



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 01:58 PM UTC

PDB ID : 5T9N / pdb_00005t9n
EMDB ID : EMD-8373
Title : Structure of rabbit RyR1 (Ca²⁺-only dataset, class 2)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-09
Resolution : 3.80 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:

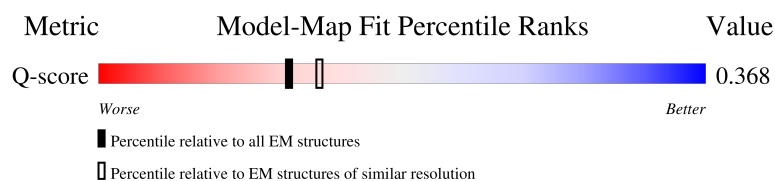
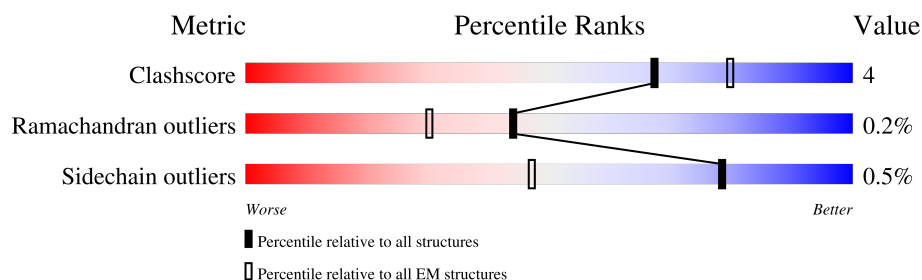
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.80 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	10198 (3.30 - 4.30)

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	9% 88% 11%
1	F	108	7% 86% 13%
1	H	108	9% 88% 11%
1	J	108	9% 88% 11%

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Mol	Chain	Length	Quality of chain
2	B	4676	18% 81% 8% 11%
2	E	4676	18% 81% 8% 11%
2	G	4676	18% 81% 8% 11%
2	I	4676	18% 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	

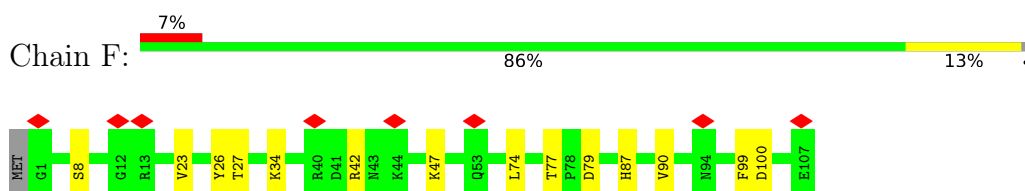
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

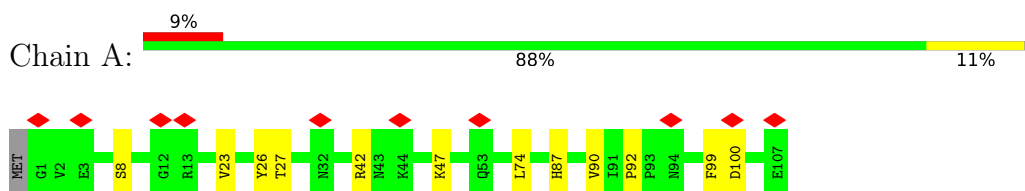
3 Residue-property plots

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.

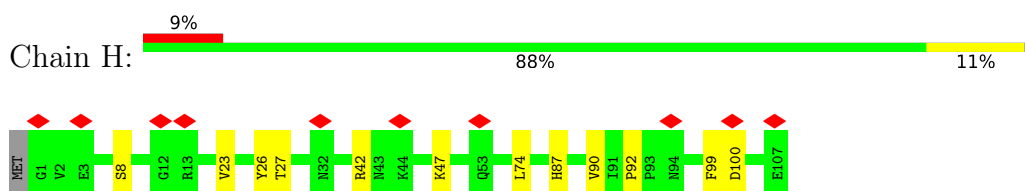
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



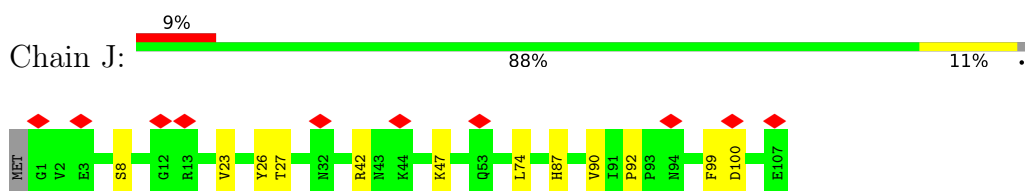
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



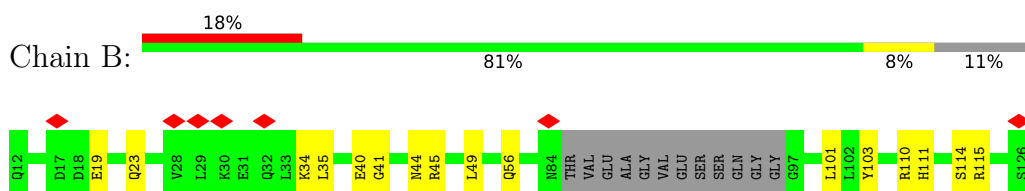
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

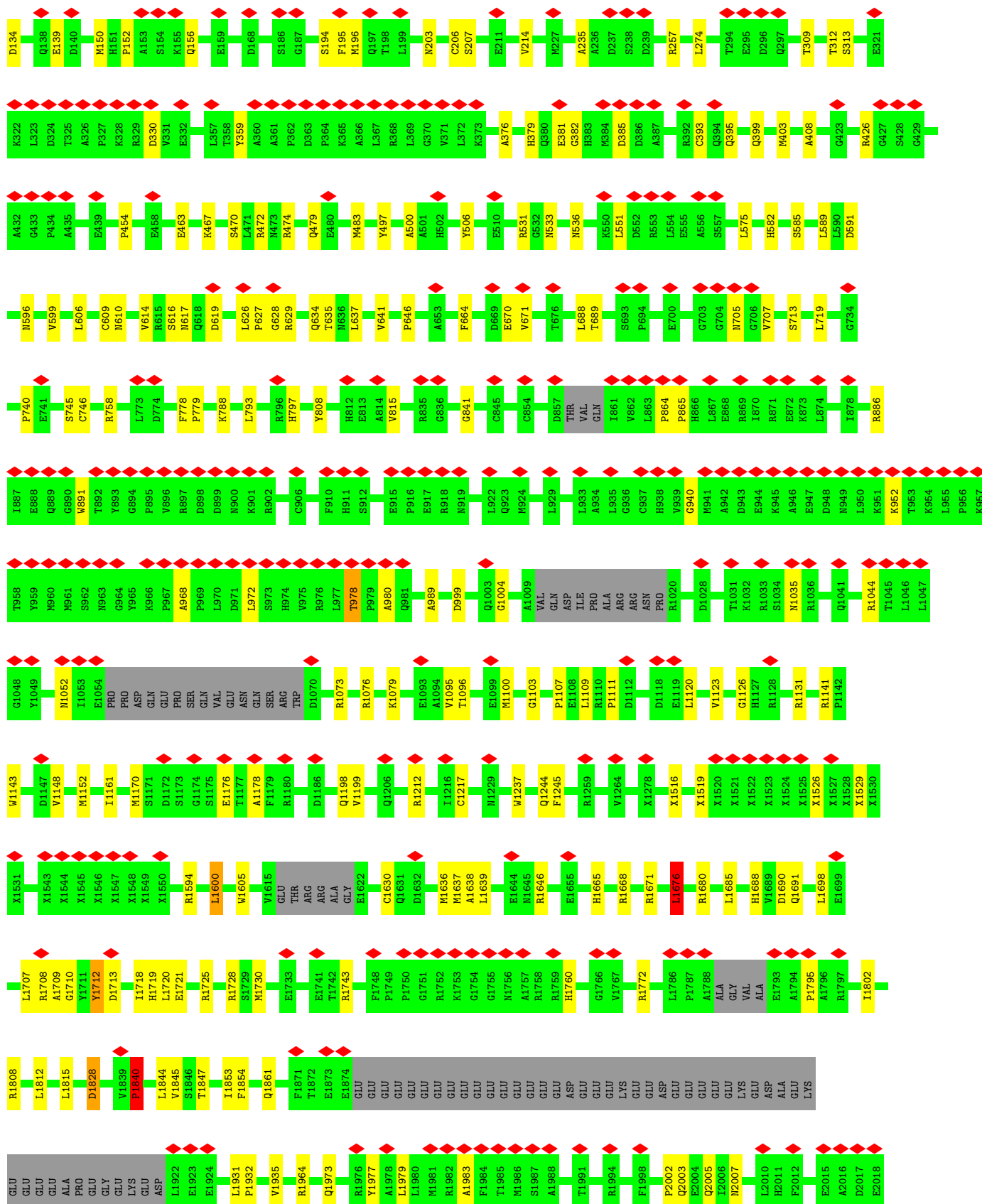


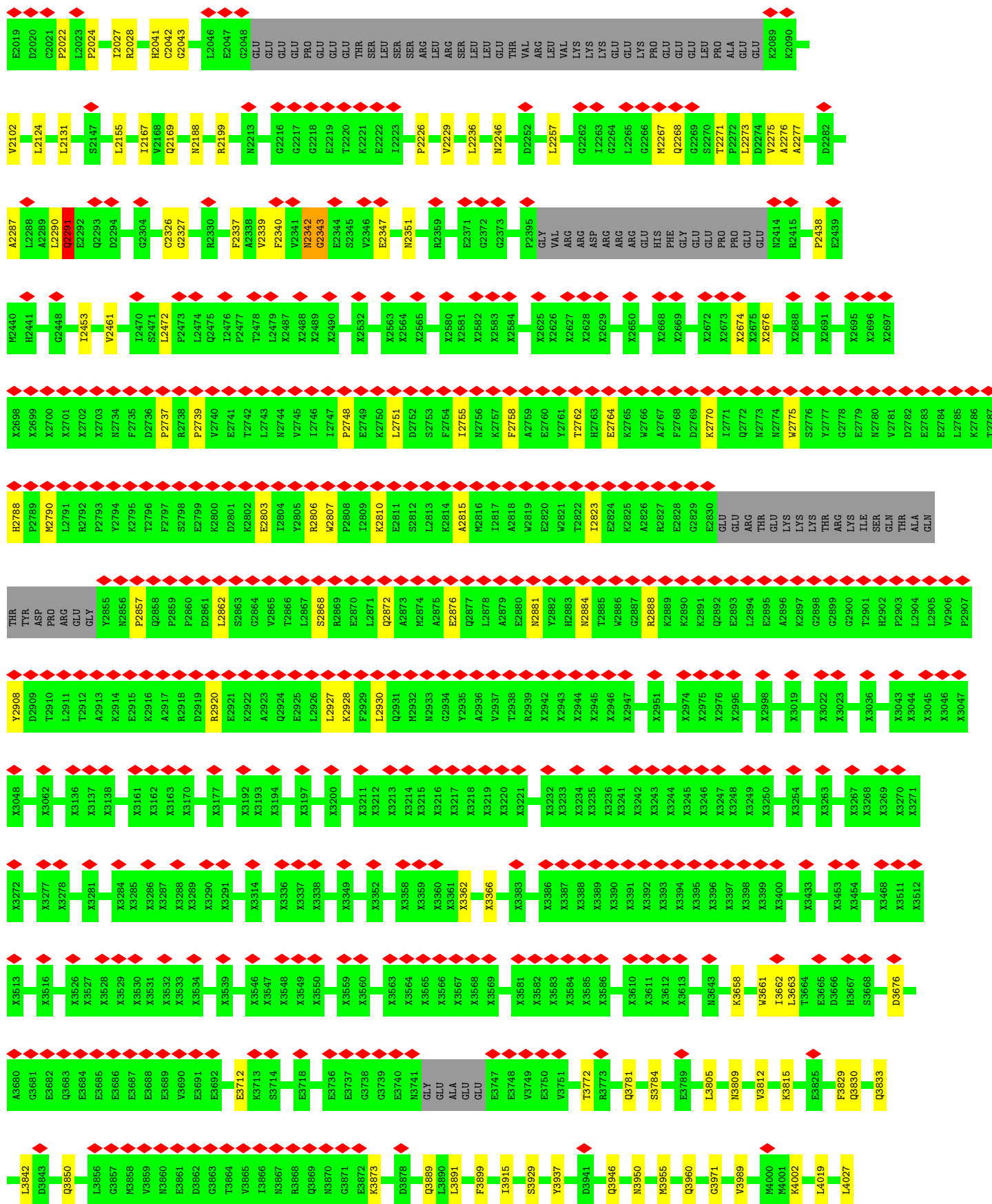
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

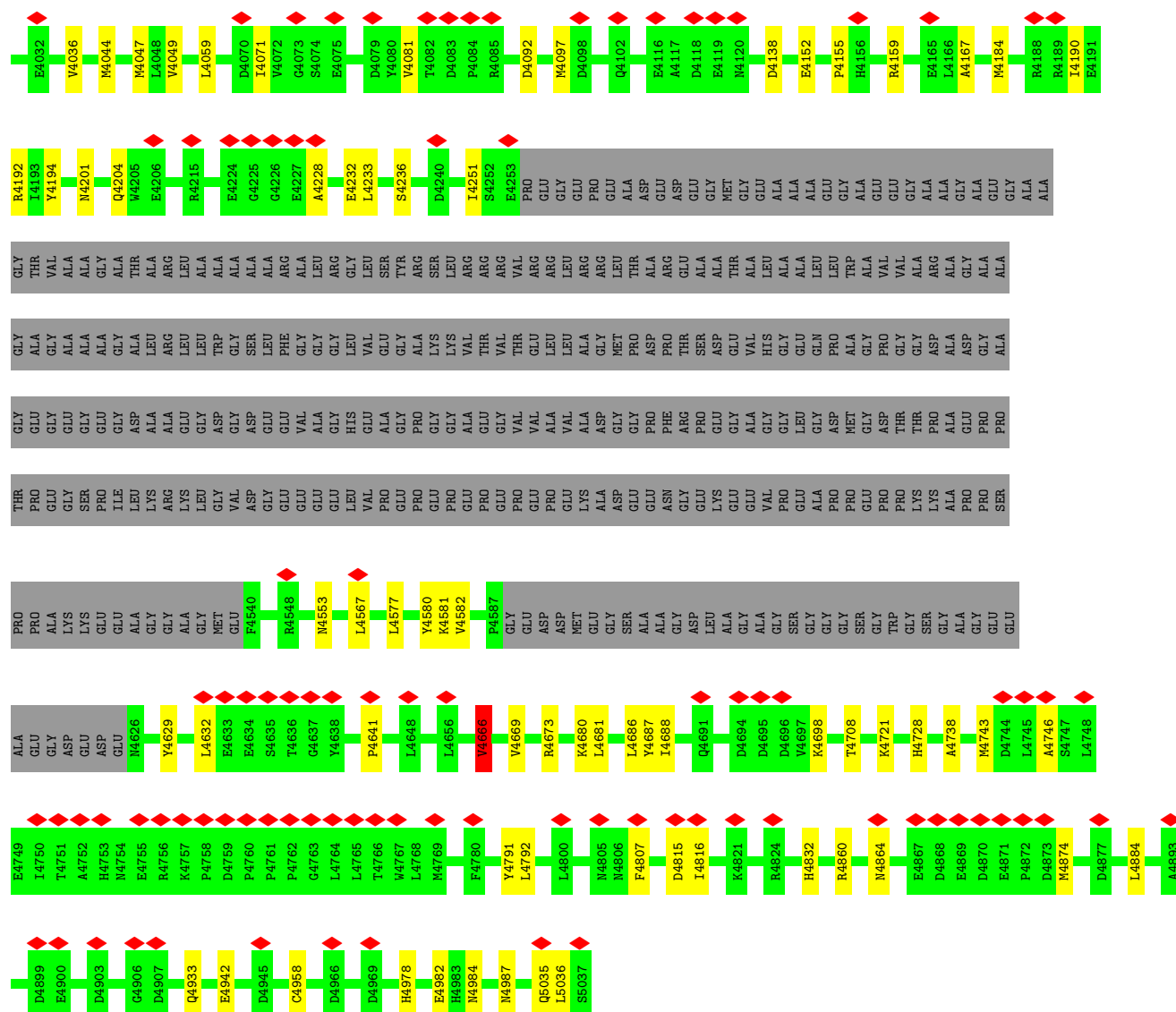


- Molecule 2: Ryanodine receptor 1

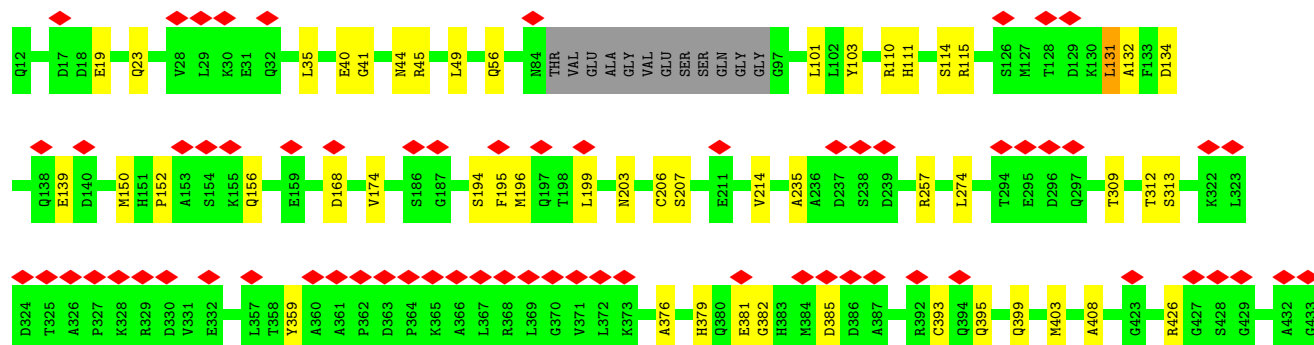
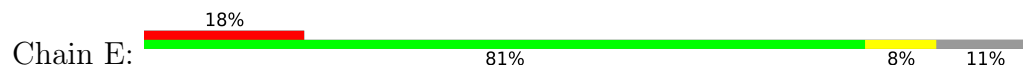






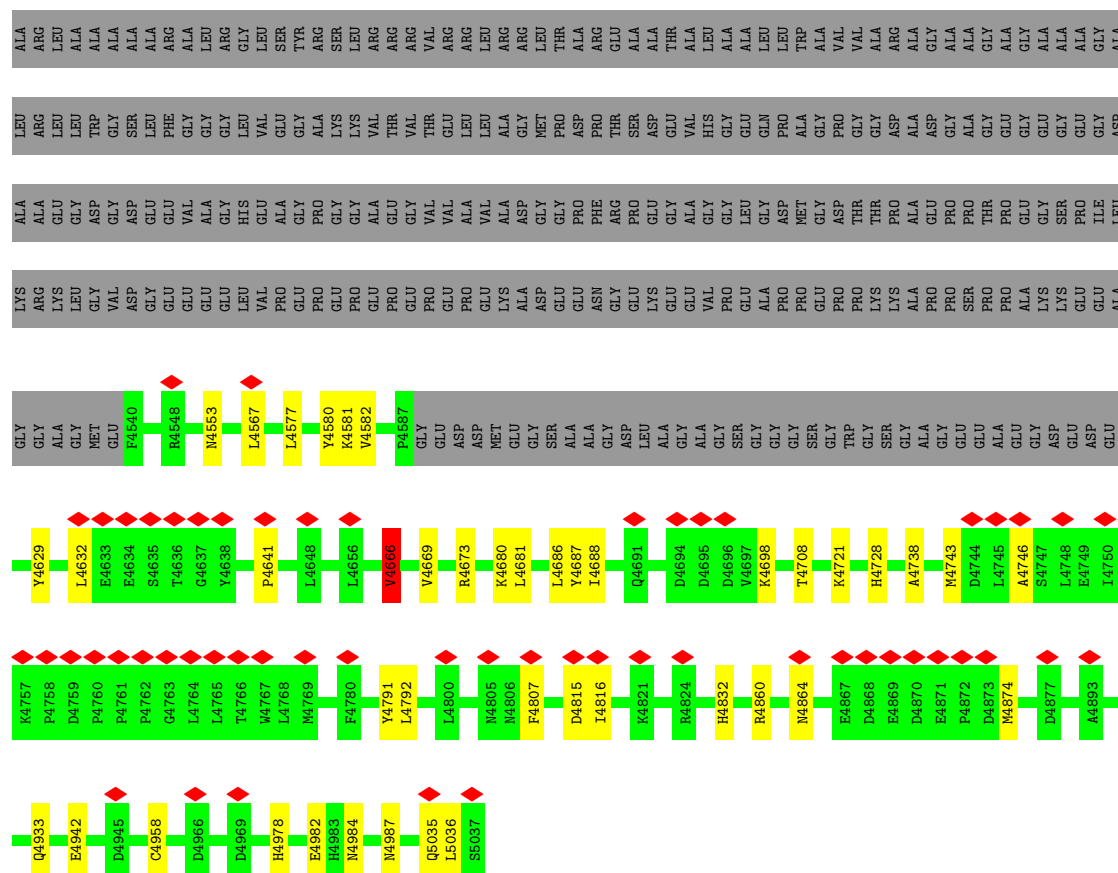


• Molecule 2: Ryanodine receptor 1

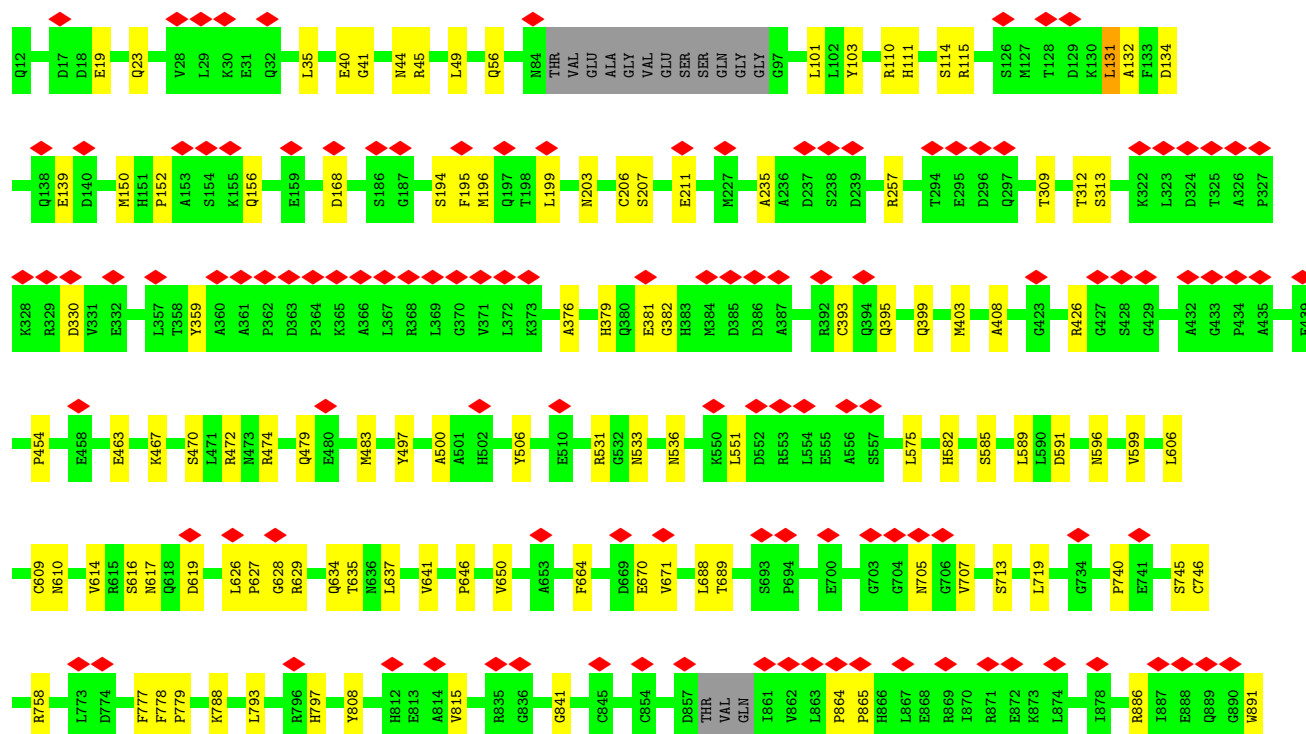
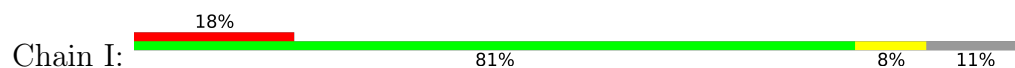








• Molecule 2: Ryanodine receptor 1

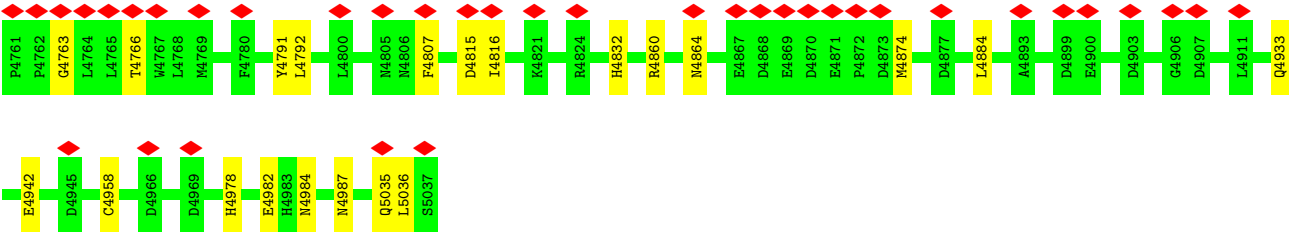








E4633	E4634	S4635	T4636	G4637	Y4638	P4641	L4648	L4656	Y4666	V4669	R4673	K4680	L4681	L4686	Y4687	I4688	Q4691	D4694	D4695	D4696	V4697	K4698	T4708	K4721	H4728	A4738	M4743	D4744	L4745	A4746	S4747	L4748	E4749	I4750	T4751	A4752	H4753	N4754	E4755	K4757	P4758	D4759	P4760							
GLY	VAL	ASP	GLY	GLY	GLY	VAL	PRO	GLY	PRO	PRO	GLY	PRO	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	PRO	GLY	PRO	PRO	PRO	PRO	PRO	PRO	PRO	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY					
ALA	ALA	ALA	ALA	ARG	ALA	LEU	ARG	GLY	LEU	VAL	GLY	TRP	ALA	ARG	GLY	LEU	VAL	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY					
ASP	GLY	ASP	GLY	GLY	VAL	GLY	HIS	GLY	LEU	VAL	GLY	TRP	GLY	VAL	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY					
GLY	VAL	ASP	GLY	GLY	GLY	VAL	PRO	GLY	PRO	PRO	GLY	TRP	ALA	ARG	GLY	LEU	VAL	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY					
MET	GLU	F4540	R4548	M4553	L4567	F4571	L4577	Y4580	K4581	V4582	P4587	GLY	ASP	ASP	MET	GLY	GLY	SER	ALA	ALA	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY					
T2912	A2913	R2914	E2915	R2916	A2917	R2918	D2919	L2920	E2921	R2922	A2923	Q2924	E2925	L2926	L2927	R2928	F2929	L2930	Q2931	R2932	N2933	G2934	V2935	A2936	V2937	T2938	R2939	X2942	X2943	X2944	X2945	X2946	X2947	X2951	X2974	X2975	X2976	X2995	X2998	X3019	X3022	X3023	X3036	X3043	X3044	X3045	X3046	X3047	X3048	X3062
X3136	X3137	X3138	X3161	X3162	X3163	X3170	X3177	X3192	X3193	X3194	X3197	X3200	X3213	X3214	X3215	X3216	X3217	X3218	X3219	X3220	X3221	X3234	X3235	X3236	X3241	X3242	X3243	X3244	X3245	X3246	X3247	X3248	X3249	X3254	X3263	X3267	X3268	X3269	X3270	X3271	X3272	X3277	X3278	X3281	X3284	X3285				
X3286	X3287	X3288	X3289	X3290	X3291	X3314	X3336	X3337	X3338	X3349	X3352	X3358	X3359	X3360	X3361	X3362	X3366	X3383	X3386	X3387	X3388	X3389	X3390	X3391	X3392	X3393	X3394	X3395	X3396	X3397	X3398	X3399	X3400	X3433	X3453	X3454	X3468	X3511	X3512	X3513	X3516	X3526	X3527	X3528	X3529	X3530				
X3531	X3532	X3533	X3534	X3539	X3546	X3547	X3548	X3549	X3550	X3559	X3560	X3563	X3564	X3565	X3566	X3567	X3568	X3569	X3581	X3582	X3583	X3584	X3585	X3586	X3610	X3611	X3612	X3613	X3658	X3661	I3662	L3663	T3664	E3665	D3666	H3667	S3668	D3676	A3680	G3681	E3682	Q3683	E3684	E3685	E3686	E3687	E3688	E3689	V3690	
E3691	E3692	E3712	K3713	S3714	E3718	E3736	E3737	E3738	E3739	E3740	E3741	GLY	GLU	ALA	GLU	E3747	E3748	V3749	E3750	V3751	T3772	R3773	Q3781	S3784	E3789	L3805	N3809	V3812	K3815	F3829	Q3830	Q3833	L3842	D3843	Q3850	L3856	G3857	M3858	V3859	N3860										
E3861	D3862	G3863	T3864	V3865	T3866	N3867	R3868	R3869	N3870	G3871	E3872	K3873	D3878	Q3889	L3890	L3891	F3899	T3915	S3929	Y3937	D3941	Q3946	N3950	N3955	Q3960	G3971	V3989	M4000	M4001	K4002	L4019	L4027	E4032	V4036	M4044	V4045	D4046	M4047	L4048	V4049										
L4059	D4070	I4071	V4072	G4073	S4074	E4075	D4079	Y4080	Y4081	T4082	D4083	P4084	R4085	D4092	M4097	D4098	Q4102	E4116	A4117	D4118	E4119	M4120	D4138	E4152	P4155	H4156	R4159	E4165	L4166	A4167	M4184	R4188	R4189	I4190	E4191	R4192	I4193	Y4194	M4201	Q4204	W4205	E4206								
R4215	E4224	G4225	G4226	E4227	A4228	E4232	L4233	S4236	I4251	S4252	E4253	PRO	GLY	GLY	GLY	PRO	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY						
ALA	ALA	ALA	ALA	ARG	ALA	LEU	ARG	GLY	LEU	VAL	GLY	TRP	ALA	ARG	GLY	LEU	VAL	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY					
ASP	GLY	ASP	GLY	GLY	VAL	GLY	HIS	GLY	LEU	VAL	GLY	TRP	GLY	VAL	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY					
GLY	VAL	ASP	GLY	GLY	GLY	VAL	PRO	GLY	PRO	PRO	GLY	TRP	ALA	ARG	GLY	LEU	VAL	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY				
MET	GLU	F4540	R4548	M4553	L4567	F4571	L4577	Y4580	K4581	V4582	P4587	GLY	ASP	ASP	MET	GLY	GLY	SER	ALA	ALA	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY				



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	0.159	Depositor
Minimum map value	-0.082	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: 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	0.46	0/1123
1	F	0.20	0/834	0.45	0/1123
1	H	0.20	0/834	0.46	0/1123
1	J	0.20	0/834	0.46	0/1123
2	B	0.24	0/25428	0.53	5/34534 (0.0%)
2	E	0.24	0/25428	0.53	5/34534 (0.0%)
2	G	0.24	0/25428	0.53	5/34534 (0.0%)
2	I	0.24	0/25428	0.53	5/34534 (0.0%)
All	All	0.23	0/105048	0.53	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	17
2	E	0	17
2	G	0	17
2	I	0	17
All	All	0	72

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	4666	VAL	CA-C-N	-7.48	110.49	119.84
2	G	4666	VAL	C-N-CA	-7.48	110.49	119.84
2	B	4666	VAL	CA-C-N	-7.47	110.51	119.84
2	B	4666	VAL	C-N-CA	-7.47	110.51	119.84
2	E	4666	VAL	CA-C-N	-7.46	110.51	119.84
2	E	4666	VAL	C-N-CA	-7.46	110.51	119.84
2	I	4666	VAL	CA-C-N	-7.46	110.51	119.84
2	I	4666	VAL	C-N-CA	-7.46	110.51	119.84
2	I	1828	ASP	CA-C-N	6.18	126.20	119.89
2	I	1828	ASP	C-N-CA	6.18	126.20	119.89
2	G	1828	ASP	CA-C-N	6.16	126.17	119.89
2	G	1828	ASP	C-N-CA	6.16	126.17	119.89
2	E	1828	ASP	CA-C-N	6.15	126.17	119.89
2	E	1828	ASP	C-N-CA	6.15	126.17	119.89
2	B	1828	ASP	CA-C-N	6.12	126.13	119.89
2	B	1828	ASP	C-N-CA	6.12	126.13	119.89
2	E	131	LEU	CA-CB-CG	5.21	134.52	116.30
2	B	131	LEU	CA-CB-CG	5.20	134.49	116.30
2	I	131	LEU	CA-CB-CG	5.20	134.49	116.30
2	G	131	LEU	CA-CB-CG	5.20	134.49	116.30

There are no chirality outliers.

All (72) 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	1690	ASP	Peptide
2	B	1712	TYR	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	1840	PRO	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

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Mol	Chain	Res	Type	Group
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1690	ASP	Peptide
2	E	1712	TYR	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide
2	E	1840	PRO	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	1690	ASP	Peptide
2	G	1712	TYR	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	Peptide
2	G	1840	PRO	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	1690	ASP	Peptide
2	I	1712	TYR	Peptide
2	I	1795	PRO	Peptide
2	I	1828	ASP	Peptide

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Mol	Chain	Res	Type	Group
2	I	1840	PRO	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	8	0
1	H	818	0	824	6	0
1	J	818	0	824	6	0
2	B	29369	0	24723	211	0
2	E	29369	0	24722	206	0
2	G	29369	0	24722	209	0
2	I	29369	0	24722	213	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	102185	843	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 (843) 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:4958:CYS:SG	2:I:4978:HIS:CD2	2.67	0.87
2:G:4958:CYS:SG	2:G:4978:HIS:CD2	2.67	0.87
2:E:4958:CYS:SG	2:E:4978:HIS:CD2	2.67	0.87
2:B:4958:CYS:SG	2:B:4978:HIS:CD2	2.67	0.87
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.75	0.68
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.75	0.68
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.27	0.68
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.27	0.67
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.75	0.67
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.77	0.67
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.77	0.67
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.27	0.67
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.77	0.66
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.78	0.66
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.27	0.66
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.77	0.66
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.78	0.66
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.76	0.65
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.78	0.65
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.77	0.65
2:B:2764:GLU:HG3	2:B:2857:PRO:HB2	1.79	0.65
2:G:2764:GLU:HG3	2:G:2857:PRO:HB2	1.79	0.65
2:I:2764:GLU:HG3	2:I:2857:PRO:HB2	1.79	0.64
2:E:2764:GLU:HG3	2:E:2857:PRO:HB2	1.79	0.64
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.81	0.62
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.82	0.62
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.82	0.62
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.82	0.62
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.34	0.61
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.65	0.61
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.33	0.61
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.33	0.61
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.33	0.61
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.82	0.61
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.65	0.61
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.34	0.61
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.65	0.61
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.65	0.60
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.34	0.60
2:E:670:GLU:HG3	2:E:788:LYS:H	1.66	0.60
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:670:GLU:HG3	2:G:788:LYS:H	1.66	0.60
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.34	0.60
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.34	0.60
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.34	0.60
2:B:670:GLU:HG3	2:B:788:LYS:H	1.66	0.60
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.34	0.60
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.34	0.60
2:I:670:GLU:HG3	2:I:788:LYS:H	1.66	0.59
2:E:2131:LEU:HB3	2:E:3662:ILE:HD13	1.85	0.59
2:G:2131:LEU:HB3	2:G:3662:ILE:HD13	1.85	0.59
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.83	0.59
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.84	0.59
2:B:2287:ALA:HA	2:B:2290:LEU:HD13	1.84	0.59
2:G:101:LEU:HB3	2:G:150:MET:HE1	1.85	0.59
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.85	0.59
2:G:4184:MET:HB3	2:G:4190:ILE:HD13	1.85	0.59
2:E:2287:ALA:HA	2:E:2290:LEU:HD13	1.85	0.59
2:I:2131:LEU:HB3	2:I:3662:ILE:HD13	1.85	0.59
2:B:2131:LEU:HB3	2:B:3662:ILE:HD13	1.85	0.58
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.85	0.58
2:G:2287:ALA:HA	2:G:2290:LEU:HD13	1.85	0.58
2:B:4184:MET:HB3	2:B:4190:ILE:HD13	1.85	0.58
2:E:4184:MET:HB3	2:E:4190:ILE:HD13	1.85	0.58
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.85	0.58
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.69	0.58
2:E:101:LEU:HB3	2:E:150:MET:HE1	1.85	0.58
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.68	0.58
2:B:609:CYS:SG	2:B:610:ASN:N	2.77	0.58
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.35	0.58
2:B:606:LEU:O	2:B:617:ASN:ND2	2.37	0.58
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.85	0.58
2:I:4184:MET:HB3	2:I:4190:ILE:HD13	1.85	0.58
2:I:41:GLY:O	2:I:45:ARG:NH1	2.37	0.57
2:I:609:CYS:SG	2:I:610:ASN:N	2.77	0.57
2:I:2287:ALA:HA	2:I:2290:LEU:HD13	1.84	0.57
2:E:41:GLY:O	2:E:45:ARG:NH1	2.37	0.57
2:I:111:HIS:HD2	2:I:114:SER:H	1.51	0.57
2:G:111:HIS:HD2	2:G:114:SER:H	1.51	0.57
2:G:606:LEU:O	2:G:617:ASN:ND2	2.37	0.57
1:A:27:THR:HB	1:A:100:ASP:HB3	1.87	0.57
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:GLY:O	2:B:45:ARG:NH1	2.37	0.57
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.68	0.57
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.68	0.57
2:B:101:LEU:HB3	2:B:150:MET:HE1	1.85	0.57
2:I:606:LEU:O	2:I:617:ASN:ND2	2.37	0.57
2:I:4832:HIS:NE2	2:I:4942:GLU:OE1	2.38	0.57
1:F:27:THR:HB	1:F:100:ASP:HB3	1.87	0.57
2:E:606:LEU:O	2:E:617:ASN:ND2	2.37	0.57
1:J:27:THR:HB	1:J:100:ASP:HB3	1.87	0.57
2:B:379:HIS:HD2	2:B:382:GLY:H	1.53	0.57
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.35	0.57
2:E:609:CYS:SG	2:E:610:ASN:N	2.77	0.57
2:B:4791:TYR:OH	2:B:4815:ASP:O	2.23	0.57
2:G:41:GLY:O	2:G:45:ARG:NH1	2.37	0.57
2:G:626:LEU:HG	2:G:628:GLY:H	1.70	0.57
2:I:626:LEU:HG	2:I:628:GLY:H	1.70	0.56
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.88	0.56
2:B:4832:HIS:NE2	2:B:4942:GLU:OE1	2.38	0.56
2:I:379:HIS:HD2	2:I:382:GLY:H	1.53	0.56
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.87	0.56
2:G:609:CYS:SG	2:G:610:ASN:N	2.77	0.56
2:B:111:HIS:HD2	2:B:114:SER:H	1.51	0.56
2:I:4791:TYR:OH	2:I:4815:ASP:O	2.23	0.56
1:H:27:THR:HB	1:H:100:ASP:HB3	1.87	0.56
2:B:626:LEU:HG	2:B:628:GLY:H	1.70	0.56
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.87	0.56
2:E:4791:TYR:OH	2:E:4815:ASP:O	2.23	0.56
2:I:101:LEU:HB3	2:I:150:MET:HE1	1.85	0.56
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.88	0.56
2:G:1730:MET:O	2:G:1772:ARG:NH1	2.39	0.56
2:E:111:HIS:HD2	2:E:114:SER:H	1.51	0.56
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.87	0.56
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.39	0.56
2:E:1730:MET:O	2:E:1772:ARG:NH1	2.39	0.56
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.87	0.56
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.88	0.56
2:E:626:LEU:HG	2:E:628:GLY:H	1.70	0.56
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.87	0.56
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.87	0.55
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.88	0.55
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.78	0.55
2:E:4049:VAL:HG21	2:E:4159:ARG:HD2	1.88	0.55
2:G:379:HIS:HD2	2:G:382:GLY:H	1.53	0.55
2:B:533:ASN:ND2	2:B:536:ASN:OD1	2.39	0.55
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.88	0.55
2:B:4049:VAL:HG21	2:B:4159:ARG:HD2	1.87	0.55
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.78	0.55
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.88	0.55
2:G:4791:TYR:OH	2:G:4815:ASP:O	2.23	0.55
2:B:2347:GLU:O	2:B:2351:ASN:N	2.40	0.55
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.89	0.55
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.88	0.55
2:B:1730:MET:O	2:B:1772:ARG:NH1	2.39	0.55
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.87	0.55
2:G:2347:GLU:O	2:G:2351:ASN:N	2.40	0.55
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.89	0.55
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.88	0.55
2:I:1730:MET:O	2:I:1772:ARG:NH1	2.39	0.55
2:I:4049:VAL:HG21	2:I:4159:ARG:HD2	1.88	0.55
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.39	0.55
2:G:4049:VAL:HG21	2:G:4159:ARG:HD2	1.88	0.55
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.35	0.54
2:E:379:HIS:HD2	2:E:382:GLY:H	1.53	0.54
2:G:4152:GLU:OE1	2:G:4192:ARG:NH2	2.41	0.54
2:E:4832:HIS:NE2	2:E:4942:GLU:OE1	2.38	0.54
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.89	0.54
2:E:56:GLN:O	2:E:309:THR:OG1	2.26	0.54
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.88	0.54
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.89	0.54
2:I:2758:PHE:O	2:I:2762:THR:N	2.40	0.54
2:E:4152:GLU:OE1	2:E:4192:ARG:NH2	2.41	0.54
2:I:2347:GLU:O	2:I:2351:ASN:N	2.40	0.54
2:G:56:GLN:O	2:G:309:THR:OG1	2.26	0.54
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.88	0.54
2:G:132:ALA:HA	2:G:194:SER:HB2	1.89	0.54
2:G:3781:GLN:HA	2:G:3784:SER:HB3	1.90	0.54
2:E:35:LEU:HD13	2:E:49:LEU:HD13	1.90	0.54
2:I:132:ALA:HA	2:I:194:SER:HB2	1.89	0.54
2:G:533:ASN:ND2	2:G:536:ASN:OD1	2.39	0.54
2:B:132:ALA:HA	2:B:194:SER:HB2	1.89	0.54
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.90	0.54
2:I:4071:ILE:HG21	2:I:4097:MET:HE1	1.90	0.54
2:I:4152:GLU:OE1	2:I:4192:ARG:NH2	2.41	0.54
2:G:35:LEU:HD13	2:G:49:LEU:HD13	1.90	0.54
2:G:1148:VAL:HG21	2:G:1212:ARG:HG2	1.90	0.54
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.90	0.53
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.90	0.53
2:B:2876:GLU:OE1	2:B:2920:ARG:NH2	2.41	0.53
2:E:132:ALA:HA	2:E:194:SER:HB2	1.89	0.53
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.90	0.53
2:G:309:THR:O	2:G:313:SER:OG	2.26	0.53
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.89	0.53
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.39	0.53
2:E:3781:GLN:HA	2:E:3784:SER:HB3	1.90	0.53
2:I:309:THR:O	2:I:313:SER:OG	2.26	0.53
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.39	0.53
2:G:2758:PHE:O	2:G:2762:THR:N	2.40	0.53
2:B:4152:GLU:OE1	2:B:4192:ARG:NH2	2.41	0.53
2:I:35:LEU:HD13	2:I:49:LEU:HD13	1.90	0.53
2:I:2876:GLU:OE1	2:I:2920:ARG:NH2	2.41	0.53
2:E:1148:VAL:HG21	2:E:1212:ARG:HG2	1.90	0.53
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.90	0.53
2:B:4071:ILE:HG21	2:B:4097:MET:HE1	1.90	0.53
2:G:4071:ILE:HG21	2:G:4097:MET:HE1	1.90	0.53
2:B:1148:VAL:HG21	2:B:1212:ARG:HG2	1.90	0.53
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.41	0.53
2:E:2876:GLU:OE1	2:E:2920:ARG:NH2	2.41	0.53
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.90	0.53
2:B:3781:GLN:HA	2:B:3784:SER:HB3	1.90	0.53
2:I:454:PRO:HG2	2:I:531:ARG:HH12	1.74	0.53
2:I:619:ASP:OD1	2:I:1680:ARG:NH1	2.39	0.53
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.90	0.52
2:I:56:GLN:O	2:I:309:THR:OG1	2.26	0.52
2:B:35:LEU:HD13	2:B:49:LEU:HD13	1.90	0.52
2:B:575:LEU:HD22	2:B:609:CYS:HB3	1.91	0.52
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.90	0.52
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.42	0.52
2:I:1148:VAL:HG21	2:I:1212:ARG:HG2	1.90	0.52
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.42	0.52
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.42	0.52
2:G:23:GLN:OE1	2:G:203:ASN:ND2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2876:GLU:OE1	2:G:2920:ARG:NH2	2.41	0.52
2:B:56:GLN:O	2:B:309:THR:OG1	2.26	0.52
2:I:575:LEU:HD22	2:I:609:CYS:HB3	1.91	0.52
2:I:4933:GLN:NE2	2:G:4933:GLN:OE1	2.43	0.52
2:E:4071:ILE:HG21	2:E:4097:MET:HE1	1.90	0.52
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.75	0.52
2:G:40:GLU:HB3	2:G:44:ASN:HB3	1.91	0.52
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.39	0.52
2:B:4978:HIS:ND1	2:B:4982:GLU:OE1	2.39	0.52
2:E:309:THR:O	2:E:313:SER:OG	2.26	0.52
2:E:2758:PHE:O	2:E:2762:THR:N	2.40	0.52
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.42	0.52
2:B:40:GLU:HB3	2:B:44:ASN:HB3	1.91	0.52
2:I:23:GLN:OE1	2:I:203:ASN:ND2	2.42	0.52
2:G:575:LEU:HD22	2:G:609:CYS:HB3	1.91	0.52
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.78	0.52
2:B:23:GLN:OE1	2:B:203:ASN:ND2	2.42	0.52
2:E:575:LEU:HD22	2:E:609:CYS:HB3	1.91	0.52
2:I:393:CYS:SG	2:I:395:GLN:NE2	2.83	0.52
2:G:463:GLU:OE2	2:G:467:LYS:NZ	2.43	0.52
2:E:23:GLN:OE1	2:E:203:ASN:ND2	2.42	0.52
2:E:2257:LEU:HD11	2:E:2276:ALA:HB2	1.92	0.52
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.42	0.52
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.43	0.52
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.75	0.52
2:G:454:PRO:HG2	2:G:531:ARG:HH12	1.74	0.52
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.43	0.52
2:G:4832:HIS:NE2	2:G:4942:GLU:OE1	2.38	0.52
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.43	0.51
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.78	0.51
2:I:463:GLU:OE2	2:I:467:LYS:NZ	2.43	0.51
2:E:40:GLU:HB3	2:E:44:ASN:HB3	1.91	0.51
2:E:454:PRO:HG2	2:E:531:ARG:HH12	1.74	0.51
2:G:619:ASP:OD1	2:G:1680:ARG:NH1	2.39	0.51
2:G:689:THR:H	2:G:778:PHE:HE2	1.58	0.51
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.42	0.51
2:E:463:GLU:OE2	2:E:467:LYS:NZ	2.43	0.51
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.75	0.51
2:I:4567:LEU:HD12	2:I:4816:ILE:HD12	1.93	0.51
2:B:454:PRO:HG2	2:B:531:ARG:HH12	1.74	0.51
2:B:463:GLU:OE2	2:B:467:LYS:NZ	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.42	0.51
2:B:4567:LEU:HD12	2:B:4816:ILE:HD12	1.93	0.51
2:E:393:CYS:SG	2:E:395:GLN:NE2	2.83	0.51
2:G:393:CYS:SG	2:G:395:GLN:NE2	2.83	0.51
2:E:2347:GLU:O	2:E:2351:ASN:N	2.40	0.51
2:I:40:GLU:HB3	2:I:44:ASN:HB3	1.91	0.51
2:B:393:CYS:SG	2:B:395:GLN:NE2	2.83	0.51
2:E:4567:LEU:HD12	2:E:4816:ILE:HD12	1.93	0.51
2:I:1812:LEU:HD21	2:I:1861:GLN:HG2	1.93	0.51
2:G:1245:PHE:HD1	2:G:1600:LEU:HB3	1.76	0.51
2:G:2257:LEU:HD11	2:G:2276:ALA:HB2	1.92	0.51
2:B:1812:LEU:HD21	2:B:1861:GLN:HG2	1.93	0.51
2:E:1245:PHE:HD1	2:E:1600:LEU:HB3	1.76	0.51
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.42	0.51
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.92	0.51
2:B:2758:PHE:O	2:B:2762:THR:N	2.40	0.51
2:E:4666:VAL:HG23	2:E:4669:VAL:HB	1.93	0.51
2:B:309:THR:O	2:B:313:SER:OG	2.26	0.51
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.75	0.51
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.41	0.51
2:G:4567:LEU:HD12	2:G:4816:ILE:HD12	1.93	0.51
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.92	0.51
2:B:4933:GLN:OE1	2:E:4933:GLN:NE2	2.43	0.51
2:E:619:ASP:OD1	2:E:1680:ARG:NH1	2.39	0.51
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.43	0.51
2:I:4581:LYS:HD2	2:I:4632:LEU:HD22	1.93	0.51
2:G:1152:MET:HE1	2:G:1217:CYS:HB3	1.93	0.51
2:I:689:THR:H	2:I:778:PHE:HE2	1.58	0.50
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.41	0.50
1:A:92:PRO:HD3	2:B:627:PRO:HB2	1.92	0.50
2:B:689:THR:H	2:B:778:PHE:HE2	1.58	0.50
2:I:2257:LEU:HD11	2:I:2276:ALA:HB2	1.92	0.50
2:I:2277:ALA:HB1	2:I:2337:PHE:HD2	1.77	0.50
2:B:2257:LEU:HD11	2:B:2276:ALA:HB2	1.92	0.50
2:E:1100:MET:HE2	2:E:1198:GLN:HB3	1.94	0.50
2:G:4666:VAL:HG23	2:G:4669:VAL:HB	1.93	0.50
2:B:1100:MET:HE2	2:B:1198:GLN:HB3	1.94	0.50
2:B:1152:MET:HE1	2:B:1217:CYS:HB3	1.93	0.50
2:I:4984:ASN:ND2	2:I:4987:ASN:OD1	2.38	0.50
2:B:4666:VAL:HG23	2:B:4669:VAL:HB	1.93	0.50
2:E:1812:LEU:HD21	2:E:1861:GLN:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.77	0.50
2:B:4933:GLN:NE2	2:I:4933:GLN:OE1	2.44	0.50
2:I:4666:VAL:HG23	2:I:4669:VAL:HB	1.93	0.50
2:B:4138:ASP:OD1	2:B:4138:ASP:N	2.44	0.50
2:E:689:THR:H	2:E:778:PHE:HE2	1.58	0.50
2:E:4984:ASN:ND2	2:E:4987:ASN:OD1	2.38	0.50
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.94	0.50
2:G:1100:MET:HE2	2:G:1198:GLN:HB3	1.94	0.50
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.94	0.50
2:B:2277:ALA:HB1	2:B:2337:PHE:HD2	1.77	0.50
2:E:4581:LYS:HD2	2:E:4632:LEU:HD22	1.94	0.50
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.77	0.49
2:E:1152:MET:HE1	2:E:1217:CYS:HB3	1.94	0.49
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.46	0.49
2:I:1100:MET:HE2	2:I:1198:GLN:HB3	1.94	0.49
2:G:1170:MET:HE1	2:G:1176:GLU:HG3	1.94	0.49
2:G:1812:LEU:HD21	2:G:1861:GLN:HG2	1.93	0.49
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.94	0.49
2:B:4581:LYS:HD2	2:B:4632:LEU:HD22	1.94	0.49
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.92	0.49
2:B:2236:LEU:HD23	2:B:2275:VAL:HG21	1.94	0.49
2:G:627:PRO:O	2:G:629:ARG:NH1	2.46	0.49
2:I:1245:PHE:HD1	2:I:1600:LEU:HB3	1.76	0.49
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.92	0.49
2:E:399:GLN:HG2	2:E:403:MET:HE3	1.95	0.49
2:I:399:GLN:HG2	2:I:403:MET:HE3	1.95	0.49
2:I:1152:MET:HE1	2:I:1217:CYS:HB3	1.93	0.49
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.77	0.49
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.94	0.49
2:I:2236:LEU:HD23	2:I:2275:VAL:HG21	1.94	0.49
2:B:399:GLN:HG2	2:B:403:MET:HE3	1.95	0.49
2:I:627:PRO:O	2:I:629:ARG:NH1	2.46	0.49
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.45	0.49
2:G:4581:LYS:HD2	2:G:4632:LEU:HD22	1.93	0.49
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.95	0.49
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.77	0.49
2:B:1245:PHE:HD1	2:B:1600:LEU:HB3	1.76	0.49
2:E:1170:MET:HE1	2:E:1176:GLU:HG3	1.94	0.49
2:G:3850:GLN:HB3	2:G:3873:LYS:HD3	1.95	0.49
2:G:4864:ASN:H	2:G:4874:MET:HE3	1.78	0.49
2:B:627:PRO:O	2:B:629:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.46	0.48
2:E:3850:GLN:HB3	2:E:3873:LYS:HD3	1.95	0.48
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	1.95	0.48
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	1.95	0.48
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.95	0.48
2:E:2236:LEU:HD23	2:E:2275:VAL:HG21	1.94	0.48
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.46	0.48
2:G:2277:ALA:HB1	2:G:2337:PHE:HD2	1.77	0.48
2:E:4978:HIS:ND1	2:E:4982:GLU:OE1	2.39	0.48
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.95	0.48
2:I:1170:MET:HE1	2:I:1176:GLU:HG3	1.94	0.48
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	1.96	0.48
2:G:2236:LEU:HD23	2:G:2275:VAL:HG21	1.94	0.48
1:F:26:TYR:OH	1:F:42:ARG:NH2	2.47	0.48
2:B:619:ASP:OD1	2:B:1680:ARG:NH1	2.39	0.48
2:B:1170:MET:HE1	2:B:1176:GLU:HG3	1.94	0.48
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	1.96	0.48
2:E:4864:ASN:H	2:E:4874:MET:HE3	1.78	0.48
2:I:2267:MET:HE3	2:I:2268:GLN:HG2	1.95	0.48
2:G:999:ASP:O	2:G:1004:GLY:N	2.47	0.48
1:J:26:TYR:OH	1:J:42:ARG:NH2	2.47	0.48
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	1.96	0.48
1:J:92:PRO:HD3	2:I:627:PRO:HB2	1.95	0.48
2:B:940:GLY:O	2:B:1052:ASN:N	2.47	0.48
2:B:1808:ARG:HD3	2:B:1853:ILE:HG22	1.95	0.48
2:I:940:GLY:O	2:I:1052:ASN:N	2.47	0.48
2:I:999:ASP:O	2:I:1004:GLY:N	2.47	0.48
2:I:1131:ARG:NH1	2:I:1178:ALA:O	2.47	0.48
2:G:399:GLN:HG2	2:G:403:MET:HE3	1.95	0.48
2:G:4984:ASN:ND2	2:G:4987:ASN:OD1	2.38	0.48
2:B:1131:ARG:NH1	2:B:1178:ALA:O	2.47	0.48
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.96	0.48
2:G:1516:UNK:N	2:G:1529:UNK:O	2.47	0.48
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.87	0.48
2:B:999:ASP:O	2:B:1004:GLY:N	2.47	0.48
2:E:627:PRO:O	2:E:629:ARG:NH1	2.46	0.48
2:E:940:GLY:O	2:E:1052:ASN:N	2.47	0.48
2:E:1131:ARG:NH1	2:E:1178:ALA:O	2.47	0.48
2:E:1244:GLN:OE1	2:E:1646:ARG:NH1	2.47	0.48
2:E:1516:UNK:N	2:E:1529:UNK:O	2.47	0.48
2:I:1244:GLN:OE1	2:I:1646:ARG:NH1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	1.96	0.48
2:I:4864:ASN:H	2:I:4874:MET:HE3	1.79	0.48
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.95	0.48
1:A:26:TYR:OH	1:A:42:ARG:NH2	2.47	0.48
2:B:1516:UNK:N	2:B:1529:UNK:O	2.47	0.48
2:B:3850:GLN:HB3	2:B:3873:LYS:HD3	1.95	0.48
2:I:1516:UNK:N	2:I:1529:UNK:O	2.47	0.48
2:G:614:VAL:HA	2:G:2169:GLN:HB3	1.96	0.48
2:G:1131:ARG:NH1	2:G:1178:ALA:O	2.47	0.48
2:G:1808:ARG:HD3	2:G:1853:ILE:HG22	1.95	0.48
2:B:2267:MET:HE3	2:B:2268:GLN:HG2	1.95	0.47
2:E:359:TYR:HA	2:E:376:ALA:HA	1.96	0.47
2:E:999:ASP:O	2:E:1004:GLY:N	2.47	0.47
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.87	0.47
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.80	0.47
2:B:1244:GLN:OE1	2:B:1646:ARG:NH1	2.47	0.47
2:E:614:VAL:HA	2:E:2169:GLN:HB3	1.96	0.47
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.96	0.47
2:I:359:TYR:HA	2:I:376:ALA:HA	1.96	0.47
2:I:1808:ARG:HD3	2:I:1853:ILE:HG22	1.95	0.47
2:I:3850:GLN:HB3	2:I:3873:LYS:HD3	1.95	0.47
2:G:2868:SER:O	2:G:2872:GLN:N	2.45	0.47
1:H:26:TYR:OH	1:H:42:ARG:NH2	2.47	0.47
2:I:1720:LEU:HD12	2:I:1847:THR:HG23	1.97	0.47
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.87	0.47
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.97	0.47
2:I:2868:SER:O	2:I:2872:GLN:N	2.45	0.47
2:G:359:TYR:HA	2:G:376:ALA:HA	1.96	0.47
2:B:359:TYR:HA	2:B:376:ALA:HA	1.96	0.47
2:E:2267:MET:HE3	2:E:2268:GLN:HG2	1.95	0.47
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	1.95	0.47
2:G:793:LEU:HD12	2:G:797:HIS:H	1.80	0.47
2:G:1720:LEU:HD12	2:G:1847:THR:HG23	1.97	0.47
1:H:92:PRO:HD3	2:G:627:PRO:HB2	1.95	0.47
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.96	0.47
2:B:1126:GLY:HA3	2:B:1143:TRP:CE2	2.49	0.47
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.96	0.47
2:I:1815:LEU:HD22	2:I:1845:VAL:HG21	1.97	0.47
2:G:1244:GLN:OE1	2:G:1646:ARG:NH1	2.47	0.47
2:G:1973:GLN:O	2:G:1977:TYR:N	2.47	0.47
2:G:2267:MET:HE3	2:G:2268:GLN:HG2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	1.96	0.47
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.97	0.47
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.96	0.47
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.80	0.47
2:E:1126:GLY:HA3	2:E:1143:TRP:CE2	2.49	0.47
2:E:1808:ARG:HD3	2:E:1853:ILE:HG22	1.95	0.47
2:E:2277:ALA:HB1	2:E:2337:PHE:HD2	1.77	0.47
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	1.96	0.47
2:E:4138:ASP:OD1	2:E:4138:ASP:N	2.44	0.47
2:E:4933:GLN:OE1	2:G:4933:GLN:NE2	2.46	0.47
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.96	0.47
2:G:940:GLY:O	2:G:1052:ASN:N	2.47	0.47
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	1.95	0.47
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.87	0.47
2:E:1720:LEU:HD12	2:E:1847:THR:HG23	1.97	0.47
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	1.96	0.47
2:I:1126:GLY:HA3	2:I:1143:TRP:CE2	2.49	0.47
2:B:1815:LEU:HD22	2:B:1845:VAL:HG21	1.97	0.47
2:B:1973:GLN:O	2:B:1977:TYR:N	2.47	0.47
2:E:793:LEU:HD12	2:E:797:HIS:H	1.80	0.47
2:G:1126:GLY:HA3	2:G:1143:TRP:CE2	2.49	0.47
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.97	0.47
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.96	0.47
2:G:4152:GLU:OE1	2:G:4194:TYR:OH	2.33	0.47
2:B:4864:ASN:H	2:B:4874:MET:HE3	1.78	0.47
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.79	0.47
2:I:2908:TYR:OH	2:I:2920:ARG:NE	2.44	0.47
2:G:470:SER:O	2:G:474:ARG:NE	2.46	0.47
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.96	0.47
2:B:4152:GLU:OE1	2:B:4194:TYR:OH	2.33	0.47
2:B:1720:LEU:HD12	2:B:1847:THR:HG23	1.97	0.46
2:E:4152:GLU:OE1	2:E:4194:TYR:OH	2.33	0.46
2:G:614:VAL:HG22	2:G:616:SER:H	1.79	0.46
2:G:2155:LEU:HD13	2:G:2188:ASN:HD21	1.81	0.46
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.41	0.46
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	1.96	0.46
2:E:1973:GLN:O	2:E:1977:TYR:N	2.47	0.46
2:E:3809:ASN:HB3	2:E:3812:VAL:HG22	1.97	0.46
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.80	0.46
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.81	0.46
2:B:614:VAL:HA	2:B:2169:GLN:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:793:LEU:HD12	2:B:797:HIS:H	1.80	0.46
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.49	0.46
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.97	0.46
2:I:614:VAL:HG22	2:I:616:SER:H	1.79	0.46
2:I:4152:GLU:OE1	2:I:4194:TYR:OH	2.33	0.46
2:B:614:VAL:HG22	2:B:616:SER:H	1.79	0.46
2:G:1815:LEU:HD22	2:G:1845:VAL:HG21	1.97	0.46
2:I:2155:LEU:HD13	2:I:2188:ASN:HD21	1.81	0.46
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.81	0.46
2:B:2155:LEU:HD13	2:B:2188:ASN:HD21	1.81	0.46
2:E:1815:LEU:HD22	2:E:1845:VAL:HG21	1.97	0.46
2:E:2155:LEU:HD13	2:E:2188:ASN:HD21	1.80	0.46
2:G:1840:PRO:O	2:G:1844:LEU:N	2.48	0.46
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.81	0.46
2:B:470:SER:O	2:B:474:ARG:NE	2.45	0.46
2:E:1808:ARG:HD2	2:E:1854:PHE:HA	1.98	0.46
2:I:793:LEU:HD12	2:I:797:HIS:H	1.80	0.46
2:E:614:VAL:HG22	2:E:616:SER:H	1.79	0.46
2:E:1840:PRO:O	2:E:1844:LEU:N	2.48	0.46
2:I:614:VAL:HA	2:I:2169:GLN:HB3	1.96	0.46
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.51	0.46
2:I:1840:PRO:O	2:I:1844:LEU:N	2.48	0.46
2:G:1808:ARG:HD2	2:G:1854:PHE:HA	1.98	0.46
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.51	0.45
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.49	0.45
2:B:3809:ASN:HB3	2:B:3812:VAL:HG22	1.97	0.45
2:B:235:ALA:HA	2:B:257:ARG:HD3	1.98	0.45
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.49	0.45
2:I:235:ALA:HA	2:I:257:ARG:HD3	1.98	0.45
2:I:4708:THR:O	2:I:4721:LYS:NZ	2.48	0.45
2:G:3809:ASN:HB3	2:G:3812:VAL:HG22	1.97	0.45
2:I:379:HIS:CD2	2:I:381:GLU:H	2.35	0.45
2:I:1808:ARG:HD2	2:I:1854:PHE:HA	1.98	0.45
2:I:4978:HIS:ND1	2:I:4982:GLU:OE1	2.39	0.45
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.49	0.45
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.51	0.45
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.99	0.45
2:E:235:ALA:HA	2:E:257:ARG:HD3	1.98	0.45
2:E:2868:SER:O	2:E:2872:GLN:N	2.45	0.45
2:E:4688:ILE:HG21	2:E:4728:HIS:HB3	1.99	0.45
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1973:GLN:O	2:I:1977:TYR:N	2.47	0.45
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.51	0.45
2:I:3842:LEU:O	2:I:3929:SER:OG	2.35	0.45
2:G:379:HIS:CD2	2:G:381:GLU:H	2.35	0.45
2:G:4688:ILE:HG21	2:G:4728:HIS:HB3	1.98	0.45
2:B:134:ASP:OD1	2:B:134:ASP:N	2.49	0.45
2:B:2908:TYR:OH	2:B:2920:ARG:NE	2.44	0.45
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.51	0.45
2:I:4688:ILE:HG21	2:I:4728:HIS:HB3	1.99	0.45
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.98	0.45
2:G:4978:HIS:ND1	2:G:4982:GLU:OE1	2.39	0.45
2:I:582:HIS:O	2:I:585:SER:OG	2.29	0.45
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.99	0.45
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.51	0.45
2:B:1808:ARG:HD2	2:B:1854:PHE:HA	1.98	0.45
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.51	0.45
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.50	0.45
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.99	0.45
2:I:4036:VAL:HG11	2:I:5035:GLN:HB3	1.99	0.45
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.50	0.45
2:G:4036:VAL:HG11	2:G:5035:GLN:HB3	1.99	0.45
2:G:4738:ALA:HA	2:G:4743:MET:HE3	1.99	0.45
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.81	0.44
2:B:1840:PRO:O	2:B:1844:LEU:N	2.48	0.44
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.50	0.44
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.99	0.44
2:B:4738:ALA:HA	2:B:4743:MET:HE3	1.99	0.44
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.99	0.44
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.51	0.44
2:I:3809:ASN:HB3	2:I:3812:VAL:HG22	1.97	0.44
2:I:4138:ASP:OD1	2:I:4138:ASP:N	2.44	0.44
2:G:3842:LEU:O	2:G:3929:SER:OG	2.35	0.44
2:B:2862:LEU:HB3	2:B:2928:LYS:HB3	1.99	0.44
2:B:4036:VAL:HG11	2:B:5035:GLN:HB3	1.99	0.44
2:B:4059:LEU:HD13	2:B:4167:ALA:HB2	1.99	0.44
2:B:4688:ILE:HG21	2:B:4728:HIS:HB3	1.99	0.44
2:E:2862:LEU:HB3	2:E:2928:LYS:HB3	1.99	0.44
2:E:4059:LEU:HD13	2:E:4167:ALA:HB2	1.99	0.44
2:E:4738:ALA:HA	2:E:4743:MET:HE3	1.99	0.44
2:I:4681:LEU:HD21	2:I:4687:TYR:HD2	1.82	0.44
2:G:4577:LEU:HG	2:G:4580:TYR:HE2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4680:LYS:HD3	2:B:4686:LEU:HD22	1.99	0.44
2:E:134:ASP:N	2:E:134:ASP:OD1	2.49	0.44
2:E:4036:VAL:HG11	2:E:5035:GLN:HB3	1.99	0.44
2:E:4681:LEU:HD21	2:E:4687:TYR:HD2	1.82	0.44
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.99	0.44
2:I:4738:ALA:HA	2:I:4743:MET:HE3	1.99	0.44
2:G:134:ASP:OD1	2:G:134:ASP:N	2.49	0.44
2:G:235:ALA:HA	2:G:257:ARG:HD3	1.98	0.44
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.99	0.44
2:B:3842:LEU:O	2:B:3929:SER:OG	2.35	0.44
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.98	0.44
2:I:2862:LEU:HB3	2:I:2928:LYS:HB3	1.99	0.44
2:I:4155:PRO:HD2	2:I:5036:LEU:HD23	2.00	0.44
2:G:4138:ASP:OD1	2:G:4138:ASP:N	2.44	0.44
2:B:379:HIS:CD2	2:B:381:GLU:H	2.35	0.44
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.98	0.44
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	2.00	0.44
2:B:4629:TYR:OH	2:I:4860:ARG:NH2	2.49	0.44
2:E:978:THR:HB	2:E:980:ALA:H	1.82	0.44
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.50	0.44
2:G:4155:PRO:HD2	2:G:5036:LEU:HD23	2.00	0.44
2:G:4680:LYS:HD3	2:G:4686:LEU:HD22	1.99	0.44
2:B:385:ASP:HB2	2:I:156:GLN:HE21	1.83	0.44
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.99	0.44
2:B:4681:LEU:HD21	2:B:4687:TYR:HD2	1.82	0.44
2:E:379:HIS:CD2	2:E:381:GLU:H	2.35	0.44
2:I:4059:LEU:HD13	2:I:4167:ALA:HB2	1.99	0.44
2:I:4228:ALA:O	2:I:4232:GLU:N	2.51	0.44
2:G:1096:THR:HG23	2:G:1199:VAL:HG22	2.00	0.44
2:G:4092:ASP:OD1	2:G:4092:ASP:N	2.51	0.44
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.99	0.44
2:I:4680:LYS:HD3	2:I:4686:LEU:HD22	1.99	0.44
2:B:1096:THR:HG23	2:B:1199:VAL:HG22	2.00	0.44
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	2.00	0.44
2:B:4228:ALA:O	2:B:4232:GLU:N	2.51	0.44
2:B:4708:THR:O	2:B:4721:LYS:NZ	2.48	0.44
2:E:4233:LEU:HA	2:E:4236:SER:HB3	2.00	0.44
2:I:470:SER:O	2:I:474:ARG:NE	2.46	0.44
2:I:1694:LEU:O	2:I:1712:TYR:OH	2.26	0.44
2:G:978:THR:HB	2:G:980:ALA:H	1.82	0.44
2:E:4680:LYS:HD3	2:E:4686:LEU:HD22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	2.00	0.43
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	2.00	0.43
2:I:4577:LEU:HG	2:I:4580:TYR:HE2	1.83	0.43
2:G:2024:PRO:O	2:G:2028:ARG:NE	2.47	0.43
2:G:4681:LEU:HD21	2:G:4687:TYR:HD2	1.82	0.43
2:B:4577:LEU:HG	2:B:4580:TYR:HE2	1.83	0.43
2:E:3842:LEU:O	2:E:3929:SER:OG	2.35	0.43
2:I:408:ALA:HB2	2:I:483:MET:HE1	2.01	0.43
2:G:408:ALA:HB2	2:G:483:MET:HE1	2.01	0.43
2:B:596:ASN:HB3	2:B:599:VAL:HG22	2.01	0.43
2:B:978:THR:HB	2:B:980:ALA:H	1.82	0.43
2:B:4233:LEU:HA	2:B:4236:SER:HB3	2.00	0.43
2:E:1096:THR:HG23	2:E:1199:VAL:HG22	2.00	0.43
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	2.00	0.43
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.99	0.43
2:I:596:ASN:HB3	2:I:599:VAL:HG22	2.00	0.43
2:I:2024:PRO:O	2:I:2028:ARG:NE	2.47	0.43
2:G:596:ASN:HB3	2:G:599:VAL:HG22	2.00	0.43
2:G:4228:ALA:O	2:G:4232:GLU:N	2.51	0.43
2:E:1931:LEU:HB3	2:E:1935:VAL:HB	2.00	0.43
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	2.00	0.43
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	2.01	0.43
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	2.00	0.43
2:G:2908:TYR:OH	2:G:2920:ARG:NE	2.44	0.43
2:G:3989:VAL:HG12	2:G:4047:MET:HE1	2.01	0.43
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	2.01	0.43
2:I:134:ASP:OD1	2:I:134:ASP:N	2.49	0.43
2:I:1096:THR:HG23	2:I:1199:VAL:HG22	2.00	0.43
2:I:1979:LEU:HA	2:I:1983:ALA:HB3	2.01	0.43
2:E:426:ARG:HB2	2:E:506:TYR:HA	2.01	0.43
2:E:1076:ARG:HD3	2:E:1237:TRP:HB2	2.00	0.43
2:G:2862:LEU:HB3	2:G:2928:LYS:HB3	1.99	0.43
2:B:426:ARG:HB2	2:B:506:TYR:HA	2.01	0.43
2:E:4251:ILE:HG22	2:E:4553:ASN:HD22	1.84	0.43
2:I:637:LEU:HD23	2:I:1637:MET:HB3	2.01	0.43
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	2.01	0.43
1:F:34:LYS:HD3	2:E:629:ARG:HD2	2.00	0.43
2:B:195:PHE:HB3	2:B:196:MET:HG2	2.00	0.43
2:B:206:CYS:SG	2:B:207:SER:N	2.92	0.43
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.99	0.43
2:B:1979:LEU:HA	2:B:1983:ALA:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2199:ARG:NH2	2:B:2246:ASN:OD1	2.52	0.43
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	2.01	0.43
2:E:4155:PRO:HD2	2:E:5036:LEU:HD23	1.99	0.43
2:E:4577:LEU:HG	2:E:4580:TYR:HE2	1.83	0.43
2:E:4914:VAL:HG21	2:G:4884:LEU:HD11	2.01	0.43
2:G:637:LEU:HD23	2:G:1637:MET:HB3	2.01	0.43
2:G:1931:LEU:HB3	2:G:1935:VAL:HB	2.01	0.43
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.99	0.43
2:G:4708:THR:O	2:G:4721:LYS:NZ	2.48	0.43
2:B:408:ALA:HB2	2:B:483:MET:HE1	2.01	0.43
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	2.00	0.43
2:I:551:LEU:HD21	2:I:589:LEU:HD13	2.01	0.43
2:I:886:ARG:HB3	2:I:891:TRP:HB2	2.01	0.43
2:G:195:PHE:HB3	2:G:196:MET:HG2	2.00	0.43
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.48	0.43
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.48	0.43
2:B:2102:VAL:HB	2:B:2124:LEU:HD12	2.01	0.43
2:E:156:GLN:HE21	2:G:385:ASP:HB2	1.84	0.43
2:E:408:ALA:HB2	2:E:483:MET:HE1	2.01	0.43
2:E:596:ASN:HB3	2:E:599:VAL:HG22	2.00	0.43
2:I:2102:VAL:HB	2:I:2124:LEU:HD12	2.01	0.43
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.84	0.43
2:G:1076:ARG:HD3	2:G:1237:TRP:HB2	2.00	0.43
2:G:1707:LEU:O	2:G:1709:ALA:N	2.52	0.43
2:B:4155:PRO:HD2	2:B:5036:LEU:HD23	1.99	0.42
2:E:174:VAL:O	2:G:2452:ARG:NH1	2.52	0.42
2:E:206:CYS:SG	2:E:207:SER:N	2.92	0.42
2:E:3989:VAL:HG12	2:E:4047:MET:HE1	2.01	0.42
2:I:4092:ASP:OD1	2:I:4092:ASP:N	2.51	0.42
2:I:4233:LEU:HA	2:I:4236:SER:HB3	2.00	0.42
2:G:206:CYS:SG	2:G:207:SER:N	2.92	0.42
2:G:629:ARG:HD3	2:G:634:GLN:HG2	2.01	0.42
2:G:4059:LEU:HD13	2:G:4167:ALA:HB2	1.99	0.42
2:B:1076:ARG:HD3	2:B:1237:TRP:HB2	2.00	0.42
2:E:195:PHE:HB3	2:E:196:MET:HG2	2.00	0.42
2:E:1979:LEU:HA	2:E:1983:ALA:HB3	2.00	0.42
2:E:2199:ARG:NH2	2:E:2246:ASN:OD1	2.52	0.42
2:E:2908:TYR:OH	2:E:2920:ARG:NE	2.44	0.42
2:E:4092:ASP:N	2:E:4092:ASP:OD1	2.51	0.42
2:G:4027:LEU:HD22	2:G:4044:MET:HE2	2.02	0.42
2:B:1636:MET:HE2	2:B:1638:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.53	0.42
2:B:4027:LEU:HD22	2:B:4044:MET:HE2	2.02	0.42
2:I:195:PHE:HB3	2:I:196:MET:HG2	2.00	0.42
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.51	0.42
2:I:3989:VAL:HG12	2:I:4047:MET:HE1	2.01	0.42
2:I:4251:ILE:HG22	2:I:4553:ASN:HD22	1.84	0.42
2:G:582:HIS:O	2:G:585:SER:OG	2.29	0.42
2:G:886:ARG:HB3	2:G:891:TRP:HB2	2.01	0.42
2:G:3362:UNK:O	2:G:3366:UNK:N	2.53	0.42
2:B:637:LEU:HD23	2:B:1637:MET:HB3	2.01	0.42
2:B:2342:ASN:OD1	2:B:2342:ASN:N	2.41	0.42
2:B:4984:ASN:ND2	2:B:4987:ASN:OD1	2.38	0.42
2:E:3362:UNK:O	2:E:3366:UNK:N	2.53	0.42
2:I:4027:LEU:HD22	2:I:4044:MET:HE2	2.02	0.42
2:G:4251:ILE:HG22	2:G:4553:ASN:HD22	1.84	0.42
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	2.01	0.42
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.84	0.42
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.53	0.42
2:I:206:CYS:SG	2:I:207:SER:N	2.92	0.42
2:I:978:THR:HB	2:I:980:ALA:H	1.82	0.42
2:I:2199:ARG:NH2	2:I:2246:ASN:OD1	2.52	0.42
2:I:3362:UNK:O	2:I:3366:UNK:N	2.53	0.42
2:G:2199:ARG:NH2	2:G:2246:ASN:OD1	2.52	0.42
2:G:4233:LEU:HA	2:G:4236:SER:HB3	2.00	0.42
2:B:19:GLU:HB2	2:B:206:CYS:HB3	2.01	0.42
2:B:629:ARG:HD3	2:B:634:GLN:HG2	2.01	0.42
2:B:1760:HIS:HE1	2:B:2041:HIS:HA	1.85	0.42
2:B:1931:LEU:HB3	2:B:1935:VAL:HB	2.01	0.42
2:E:1707:LEU:O	2:E:1709:ALA:N	2.52	0.42
2:E:4228:ALA:O	2:E:4232:GLU:N	2.51	0.42
2:E:4708:THR:O	2:E:4721:LYS:NZ	2.48	0.42
2:G:479:GLN:HE21	2:G:536:ASN:ND2	2.18	0.42
2:G:1636:MET:HE2	2:G:1638:ALA:HB2	2.01	0.42
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.85	0.42
2:B:551:LEU:HD21	2:B:589:LEU:HD13	2.01	0.42
2:B:1707:LEU:O	2:B:1709:ALA:N	2.52	0.42
2:E:551:LEU:HD21	2:E:589:LEU:HD13	2.01	0.42
2:I:1707:LEU:O	2:I:1709:ALA:N	2.52	0.42
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.53	0.42
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	2.00	0.42
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:19:GLU:HB2	2:G:206:CYS:HB3	2.01	0.42
2:G:3662:ILE:H	2:G:3662:ILE:HG13	1.73	0.42
2:B:886:ARG:HB3	2:B:891:TRP:HB2	2.01	0.42
2:B:1671:ARG:NH2	2:B:1713:ASP:HB3	2.35	0.42
2:E:168:ASP:HB3	2:E:199:LEU:HD22	2.02	0.42
2:E:479:GLN:HE21	2:E:536:ASN:ND2	2.18	0.42
2:E:2102:VAL:HB	2:E:2124:LEU:HD12	2.01	0.42
2:E:4027:LEU:HD22	2:E:4044:MET:HE2	2.02	0.42
2:I:479:GLN:HE21	2:I:536:ASN:ND2	2.18	0.42
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.85	0.42
2:I:3891:LEU:HB3	2:I:3899:PHE:CE2	2.55	0.42
2:G:1979:LEU:HA	2:G:1983:ALA:HB3	2.00	0.42
2:G:2102:VAL:HB	2:G:2124:LEU:HD12	2.01	0.42
2:B:479:GLN:HE21	2:B:536:ASN:ND2	2.18	0.41
2:B:864:PRO:HA	2:B:865:PRO:HD3	1.92	0.41
2:B:3676:ASP:OD1	2:B:3676:ASP:N	2.53	0.41
2:B:3989:VAL:HG12	2:B:4047:MET:HE1	2.01	0.41
2:B:4092:ASP:OD1	2:B:4092:ASP:N	2.51	0.41
2:E:637:LEU:HD23	2:E:1637:MET:HB3	2.01	0.41
2:I:19:GLU:HB2	2:I:206:CYS:HB3	2.01	0.41
2:G:551:LEU:HD21	2:G:589:LEU:HD13	2.01	0.41
2:G:4763:GLY:O	2:G:4766:THR:OG1	2.32	0.41
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.84	0.41
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.85	0.41
2:B:3362:UNK:O	2:B:3366:UNK:N	2.53	0.41
2:I:1931:LEU:HB3	2:I:1935:VAL:HB	2.00	0.41
2:G:168:ASP:HB3	2:G:199:LEU:HD22	2.02	0.41
2:G:426:ARG:HB2	2:G:506:TYR:HA	2.01	0.41
2:G:1671:ARG:NH2	2:G:1713:ASP:HB3	2.35	0.41
2:G:4815:ASP:OD1	2:G:4815:ASP:N	2.53	0.41
2:B:4860:ARG:NH2	2:E:4629:TYR:OH	2.50	0.41
2:E:629:ARG:HD3	2:E:634:GLN:HG2	2.01	0.41
2:E:2788:HIS:CE1	2:E:2790:MET:HB2	2.56	0.41
2:B:156:GLN:HE21	2:E:385:ASP:HB2	1.85	0.41
2:B:1676:LEU:HD23	2:B:2167:ILE:HG23	2.03	0.41
2:B:3891:LEU:HB3	2:B:3899:PHE:CE2	2.55	0.41
2:B:4884:LEU:HD11	2:I:4914:VAL:HG21	2.03	0.41
2:E:19:GLU:HB2	2:E:206:CYS:HB3	2.01	0.41
2:E:1636:MET:HE2	2:E:1638:ALA:HB2	2.01	0.41
2:E:2337:PHE:HA	2:E:2340:PHE:HB2	2.02	0.41
2:E:3891:LEU:HB3	2:E:3899:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:426:ARG:HB2	2:I:506:TYR:HA	2.01	0.41
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.84	0.41
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	2.01	0.41
2:I:1760:HIS:HE1	2:I:2041:HIS:HA	1.85	0.41
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.85	0.41
2:B:2024:PRO:HB2	2:B:2027:ILE:HG12	2.02	0.41
2:B:2788:HIS:CE1	2:B:2790:MET:HB2	2.56	0.41
2:E:591:ASP:O	2:E:1594:ARG:NH2	2.54	0.41
2:E:886:ARG:HB3	2:E:891:TRP:HB2	2.01	0.41
2:G:2024:PRO:HB2	2:G:2027:ILE:HG12	2.02	0.41
2:G:2337:PHE:HA	2:G:2340:PHE:HB2	2.03	0.41
2:G:4201:ASN:HA	2:G:4204:GLN:HB3	2.03	0.41
2:B:1665:HIS:HA	2:B:1668:ARG:HG2	2.02	0.41
2:B:3829:PHE:HD1	2:B:3915:ILE:HD11	1.86	0.41
2:E:2290:LEU:HG	2:E:2291:GLN:H	1.85	0.41
2:E:2815:ALA:HB3	2:E:2881:ASN:HD21	1.86	0.41
2:I:330:ASP:OD1	2:I:330:ASP:N	2.54	0.41
2:I:2290:LEU:HG	2:I:2291:GLN:H	1.86	0.41
2:I:3829:PHE:HD1	2:I:3915:ILE:HD11	1.86	0.41
2:I:3927:GLN:NE2	2:I:3988:ALA:O	2.50	0.41
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	2.02	0.41
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.53	0.41
2:B:2868:SER:O	2:B:2872:GLN:N	2.45	0.41
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	2.02	0.41
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.85	0.41
2:I:1636:MET:HE2	2:I:1638:ALA:HB2	2.01	0.41
2:I:1665:HIS:HA	2:I:1668:ARG:HG2	2.02	0.41
2:I:1676:LEU:HD23	2:I:2167:ILE:HG23	2.03	0.41
2:I:2788:HIS:CE1	2:I:2790:MET:HB2	2.56	0.41
2:B:214:VAL:HG12	2:B:274:LEU:HD12	2.03	0.41
2:B:4251:ILE:HG22	2:B:4553:ASN:HD22	1.84	0.41
2:E:1671:ARG:NH2	2:E:1713:ASP:HB3	2.35	0.41
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	2.01	0.41
2:G:3891:LEU:HB3	2:G:3899:PHE:CE2	2.55	0.41
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	2.02	0.41
2:B:2024:PRO:O	2:B:2028:ARG:NE	2.47	0.41
2:B:2188:ASN:OD1	2:B:2188:ASN:N	2.54	0.41
2:B:2290:LEU:HG	2:B:2291:GLN:H	1.86	0.41
2:B:2815:ALA:HB3	2:B:2881:ASN:HD21	1.86	0.41
2:E:470:SER:O	2:E:474:ARG:NE	2.46	0.41
2:E:1641:ILE:HA	2:E:1642:PRO:HD3	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1665:HIS:HA	2:E:1668:ARG:HG2	2.02	0.41
2:E:1676:LEU:HD23	2:E:2167:ILE:HG23	2.03	0.41
2:E:1760:HIS:HE1	2:E:2041:HIS:HA	1.85	0.41
2:E:2024:PRO:O	2:E:2028:ARG:NE	2.47	0.41
2:I:591:ASP:O	2:I:1594:ARG:NH2	2.54	0.41
2:I:629:ARG:HD3	2:I:634:GLN:HG2	2.01	0.41
2:I:1141:ARG:H	2:I:1141:ARG:HD2	1.86	0.41
2:I:2024:PRO:HB2	2:I:2027:ILE:HG12	2.02	0.41
2:I:4201:ASN:HA	2:I:4204:GLN:HB3	2.03	0.41
2:G:330:ASP:OD1	2:G:330:ASP:N	2.54	0.41
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	2.02	0.41
2:G:1676:LEU:HD23	2:G:2167:ILE:HG23	2.03	0.41
2:G:2788:HIS:CE1	2:G:2790:MET:HB2	2.55	0.41
1:F:77:THR:OG1	1:F:79:ASP:OD1	2.33	0.41
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.52	0.41
2:B:2337:PHE:HA	2:B:2340:PHE:HB2	2.02	0.41
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.85	0.41
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	2.03	0.41
2:I:1725:ARG:HH21	2:I:1725:ARG:HD2	1.71	0.41
2:I:2452:ARG:NH1	2:G:174:VAL:O	2.54	0.41
2:I:3676:ASP:N	2:I:3676:ASP:OD1	2.53	0.41
2:G:2815:ALA:HB3	2:G:2881:ASN:HD21	1.86	0.41
2:B:330:ASP:OD1	2:B:330:ASP:N	2.54	0.40
2:B:1141:ARG:HD2	2:B:1141:ARG:H	1.86	0.40
2:E:214:VAL:HG12	2:E:274:LEU:HD12	2.03	0.40
2:E:2024:PRO:HB2	2:E:2027:ILE:HG12	2.02	0.40
2:I:1671:ARG:NH2	2:I:1713:ASP:HB3	2.36	0.40
2:G:1658:ASP:N	2:G:1658:ASP:OD1	2.54	0.40
2:G:3829:PHE:HD1	2:G:3915:ILE:HD11	1.86	0.40
2:B:1131:ARG:HH12	2:B:1178:ALA:HB3	1.86	0.40
2:E:1141:ARG:HD2	2:E:1141:ARG:H	1.86	0.40
2:E:3844:LEU:HD23	2:E:3844:LEU:HA	1.92	0.40
2:I:168:ASP:HB3	2:I:199:LEU:HD22	2.02	0.40
2:I:2815:ALA:HB3	2:I:2881:ASN:HD21	1.86	0.40
2:I:3662:ILE:H	2:I:3662:ILE:HG13	1.73	0.40
2:G:1141:ARG:H	2:G:1141:ARG:HD2	1.86	0.40
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.51	0.40
2:B:591:ASP:O	2:B:1594:ARG:NH2	2.54	0.40
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	2.03	0.40
2:E:3829:PHE:HD1	2:E:3915:ILE:HD11	1.86	0.40
2:I:211:GLU:OE2	2:I:3907:THR:OG1	2.31	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:650:VAL:HB	2:I:777:PHE:HB2	2.04	0.40
2:I:1131:ARG:HH12	2:I:1178:ALA:HB3	1.86	0.40
2:G:591:ASP:O	2:G:1594:ARG:NH2	2.54	0.40
2:G:2290:LEU:HG	2:G:2291:GLN:H	1.86	0.40
2:B:23:GLN:HE21	2:B:34:LYS:HB3	1.87	0.40
2:B:582:HIS:O	2:B:585:SER:OG	2.29	0.40
2:B:841:GLY:HA2	2:B:1073:ARG:HD2	2.04	0.40
2:B:2674:UNK:O	2:B:2676:UNK:N	2.54	0.40
2:E:548:VAL:HG12	2:E:564:LEU:HD22	2.04	0.40
2:E:650:VAL:HB	2:E:777:PHE:HB2	2.04	0.40
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.48	0.40
2:I:841:GLY:HA2	2:I:1073:ARG:HD2	2.04	0.40
2:I:2337:PHE:HA	2:I:2340:PHE:HB2	2.02	0.40
2:I:2437:ALA:HA	2:I:2438:PRO:HD3	1.93	0.40
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	2.03	0.40
2:B:4201:ASN:HA	2:B:4204:GLN:HB3	2.03	0.40
2:E:2674:UNK:O	2:E:2676:UNK:N	2.54	0.40
2:I:864:PRO:HA	2:I:865:PRO:HD3	1.92	0.40
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	2.02	0.40
2:G:548:VAL:HG12	2:G:564:LEU:HD22	2.04	0.40
2:G:647:ASN:ND2	2:G:820:ARG:O	2.46	0.40
2:G:1665:HIS:HA	2:G:1668:ARG:HG2	2.02	0.40
2:G:3676:ASP:N	2:G:3676:ASP:OD1	2.53	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%)	93 (89%)	12 (11%)	0	100	100
1	F	105/108 (97%)	93 (89%)	12 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	J	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
2	B	3235/4676 (69%)	2899 (90%)	330 (10%)	6 (0%)	43	73
2	E	3235/4676 (69%)	2899 (90%)	330 (10%)	6 (0%)	43	73
2	G	3235/4676 (69%)	2898 (90%)	331 (10%)	6 (0%)	43	73
2	I	3235/4676 (69%)	2899 (90%)	330 (10%)	6 (0%)	43	73
All	All	13360/19136 (70%)	11967 (90%)	1369 (10%)	24 (0%)	44	73

All (24) 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	E	2291	GLN
2	I	2291	GLN
2	G	2291	GLN
2	B	2291	GLN
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
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%)	2480 (100%)	13 (0%)	81	81
2	E	2493/3202 (78%)	2480 (100%)	13 (0%)	81	81
2	G	2493/3202 (78%)	2480 (100%)	13 (0%)	81	81
2	I	2493/3202 (78%)	2480 (100%)	13 (0%)	81	81
All	All	10324/13164 (78%)	10272 (100%)	52 (0%)	78	81

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	688	LEU
2	B	719	LEU
2	B	815	VAL
2	B	978	THR
2	B	1600	LEU
2	B	1676	LEU
2	B	2339	VAL
2	B	2461	VAL
2	B	3663	LEU
2	B	3805	LEU
2	B	4081	VAL
2	B	4792	LEU
2	E	131	LEU
2	E	688	LEU
2	E	719	LEU
2	E	815	VAL
2	E	978	THR
2	E	1600	LEU
2	E	1676	LEU
2	E	2339	VAL
2	E	2461	VAL
2	E	3663	LEU

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Mol	Chain	Res	Type
2	E	3805	LEU
2	E	4081	VAL
2	E	4792	LEU
2	I	131	LEU
2	I	688	LEU
2	I	719	LEU
2	I	815	VAL
2	I	978	THR
2	I	1600	LEU
2	I	1676	LEU
2	I	2339	VAL
2	I	2461	VAL
2	I	3663	LEU
2	I	3805	LEU
2	I	4081	VAL
2	I	4792	LEU
2	G	131	LEU
2	G	688	LEU
2	G	719	LEU
2	G	815	VAL
2	G	978	THR
2	G	1600	LEU
2	G	1676	LEU
2	G	2339	VAL
2	G	2461	VAL
2	G	3663	LEU
2	G	3805	LEU
2	G	4081	VAL
2	G	4792	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (179) 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	23	GLN
2	B	105	HIS
2	B	113	HIS
2	B	156	GLN
2	B	203	ASN

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Mol	Chain	Res	Type
2	B	379	HIS
2	B	383	HIS
2	B	405	HIS
2	B	479	GLN
2	B	582	HIS
2	B	634	GLN
2	B	877	ASN
2	B	1640	HIS
2	B	1691	GLN
2	B	1693	GLN
2	B	1775	HIS
2	B	1861	GLN
2	B	2005	GLN
2	B	2035	HIS
2	B	2194	HIS
2	B	2260	ASN
2	B	2773	ASN
2	B	2788	HIS
2	B	3704	HIS
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	4109	GLN
2	B	4120	ASN
2	B	4201	ASN
2	B	4204	GLN
2	B	4246	GLN
2	B	4553	ASN
2	B	4700	GLN
2	B	4776	GLN
2	B	4933	GLN
2	B	5003	HIS
2	B	5031	GLN
2	E	23	GLN
2	E	105	HIS
2	E	113	HIS
2	E	156	GLN
2	E	203	ASN
2	E	379	HIS

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Mol	Chain	Res	Type
2	E	383	HIS
2	E	395	GLN
2	E	405	HIS
2	E	479	GLN
2	E	582	HIS
2	E	634	GLN
2	E	866	HIS
2	E	877	ASN
2	E	1640	HIS
2	E	1688	HIS
2	E	1691	GLN
2	E	1693	GLN
2	E	1775	HIS
2	E	1861	GLN
2	E	2005	GLN
2	E	2035	HIS
2	E	2194	HIS
2	E	2260	ASN
2	E	2773	ASN
2	E	2788	HIS
2	E	3704	HIS
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	4109	GLN
2	E	4120	ASN
2	E	4201	ASN
2	E	4204	GLN
2	E	4553	ASN
2	E	4691	GLN
2	E	4700	GLN
2	E	4776	GLN
2	E	4806	ASN
2	E	4933	GLN
2	E	4949	GLN
2	E	5003	HIS
2	E	5031	GLN
2	I	23	GLN
2	I	105	HIS

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Mol	Chain	Res	Type
2	I	113	HIS
2	I	156	GLN
2	I	203	ASN
2	I	273	HIS
2	I	379	HIS
2	I	383	HIS
2	I	395	GLN
2	I	405	HIS
2	I	479	GLN
2	I	520	ASN
2	I	582	HIS
2	I	634	GLN
2	I	866	HIS
2	I	877	ASN
2	I	1611	HIS
2	I	1640	HIS
2	I	1691	GLN
2	I	1693	GLN
2	I	1861	GLN
2	I	2005	GLN
2	I	2035	HIS
2	I	2194	HIS
2	I	2260	ASN
2	I	2773	ASN
2	I	2788	HIS
2	I	2881	ASN
2	I	3704	HIS
2	I	3771	HIS
2	I	3814	GLN
2	I	3895	HIS
2	I	3896	ASN
2	I	3909	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	4034	ASN
2	I	4109	GLN
2	I	4120	ASN
2	I	4204	GLN
2	I	4246	GLN
2	I	4553	ASN
2	I	4691	GLN
2	I	4776	GLN

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Mol	Chain	Res	Type
2	I	4806	ASN
2	I	4864	ASN
2	I	4933	GLN
2	I	5003	HIS
2	I	5031	GLN
2	G	23	GLN
2	G	105	HIS
2	G	156	GLN
2	G	203	ASN
2	G	379	HIS
2	G	383	HIS
2	G	405	HIS
2	G	479	GLN
2	G	520	ASN
2	G	582	HIS
2	G	634	GLN
2	G	866	HIS
2	G	877	ASN
2	G	1691	GLN
2	G	1693	GLN
2	G	1861	GLN
2	G	2005	GLN
2	G	2035	HIS
2	G	2194	HIS
2	G	2260	ASN
2	G	2773	ASN
2	G	2788	HIS
2	G	3704	HIS
2	G	3814	GLN
2	G	3895	HIS
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	4034	ASN
2	G	4109	GLN
2	G	4120	ASN
2	G	4133	GLN
2	G	4204	GLN
2	G	4246	GLN
2	G	4553	ASN
2	G	4776	GLN
2	G	4933	GLN

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Mol	Chain	Res	Type
2	G	5003	HIS
2	G	5031	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

Continued on next page...

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Mol	Chain	Number of breaks
2	B	12
2	E	12
2	G	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	43.02
1	B	3613:UNK	C	3639:THR	N	43.01
1	E	3613:UNK	C	3639:THR	N	43.01
1	G	3613:UNK	C	3639:THR	N	42.96
1	B	3163:UNK	C	3170:UNK	N	16.39
1	E	3163:UNK	C	3170:UNK	N	16.39
1	I	3163:UNK	C	3170:UNK	N	16.39
1	G	3163:UNK	C	3170:UNK	N	16.39
1	B	3468:UNK	C	3511:UNK	N	15.14
1	E	3468:UNK	C	3511:UNK	N	15.14
1	I	3468:UNK	C	3511:UNK	N	15.14
1	G	3468:UNK	C	3511:UNK	N	15.14
1	E	3063:UNK	C	3134:UNK	N	14.90
1	B	3063:UNK	C	3134:UNK	N	14.89
1	I	3063:UNK	C	3134:UNK	N	14.89
1	G	3063:UNK	C	3134:UNK	N	14.89
1	G	2703:UNK	C	2734:ASN	N	14.64
1	B	2703:UNK	C	2734:ASN	N	14.61
1	E	2703:UNK	C	2734:ASN	N	14.59
1	I	2703:UNK	C	2734:ASN	N	14.59
1	B	3236:UNK	C	3241:UNK	N	13.53
1	E	3236:UNK	C	3241:UNK	N	13.53
1	I	3236:UNK	C	3241:UNK	N	13.53
1	G	3236:UNK	C	3241:UNK	N	13.53
1	G	1564:UNK	C	1573:MET	N	12.52
1	B	1564:UNK	C	1573:MET	N	12.51
1	I	1564:UNK	C	1573:MET	N	12.51
1	E	1564:UNK	C	1573:MET	N	12.49
1	B	2976:UNK	C	2995:UNK	N	12.26
1	E	2976:UNK	C	2995:UNK	N	12.26
1	I	2976:UNK	C	2995:UNK	N	12.26
1	G	2976:UNK	C	2995:UNK	N	12.26
1	E	3254:UNK	C	3261:UNK	N	8.39
1	I	3254:UNK	C	3261:UNK	N	8.39
1	B	3254:UNK	C	3261:UNK	N	8.38
1	G	3254:UNK	C	3261:UNK	N	8.38

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1297:UNK	C	1430:UNK	N	5.79
1	I	1297:UNK	C	1430:UNK	N	5.79
1	G	1297:UNK	C	1430:UNK	N	5.79
1	E	1297:UNK	C	1430:UNK	N	5.77
1	G	2939:ARG	C	2942:UNK	N	3.40
1	B	2939:ARG	C	2942:UNK	N	3.37
1	E	2939:ARG	C	2942:UNK	N	3.36
1	I	2939:ARG	C	2942:UNK	N	3.36
1	E	2479:LEU	C	2487:UNK	N	3.29
1	I	2479:LEU	C	2487:UNK	N	3.29
1	B	2479:LEU	C	2487:UNK	N	3.28
1	G	2479:LEU	C	2487:UNK	N	3.25

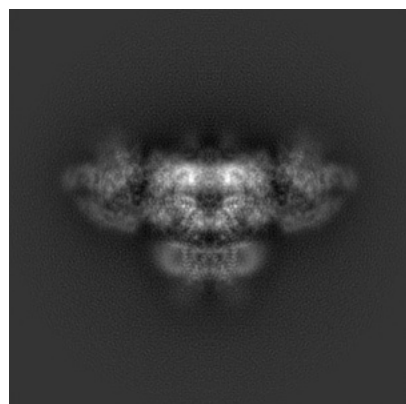
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8373. These allow visual inspection of the internal detail of the map and identification of artifacts.

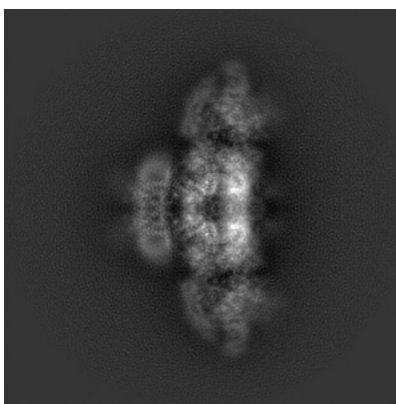
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

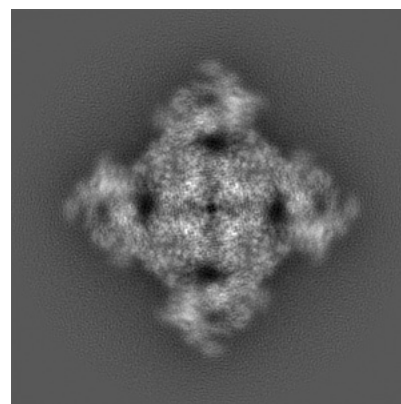
6.1.1 Primary map



X

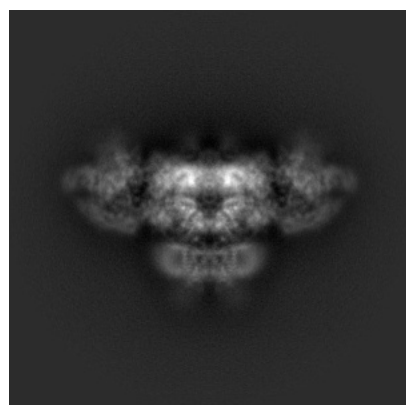


Y

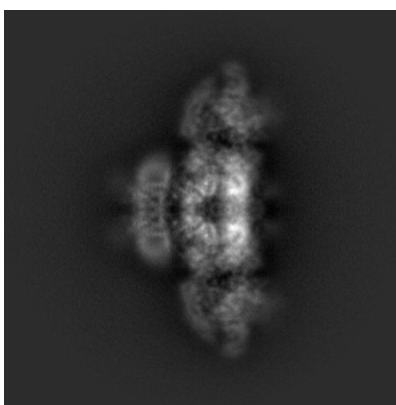


Z

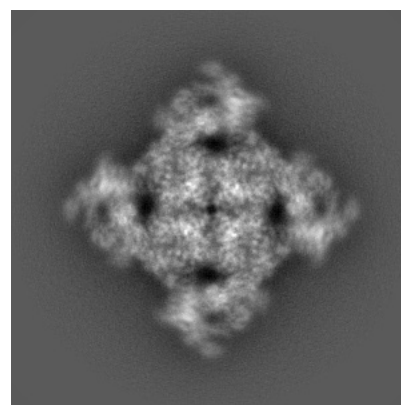
6.1.2 Raw map



X



Y

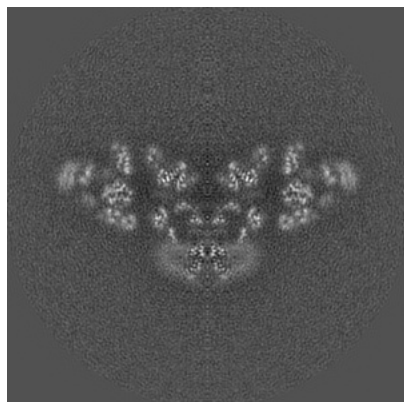


Z

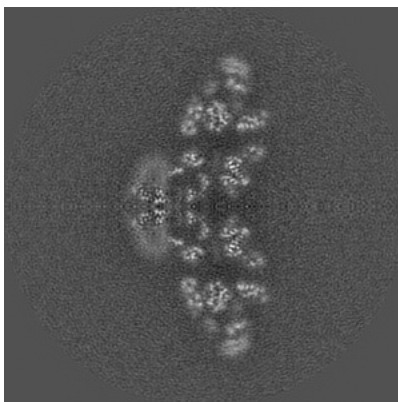
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

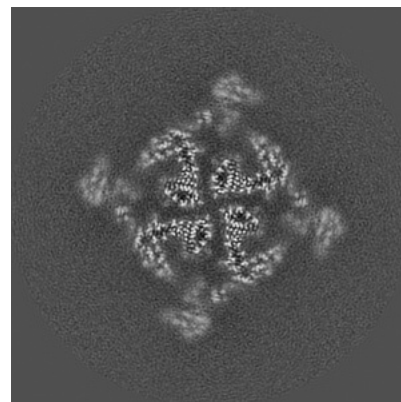
6.2.1 Primary map



X Index: 200

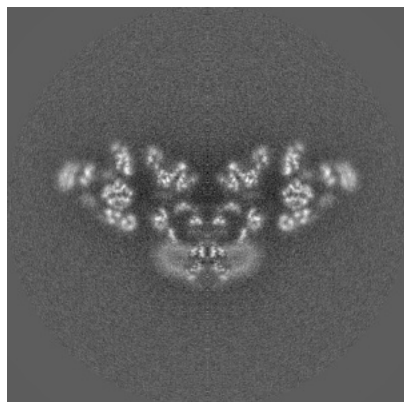


Y Index: 200

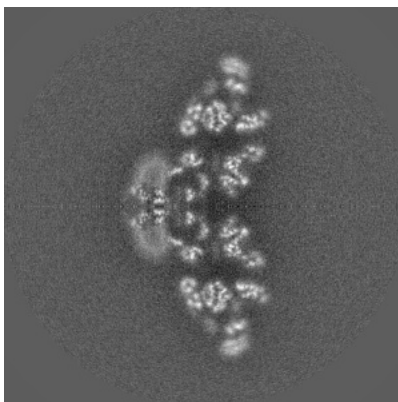


Z Index: 200

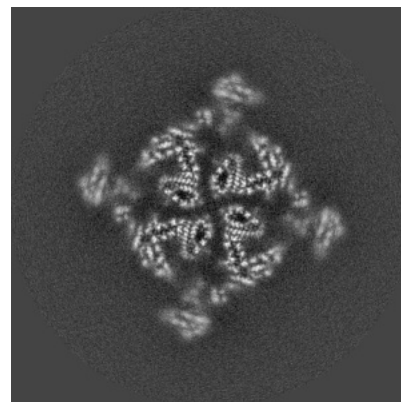
6.2.2 Raw map



X Index: 200



Y Index: 200

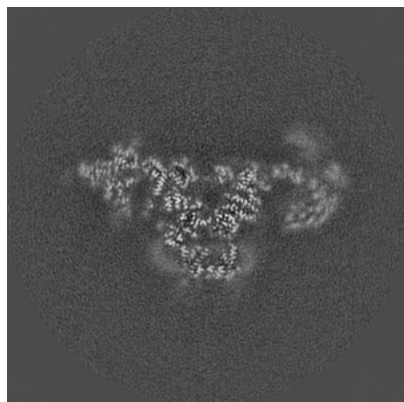


Z Index: 200

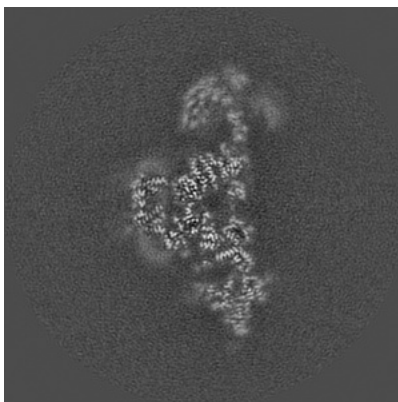
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

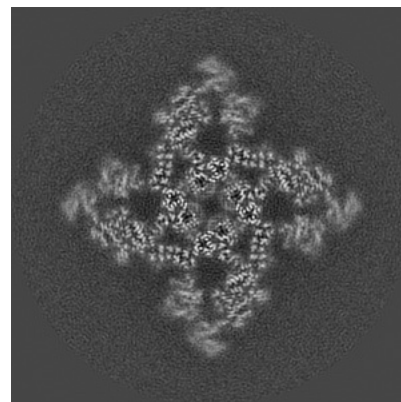
6.3.1 Primary map



X Index: 216

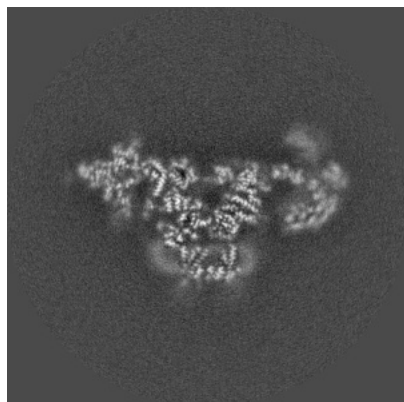


Y Index: 184

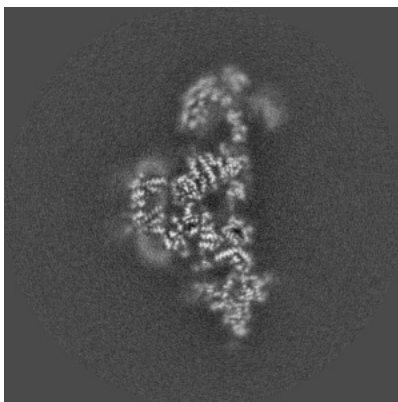


Z Index: 227

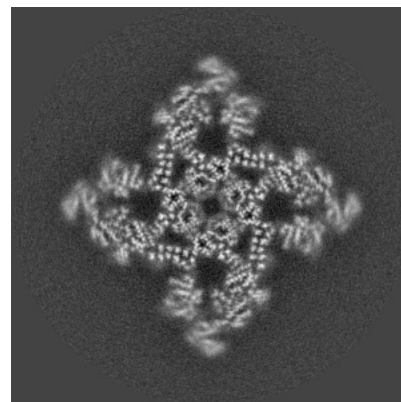
6.3.2 Raw map



X Index: 216



Y Index: 184

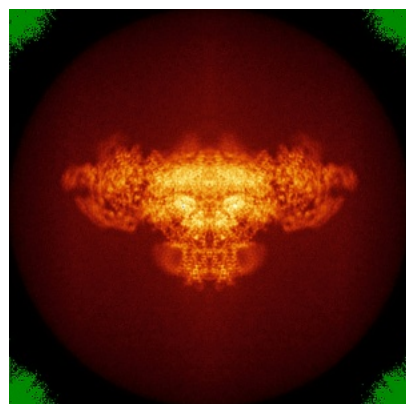


Z Index: 227

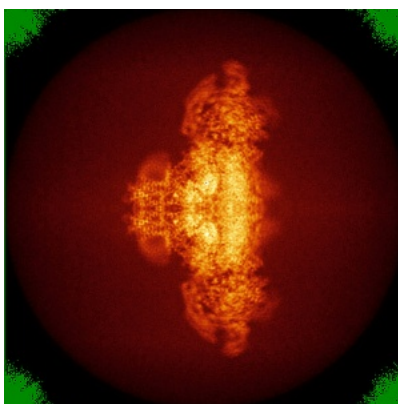
The images above show the largest variance slices of the map in three orthogonal directions.

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

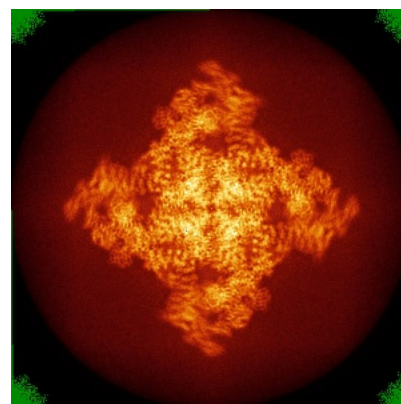
6.4.1 Primary map



X

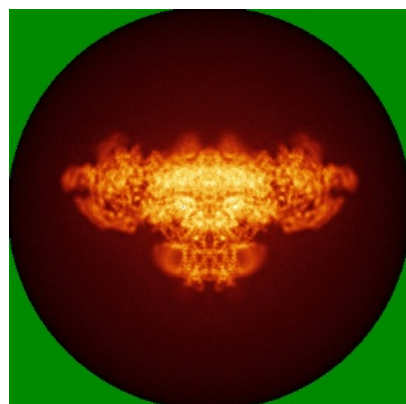


Y

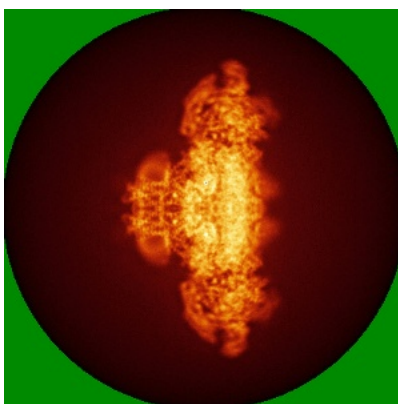


Z

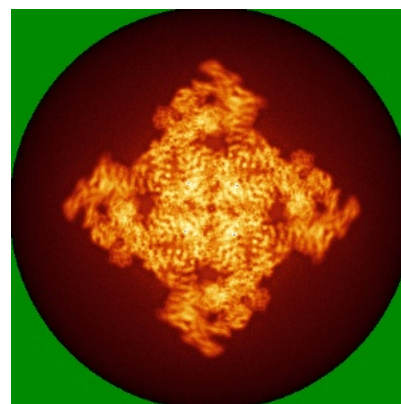
6.4.2 Raw map



X



Y

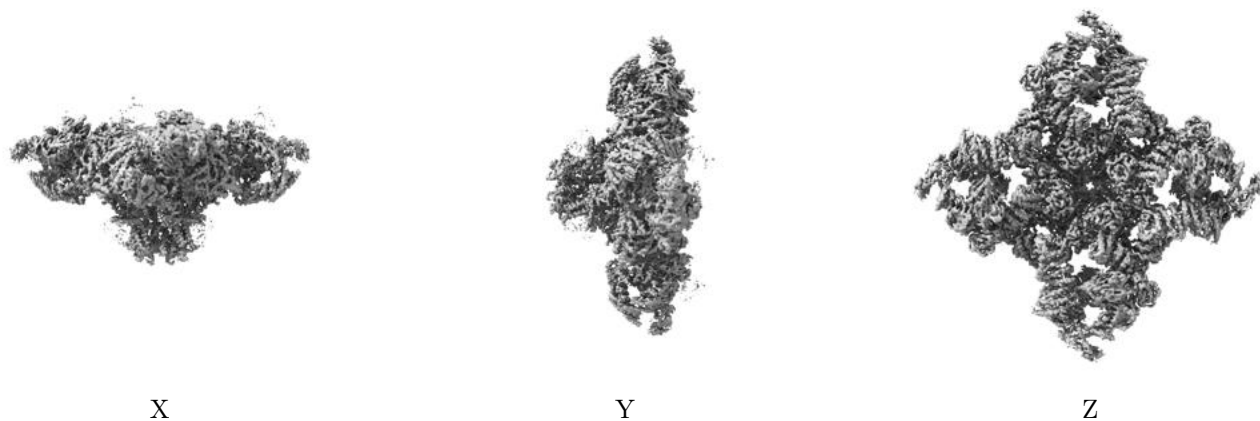


Z

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.

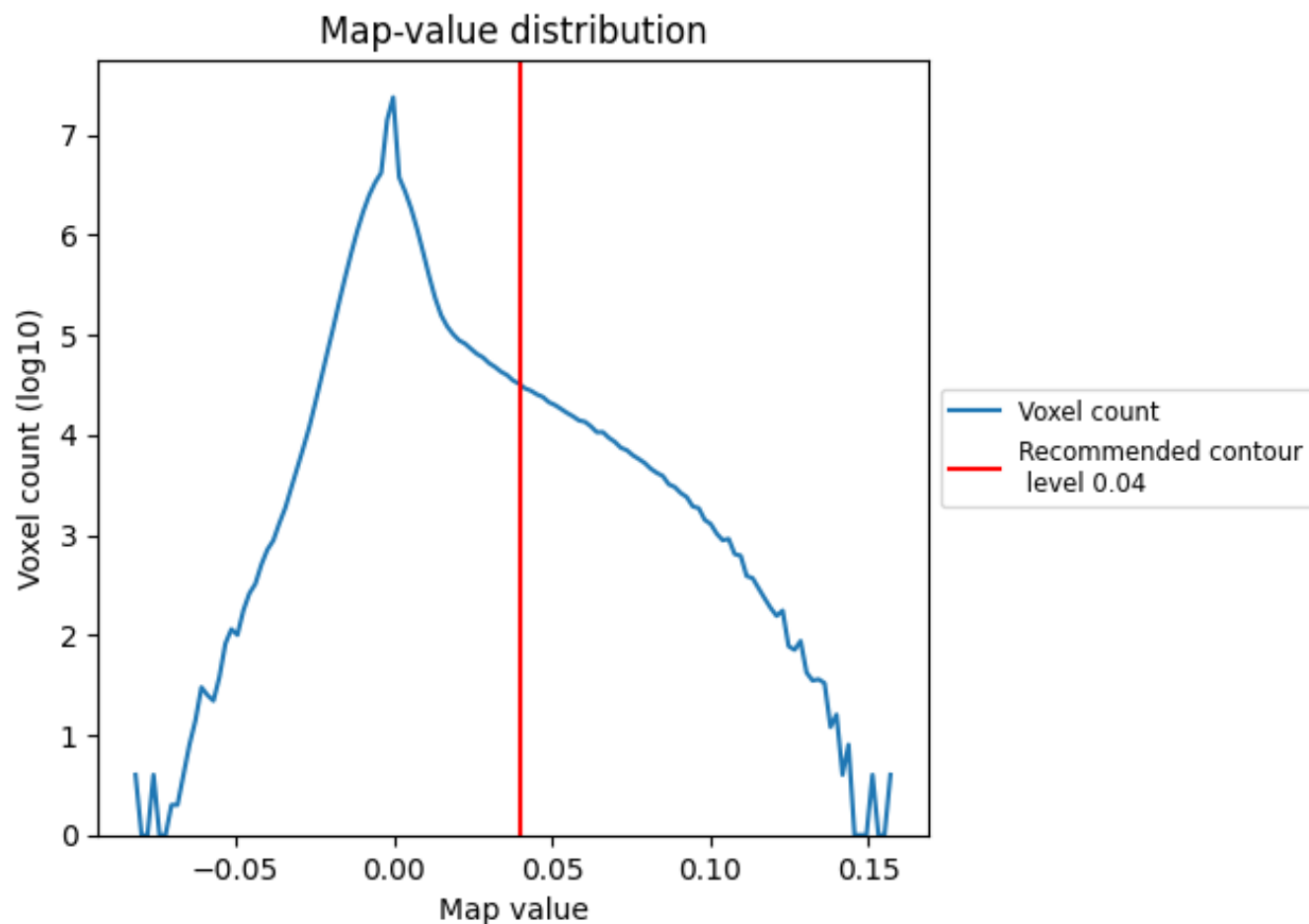
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

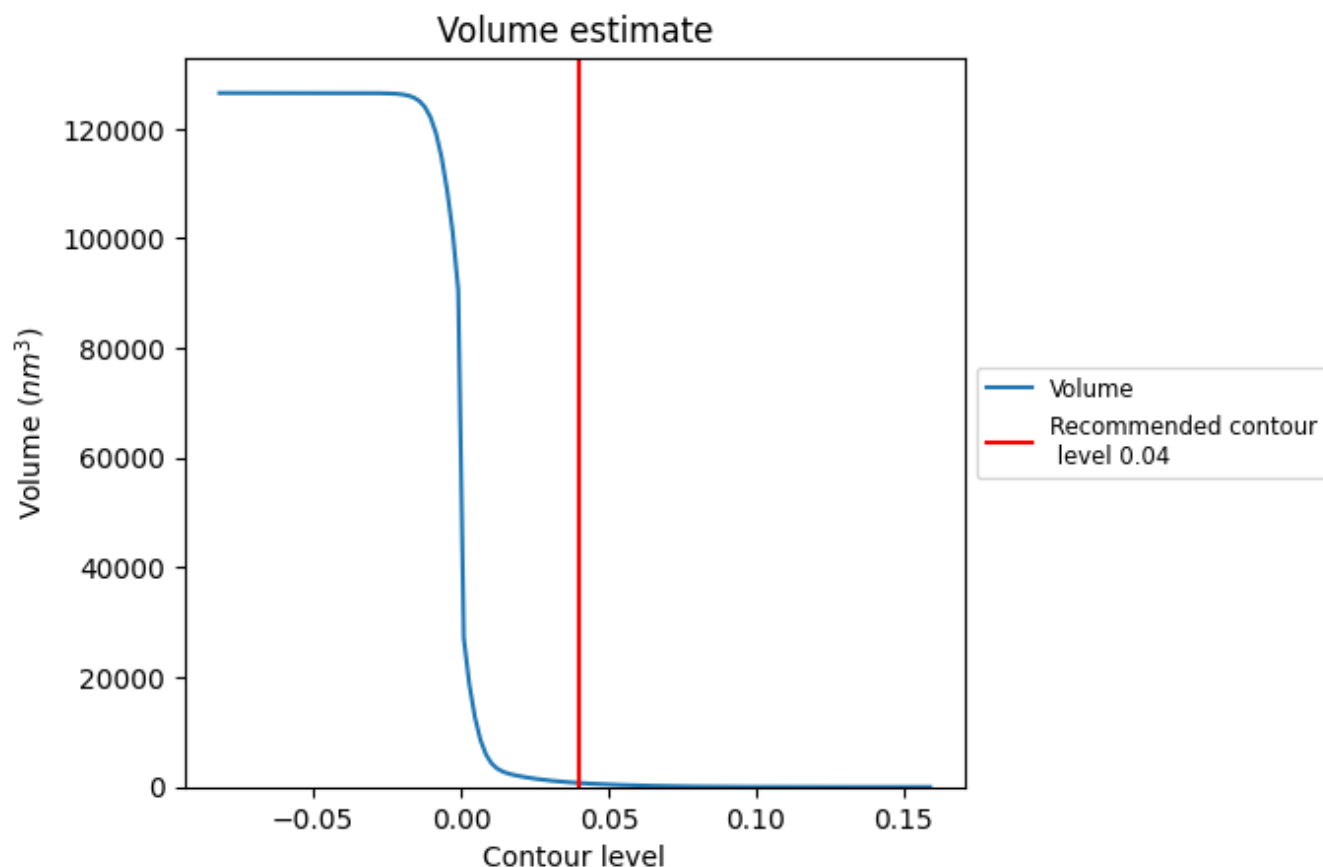
This section contains the results of statistical analysis of the map.

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.

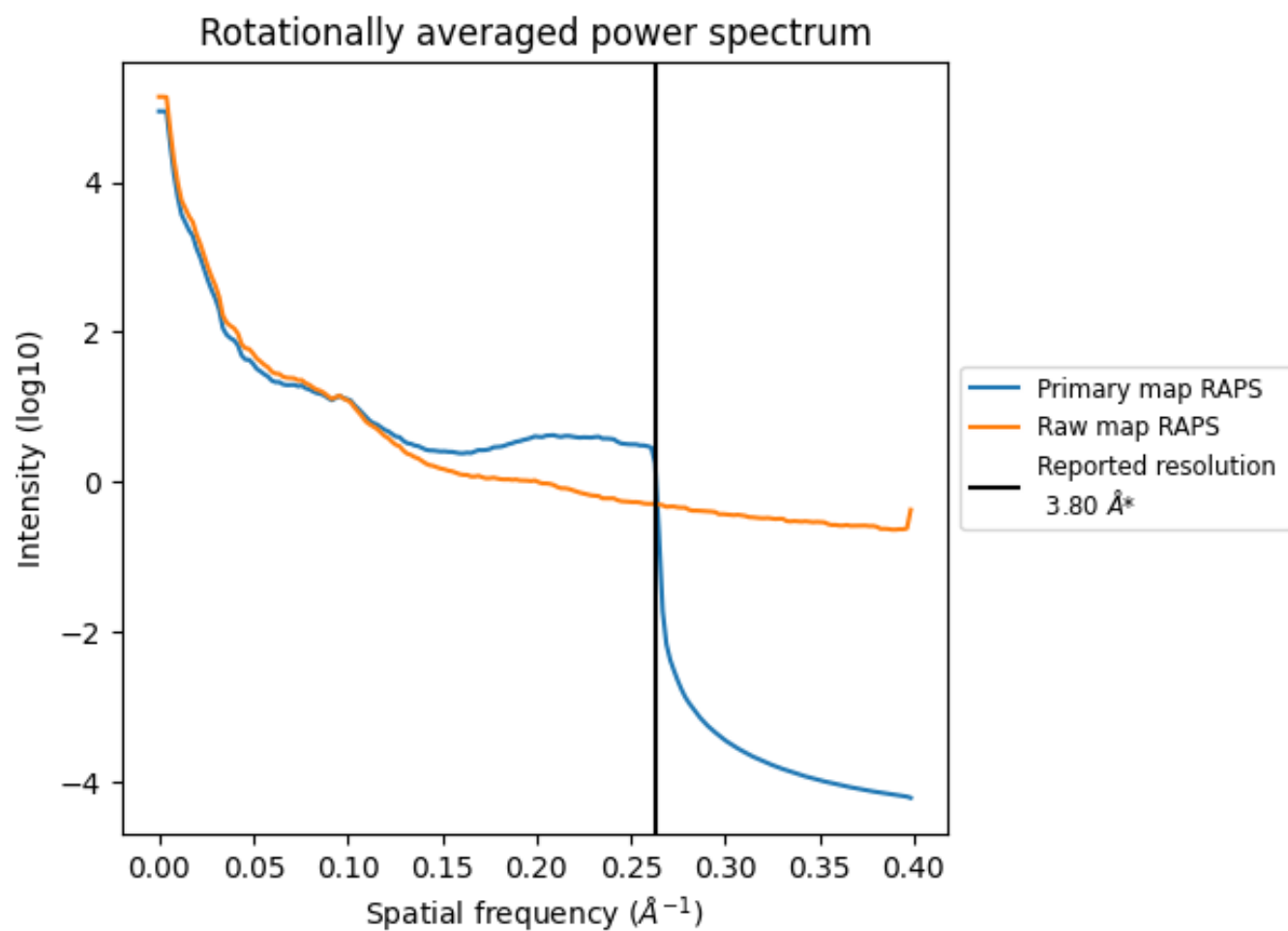
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 729 nm³; this corresponds to an approximate mass of 658 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 ⓘ

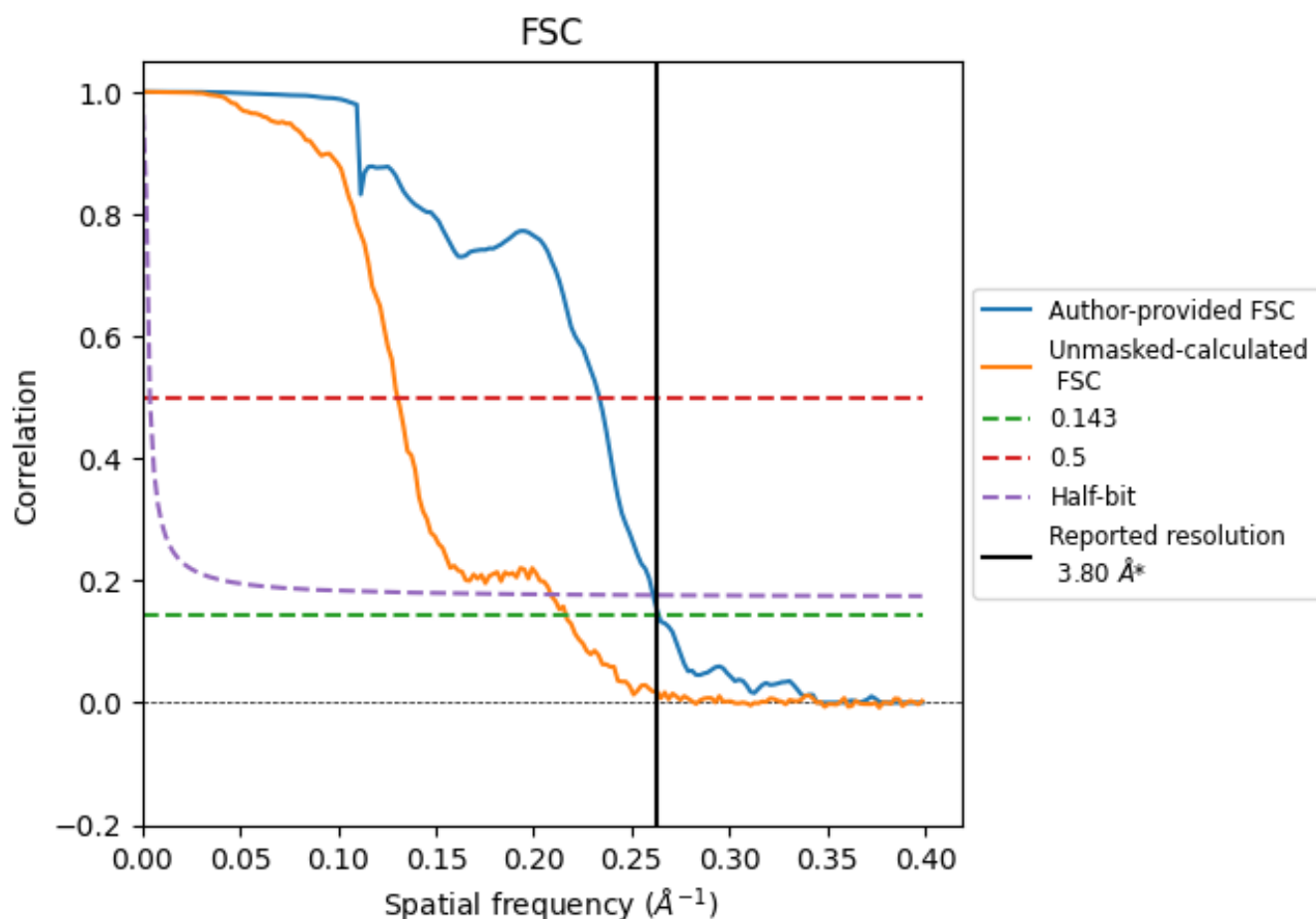


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

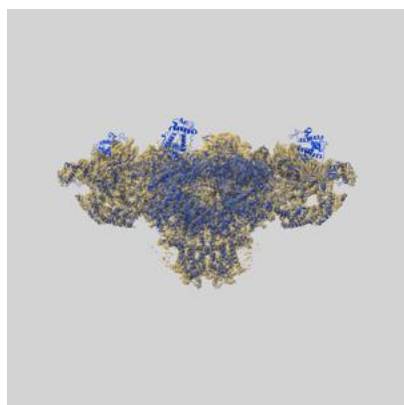
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.79	4.28	3.83
Unmasked-calculated*	4.62	7.67	4.79

*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 4.62 differs from the reported value 3.8 by more than 10 %

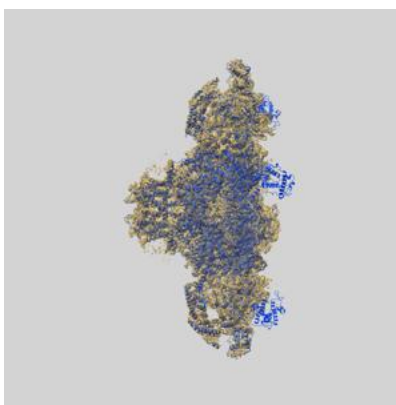
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8373 and PDB model 5T9N. Per-residue inclusion information can be found in section [3](#) on page [6](#).

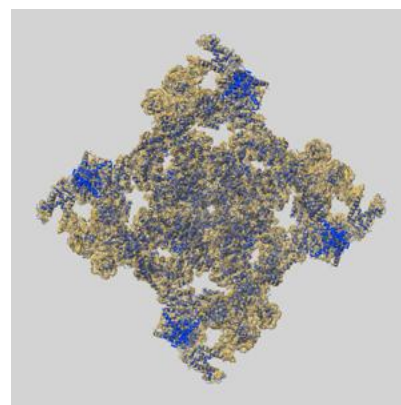
9.1 Map-model overlay [i](#)



X



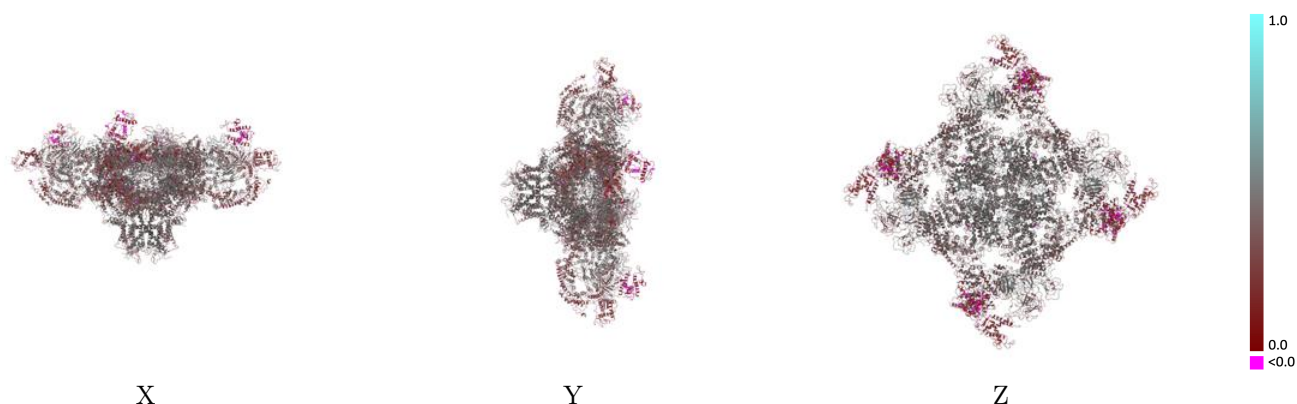
Y



Z

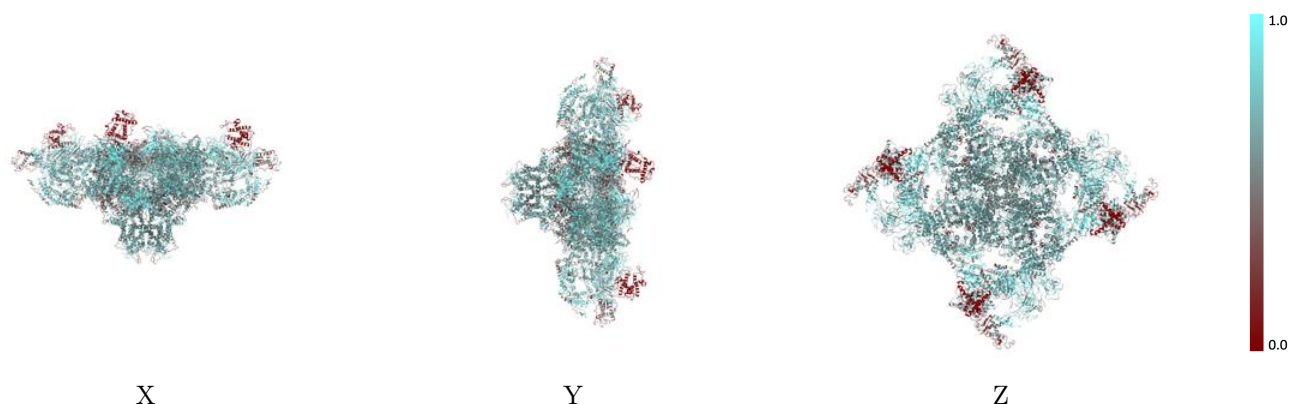
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



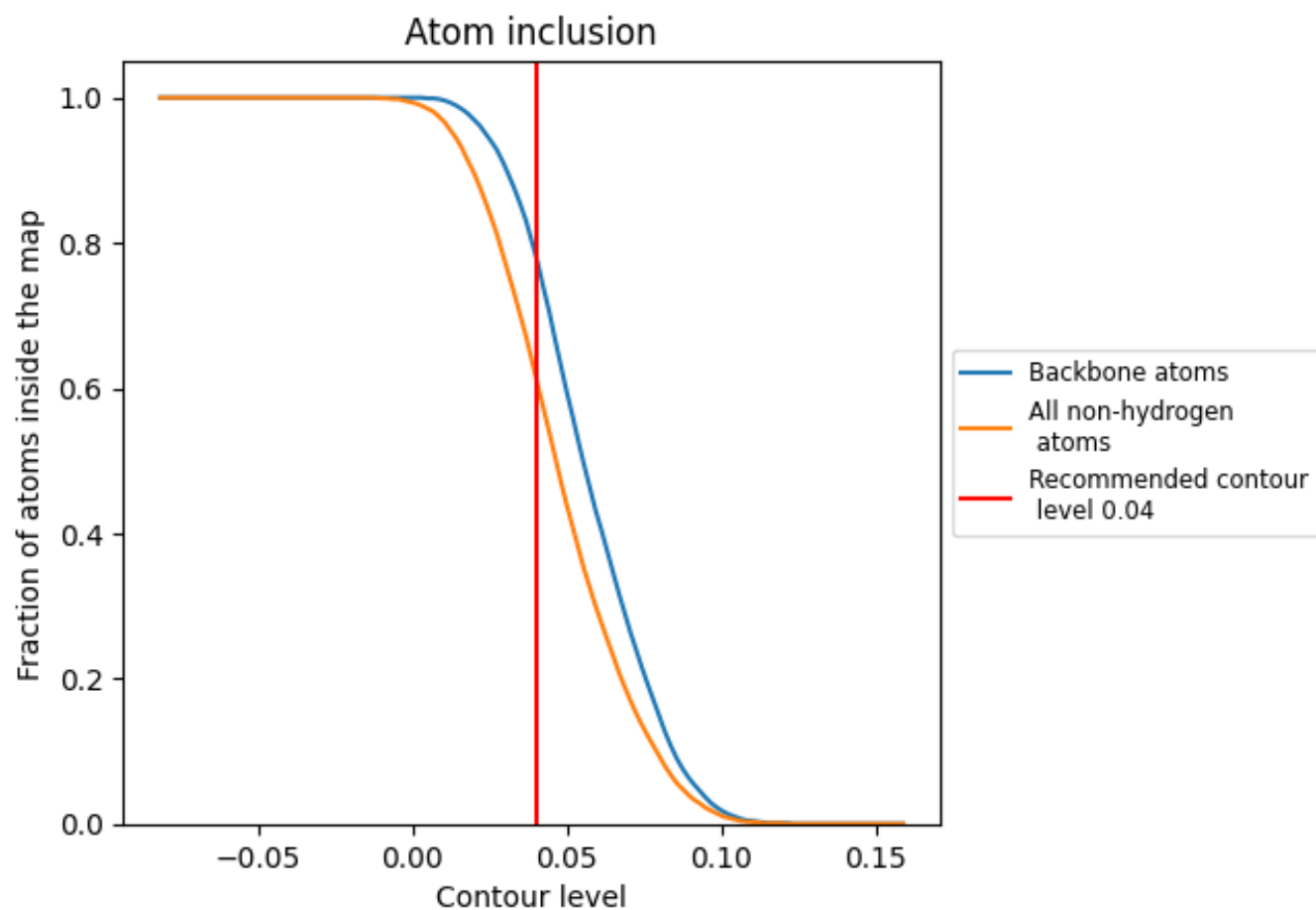
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 78% of all backbone atoms, 62% 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	0.6150	0.3680
A	0.6350	0.3810
B	0.6150	0.3680
E	0.6150	0.3670
F	0.6340	0.3870
G	0.6150	0.3680
H	0.6390	0.3850
I	0.6150	0.3680
J	0.6380	0.3820

1.0

0.0

<0.0