1	2:B:2790:MET:HB2	1.84	0.42
2:B:2827:ARG:H	2:B:2934:GLY:HA3	1.85	0.42
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.49	0.42
2:I:315:CYS:SG	2:I:316:PHE:N	2.92	0.42
2:I:2215:LEU:HD21	2:I:2272:PRO:HG3	2.02	0.42
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	2.01	0.42
2:G:3804:ILE:HG22	2:G:3812:VAL:HG21	2.01	0.42
2:G:4922:PHE:HA	2:G:4926:VAL:HG12	2.01	0.42
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.52	0.42
2:B:4142:ASN:HA	2:B:4145:VAL:HG12	2.01	0.42
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.52	0.42
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	2.01	0.42
2:I:4922:PHE:HA	2:I:4926:VAL:HG12	2.01	0.42
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.52	0.42
2:G:4142:ASN:HA	2:G:4145:VAL:HG12	2.01	0.42
2:B:635:THR:HG23	2:B:1693:GLN:HE22	1.84	0.42
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	2.00	0.42
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	2.01	0.42
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	2.00	0.42
2:E:315:CYS:SG	2:E:316:PHE:N	2.92	0.42
2:E:710:ASP:N	2:E:710:ASP:OD1	2.52	0.42
2:E:2827:ARG:H	2:E:2934:GLY:HA3	1.85	0.42
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	2.01	0.42
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	2.01	0.42
2:G:282:ILE:HD12	2:G:314:PHE:HD2	1.85	0.42
2:G:1099:GLU:OE2	2:G:1127:HIS:ND1	2.38	0.42
2:G:2788:HIS:CE1	2:G:2790:MET:HB2	2.55	0.42
2:G:2788:HIS:HE1	2:G:2790:MET:HB2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3905:THR:HA	2:B:3912:THR:HG23	2.01	0.42
2:B:4922:PHE:HA	2:B:4926:VAL:HG12	2.01	0.42
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	2.01	0.42
2:E:2788:HIS:CE1	2:E:2790:MET:HB2	2.54	0.42
2:I:635:THR:HG23	2:I:1693:GLN:HE22	1.84	0.42
2:I:886:ARG:HB3	2:I:891:TRP:HB2	2.02	0.42
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	2.00	0.42
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.54	0.42
2:I:2788:HIS:CE1	2:I:2790:MET:HB2	2.55	0.42
2:B:282:ILE:HD12	2:B:314:PHE:HD2	1.85	0.42
2:B:2215:LEU:HD21	2:B:2272:PRO:HG3	2.02	0.42
2:B:3891:LEU:HB3	2:B:3899:PHE:CE2	2.55	0.42
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.54	0.42
2:I:1126:GLY:HA3	2:I:1143:TRP:CE2	2.54	0.42
2:I:3676:ASP:OD1	2:I:3676:ASP:N	2.52	0.42
2:I:5027:CYS:O	2:I:5029:ARG:N	2.48	0.42
2:G:3891:LEU:HB3	2:G:3899:PHE:CE2	2.55	0.42
1:H:54:GLU:O	2:G:1785:ALA:N	2.53	0.42
2:B:599:VAL:HG23	2:B:600:LEU:HD12	2.02	0.42
2:B:642:THR:HG23	2:B:1613:LEU:HD12	2.02	0.42
2:B:2339:VAL:HG12	2:B:2345:SER:H	1.85	0.42
2:E:2290:LEU:HD21	2:E:2349:ASN:HA	2.01	0.42
2:E:3891:LEU:HB3	2:E:3899:PHE:CE2	2.55	0.42
2:G:886:ARG:HB3	2:G:891:TRP:HB2	2.02	0.42
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	2.01	0.42
2:G:3676:ASP:OD1	2:G:3676:ASP:N	2.52	0.42
2:B:1727:ARG:HH12	2:B:1772:ARG:HB3	1.85	0.41
2:B:2290:LEU:HD21	2:B:2349:ASN:HA	2.01	0.41
2:B:2346:VAL:O	2:B:2349:ASN:ND2	2.53	0.41
2:E:282:ILE:HD12	2:E:314:PHE:HD2	1.85	0.41
2:E:864:PRO:HA	2:E:865:PRO:HD3	1.89	0.41
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.49	0.41
2:I:2290:LEU:HD21	2:I:2349:ASN:HA	2.01	0.41
2:G:1126:GLY:HA3	2:G:1143:TRP:CE2	2.54	0.41
2:G:2215:LEU:HD21	2:G:2272:PRO:HG3	2.02	0.41
2:B:1099:GLU:OE2	2:B:1127:HIS:ND1	2.38	0.41
2:E:395:GLN:HG3	2:E:397:GLU:H	1.85	0.41
2:E:474:ARG:HH11	2:E:474:ARG:HD2	1.75	0.41
2:E:1245:PHE:CD1	2:E:1600:LEU:HB3	2.54	0.41
2:I:282:ILE:HD12	2:I:314:PHE:HD2	1.85	0.41
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2155:LEU:HD13	2:B:2188:ASN:HD21	1.85	0.41
2:B:2288:LEU:O	2:B:3873:LYS:NZ	2.41	0.41
2:B:2788:HIS:CE1	2:B:2790:MET:HB2	2.54	0.41
2:E:2215:LEU:HD21	2:E:2272:PRO:HG3	2.02	0.41
2:E:2346:VAL:O	2:E:2349:ASN:ND2	2.53	0.41
2:I:1141:ARG:HD2	2:I:1141:ARG:H	1.86	0.41
2:I:1245:PHE:CD1	2:I:1600:LEU:HB3	2.54	0.41
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.25	0.41
2:I:3844:LEU:HA	2:I:3844:LEU:HD23	1.88	0.41
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	2.02	0.41
2:G:582:HIS:O	2:G:585:SER:OG	2.28	0.41
2:G:1141:ARG:HD2	2:G:1141:ARG:H	1.86	0.41
2:G:3844:LEU:HD23	2:G:3844:LEU:HA	1.88	0.41
2:B:3804:ILE:HG22	2:B:3812:VAL:HG21	2.01	0.41
2:B:4152:GLU:OE2	2:B:4180:ARG:NH1	2.50	0.41
2:I:1727:ARG:HH12	2:I:1772:ARG:HB3	1.85	0.41
2:I:2339:VAL:HG12	2:I:2345:SER:H	1.85	0.41
2:G:426:ARG:HB2	2:G:506:TYR:HA	2.03	0.41
2:G:599:VAL:HG23	2:G:600:LEU:HD12	2.02	0.41
2:G:1840:PRO:HB3	2:G:1843:LYS:HB3	2.02	0.41
2:G:2208:MET:HE1	2:G:2253:HIS:HB3	2.02	0.41
2:G:2290:LEU:HD21	2:G:2349:ASN:HA	2.01	0.41
2:B:315:CYS:SG	2:B:316:PHE:N	2.92	0.41
2:B:3842:LEU:O	2:B:3929:SER:OG	2.39	0.41
2:E:1727:ARG:HH12	2:E:1772:ARG:HB3	1.85	0.41
2:I:426:ARG:HB2	2:I:506:TYR:HA	2.03	0.41
2:I:642:THR:HG23	2:I:1613:LEU:HD12	2.02	0.41
2:B:3844:LEU:HA	2:B:3844:LEU:HD23	1.88	0.41
2:E:2288:LEU:O	2:E:3873:LYS:NZ	2.41	0.41
2:E:3804:ILE:HG22	2:E:3812:VAL:HG21	2.01	0.41
2:E:3905:THR:HA	2:E:3912:THR:HG23	2.01	0.41
2:E:4922:PHE:HA	2:E:4926:VAL:HG12	2.01	0.41
2:I:3891:LEU:HB3	2:I:3899:PHE:CE2	2.55	0.41
2:G:395:GLN:HG3	2:G:397:GLU:H	1.85	0.41
2:G:4232:GLU:OE1	2:G:5019:TRP:NE1	2.53	0.41
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	2.01	0.41
2:E:3658:LYS:HA	2:E:3661:TRP:CE2	2.56	0.41
2:E:3842:LEU:O	2:E:3929:SER:OG	2.39	0.41
2:I:2346:VAL:O	2:I:2349:ASN:ND2	2.53	0.41
2:I:3658:LYS:HA	2:I:3661:TRP:CE2	2.56	0.41
2:G:642:THR:HG23	2:G:1613:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:647:ASN:OD1	2:G:647:ASN:N	2.53	0.41
2:G:1727:ARG:HH12	2:G:1772:ARG:HB3	1.85	0.41
2:G:2155:LEU:HD13	2:G:2188:ASN:HD21	1.85	0.41
2:G:2346:VAL:O	2:G:2349:ASN:ND2	2.53	0.41
2:B:214:VAL:HG12	2:B:274:LEU:HD12	2.03	0.41
2:B:772:ASN:OD1	2:B:772:ASN:N	2.54	0.41
2:E:214:VAL:HG22	2:E:341:TYR:CE1	2.56	0.41
2:E:214:VAL:HG12	2:E:274:LEU:HD12	2.03	0.41
2:E:2155:LEU:HD13	2:E:2188:ASN:HD21	1.86	0.41
2:E:4570:ALA:HA	2:E:4573:ILE:HG22	2.03	0.41
2:I:404:ILE:HG21	2:I:481:GLU:HG3	2.03	0.41
2:I:1041:GLN:O	2:I:1045:THR:OG1	2.33	0.41
2:G:1245:PHE:CD1	2:G:1600:LEU:HB3	2.54	0.41
2:B:214:VAL:HG22	2:B:341:TYR:CE1	2.56	0.41
2:B:404:ILE:HG21	2:B:481:GLU:HG3	2.03	0.41
2:B:886:ARG:HB3	2:B:891:TRP:HB2	2.02	0.41
2:B:1141:ARG:H	2:B:1141:ARG:HD2	1.86	0.41
2:B:1245:PHE:CD1	2:B:1600:LEU:HB3	2.54	0.41
2:B:1725:ARG:HH21	2:B:1725:ARG:HD2	1.72	0.41
2:E:1141:ARG:H	2:E:1141:ARG:HD2	1.86	0.41
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.25	0.41
2:E:2208:MET:HE1	2:E:2253:HIS:HB3	2.02	0.41
2:E:3676:ASP:OD1	2:E:3676:ASP:N	2.52	0.41
2:E:4247:ILE:HD12	2:E:4247:ILE:HA	1.98	0.41
2:I:134:ASP:OD1	2:I:134:ASP:N	2.51	0.41
2:I:214:VAL:HG22	2:I:341:TYR:CE1	2.56	0.41
2:I:408:ALA:HB2	2:I:483:MET:HE1	2.03	0.41
2:I:865:PRO:HA	2:I:868:GLU:HB2	2.03	0.41
2:I:2155:LEU:HD13	2:I:2188:ASN:HD21	1.86	0.41
2:I:2208:MET:HE1	2:I:2253:HIS:HB3	2.02	0.41
2:G:710:ASP:OD1	2:G:710:ASP:N	2.52	0.41
2:G:865:PRO:HA	2:G:868:GLU:HB2	2.03	0.41
2:G:2339:VAL:HG12	2:G:2345:SER:H	1.85	0.41
2:B:426:ARG:HB2	2:B:506:TYR:HA	2.03	0.41
2:B:4570:ALA:HA	2:B:4573:ILE:HG22	2.03	0.41
2:E:599:VAL:HG23	2:E:600:LEU:HD12	2.02	0.41
2:E:1840:PRO:HB3	2:E:1843:LYS:HB3	2.02	0.41
2:E:1972:ASN:HD21	2:E:2024:PRO:HB3	1.86	0.41
2:E:2155:LEU:HD21	2:E:2198:MET:HE1	2.03	0.41
2:E:4865:LYS:HA	2:E:4865:LYS:HD2	1.90	0.41
2:I:395:GLN:HG3	2:I:397:GLU:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:767:VAL:HG12	2:I:769:GLU:HG3	2.03	0.41
2:I:2095:GLN:NE2	2:I:2127:GLN:O	2.54	0.41
2:B:395:GLN:HG3	2:B:397:GLU:H	1.85	0.40
2:E:426:ARG:HB2	2:E:506:TYR:HA	2.03	0.40
2:E:1725:ARG:HH21	2:E:1725:ARG:HD2	1.71	0.40
2:E:2095:GLN:NE2	2:E:2127:GLN:O	2.54	0.40
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	2.02	0.40
2:I:4172:GLU:OE1	2:I:4175:ARG:NH1	2.55	0.40
2:I:4570:ALA:HA	2:I:4573:ILE:HG22	2.03	0.40
2:G:767:VAL:HG12	2:G:769:GLU:HG3	2.03	0.40
2:E:688:LEU:HB3	2:E:777:PHE:CE1	2.57	0.40
2:E:1671:ARG:NH2	2:E:1713:ASP:HB3	2.36	0.40
2:G:214:VAL:HG22	2:G:341:TYR:CE1	2.56	0.40
2:G:1694:LEU:O	2:G:1712:TYR:OH	2.23	0.40
2:G:3658:LYS:HA	2:G:3661:TRP:CE2	2.56	0.40
2:B:688:LEU:HB3	2:B:777:PHE:CE1	2.57	0.40
2:B:4138:ASP:OD1	2:B:4138:ASP:N	2.51	0.40
2:B:4863:TYR:HA	2:B:4901:ILE:HG23	2.04	0.40
2:E:642:THR:HG23	2:E:1613:LEU:HD12	2.03	0.40
2:I:4152:GLU:OE2	2:I:4180:ARG:NH1	2.50	0.40
2:I:4251:ILE:HG22	2:I:4553:ASN:HD22	1.87	0.40
2:I:5036:LEU:HD12	2:I:5036:LEU:HA	1.91	0.40
2:G:4251:ILE:HG22	2:G:4553:ASN:HD22	1.87	0.40
2:B:408:ALA:HB2	2:B:483:MET:HE1	2.02	0.40
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	2.03	0.40
2:B:1972:ASN:HD21	2:B:2024:PRO:HB3	1.86	0.40
2:B:2155:LEU:HD21	2:B:2198:MET:HE1	2.03	0.40
2:B:2878:LEU:HD23	2:B:2878:LEU:HA	1.94	0.40
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	2.02	0.40
2:E:4791:TYR:OH	2:E:4815:ASP:O	2.33	0.40
2:I:454:PRO:HG2	2:I:531:ARG:HH12	1.87	0.40
2:I:649:PHE:HB3	2:I:776:LEU:HB3	2.04	0.40
2:G:864:PRO:HA	2:G:865:PRO:HD3	1.89	0.40
2:G:2095:GLN:NE2	2:G:2127:GLN:O	2.54	0.40
2:G:4172:GLU:OE1	2:G:4175:ARG:NH1	2.55	0.40
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	2.02	0.40
2:B:4172:GLU:OE1	2:B:4175:ARG:NH1	2.55	0.40
2:E:886:ARG:HB3	2:E:891:TRP:HB2	2.02	0.40
2:E:1171:SER:HG	2:E:1175:SER:H	1.63	0.40
2:E:4017:LEU:HD23	2:E:4017:LEU:HA	1.87	0.40
2:I:1658:ASP:N	2:I:1658:ASP:OD1	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3787:LYS:HB2	2:I:3831:SER:HA	2.04	0.40
2:I:4863:TYR:HA	2:I:4901:ILE:HG23	2.04	0.40
2:G:408:ALA:HB2	2:G:483:MET:HE1	2.03	0.40
2:G:1651:LEU:HA	2:G:1651:LEU:HD23	1.86	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%)	91 (87%)	14 (13%)	0	100	100
1	F	105/108 (97%)	91 (87%)	14 (13%)	0	100	100
1	H	105/108 (97%)	91 (87%)	14 (13%)	0	100	100
1	J	105/108 (97%)	91 (87%)	14 (13%)	0	100	100
2	B	3237/4676 (69%)	2857 (88%)	371 (12%)	9 (0%)	36	65
2	E	3237/4676 (69%)	2859 (88%)	369 (11%)	9 (0%)	36	65
2	G	3237/4676 (69%)	2858 (88%)	370 (11%)	9 (0%)	36	65
2	I	3237/4676 (69%)	2859 (88%)	369 (11%)	9 (0%)	36	65
All	All	13368/19136 (70%)	11797 (88%)	1535 (12%)	36 (0%)	37	65

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	B	1932	PRO
2	E	1708	ARG
2	E	1932	PRO
2	I	1708	ARG
2	I	1932	PRO

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Mol	Chain	Res	Type
2	G	1708	ARG
2	G	1932	PRO
2	B	1840	PRO
2	B	4641	PRO
2	B	5028	PHE
2	E	1840	PRO
2	E	4641	PRO
2	E	5028	PHE
2	I	1840	PRO
2	I	4641	PRO
2	I	5028	PHE
2	G	1840	PRO
2	G	4641	PRO
2	G	5028	PHE
2	B	2291	GLN
2	E	2291	GLN
2	I	2291	GLN
2	G	2291	GLN
2	B	4640	GLU
2	E	4135	PRO
2	E	4640	GLU
2	I	4135	PRO
2	I	4640	GLU
2	G	4640	GLU
2	B	4135	PRO
2	G	4135	PRO
2	B	2343	GLY
2	E	2343	GLY
2	I	2343	GLY
2	G	2343	GLY

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	2482 (100%)	11 (0%)	84	81
2	E	2493/3202 (78%)	2482 (100%)	11 (0%)	84	81
2	G	2493/3202 (78%)	2481 (100%)	12 (0%)	81	80
2	I	2493/3202 (78%)	2481 (100%)	12 (0%)	81	80
All	All	10324/13164 (78%)	10278 (100%)	46 (0%)	81	81

All (46) 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	1676	LEU
2	B	2339	VAL
2	B	2342	ASN
2	B	3663	LEU
2	B	3805	LEU
2	B	3896	ASN
2	B	4081	VAL
2	E	131	LEU
2	E	719	LEU
2	E	815	VAL
2	E	1600	LEU
2	E	1676	LEU
2	E	2339	VAL
2	E	2342	ASN
2	E	3663	LEU
2	E	3805	LEU
2	E	3896	ASN
2	E	4081	VAL
2	I	131	LEU
2	I	719	LEU
2	I	815	VAL
2	I	1600	LEU
2	I	1676	LEU
2	I	1720	LEU

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Mol	Chain	Res	Type
2	I	2339	VAL
2	I	2342	ASN
2	I	3663	LEU
2	I	3805	LEU
2	I	3896	ASN
2	I	4081	VAL
2	G	131	LEU
2	G	719	LEU
2	G	815	VAL
2	G	1600	LEU
2	G	1676	LEU
2	G	1720	LEU
2	G	2339	VAL
2	G	2342	ASN
2	G	3663	LEU
2	G	3805	LEU
2	G	3896	ASN
2	G	4081	VAL

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
1	H	87	HIS
1	J	87	HIS
2	B	57	ASN
2	B	105	HIS
2	B	111	HIS
2	B	113	HIS
2	B	156	GLN
2	B	201	ASN
2	B	203	ASN
2	B	224	HIS
2	B	379	HIS
2	B	383	HIS
2	B	395	GLN
2	B	465	GLN
2	B	479	GLN
2	B	520	ASN
2	B	725	HIS
2	B	866	HIS

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Mol	Chain	Res	Type
2	B	877	ASN
2	B	1220	GLN
2	B	1254	HIS
2	B	1598	GLN
2	B	1611	HIS
2	B	1640	HIS
2	B	1663	HIS
2	B	1688	HIS
2	B	1691	GLN
2	B	1693	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	1776	HIS
2	B	1952	GLN
2	B	1972	ASN
2	B	2005	GLN
2	B	2127	GLN
2	B	2260	ASN
2	B	2291	GLN
2	B	2773	ASN
2	B	2881	ASN
2	B	2931	GLN
2	B	3761	GLN
2	B	3814	GLN
2	B	3895	HIS
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	4034	ASN
2	B	4078	GLN
2	B	4102	GLN
2	B	4109	GLN
2	B	4120	ASN
2	B	4246	GLN
2	B	4553	ASN
2	B	4691	GLN
2	B	4700	GLN
2	B	4728	HIS
2	B	4776	GLN
2	B	4864	ASN
2	B	4949	GLN
2	B	5031	GLN

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Mol	Chain	Res	Type
2	E	105	HIS
2	E	113	HIS
2	E	156	GLN
2	E	201	ASN
2	E	203	ASN
2	E	224	HIS
2	E	379	HIS
2	E	383	HIS
2	E	395	GLN
2	E	465	GLN
2	E	479	GLN
2	E	582	HIS
2	E	725	HIS
2	E	877	ASN
2	E	1220	GLN
2	E	1254	HIS
2	E	1598	GLN
2	E	1611	HIS
2	E	1640	HIS
2	E	1663	HIS
2	E	1688	HIS
2	E	1691	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	1776	HIS
2	E	1952	GLN
2	E	1972	ASN
2	E	2005	GLN
2	E	2127	GLN
2	E	2260	ASN
2	E	2773	ASN
2	E	2881	ASN
2	E	3761	GLN
2	E	3766	GLN
2	E	3814	GLN
2	E	3895	HIS
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	4034	ASN
2	E	4078	GLN
2	E	4102	GLN

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Mol	Chain	Res	Type
2	E	4109	GLN
2	E	4120	ASN
2	E	4246	GLN
2	E	4553	ASN
2	E	4691	GLN
2	E	4700	GLN
2	E	4728	HIS
2	E	4776	GLN
2	E	4864	ASN
2	E	4949	GLN
2	E	5031	GLN
2	I	57	ASN
2	I	113	HIS
2	I	151	HIS
2	I	156	GLN
2	I	201	ASN
2	I	203	ASN
2	I	224	HIS
2	I	308	HIS
2	I	379	HIS
2	I	383	HIS
2	I	395	GLN
2	I	465	GLN
2	I	479	GLN
2	I	520	ASN
2	I	582	HIS
2	I	725	HIS
2	I	877	ASN
2	I	1220	GLN
2	I	1254	HIS
2	I	1598	GLN
2	I	1611	HIS
2	I	1663	HIS
2	I	1688	HIS
2	I	1691	GLN
2	I	1719	HIS
2	I	1775	HIS
2	I	1776	HIS
2	I	1952	GLN
2	I	1972	ASN
2	I	2005	GLN
2	I	2127	GLN

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Mol	Chain	Res	Type
2	I	2260	ASN
2	I	2773	ASN
2	I	2881	ASN
2	I	3761	GLN
2	I	3814	GLN
2	I	3895	HIS
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	3994	HIS
2	I	4034	ASN
2	I	4078	GLN
2	I	4102	GLN
2	I	4109	GLN
2	I	4120	ASN
2	I	4246	GLN
2	I	4553	ASN
2	I	4691	GLN
2	I	4700	GLN
2	I	4728	HIS
2	I	4776	GLN
2	I	4864	ASN
2	I	4949	GLN
2	I	5031	GLN
2	G	57	ASN
2	G	105	HIS
2	G	113	HIS
2	G	156	GLN
2	G	201	ASN
2	G	203	ASN
2	G	224	HIS
2	G	308	HIS
2	G	379	HIS
2	G	383	HIS
2	G	395	GLN
2	G	465	GLN
2	G	479	GLN
2	G	520	ASN
2	G	582	HIS
2	G	725	HIS
2	G	877	ASN
2	G	1220	GLN

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Mol	Chain	Res	Type
2	G	1254	HIS
2	G	1598	GLN
2	G	1663	HIS
2	G	1691	GLN
2	G	1719	HIS
2	G	1775	HIS
2	G	1776	HIS
2	G	1952	GLN
2	G	1972	ASN
2	G	2005	GLN
2	G	2127	GLN
2	G	2260	ASN
2	G	2291	GLN
2	G	2773	ASN
2	G	2881	ASN
2	G	3761	GLN
2	G	3814	GLN
2	G	3895	HIS
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	3994	HIS
2	G	4034	ASN
2	G	4078	GLN
2	G	4109	GLN
2	G	4120	ASN
2	G	4153	HIS
2	G	4246	GLN
2	G	4553	ASN
2	G	4691	GLN
2	G	4700	GLN
2	G	4728	HIS
2	G	4776	GLN
2	G	4864	ASN
2	G	4949	GLN
2	G	5031	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

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

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3613:UNK	C	3639:THR	N	42.64
1	G	3613:UNK	C	3639:THR	N	42.57
1	I	3613:UNK	C	3639:THR	N	42.56
1	E	3613:UNK	C	3639:THR	N	42.54

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	3163:UNK	C	3170:UNK	N	16.55
1	I	3163:UNK	C	3170:UNK	N	16.55
1	G	3163:UNK	C	3170:UNK	N	16.55
1	B	3163:UNK	C	3170:UNK	N	16.52
1	E	3468:UNK	C	3511:UNK	N	15.29
1	I	3468:UNK	C	3511:UNK	N	15.29
1	G	3468:UNK	C	3511:UNK	N	15.29
1	B	3468:UNK	C	3511:UNK	N	15.27
1	E	3063:UNK	C	3134:UNK	N	14.87
1	G	3063:UNK	C	3134:UNK	N	14.87
1	I	3063:UNK	C	3134:UNK	N	14.86
1	B	3063:UNK	C	3134:UNK	N	14.83
1	E	2703:UNK	C	2734:ASN	N	14.48
1	I	2703:UNK	C	2734:ASN	N	14.47
1	G	2703:UNK	C	2734:ASN	N	14.44
1	B	2703:UNK	C	2734:ASN	N	14.41
1	B	3236:UNK	C	3241:UNK	N	13.70
1	G	3236:UNK	C	3241:UNK	N	13.62
1	I	3236:UNK	C	3241:UNK	N	13.61
1	E	3236:UNK	C	3241:UNK	N	13.60
1	E	1564:UNK	C	1573:MET	N	12.83
1	I	1564:UNK	C	1573:MET	N	12.83
1	G	1564:UNK	C	1573:MET	N	12.81
1	B	1564:UNK	C	1573:MET	N	12.75
1	E	2976:UNK	C	2995:UNK	N	12.39
1	I	2976:UNK	C	2995:UNK	N	12.39
1	G	2976:UNK	C	2995:UNK	N	12.39
1	B	2976:UNK	C	2995:UNK	N	12.36
1	E	3254:UNK	C	3261:UNK	N	8.63
1	I	3254:UNK	C	3261:UNK	N	8.62
1	G	3254:UNK	C	3261:UNK	N	8.62
1	B	3254:UNK	C	3261:UNK	N	8.56
1	B	1297:UNK	C	1430:UNK	N	5.72
1	E	1297:UNK	C	1430:UNK	N	5.72
1	I	1297:UNK	C	1430:UNK	N	5.72
1	G	1297:UNK	C	1430:UNK	N	5.72
1	B	2479:LEU	C	2487:UNK	N	3.59
1	G	2479:LEU	C	2487:UNK	N	3.53
1	I	2479:LEU	C	2487:UNK	N	3.52
1	E	2479:LEU	C	2487:UNK	N	3.51
1	E	2939:ARG	C	2942:UNK	N	3.37
1	I	2939:ARG	C	2942:UNK	N	3.34

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	2939:ARG	C	2942:UNK	N	3.33
1	B	2939:ARG	C	2942:UNK	N	3.26

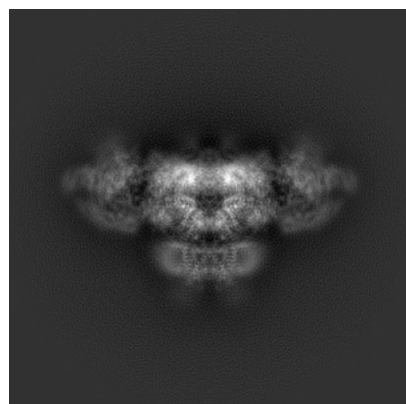
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8342. These allow visual inspection of the internal detail of the map and identification of artifacts.

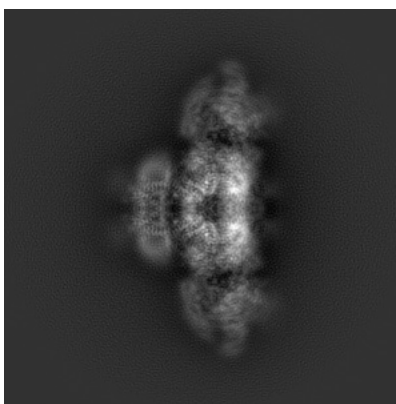
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

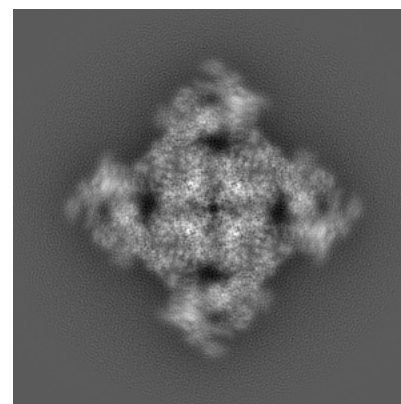
6.1.1 Primary map



X



Y

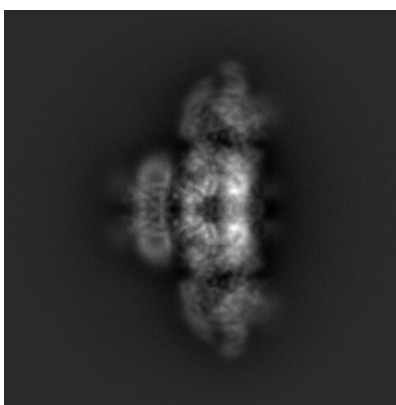


Z

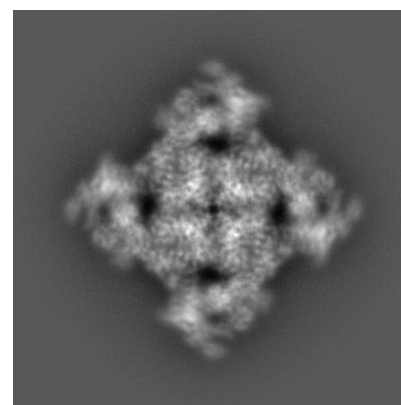
6.1.2 Raw map



X



Y

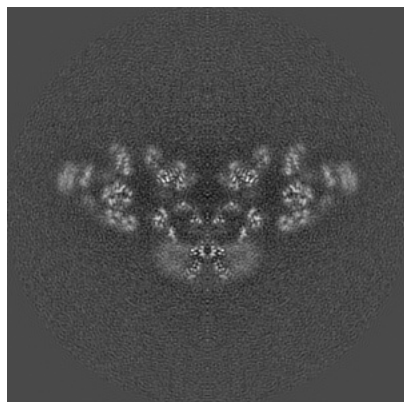


Z

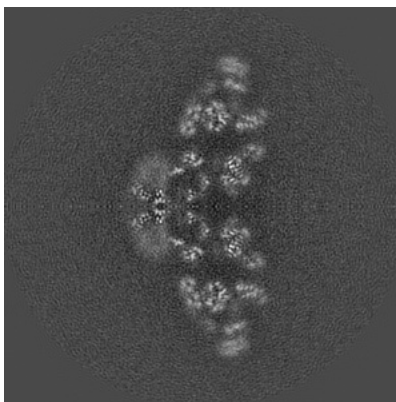
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

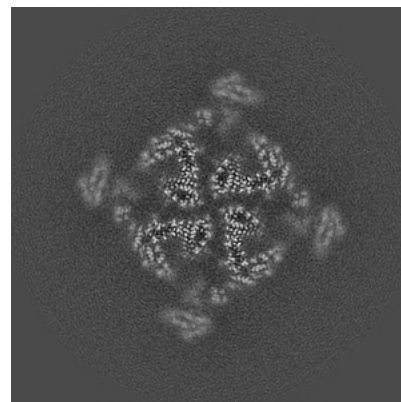
6.2.1 Primary map



X Index: 200

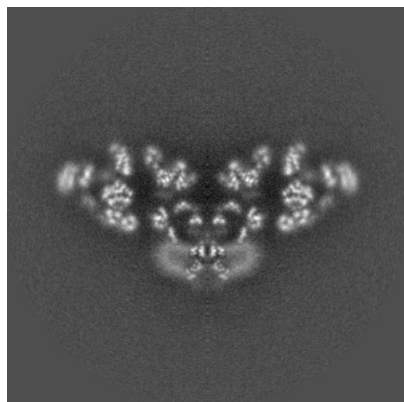


Y Index: 200

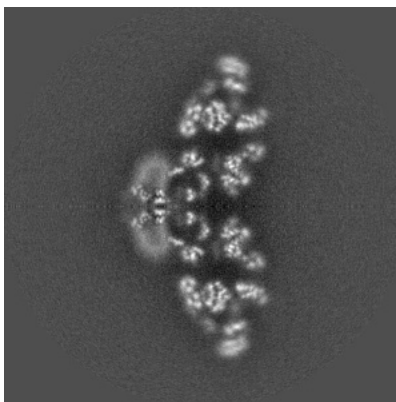


Z Index: 200

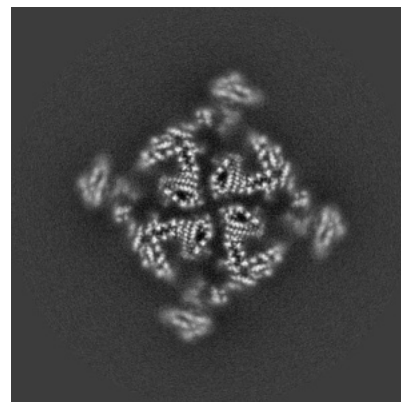
6.2.2 Raw map



X Index: 200



Y Index: 200

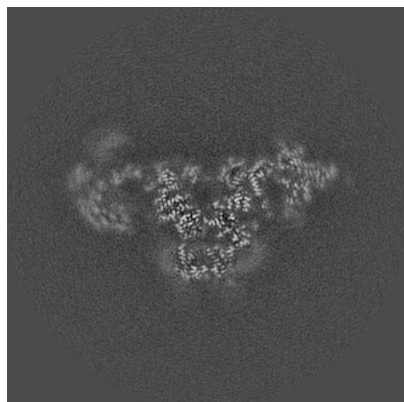


Z Index: 200

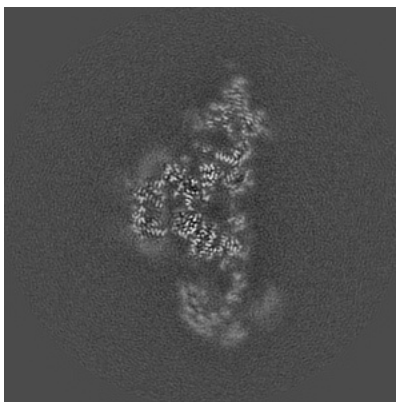
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

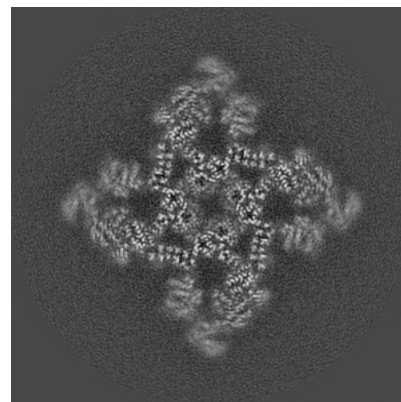
6.3.1 Primary map



X Index: 184

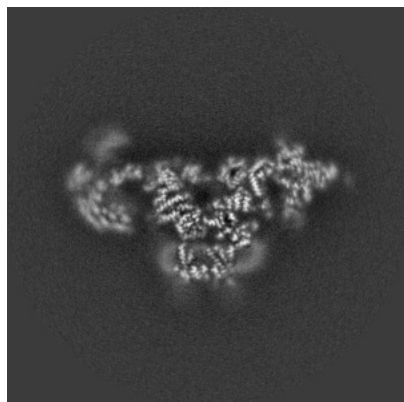


Y Index: 216

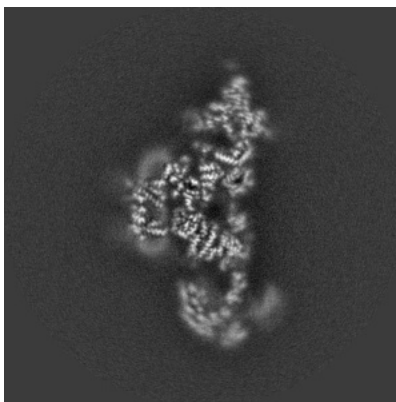


Z Index: 227

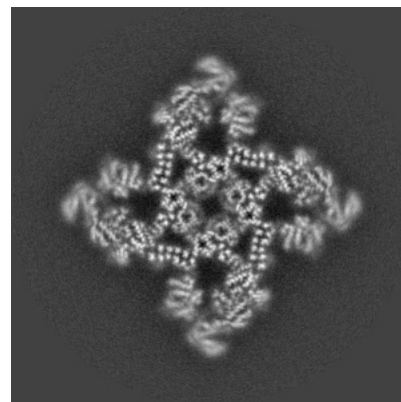
6.3.2 Raw map



X Index: 184



Y Index: 216

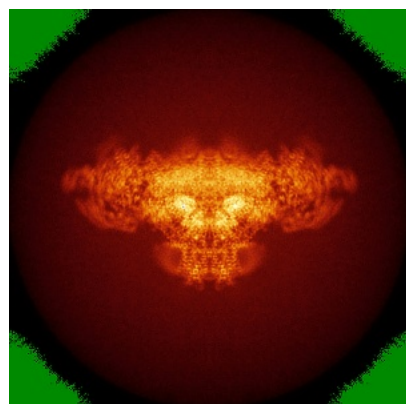


Z Index: 227

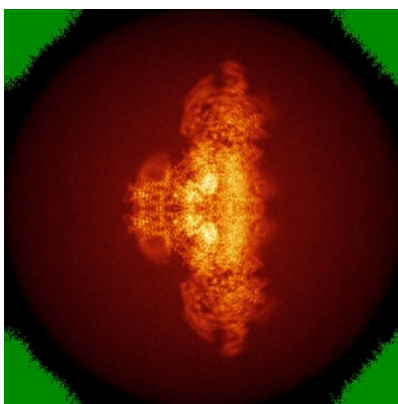
The images above show the largest variance slices of the map in three orthogonal directions.

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

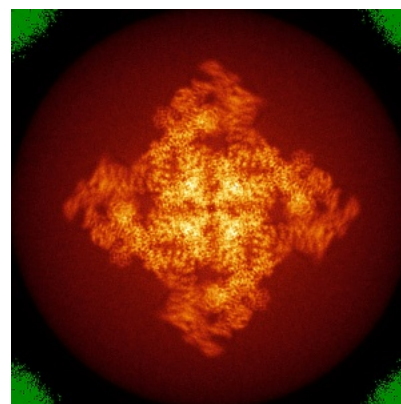
6.4.1 Primary map



X



Y

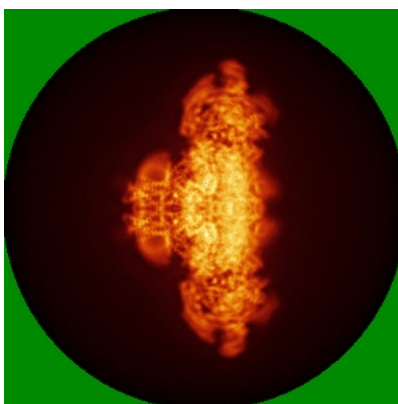


Z

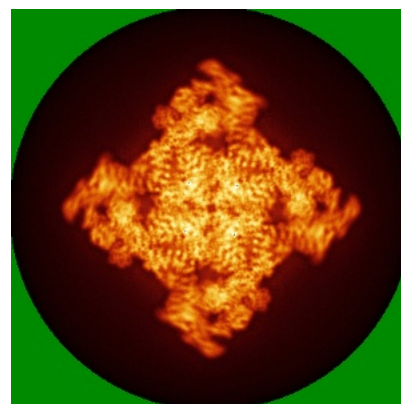
6.4.2 Raw map



X



Y

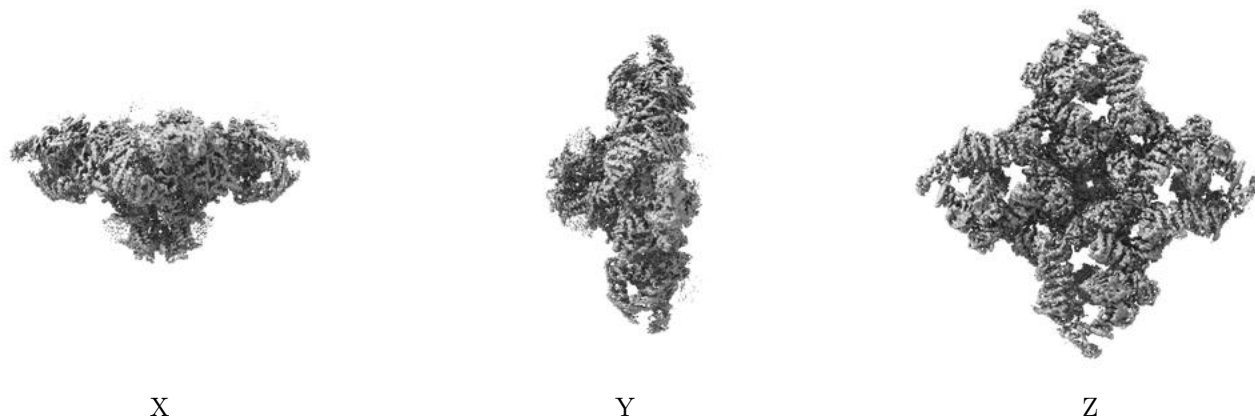


Z

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.

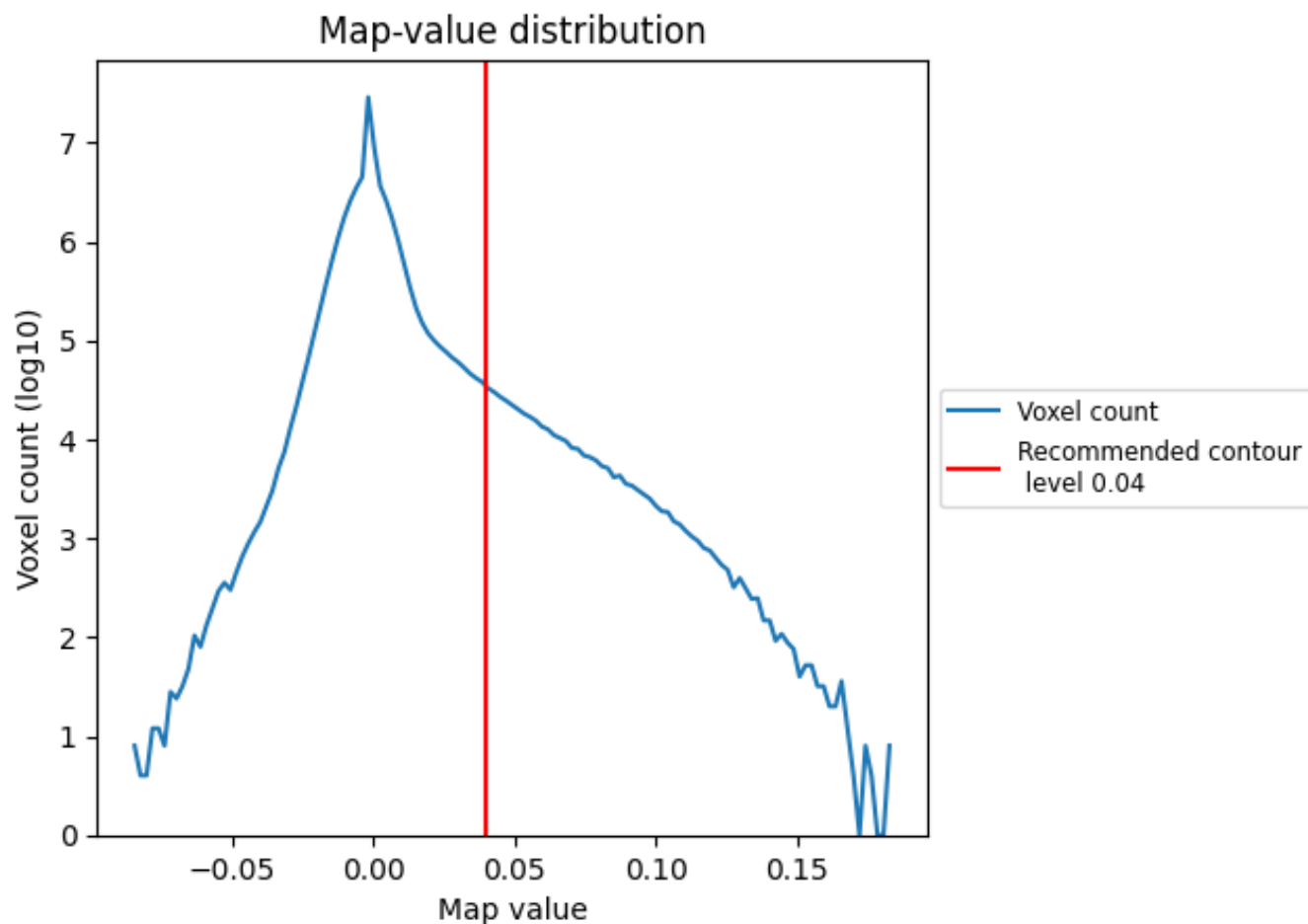
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

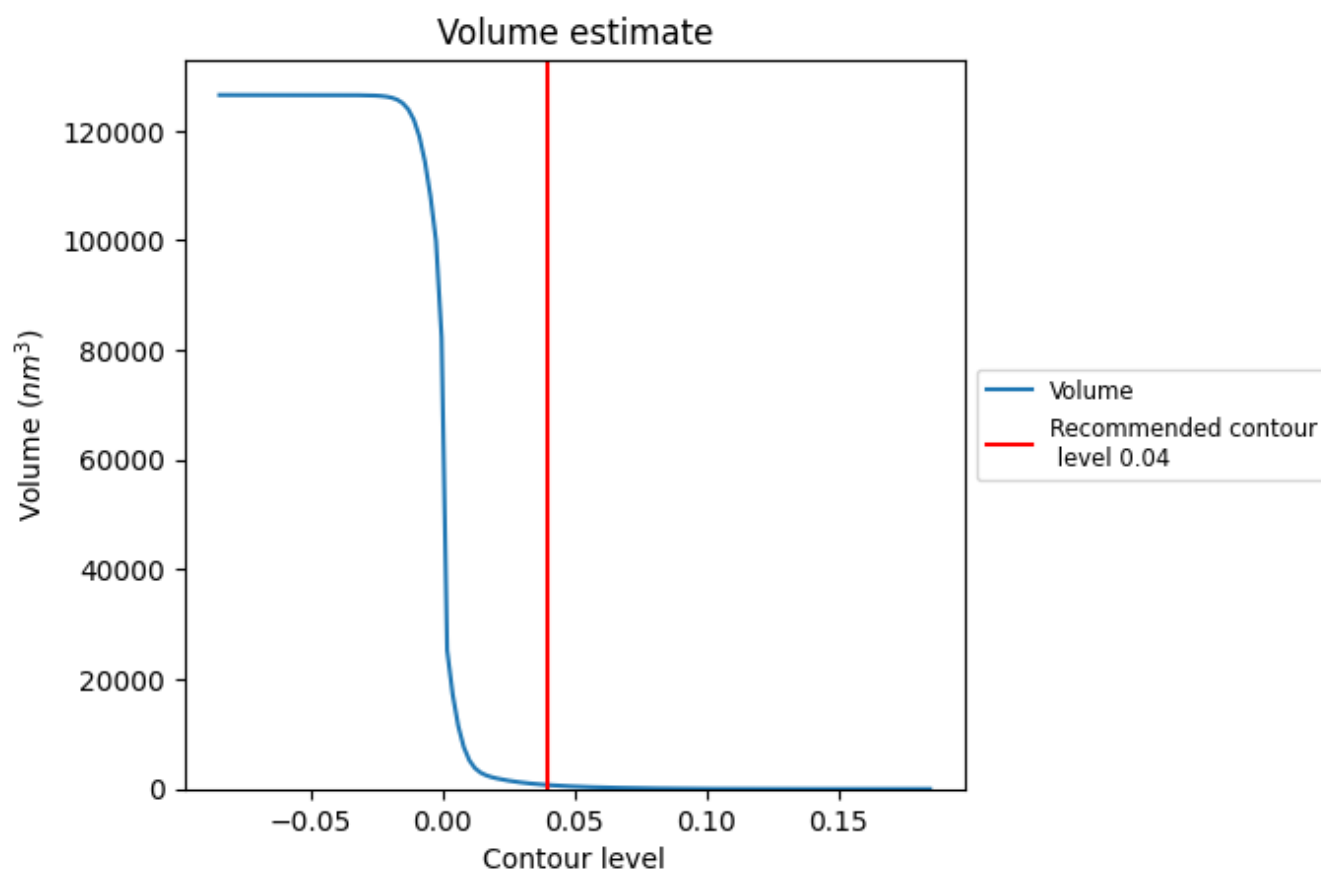
This section contains the results of statistical analysis of the map.

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.

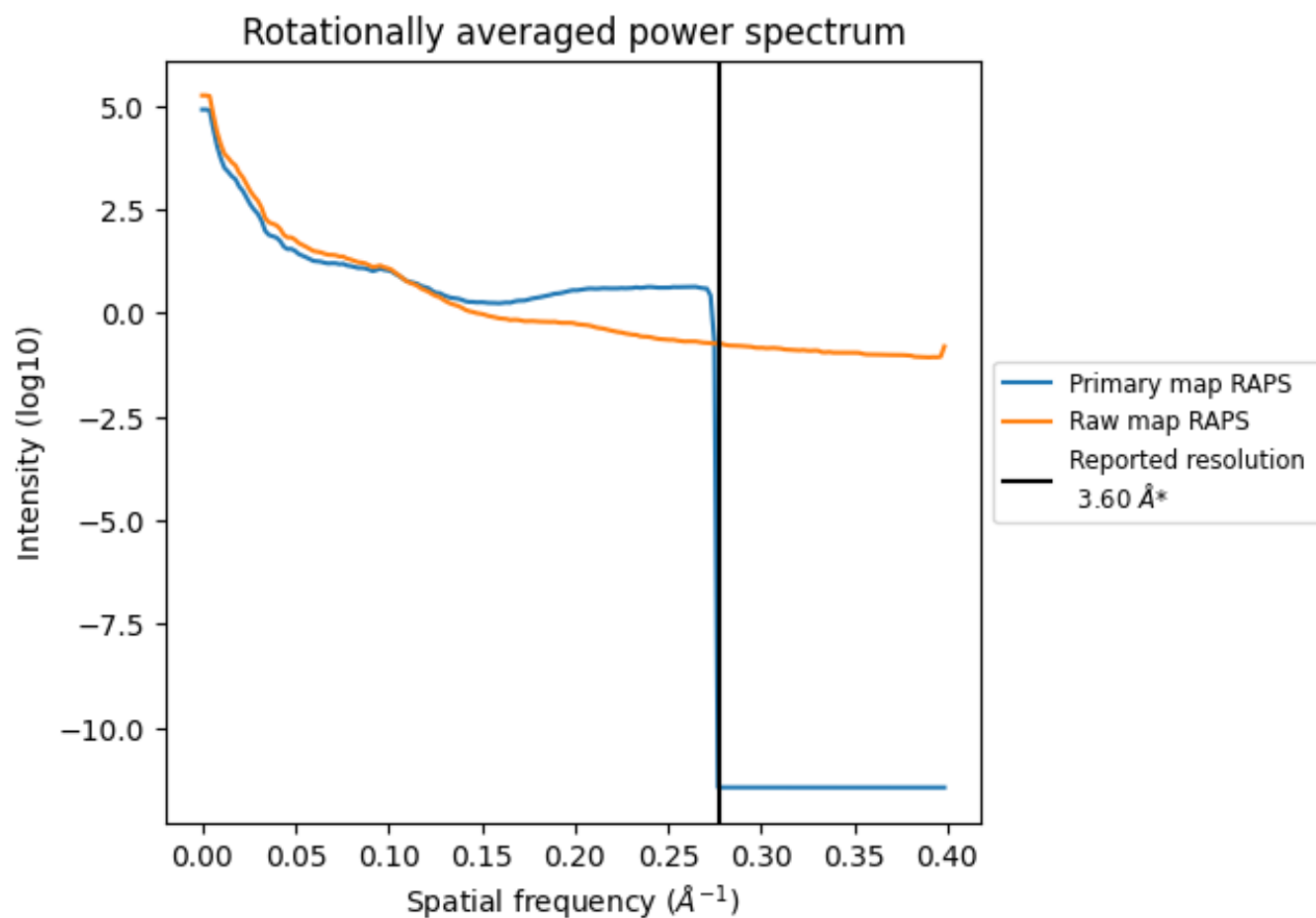
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 716 nm³; this corresponds to an approximate mass of 647 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 ⓘ

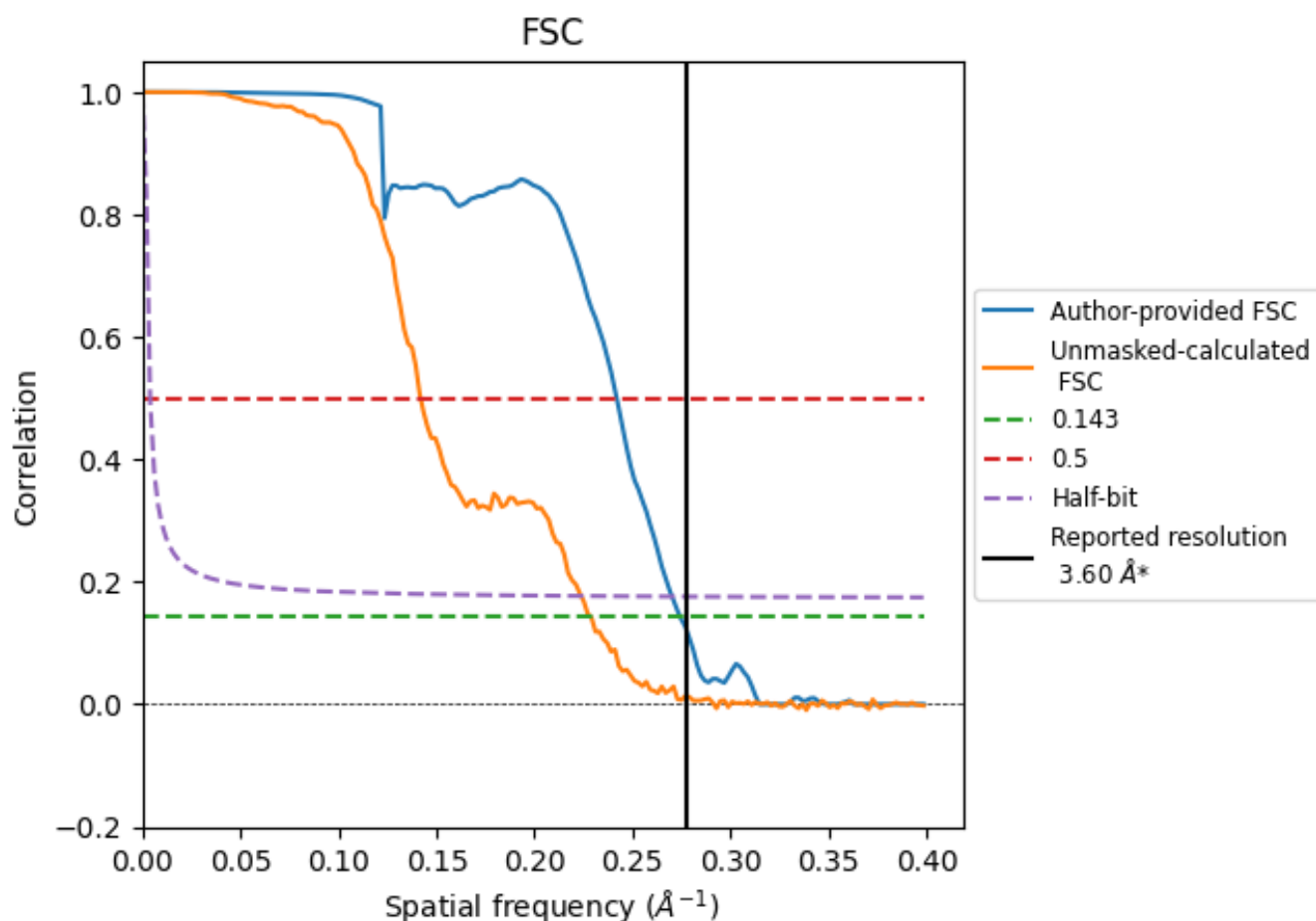


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 $0.278 \text{ \AA}^{-1}$

8.2 Resolution estimates

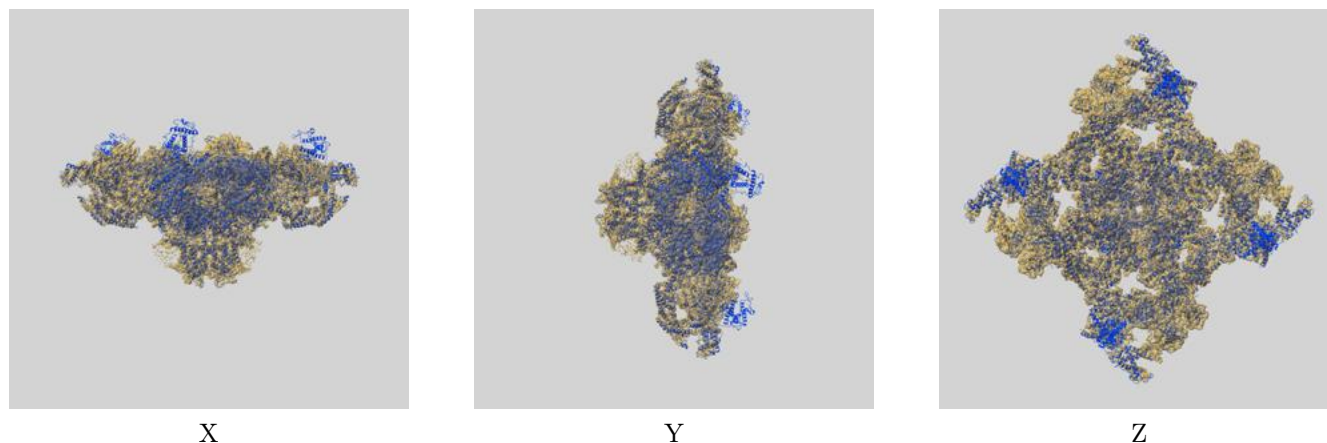
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.65	4.13	3.70
Unmasked-calculated*	4.38	7.05	4.47

*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 4.38 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

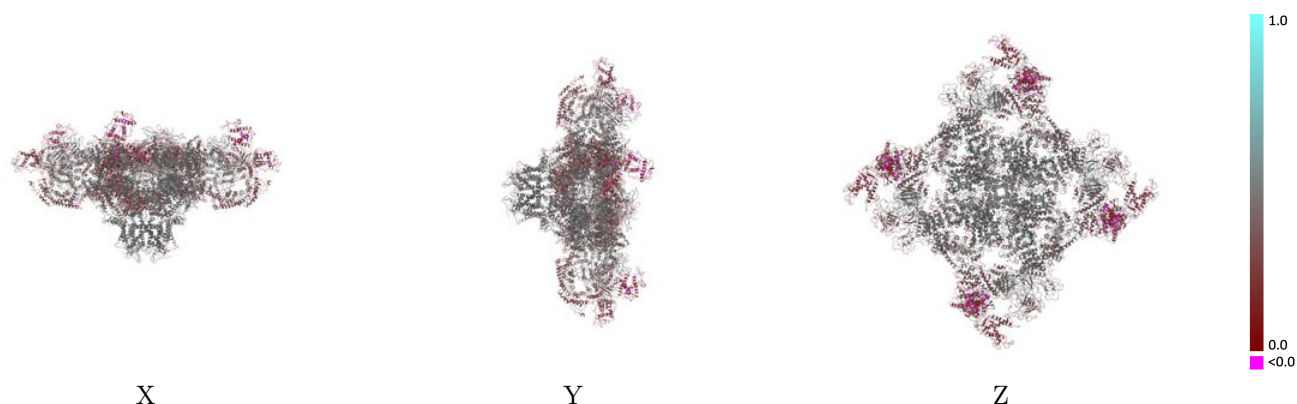
This section contains information regarding the fit between EMDB map EMD-8342 and PDB model 5T15. Per-residue inclusion information can be found in section [3](#) on page [6](#).

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](#)

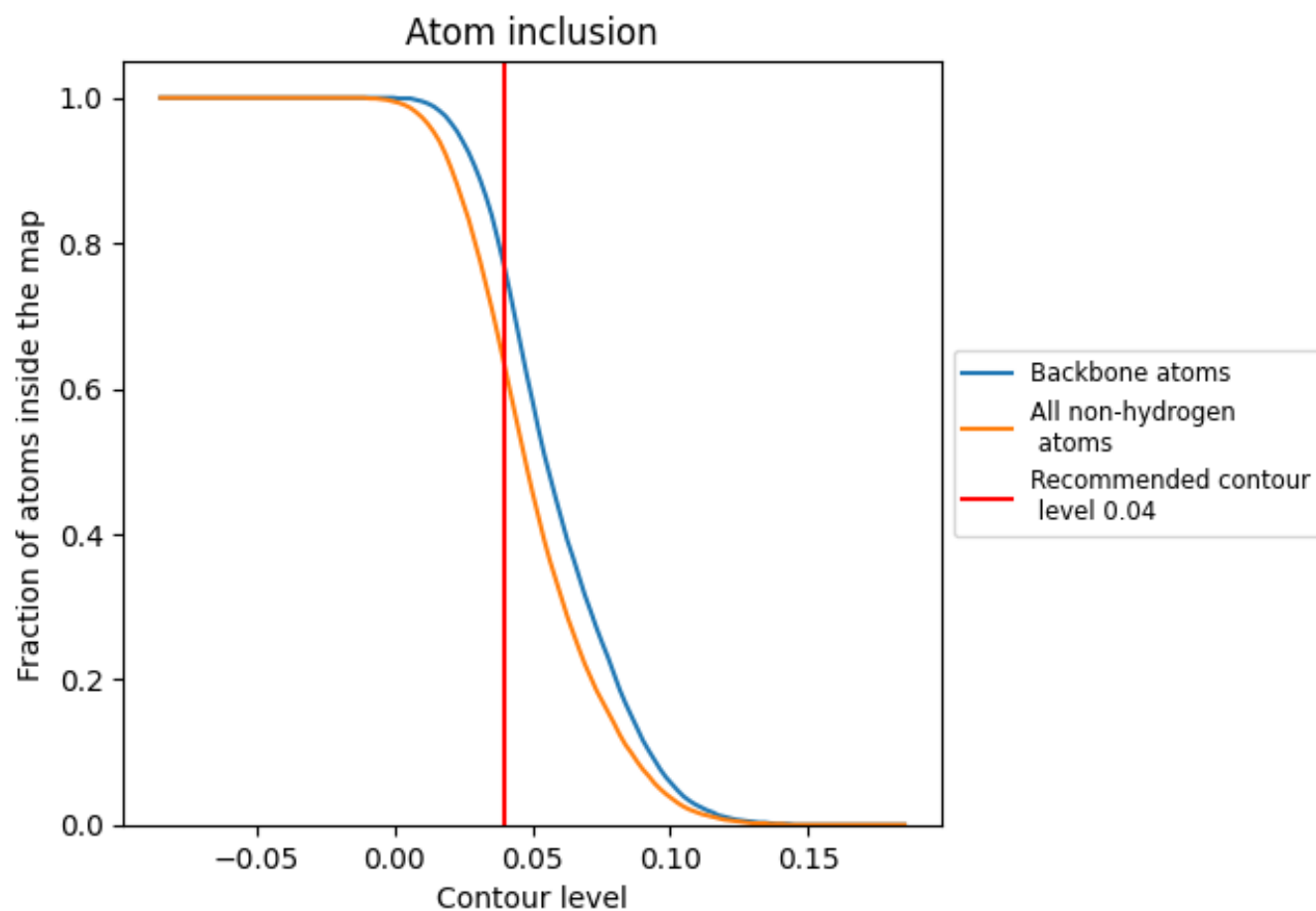


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 63% 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	0.6300	0.3980
A	0.6390	0.4060
B	0.6300	0.3980
E	0.6300	0.3980
F	0.6440	0.4120
G	0.6300	0.3980
H	0.6460	0.4120
I	0.6300	0.3980
J	0.6410	0.4090

1.0

0.0

<0.0