



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 07:57 AM UTC

PDB ID : 7AA5 / pdb_00007aa5
EMDB ID : EMD-11690
Title : Human TRPV4 structure in presence of 4a-PDD
Authors : Botte, M.; Ulrich, A.K.G.; Adaixo, R.; Gnutt, D.; Brockmann, A.; Bucher, D.; Chami, M.; Bocquet, M.; Ebbinghaus-Kintscher, U.; Puetter, V.; Becker, A.; Egner, U.; Stahlberg, H.; Hennig, M.; Holton, S.J.
Deposited on : 2020-09-03
Resolution : 4.18 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

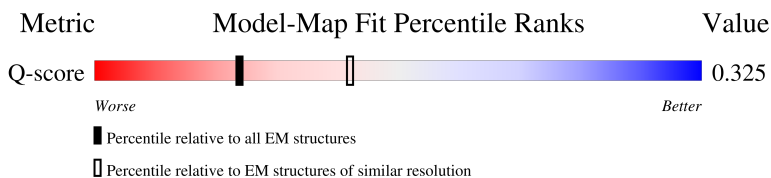
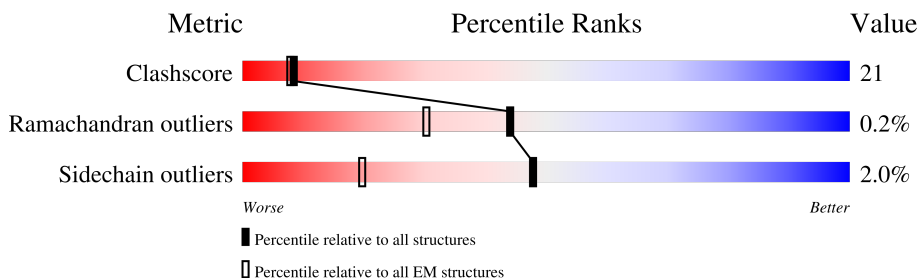
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.18 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	5389 (3.68 - 4.68)

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	935	 6% 36% 28% 35%
1	B	935	 6% 36% 29% 35%
1	C	935	 5% 36% 29% 35%
1	D	935	 6% 36% 28% 35%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19705 atoms, of which 8 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 Transient receptor potential cation channel subfamily V member 4, Green fluorescent protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	612	Total	C	H	N	O	S	0	0
			4926	3201	2	817	879	27		
1	B	612	Total	C	H	N	O	S	0	0
			4926	3201	2	817	879	27		
1	C	612	Total	C	H	N	O	S	0	0
			4926	3201	2	817	879	27		
1	D	612	Total	C	H	N	O	S	0	0
			4926	3201	2	817	879	27		

There are 264 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	116	MET	-	initiating methionine	UNP Q9HBA0
A	117	ASP	-	expression tag	UNP Q9HBA0
A	118	TYR	-	expression tag	UNP Q9HBA0
A	119	LYS	-	expression tag	UNP Q9HBA0
A	120	ASP	-	expression tag	UNP Q9HBA0
A	121	ASP	-	expression tag	UNP Q9HBA0
A	122	ASP	-	expression tag	UNP Q9HBA0
A	123	ASP	-	expression tag	UNP Q9HBA0
A	124	LYS	-	expression tag	UNP Q9HBA0
A	125	SER	-	expression tag	UNP Q9HBA0
A	126	SER	-	expression tag	UNP Q9HBA0
A	127	MET	-	expression tag	UNP Q9HBA0
A	128	GLY	-	expression tag	UNP Q9HBA0
A	129	SER	-	expression tag	UNP Q9HBA0
A	130	ARG	-	expression tag	UNP Q9HBA0
A	131	THR	-	expression tag	UNP Q9HBA0
A	132	SER	-	expression tag	UNP Q9HBA0
A	133	LEU	-	expression tag	UNP Q9HBA0
A	134	TYR	-	expression tag	UNP Q9HBA0
A	135	LYS	-	expression tag	UNP Q9HBA0
A	136	LYS	-	expression tag	UNP Q9HBA0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	137	ALA	-	expression tag	UNP Q9HBA0
A	138	GLY	-	expression tag	UNP Q9HBA0
A	139	SER	-	expression tag	UNP Q9HBA0
A	140	LEU	-	expression tag	UNP Q9HBA0
A	141	GLU	-	expression tag	UNP Q9HBA0
A	142	VAL	-	expression tag	UNP Q9HBA0
A	143	LEU	-	expression tag	UNP Q9HBA0
A	144	PHE	-	expression tag	UNP Q9HBA0
A	145	GLN	-	expression tag	UNP Q9HBA0
A	146	GLY	-	expression tag	UNP Q9HBA0
A	147	PRO	-	expression tag	UNP Q9HBA0
A	651	ASP	ASN	conflict	UNP Q9HBA0
A	788	GLU	-	linker	UNP Q9HBA0
A	789	ASN	-	linker	UNP Q9HBA0
A	790	LEU	-	linker	UNP Q9HBA0
A	791	TYR	-	linker	UNP Q9HBA0
A	792	PHE	-	linker	UNP Q9HBA0
A	793	GLN	-	linker	UNP Q9HBA0
A	794	GLY	-	linker	UNP Q9HBA0
A	795	ALA	-	linker	UNP Q9HBA0
A	796	ALA	-	linker	UNP Q9HBA0
A	797	GLY	-	linker	UNP Q9HBA0
A	798	SER	-	linker	UNP Q9HBA0
A	799	GLY	-	linker	UNP Q9HBA0
A	800	GLU	-	linker	UNP Q9HBA0
A	801	PHE	-	linker	UNP Q9HBA0
A	863	LEU	PHE	conflict	UNP P42212
A	864	THR	SER	conflict	UNP P42212
A	879	ARG	GLN	conflict	UNP P42212
A	898	SER	PHE	conflict	UNP P42212
A	952	THR	MET	conflict	UNP P42212
A	962	ALA	VAL	conflict	UNP P42212
A	1038	ALA	-	expression tag	UNP P42212
A	1039	SER	-	expression tag	UNP P42212
A	1040	GLY	-	expression tag	UNP P42212
A	1041	HIS	-	expression tag	UNP P42212
A	1042	HIS	-	expression tag	UNP P42212
A	1043	HIS	-	expression tag	UNP P42212
A	1044	HIS	-	expression tag	UNP P42212
A	1045	HIS	-	expression tag	UNP P42212
A	1046	HIS	-	expression tag	UNP P42212
A	1047	HIS	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1048	HIS	-	expression tag	UNP P42212
A	1049	HIS	-	expression tag	UNP P42212
A	1050	HIS	-	expression tag	UNP P42212
B	116	MET	-	initiating methionine	UNP Q9HBA0
B	117	ASP	-	expression tag	UNP Q9HBA0
B	118	TYR	-	expression tag	UNP Q9HBA0
B	119	LYS	-	expression tag	UNP Q9HBA0
B	120	ASP	-	expression tag	UNP Q9HBA0
B	121	ASP	-	expression tag	UNP Q9HBA0
B	122	ASP	-	expression tag	UNP Q9HBA0
B	123	ASP	-	expression tag	UNP Q9HBA0
B	124	LYS	-	expression tag	UNP Q9HBA0
B	125	SER	-	expression tag	UNP Q9HBA0
B	126	SER	-	expression tag	UNP Q9HBA0
B	127	MET	-	expression tag	UNP Q9HBA0
B	128	GLY	-	expression tag	UNP Q9HBA0
B	129	SER	-	expression tag	UNP Q9HBA0
B	130	ARG	-	expression tag	UNP Q9HBA0
B	131	THR	-	expression tag	UNP Q9HBA0
B	132	SER	-	expression tag	UNP Q9HBA0
B	133	LEU	-	expression tag	UNP Q9HBA0
B	134	TYR	-	expression tag	UNP Q9HBA0
B	135	LYS	-	expression tag	UNP Q9HBA0
B	136	LYS	-	expression tag	UNP Q9HBA0
B	137	ALA	-	expression tag	UNP Q9HBA0
B	138	GLY	-	expression tag	UNP Q9HBA0
B	139	SER	-	expression tag	UNP Q9HBA0
B	140	LEU	-	expression tag	UNP Q9HBA0
B	141	GLU	-	expression tag	UNP Q9HBA0
B	142	VAL	-	expression tag	UNP Q9HBA0
B	143	LEU	-	expression tag	UNP Q9HBA0
B	144	PHE	-	expression tag	UNP Q9HBA0
B	145	GLN	-	expression tag	UNP Q9HBA0
B	146	GLY	-	expression tag	UNP Q9HBA0
B	147	PRO	-	expression tag	UNP Q9HBA0
B	651	ASP	ASN	conflict	UNP Q9HBA0
B	788	GLU	-	linker	UNP Q9HBA0
B	789	ASN	-	linker	UNP Q9HBA0
B	790	LEU	-	linker	UNP Q9HBA0
B	791	TYR	-	linker	UNP Q9HBA0
B	792	PHE	-	linker	UNP Q9HBA0
B	793	GLN	-	linker	UNP Q9HBA0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	794	GLY	-	linker	UNP Q9HBA0
B	795	ALA	-	linker	UNP Q9HBA0
B	796	ALA	-	linker	UNP Q9HBA0
B	797	GLY	-	linker	UNP Q9HBA0
B	798	SER	-	linker	UNP Q9HBA0
B	799	GLY	-	linker	UNP Q9HBA0
B	800	GLU	-	linker	UNP Q9HBA0
B	801	PHE	-	linker	UNP Q9HBA0
B	863	LEU	PHE	conflict	UNP P42212
B	864	THR	SER	conflict	UNP P42212
B	879	ARG	GLN	conflict	UNP P42212
B	898	SER	PHE	conflict	UNP P42212
B	952	THR	MET	conflict	UNP P42212
B	962	ALA	VAL	conflict	UNP P42212
B	1038	ALA	-	expression tag	UNP P42212
B	1039	SER	-	expression tag	UNP P42212
B	1040	GLY	-	expression tag	UNP P42212
B	1041	HIS	-	expression tag	UNP P42212
B	1042	HIS	-	expression tag	UNP P42212
B	1043	HIS	-	expression tag	UNP P42212
B	1044	HIS	-	expression tag	UNP P42212
B	1045	HIS	-	expression tag	UNP P42212
B	1046	HIS	-	expression tag	UNP P42212
B	1047	HIS	-	expression tag	UNP P42212
B	1048	HIS	-	expression tag	UNP P42212
B	1049	HIS	-	expression tag	UNP P42212
B	1050	HIS	-	expression tag	UNP P42212
C	116	MET	-	initiating methionine	UNP Q9HBA0
C	117	ASP	-	expression tag	UNP Q9HBA0
C	118	TYR	-	expression tag	UNP Q9HBA0
C	119	LYS	-	expression tag	UNP Q9HBA0
C	120	ASP	-	expression tag	UNP Q9HBA0
C	121	ASP	-	expression tag	UNP Q9HBA0
C	122	ASP	-	expression tag	UNP Q9HBA0
C	123	ASP	-	expression tag	UNP Q9HBA0
C	124	LYS	-	expression tag	UNP Q9HBA0
C	125	SER	-	expression tag	UNP Q9HBA0
C	126	SER	-	expression tag	UNP Q9HBA0
C	127	MET	-	expression tag	UNP Q9HBA0
C	128	GLY	-	expression tag	UNP Q9HBA0
C	129	SER	-	expression tag	UNP Q9HBA0
C	130	ARG	-	expression tag	UNP Q9HBA0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	131	THR	-	expression tag	UNP Q9HBA0
C	132	SER	-	expression tag	UNP Q9HBA0
C	133	LEU	-	expression tag	UNP Q9HBA0
C	134	TYR	-	expression tag	UNP Q9HBA0
C	135	LYS	-	expression tag	UNP Q9HBA0
C	136	LYS	-	expression tag	UNP Q9HBA0
C	137	ALA	-	expression tag	UNP Q9HBA0
C	138	GLY	-	expression tag	UNP Q9HBA0
C	139	SER	-	expression tag	UNP Q9HBA0
C	140	LEU	-	expression tag	UNP Q9HBA0
C	141	GLU	-	expression tag	UNP Q9HBA0
C	142	VAL	-	expression tag	UNP Q9HBA0
C	143	LEU	-	expression tag	UNP Q9HBA0
C	144	PHE	-	expression tag	UNP Q9HBA0
C	145	GLN	-	expression tag	UNP Q9HBA0
C	146	GLY	-	expression tag	UNP Q9HBA0
C	147	PRO	-	expression tag	UNP Q9HBA0
C	651	ASP	ASN	conflict	UNP Q9HBA0
C	788	GLU	-	linker	UNP Q9HBA0
C	789	ASN	-	linker	UNP Q9HBA0
C	790	LEU	-	linker	UNP Q9HBA0
C	791	TYR	-	linker	UNP Q9HBA0
C	792	PHE	-	linker	UNP Q9HBA0
C	793	GLN	-	linker	UNP Q9HBA0
C	794	GLY	-	linker	UNP Q9HBA0
C	795	ALA	-	linker	UNP Q9HBA0
C	796	ALA	-	linker	UNP Q9HBA0
C	797	GLY	-	linker	UNP Q9HBA0
C	798	SER	-	linker	UNP Q9HBA0
C	799	GLY	-	linker	UNP Q9HBA0
C	800	GLU	-	linker	UNP Q9HBA0
C	801	PHE	-	linker	UNP Q9HBA0
C	863	LEU	PHE	conflict	UNP P42212
C	864	THR	SER	conflict	UNP P42212
C	879	ARG	GLN	conflict	UNP P42212
C	898	SER	PHE	conflict	UNP P42212
C	952	THR	MET	conflict	UNP P42212
C	962	ALA	VAL	conflict	UNP P42212
C	1038	ALA	-	expression tag	UNP P42212
C	1039	SER	-	expression tag	UNP P42212
C	1040	GLY	-	expression tag	UNP P42212
C	1041	HIS	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1042	HIS	-	expression tag	UNP P42212
C	1043	HIS	-	expression tag	UNP P42212
C	1044	HIS	-	expression tag	UNP P42212
C	1045	HIS	-	expression tag	UNP P42212
C	1046	HIS	-	expression tag	UNP P42212
C	1047	HIS	-	expression tag	UNP P42212
C	1048	HIS	-	expression tag	UNP P42212
C	1049	HIS	-	expression tag	UNP P42212
C	1050	HIS	-	expression tag	UNP P42212
D	116	MET	-	initiating methionine	UNP Q9HBA0
D	117	ASP	-	expression tag	UNP Q9HBA0
D	118	TYR	-	expression tag	UNP Q9HBA0
D	119	LYS	-	expression tag	UNP Q9HBA0
D	120	ASP	-	expression tag	UNP Q9HBA0
D	121	ASP	-	expression tag	UNP Q9HBA0
D	122	ASP	-	expression tag	UNP Q9HBA0
D	123	ASP	-	expression tag	UNP Q9HBA0
D	124	LYS	-	expression tag	UNP Q9HBA0
D	125	SER	-	expression tag	UNP Q9HBA0
D	126	SER	-	expression tag	UNP Q9HBA0
D	127	MET	-	expression tag	UNP Q9HBA0
D	128	GLY	-	expression tag	UNP Q9HBA0
D	129	SER	-	expression tag	UNP Q9HBA0
D	130	ARG	-	expression tag	UNP Q9HBA0
D	131	THR	-	expression tag	UNP Q9HBA0
D	132	SER	-	expression tag	UNP Q9HBA0
D	133	LEU	-	expression tag	UNP Q9HBA0
D	134	TYR	-	expression tag	UNP Q9HBA0
D	135	LYS	-	expression tag	UNP Q9HBA0
D	136	LYS	-	expression tag	UNP Q9HBA0
D	137	ALA	-	expression tag	UNP Q9HBA0
D	138	GLY	-	expression tag	UNP Q9HBA0
D	139	SER	-	expression tag	UNP Q9HBA0
D	140	LEU	-	expression tag	UNP Q9HBA0
D	141	GLU	-	expression tag	UNP Q9HBA0
D	142	VAL	-	expression tag	UNP Q9HBA0
D	143	LEU	-	expression tag	UNP Q9HBA0
D	144	PHE	-	expression tag	UNP Q9HBA0
D	145	GLN	-	expression tag	UNP Q9HBA0
D	146	GLY	-	expression tag	UNP Q9HBA0
D	147	PRO	-	expression tag	UNP Q9HBA0
D	651	ASP	ASN	conflict	UNP Q9HBA0

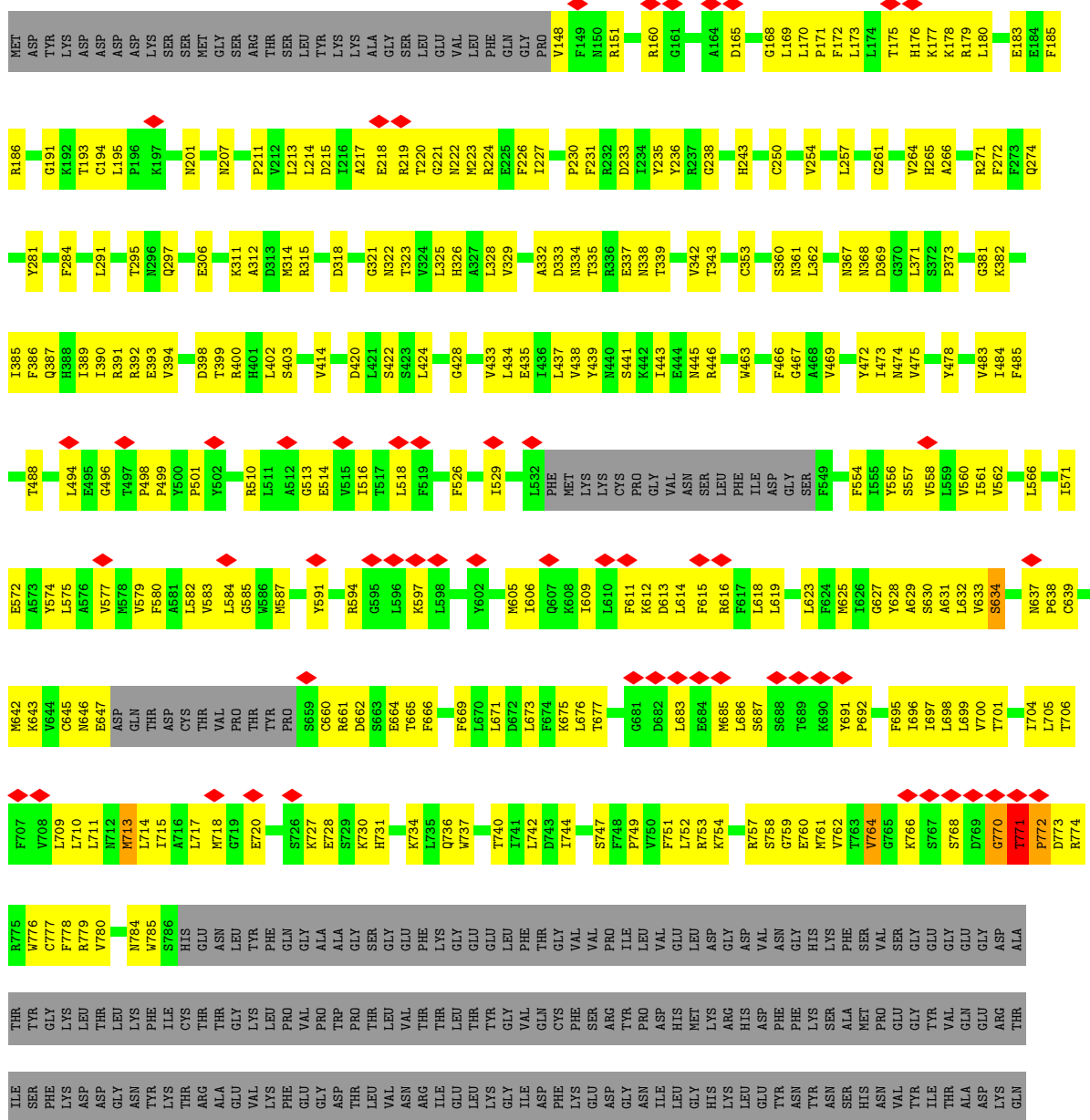
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Chain	Residue	Modelled	Actual	Comment	Reference
D	788	GLU	-	linker	UNP Q9HBA0
D	789	ASN	-	linker	UNP Q9HBA0
D	790	LEU	-	linker	UNP Q9HBA0
D	791	TYR	-	linker	UNP Q9HBA0
D	792	PHE	-	linker	UNP Q9HBA0
D	793	GLN	-	linker	UNP Q9HBA0
D	794	GLY	-	linker	UNP Q9HBA0
D	795	ALA	-	linker	UNP Q9HBA0
D	796	ALA	-	linker	UNP Q9HBA0
D	797	GLY	-	linker	UNP Q9HBA0
D	798	SER	-	linker	UNP Q9HBA0
D	799	GLY	-	linker	UNP Q9HBA0
D	800	GLU	-	linker	UNP Q9HBA0
D	801	PHE	-	linker	UNP Q9HBA0
D	863	LEU	PHE	conflict	UNP P42212
D	864	THR	SER	conflict	UNP P42212
D	879	ARG	GLN	conflict	UNP P42212
D	898	SER	PHE	conflict	UNP P42212
D	952	THR	MET	conflict	UNP P42212
D	962	ALA	VAL	conflict	UNP P42212
D	1038	ALA	-	expression tag	UNP P42212
D	1039	SER	-	expression tag	UNP P42212
D	1040	GLY	-	expression tag	UNP P42212
D	1041	HIS	-	expression tag	UNP P42212
D	1042	HIS	-	expression tag	UNP P42212
D	1043	HIS	-	expression tag	UNP P42212
D	1044	HIS	-	expression tag	UNP P42212
D	1045	HIS	-	expression tag	UNP P42212
D	1046	HIS	-	expression tag	UNP P42212
D	1047	HIS	-	expression tag	UNP P42212
D	1048	HIS	-	expression tag	UNP P42212
D	1049	HIS	-	expression tag	UNP P42212
D	1050	HIS	-	expression tag	UNP P42212

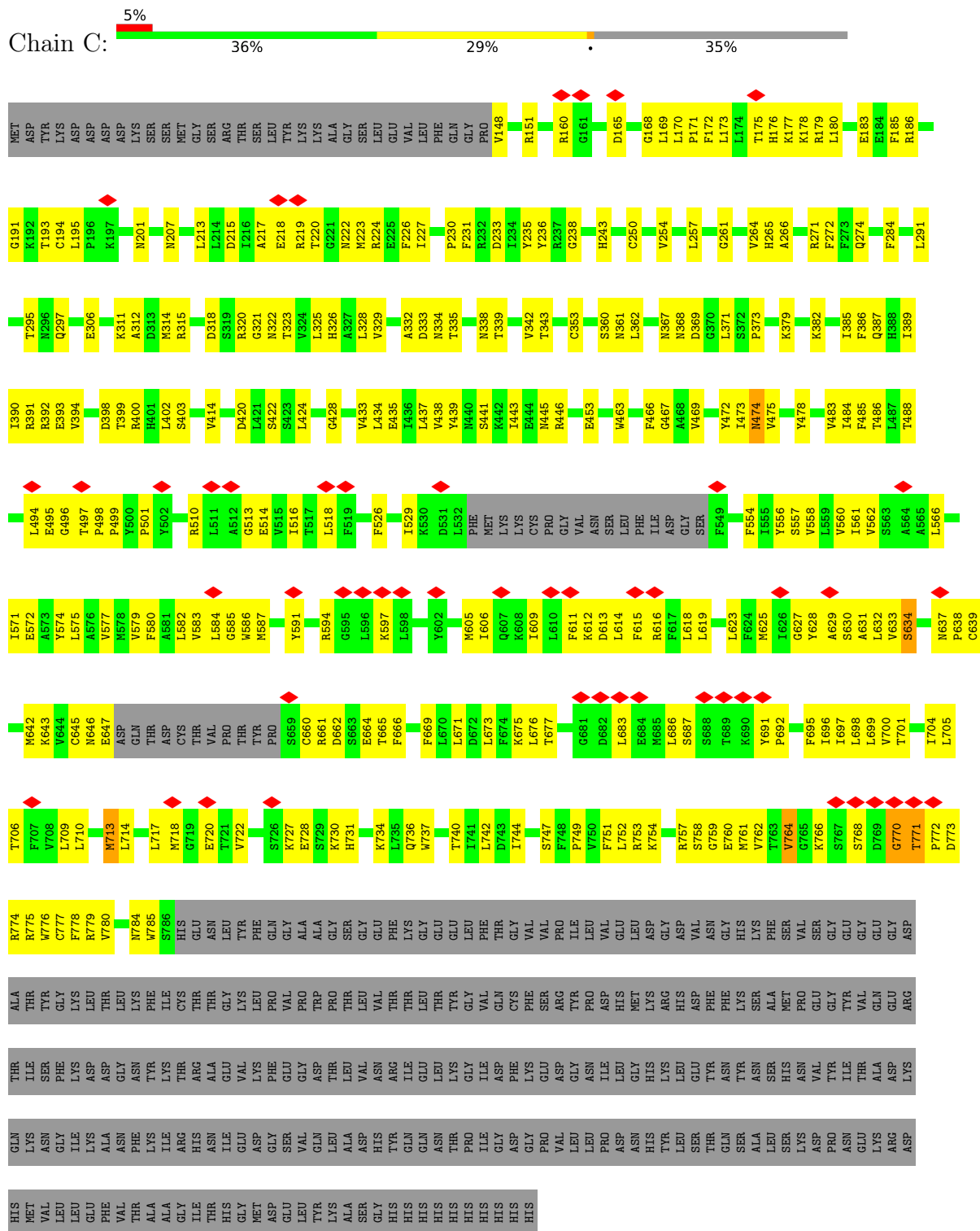
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

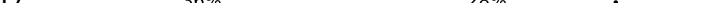
Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total Ca 1 1	0



LYS	ASN	GLY	ILE	LYS	ALA	ASN	PHE	THR	ALA	ILE	ARG	HIS	ASN	ILE	GLU	ASP	GLY	SER	VAL	GLN	LEU	LEU	ASP	ALA	ALA	ASP	HIS	TYR	GLN	GLN	ASN	THR	HIS	PRO	PRO	VAL	VAL	LEU	LEU	PRO	ASP	ASN	HIS	TYR	LEU	SER	THR	GLN	SER	ALA	LEU	SER	LYS	PRO	PRO	GLU	ARG	LYS	ASP	HIS
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- Molecule 1: Transient receptor potential channel subfamily V member 4, Green fluorescent protein



- Chain D:  6% 36% 28% 35%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	51215	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	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	0.739	Depositor
Minimum map value	-0.363	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.148	Depositor
Map size (Å)	327.168, 327.168, 327.168	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.639, 0.639, 0.639	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.23	0/5034	0.52	6/6822 (0.1%)
1	B	0.40	3/5034 (0.1%)	0.60	8/6822 (0.1%)
1	C	0.29	1/5034 (0.0%)	0.60	7/6822 (0.1%)
1	D	0.40	3/5034 (0.1%)	0.60	8/6822 (0.1%)
All	All	0.34	7/20136 (0.0%)	0.58	29/27288 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	C	0	2
1	D	0	3
All	All	0	10

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	772	PRO	N-CD	17.22	1.71	1.47
1	B	772	PRO	N-CD	17.20	1.71	1.47
1	D	772	PRO	N-CA	-13.84	1.29	1.47
1	B	772	PRO	N-CA	-13.80	1.29	1.47
1	C	772	PRO	N-CD	11.16	1.63	1.47
1	B	771	THR	C-N	7.87	1.52	1.33
1	D	771	THR	C-N	7.86	1.52	1.33

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	771	THR	CA-C-N	-16.10	99.71	119.84
1	C	771	THR	C-N-CA	-16.10	99.71	119.84
1	B	771	THR	CA-C-O	-14.05	100.91	120.16
1	D	771	THR	CA-C-O	-14.04	100.93	120.16
1	D	771	THR	CA-C-N	-14.01	102.33	119.84
1	D	771	THR	C-N-CA	-14.01	102.33	119.84
1	B	771	THR	CA-C-N	-14.00	102.34	119.84
1	B	771	THR	C-N-CA	-14.00	102.34	119.84
1	C	771	THR	CA-C-O	-13.17	102.11	120.16
1	C	764	VAL	N-CA-C	-9.49	104.08	113.20
1	A	764	VAL	N-CA-C	-9.44	104.13	113.20
1	D	764	VAL	N-CA-C	-9.44	104.14	113.20
1	B	764	VAL	N-CA-C	-9.41	104.17	113.20
1	D	772	PRO	N-CA-CB	8.97	112.67	103.25
1	B	772	PRO	N-CA-CB	8.95	112.64	103.25
1	D	771	THR	CB-CA-C	-8.78	92.87	110.17
1	B	771	THR	CB-CA-C	-8.78	92.88	110.17
1	A	770	GLY	O-C-N	7.42	132.35	122.70
1	C	771	THR	C-N-CD	7.30	154.93	125.00
1	A	771	THR	CA-C-O	-7.14	110.38	120.16
1	C	771	THR	O-C-N	7.08	129.47	121.32
1	A	770	GLY	CA-C-N	6.49	137.64	121.80
1	A	770	GLY	C-N-CA	6.49	137.64	121.80
1	D	771	THR	O-C-N	5.91	128.11	121.32
1	B	771	THR	O-C-N	5.89	128.09	121.32
1	D	771	THR	C-N-CD	5.58	147.87	125.00
1	B	771	THR	C-N-CD	5.57	147.85	125.00
1	C	772	PRO	CA-N-CD	-5.31	104.57	112.00
1	A	771	THR	CA-CB-CG2	5.29	119.49	110.50

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	768	SER	Peptide
1	A	770	GLY	Peptide
1	B	768	SER	Peptide
1	B	770	GLY	Peptide
1	B	771	THR	Peptide
1	C	768	SER	Peptide
1	C	770	GLY	Peptide
1	D	768	SER	Peptide
1	D	770	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	D	771	THR	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	4924	2	4999	218	0
1	B	4924	2	4999	220	0
1	C	4924	2	4999	231	0
1	D	4924	2	4999	235	0
2	A	1	0	0	0	0
All	All	19697	8	19996	852	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 21.

All (852) 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)
1:D:772:PRO:N	1:D:772:PRO:CD	1.71	1.45
1:B:772:PRO:N	1:B:772:PRO:CD	1.71	1.38
1:C:496:GLY:H	1:D:637:ASN:HB3	1.35	0.90
1:A:771:THR:HB	1:A:772:PRO:HD3	1.59	0.84
1:A:639:CYS:HB3	1:A:692:PRO:HB3	1.61	0.83
1:C:639:CYS:HB3	1:C:692:PRO:HB3	1.61	0.82
1:B:639:CYS:HB3	1:B:692:PRO:HB3	1.61	0.81
1:D:639:CYS:HB3	1:D:692:PRO:HB3	1.61	0.80
1:A:771:THR:HB	1:A:772:PRO:CD	2.12	0.79
1:C:484:ILE:HG21	1:C:516:ILE:HD11	1.66	0.77
1:D:484:ILE:HG21	1:D:516:ILE:HD11	1.66	0.77
1:A:484:ILE:HG21	1:A:516:ILE:HD11	1.66	0.76
1:A:579:VAL:HG23	1:C:631:ALA:HB1	1.67	0.76
1:A:637:ASN:HD21	1:B:494:LEU:HD22	1.51	0.75
1:B:484:ILE:HG21	1:B:516:ILE:HD11	1.66	0.75
1:A:314:MET:SD	1:A:314:MET:N	2.59	0.74
1:C:314:MET:SD	1:C:314:MET:N	2.59	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:MET:SD	1:B:314:MET:N	2.59	0.72
1:C:496:GLY:N	1:D:637:ASN:HB3	2.04	0.72
1:D:193:THR:HG22	1:D:194:CYS:H	1.56	0.71
1:A:193:THR:HG22	1:A:194:CYS:H	1.56	0.71
1:B:193:THR:HG22	1:B:194:CYS:H	1.56	0.71
1:B:631:ALA:HB1	1:D:579:VAL:HG23	1.72	0.71
1:C:193:THR:HG22	1:C:194:CYS:H	1.56	0.70
1:C:318:ASP:OD1	1:C:322:ASN:N	2.24	0.70
1:C:233:ASP:OD1	1:C:236:TYR:N	2.24	0.70
1:A:233:ASP:OD1	1:A:236:TYR:N	2.24	0.70
1:A:318:ASP:OD1	1:A:322:ASN:N	2.24	0.70
1:D:318:ASP:OD1	1:D:322:ASN:N	2.24	0.70
1:D:323:THR:H	1:D:326:HIS:CD2	2.10	0.70
1:A:323:THR:H	1:A:326:HIS:CD2	2.10	0.70
1:B:318:ASP:OD1	1:B:322:ASN:N	2.24	0.69
1:C:224:ARG:NH1	1:C:261:GLY:O	2.25	0.69
1:C:323:THR:H	1:C:326:HIS:CD2	2.10	0.69
1:D:233:ASP:OD1	1:D:236:TYR:N	2.24	0.69
1:B:233:ASP:OD1	1:B:236:TYR:N	2.24	0.69
1:B:323:THR:H	1:B:326:HIS:CD2	2.10	0.69
1:B:224:ARG:NH1	1:B:261:GLY:O	2.26	0.69
1:A:224:ARG:NH1	1:A:261:GLY:O	2.25	0.69
1:D:224:ARG:NH1	1:D:261:GLY:O	2.25	0.68
1:A:496:GLY:H	1:C:637:ASN:HB3	1.59	0.68
1:A:637:ASN:HB3	1:B:496:GLY:H	1.59	0.68
1:B:673:LEU:HA	1:B:676:LEU:HD12	1.76	0.67
1:D:314:MET:SD	1:D:314:MET:N	2.59	0.67
1:C:495:GLU:N	1:D:637:ASN:OD1	2.25	0.67
1:A:673:LEU:HA	1:A:676:LEU:HD12	1.76	0.67
1:C:148:VAL:HG21	1:C:169:LEU:HB3	1.77	0.67
1:D:339:THR:O	1:D:343:THR:OG1	2.12	0.67
1:B:339:THR:O	1:B:343:THR:OG1	2.12	0.66
1:A:148:VAL:HG21	1:A:169:LEU:HB3	1.77	0.66
1:D:148:VAL:HG21	1:D:169:LEU:HB3	1.77	0.66
1:D:673:LEU:HA	1:D:676:LEU:HD12	1.76	0.66
1:A:580:PHE:HE1	1:C:698:LEU:HD11	1.59	0.66
1:C:390:ILE:HG23	1:C:391:ARG:HD3	1.78	0.66
1:B:148:VAL:HG21	1:B:169:LEU:HB3	1.77	0.66
1:D:390:ILE:HG23	1:D:391:ARG:HD3	1.78	0.65
1:C:673:LEU:HA	1:C:676:LEU:HD12	1.76	0.65
1:A:390:ILE:HG23	1:A:391:ARG:HD3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:THR:O	1:A:343:THR:OG1	2.12	0.64
1:B:390:ILE:HG23	1:B:391:ARG:HD3	1.78	0.64
1:C:339:THR:O	1:C:343:THR:OG1	2.12	0.64
1:A:615:PHE:O	1:A:619:LEU:HG	1.99	0.63
1:B:685:MET:H	1:D:675:LYS:HE2	1.65	0.62
1:C:494:LEU:HD22	1:D:637:ASN:HD21	1.64	0.62
1:B:623:LEU:HD12	1:D:586:TRP:CH2	2.35	0.62
1:B:443:ILE:HG22	1:B:445:ASN:H	1.65	0.61
1:D:615:PHE:O	1:D:619:LEU:HG	2.00	0.61
1:B:615:PHE:O	1:B:619:LEU:HG	2.00	0.61
1:C:615:PHE:O	1:C:619:LEU:HG	1.99	0.61
1:A:443:ILE:HG22	1:A:445:ASN:H	1.65	0.61
1:B:338:ASN:OD1	1:D:785:TRP:NE1	2.34	0.61
1:B:758:SER:OG	1:B:759:GLY:N	2.35	0.60
1:D:443:ILE:HG22	1:D:445:ASN:H	1.65	0.60
1:A:422:SER:HB3	1:A:770:GLY:HA3	1.84	0.60
1:C:387:GLN:O	1:C:391:ARG:NE	2.29	0.60
1:D:673:LEU:O	1:D:677:THR:HG23	2.02	0.60
1:B:673:LEU:O	1:B:677:THR:HG23	2.02	0.60
1:B:264:VAL:HB	1:B:312:ALA:HB2	1.84	0.60
1:B:170:LEU:HD12	1:B:219:ARG:HG3	1.83	0.60
1:C:170:LEU:HD12	1:C:219:ARG:HG3	1.83	0.60
1:C:201:ASN:O	1:C:207:ASN:ND2	2.35	0.60
1:C:758:SER:HA	1:C:776:TRP:CD1	2.37	0.60
1:D:758:SER:OG	1:D:759:GLY:N	2.35	0.60
1:C:579:VAL:HG23	1:D:631:ALA:HB1	1.83	0.60
1:D:488:THR:HG21	1:D:513:GLY:HA3	1.84	0.60
1:C:264:VAL:HB	1:C:312:ALA:HB2	1.84	0.60
1:D:264:VAL:HB	1:D:312:ALA:HB2	1.84	0.60
1:A:201:ASN:O	1:A:207:ASN:ND2	2.35	0.59
1:A:758:SER:OG	1:A:759:GLY:N	2.35	0.59
1:B:488:THR:HG21	1:B:513:GLY:HA3	1.84	0.59
1:B:758:SER:HA	1:B:776:TRP:CD1	2.37	0.59
1:A:744:ILE:O	1:A:747:SER:OG	2.21	0.59
1:D:160:ARG:NH1	1:D:165:ASP:OD2	2.36	0.59
1:B:201:ASN:O	1:B:207:ASN:ND2	2.35	0.59
1:C:752:LEU:HB2	1:C:754:LYS:HE3	1.84	0.59
1:D:170:LEU:HD12	1:D:219:ARG:HG3	1.83	0.59
1:A:160:ARG:NH1	1:A:165:ASP:OD2	2.36	0.59
1:A:264:VAL:HB	1:A:312:ALA:HB2	1.84	0.59
1:A:758:SER:HA	1:A:776:TRP:CD1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:714:LEU:HD13	1:B:717:LEU:HD23	1.84	0.59
1:C:673:LEU:O	1:C:677:THR:HG23	2.02	0.59
1:A:714:LEU:HD13	1:A:717:LEU:HD23	1.84	0.59
1:D:752:LEU:HB2	1:D:754:LYS:HE3	1.84	0.59
1:D:758:SER:HA	1:D:776:TRP:CD1	2.37	0.59
1:A:466:PHE:HE2	1:A:754:LYS:HA	1.68	0.59
1:A:170:LEU:HD12	1:A:219:ARG:HG3	1.83	0.59
1:A:231:PHE:N	1:A:238:GLY:O	2.36	0.59
1:B:466:PHE:HE2	1:B:754:LYS:HA	1.68	0.59
1:C:443:ILE:HG22	1:C:445:ASN:H	1.65	0.59
1:C:744:ILE:O	1:C:747:SER:OG	2.21	0.59
1:B:387:GLN:O	1:B:391:ARG:NE	2.29	0.59
1:B:744:ILE:O	1:B:747:SER:OG	2.21	0.59
1:A:387:GLN:O	1:A:391:ARG:NE	2.29	0.59
1:A:673:LEU:O	1:A:677:THR:HG23	2.02	0.59
1:D:201:ASN:O	1:D:207:ASN:ND2	2.35	0.59
1:A:488:THR:HG21	1:A:513:GLY:HA3	1.84	0.59
1:D:744:ILE:O	1:D:747:SER:OG	2.21	0.59
1:A:630:SER:O	1:A:634:SER:OG	2.21	0.58
1:C:749:PRO:HB3	1:C:751:PHE:CE1	2.38	0.58
1:A:526:PHE:HA	1:A:529:ILE:HG12	1.85	0.58
1:B:160:ARG:NH1	1:B:165:ASP:OD2	2.36	0.58
1:B:231:PHE:N	1:B:238:GLY:O	2.36	0.58
1:C:160:ARG:NH1	1:C:165:ASP:OD2	2.36	0.58
1:D:714:LEU:HD13	1:D:717:LEU:HD23	1.84	0.58
1:A:586:TRP:HZ3	1:C:623:LEU:HB3	1.69	0.58
1:B:526:PHE:HA	1:B:529:ILE:HG12	1.85	0.58
1:B:749:PRO:HB3	1:B:751:PHE:CE1	2.38	0.58
1:D:478:TYR:OH	1:D:585:GLY:O	2.21	0.58
1:A:749:PRO:HB3	1:A:751:PHE:CE1	2.38	0.58
1:A:580:PHE:CE1	1:C:698:LEU:HD11	2.38	0.58
1:C:526:PHE:HA	1:C:529:ILE:HG12	1.85	0.58
1:C:714:LEU:HD13	1:C:717:LEU:HD23	1.84	0.58
1:A:686:LEU:HD21	1:A:691:TYR:CE1	2.39	0.58
1:A:752:LEU:HB2	1:A:754:LYS:HE3	1.84	0.58
1:B:686:LEU:HD21	1:B:691:TYR:CE1	2.39	0.58
1:C:478:TYR:OH	1:C:585:GLY:O	2.21	0.58
1:C:773:ASP:OD1	1:C:774:ARG:N	2.36	0.58
1:B:773:ASP:OD1	1:B:774:ARG:N	2.37	0.58
1:D:231:PHE:N	1:D:238:GLY:O	2.36	0.58
1:C:466:PHE:HE2	1:C:754:LYS:HA	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:758:SER:OG	1:C:759:GLY:N	2.35	0.58
1:D:466:PHE:HE2	1:D:754:LYS:HA	1.68	0.58
1:D:526:PHE:HA	1:D:529:ILE:HG12	1.85	0.58
1:D:749:PRO:HB3	1:D:751:PHE:CE1	2.38	0.58
1:B:478:TYR:OH	1:B:585:GLY:O	2.21	0.57
1:D:387:GLN:O	1:D:391:ARG:NE	2.29	0.57
1:D:422:SER:HB3	1:D:770:GLY:HA3	1.86	0.57
1:B:422:SER:HB3	1:B:770:GLY:HA3	1.86	0.57
1:D:665:THR:OG1	1:D:666:PHE:N	2.36	0.57
1:B:665:THR:OG1	1:B:666:PHE:N	2.36	0.57
1:B:752:LEU:HB2	1:B:754:LYS:HE3	1.84	0.57
1:C:488:THR:HG21	1:C:513:GLY:HA3	1.84	0.57
1:A:706:THR:HA	1:A:710:LEU:HD23	1.87	0.57
1:C:665:THR:OG1	1:C:666:PHE:N	2.36	0.57
1:C:686:LEU:HD21	1:C:691:TYR:CE1	2.39	0.57
1:D:686:LEU:HD21	1:D:691:TYR:CE1	2.39	0.57
1:B:623:LEU:HB3	1:D:586:TRP:HZ3	1.68	0.57
1:C:785:TRP:NE1	1:D:338:ASN:OD1	2.38	0.57
1:A:586:TRP:CZ3	1:C:623:LEU:HB3	2.39	0.56
1:B:706:THR:HA	1:B:710:LEU:HD23	1.87	0.56
1:C:706:THR:HA	1:C:710:LEU:HD23	1.87	0.56
1:A:478:TYR:OH	1:A:585:GLY:O	2.21	0.56
1:A:773:ASP:OD1	1:A:774:ARG:N	2.37	0.56
1:A:728:GLU:HA	1:A:731:HIS:HB3	1.87	0.56
1:C:728:GLU:HA	1:C:731:HIS:HB3	1.87	0.56
1:D:583:VAL:HG22	1:D:587:MET:HE2	1.88	0.56
1:D:706:THR:HA	1:D:710:LEU:HD23	1.87	0.56
1:D:773:ASP:OD1	1:D:774:ARG:N	2.37	0.56
1:C:422:SER:HB3	1:C:770:GLY:HA3	1.87	0.56
1:B:183:GLU:OE1	1:B:183:GLU:N	2.33	0.56
1:C:496:GLY:H	1:D:637:ASN:CB	2.13	0.56
1:A:329:VAL:O	1:A:382:LYS:NZ	2.38	0.56
1:B:583:VAL:HG22	1:B:587:MET:HE2	1.88	0.56
1:C:231:PHE:N	1:C:238:GLY:O	2.36	0.56
1:B:757:ARG:HH21	1:B:779:ARG:HG2	1.71	0.56
1:C:586:TRP:CZ3	1:D:623:LEU:HB3	2.41	0.56
1:D:728:GLU:HA	1:D:731:HIS:HB3	1.87	0.56
1:C:217:ALA:O	1:C:220:THR:OG1	2.20	0.56
1:A:151:ARG:HB2	1:A:185:PHE:HA	1.88	0.56
1:C:611:PHE:HB3	1:C:612:LYS:HD2	1.88	0.56
1:D:609:ILE:HD12	1:D:613:ASP:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:757:ARG:HH21	1:A:779:ARG:HG2	1.71	0.55
1:A:778:PHE:HE2	1:A:780:VAL:HB	1.71	0.55
1:B:611:PHE:HB3	1:B:612:LYS:HD2	1.88	0.55
1:C:392:ARG:NH1	1:C:402:LEU:O	2.39	0.55
1:C:669:PHE:O	1:C:673:LEU:HB2	2.06	0.55
1:D:392:ARG:NH1	1:D:402:LEU:O	2.39	0.55
1:D:630:SER:O	1:D:634:SER:OG	2.21	0.55
1:A:669:PHE:O	1:A:673:LEU:HB2	2.06	0.55
1:C:757:ARG:HH21	1:C:779:ARG:HG2	1.71	0.55
1:D:757:ARG:HH21	1:D:779:ARG:HG2	1.71	0.55
1:A:173:LEU:HD23	1:A:178:LYS:HB2	1.88	0.55
1:A:556:TYR:O	1:A:560:VAL:HG23	2.06	0.55
1:B:217:ALA:O	1:B:220:THR:OG1	2.20	0.55
1:B:392:ARG:NH1	1:B:402:LEU:O	2.39	0.55
1:D:151:ARG:HB2	1:D:185:PHE:HA	1.89	0.55
1:D:186:ARG:NE	1:D:191:GLY:O	2.38	0.55
1:A:583:VAL:HG22	1:A:587:MET:HE2	1.88	0.55
1:B:186:ARG:NE	1:B:191:GLY:O	2.38	0.55
1:B:438:VAL:HG11	1:B:742:LEU:HD12	1.88	0.55
1:B:556:TYR:O	1:B:560:VAL:HG23	2.06	0.55
1:C:151:ARG:HB2	1:C:185:PHE:HA	1.89	0.55
1:D:438:VAL:HG11	1:D:742:LEU:HD12	1.88	0.55
1:A:609:ILE:HD12	1:A:613:ASP:HB2	1.88	0.55
1:B:173:LEU:HD23	1:B:178:LYS:HB2	1.88	0.55
1:A:392:ARG:NH1	1:A:402:LEU:O	2.39	0.55
1:B:609:ILE:HD12	1:B:613:ASP:HB2	1.88	0.55
1:B:728:GLU:HA	1:B:731:HIS:HB3	1.87	0.55
1:C:306:GLU:HA	1:C:311:LYS:HD2	1.89	0.55
1:C:424:LEU:HA	1:C:433:VAL:HG12	1.89	0.55
1:D:306:GLU:HA	1:D:311:LYS:HD2	1.89	0.55
1:D:778:PHE:HE2	1:D:780:VAL:HB	1.71	0.55
1:A:424:LEU:HA	1:A:433:VAL:HG12	1.89	0.55
1:A:611:PHE:HB3	1:A:612:LYS:HD2	1.88	0.55
1:C:183:GLU:OE1	1:C:183:GLU:N	2.33	0.55
1:D:329:VAL:O	1:D:382:LYS:NZ	2.38	0.55
1:D:611:PHE:HB3	1:D:612:LYS:HD2	1.88	0.55
1:A:306:GLU:HA	1:A:311:LYS:HD2	1.89	0.55
1:B:151:ARG:HB2	1:B:185:PHE:HA	1.89	0.55
1:B:315:ARG:NH1	1:B:353:CYS:SG	2.75	0.55
1:D:646:ASN:OD1	1:D:647:GLU:N	2.40	0.55
1:B:669:PHE:O	1:B:673:LEU:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:438:VAL:HG11	1:C:742:LEU:HD12	1.88	0.55
1:C:556:TYR:O	1:C:560:VAL:HG23	2.06	0.55
1:C:646:ASN:OD1	1:C:647:GLU:N	2.40	0.55
1:C:778:PHE:HE2	1:C:780:VAL:HB	1.71	0.55
1:D:669:PHE:O	1:D:673:LEU:HB2	2.06	0.55
1:D:556:TYR:O	1:D:560:VAL:HG23	2.06	0.54
1:A:438:VAL:HG11	1:A:742:LEU:HD12	1.88	0.54
1:C:315:ARG:NH1	1:C:353:CYS:SG	2.75	0.54
1:C:583:VAL:HG22	1:C:587:MET:HE2	1.88	0.54
1:C:597:LYS:HB3	1:D:616:ARG:NH1	2.22	0.54
1:B:173:LEU:O	1:B:178:LYS:N	2.40	0.54
1:B:333:ASP:OD2	1:B:334:ASN:N	2.36	0.54
1:C:329:VAL:O	1:C:382:LYS:NZ	2.38	0.54
1:C:173:LEU:HD23	1:C:178:LYS:HB2	1.88	0.54
1:B:778:PHE:HE2	1:B:780:VAL:HB	1.71	0.54
1:A:705:LEU:HA	1:A:709:LEU:HD13	1.90	0.54
1:B:623:LEU:HD12	1:D:586:TRP:HH2	1.71	0.54
1:D:315:ARG:NH1	1:D:353:CYS:SG	2.75	0.54
1:B:306:GLU:HA	1:B:311:LYS:HD2	1.89	0.54
1:B:424:LEU:HA	1:B:433:VAL:HG12	1.89	0.54
1:C:609:ILE:HD12	1:C:613:ASP:HB2	1.88	0.54
1:D:761:MET:HE1	1:D:774:ARG:HG2	1.90	0.54
1:B:176:HIS:O	1:B:177:LYS:HG3	2.08	0.54
1:D:173:LEU:HD23	1:D:178:LYS:HB2	1.88	0.54
1:A:315:ARG:NH1	1:A:353:CYS:SG	2.75	0.54
1:B:761:MET:HE1	1:B:774:ARG:HG2	1.90	0.54
1:D:424:LEU:HA	1:D:433:VAL:HG12	1.89	0.54
1:A:173:LEU:O	1:A:178:LYS:N	2.40	0.53
1:A:284:PHE:CG	1:A:291:LEU:HD13	2.43	0.53
1:B:705:LEU:HA	1:B:709:LEU:HD13	1.90	0.53
1:C:323:THR:H	1:C:326:HIS:HD2	1.56	0.53
1:C:580:PHE:HE1	1:D:698:LEU:HD11	1.72	0.53
1:A:183:GLU:OE1	1:A:183:GLU:N	2.33	0.53
1:C:264:VAL:HG23	1:C:265:HIS:CD2	2.44	0.53
1:D:264:VAL:HG23	1:D:265:HIS:CD2	2.44	0.53
1:A:264:VAL:HG23	1:A:265:HIS:CD2	2.44	0.53
1:B:284:PHE:CG	1:B:291:LEU:HD13	2.43	0.53
1:D:284:PHE:CG	1:D:291:LEU:HD13	2.43	0.53
1:D:323:THR:H	1:D:326:HIS:HD2	1.56	0.53
1:C:398:ASP:OD1	1:C:399:THR:N	2.37	0.53
1:C:705:LEU:HA	1:C:709:LEU:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:LEU:O	1:D:178:LYS:N	2.40	0.53
1:A:752:LEU:O	1:A:754:LYS:HG2	2.09	0.53
1:C:752:LEU:O	1:C:754:LYS:HG2	2.09	0.53
1:D:217:ALA:O	1:D:220:THR:OG1	2.20	0.53
1:C:173:LEU:O	1:C:178:LYS:N	2.41	0.53
1:C:284:PHE:CG	1:C:291:LEU:HD13	2.43	0.53
1:C:428:GLY:N	1:C:435:GLU:OE2	2.28	0.53
1:C:761:MET:HE1	1:C:774:ARG:HG2	1.90	0.53
1:A:176:HIS:O	1:A:177:LYS:HG3	2.08	0.53
1:B:360:SER:OG	1:B:361:ASN:N	2.42	0.53
1:B:752:LEU:O	1:B:754:LYS:HG2	2.09	0.53
1:A:665:THR:OG1	1:A:666:PHE:N	2.36	0.53
1:C:586:TRP:HZ3	1:D:623:LEU:HB3	1.74	0.53
1:C:785:TRP:CE2	1:D:338:ASN:ND2	2.74	0.53
1:D:360:SER:OG	1:D:361:ASN:N	2.42	0.53
1:C:360:SER:OG	1:C:361:ASN:N	2.42	0.53
1:D:176:HIS:O	1:D:177:LYS:HG3	2.08	0.53
1:A:323:THR:H	1:A:326:HIS:HD2	1.56	0.52
1:B:148:VAL:HG21	1:B:169:LEU:HD13	1.91	0.52
1:D:398:ASP:OD1	1:D:399:THR:N	2.37	0.52
1:B:264:VAL:HG23	1:B:265:HIS:CD2	2.44	0.52
1:B:623:LEU:HB3	1:D:586:TRP:CZ3	2.44	0.52
1:C:176:HIS:O	1:C:177:LYS:HG3	2.08	0.52
1:C:186:ARG:NE	1:C:191:GLY:O	2.38	0.52
1:A:646:ASN:OD1	1:A:647:GLU:N	2.40	0.52
1:A:753:ARG:O	1:A:754:LYS:HE2	2.09	0.52
1:A:761:MET:HE1	1:A:774:ARG:HG2	1.90	0.52
1:B:329:VAL:O	1:B:382:LYS:NZ	2.38	0.52
1:B:646:ASN:OD1	1:B:647:GLU:N	2.40	0.52
1:B:661:ARG:HE	1:B:662:ASP:H	1.58	0.52
1:D:705:LEU:HA	1:D:709:LEU:HD13	1.90	0.52
1:B:554:PHE:O	1:B:558:VAL:HG23	2.10	0.52
1:C:630:SER:O	1:C:634:SER:OG	2.21	0.52
1:C:643:LYS:HD2	1:C:660:CYS:O	2.10	0.52
1:D:752:LEU:O	1:D:754:LYS:HG2	2.09	0.52
1:D:753:ARG:O	1:D:754:LYS:HE2	2.09	0.52
1:A:438:VAL:O	1:A:446:ARG:NH2	2.42	0.52
1:B:615:PHE:O	1:B:618:LEU:HG	2.10	0.52
1:C:180:LEU:HD23	1:C:226:PHE:HE1	1.75	0.52
1:C:393:GLU:HA	1:C:403:SER:HB3	1.92	0.52
1:C:554:PHE:O	1:C:558:VAL:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:691:TYR:HB2	1:D:692:PRO:HD2	1.92	0.52
1:A:661:ARG:HE	1:A:662:ASP:H	1.58	0.52
1:B:753:ARG:O	1:B:754:LYS:HE2	2.09	0.52
1:A:393:GLU:HA	1:A:403:SER:HB3	1.92	0.52
1:B:398:ASP:OD1	1:B:399:THR:N	2.37	0.52
1:A:186:ARG:NE	1:A:191:GLY:O	2.38	0.52
1:A:398:ASP:OD1	1:A:399:THR:N	2.37	0.52
1:A:643:LYS:HD2	1:A:660:CYS:O	2.10	0.52
1:D:615:PHE:O	1:D:618:LEU:HG	2.10	0.52
1:A:148:VAL:HG21	1:A:169:LEU:HD13	1.91	0.52
1:A:360:SER:OG	1:A:361:ASN:N	2.42	0.52
1:A:554:PHE:O	1:A:558:VAL:HG23	2.10	0.52
1:B:428:GLY:N	1:B:435:GLU:OE2	2.28	0.52
1:C:148:VAL:HG21	1:C:169:LEU:HD13	1.91	0.52
1:C:615:PHE:O	1:C:618:LEU:HG	2.10	0.52
1:D:643:LYS:HD2	1:D:660:CYS:O	2.10	0.52
1:C:472:TYR:HA	1:C:475:VAL:HG12	1.92	0.51
1:C:691:TYR:HB2	1:C:692:PRO:HD2	1.92	0.51
1:C:696:ILE:HD12	1:C:699:LEU:HD23	1.93	0.51
1:D:393:GLU:HA	1:D:403:SER:HB3	1.92	0.51
1:A:472:TYR:HA	1:A:475:VAL:HG12	1.92	0.51
1:B:180:LEU:HD23	1:B:226:PHE:HE1	1.75	0.51
1:B:643:LYS:HD2	1:B:660:CYS:O	2.10	0.51
1:D:554:PHE:O	1:D:558:VAL:HG23	2.10	0.51
1:A:696:ILE:HD12	1:A:699:LEU:HD23	1.93	0.51
1:D:696:ILE:HD12	1:D:699:LEU:HD23	1.93	0.51
1:A:615:PHE:O	1:A:618:LEU:HG	2.10	0.51
1:B:691:TYR:HB2	1:B:692:PRO:HD2	1.92	0.51
1:C:661:ARG:HE	1:C:662:ASP:H	1.58	0.51
1:C:753:ARG:O	1:C:754:LYS:HE2	2.09	0.51
1:B:170:LEU:HA	1:B:173:LEU:HD12	1.93	0.51
1:B:472:TYR:HA	1:B:475:VAL:HG12	1.92	0.51
1:C:740:THR:O	1:C:744:ILE:HG12	2.10	0.51
1:D:740:THR:O	1:D:744:ILE:HG12	2.10	0.51
1:A:180:LEU:HD23	1:A:226:PHE:HE1	1.75	0.51
1:B:393:GLU:HA	1:B:403:SER:HB3	1.92	0.51
1:D:148:VAL:HG21	1:D:169:LEU:HD13	1.91	0.51
1:D:180:LEU:HD23	1:D:226:PHE:HE1	1.75	0.51
1:A:170:LEU:HA	1:A:173:LEU:HD12	1.93	0.51
1:B:630:SER:O	1:B:634:SER:OG	2.21	0.51
1:C:438:VAL:O	1:C:446:ARG:NH2	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:661:ARG:HE	1:D:662:ASP:H	1.58	0.51
1:A:333:ASP:OD2	1:A:334:ASN:N	2.36	0.51
1:B:616:ARG:HH11	1:D:597:LYS:HB3	1.75	0.51
1:D:438:VAL:O	1:D:446:ARG:NH2	2.42	0.51
1:D:472:TYR:HA	1:D:475:VAL:HG12	1.92	0.51
1:B:577:VAL:HA	1:B:580:PHE:CD2	2.46	0.51
1:D:784:ASN:OD1	1:D:785:TRP:N	2.44	0.51
1:A:577:VAL:HA	1:A:580:PHE:CD2	2.46	0.51
1:A:691:TYR:HB2	1:A:692:PRO:HD2	1.92	0.51
1:B:616:ARG:NH1	1:D:597:LYS:HB3	2.26	0.51
1:B:740:THR:O	1:B:744:ILE:HG12	2.11	0.51
1:A:586:TRP:CH2	1:C:623:LEU:HD12	2.46	0.50
1:B:757:ARG:HD2	1:B:758:SER:O	2.11	0.50
1:C:577:VAL:HA	1:C:580:PHE:CD2	2.45	0.50
1:C:757:ARG:HD2	1:C:758:SER:O	2.12	0.50
1:D:326:HIS:CE1	1:D:373:PRO:HD3	2.46	0.50
1:B:326:HIS:CE1	1:B:373:PRO:HD3	2.47	0.50
1:B:438:VAL:O	1:B:446:ARG:NH2	2.43	0.50
1:B:696:ILE:HD12	1:B:699:LEU:HD23	1.93	0.50
1:C:326:HIS:CE1	1:C:373:PRO:HD3	2.47	0.50
1:D:757:ARG:HD2	1:D:758:SER:O	2.11	0.50
1:A:760:GLU:CD	1:A:764:VAL:HB	2.37	0.50
1:B:784:ASN:OD1	1:B:785:TRP:N	2.44	0.50
1:A:740:THR:O	1:A:744:ILE:HG12	2.11	0.50
1:A:428:GLY:N	1:A:435:GLU:OE2	2.28	0.50
1:D:170:LEU:HA	1:D:173:LEU:HD12	1.93	0.50
1:D:325:LEU:O	1:D:329:VAL:HG23	2.12	0.50
1:A:757:ARG:NH1	1:A:758:SER:O	2.45	0.50
1:A:784:ASN:OD1	1:A:785:TRP:N	2.44	0.50
1:C:784:ASN:OD1	1:C:785:TRP:N	2.44	0.50
1:A:631:ALA:HB1	1:B:579:VAL:HG23	1.93	0.50
1:C:170:LEU:HA	1:C:173:LEU:HD12	1.93	0.50
1:C:322:ASN:HB3	1:C:326:HIS:HB2	1.94	0.50
1:C:325:LEU:O	1:C:329:VAL:HG23	2.12	0.50
1:C:333:ASP:OD2	1:C:334:ASN:N	2.36	0.50
1:D:183:GLU:OE1	1:D:183:GLU:N	2.33	0.50
1:D:577:VAL:HA	1:D:580:PHE:CD2	2.46	0.50
1:D:760:GLU:CD	1:D:764:VAL:HB	2.37	0.50
1:A:326:HIS:CE1	1:A:373:PRO:HD3	2.46	0.49
1:B:322:ASN:HB3	1:B:326:HIS:HB2	1.94	0.49
1:C:295:THR:O	1:C:297:GLN:NE2	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:322:ASN:HB3	1:D:326:HIS:HB2	1.94	0.49
1:A:727:LYS:O	1:A:731:HIS:HB3	2.12	0.49
1:A:325:LEU:O	1:A:329:VAL:HG23	2.12	0.49
1:C:394:VAL:HB	1:C:400:ARG:HA	1.94	0.49
1:C:727:LYS:O	1:C:731:HIS:HB3	2.12	0.49
1:B:171:PRO:O	1:B:175:THR:OG1	2.26	0.49
1:B:325:LEU:O	1:B:329:VAL:HG23	2.12	0.49
1:C:194:CYS:HB3	1:C:213:LEU:HD21	1.94	0.49
1:D:394:VAL:HB	1:D:400:ARG:HA	1.94	0.49
1:D:627:GLY:O	1:D:630:SER:OG	2.26	0.49
1:A:757:ARG:HD2	1:A:758:SER:O	2.12	0.49
1:D:757:ARG:NH1	1:D:758:SER:O	2.45	0.49
1:B:323:THR:H	1:B:326:HIS:HD2	1.56	0.49
1:C:760:GLU:CD	1:C:764:VAL:HB	2.37	0.49
1:A:394:VAL:HB	1:A:400:ARG:HA	1.94	0.49
1:B:148:VAL:HG11	1:B:169:LEU:HD22	1.95	0.49
1:B:194:CYS:HB3	1:B:213:LEU:HD21	1.94	0.49
1:B:760:GLU:CD	1:B:764:VAL:HB	2.37	0.49
1:C:486:THR:HG23	1:D:630:SER:OG	2.13	0.49
1:C:627:GLY:O	1:C:630:SER:OG	2.26	0.49
1:D:295:THR:O	1:D:297:GLN:NE2	2.38	0.49
1:B:757:ARG:NH1	1:B:758:SER:O	2.45	0.49
1:C:757:ARG:NH1	1:C:758:SER:O	2.45	0.49
1:D:727:LYS:O	1:D:731:HIS:HB3	2.12	0.49
1:A:586:TRP:HH2	1:C:623:LEU:HD12	1.77	0.49
1:B:727:LYS:O	1:B:731:HIS:HB3	2.13	0.49
1:A:148:VAL:HG11	1:A:169:LEU:HD22	1.95	0.48
1:A:322:ASN:HB3	1:A:326:HIS:HB2	1.94	0.48
1:D:686:LEU:HD22	1:D:696:ILE:HG21	1.95	0.48
1:A:686:LEU:HD22	1:A:696:ILE:HG21	1.95	0.48
1:B:338:ASN:ND2	1:D:785:TRP:CE2	2.80	0.48
1:D:194:CYS:HB3	1:D:213:LEU:HD21	1.94	0.48
1:D:315:ARG:HH22	1:D:362:LEU:HD13	1.79	0.48
1:A:597:LYS:HB3	1:C:616:ARG:NH1	2.28	0.48
1:B:488:THR:HG22	1:B:510:ARG:HA	1.96	0.48
1:A:194:CYS:HB3	1:A:213:LEU:HD21	1.94	0.48
1:A:315:ARG:HH22	1:A:362:LEU:HD13	1.79	0.48
1:B:664:GLU:OE1	1:D:494:LEU:HD12	2.14	0.48
1:D:671:LEU:O	1:D:675:LYS:HG2	2.14	0.48
1:A:488:THR:HG22	1:A:510:ARG:HA	1.96	0.48
1:B:686:LEU:HD22	1:B:696:ILE:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:686:LEU:HD22	1:C:696:ILE:HG21	1.95	0.48
1:D:148:VAL:HG11	1:D:169:LEU:HD22	1.95	0.48
1:D:499:PRO:O	1:D:501:PRO:HD3	2.14	0.48
1:B:394:VAL:HB	1:B:400:ARG:HA	1.94	0.48
1:C:148:VAL:HG11	1:C:169:LEU:HD22	1.95	0.48
1:A:217:ALA:O	1:A:220:THR:OG1	2.20	0.48
1:B:315:ARG:HH22	1:B:362:LEU:HD13	1.79	0.48
1:B:367:ASN:OD1	1:B:371:LEU:N	2.36	0.48
1:B:499:PRO:O	1:B:501:PRO:HD3	2.14	0.48
1:B:671:LEU:O	1:B:675:LYS:HG2	2.14	0.48
1:B:709:LEU:O	1:B:713:MET:N	2.38	0.48
1:D:709:LEU:O	1:D:713:MET:N	2.38	0.48
1:C:215:ASP:O	1:C:219:ARG:HG2	2.14	0.47
1:C:499:PRO:O	1:C:501:PRO:HD3	2.14	0.47
1:A:183:GLU:HA	1:A:186:ARG:HD3	1.97	0.47
1:C:642:MET:HB3	1:C:692:PRO:HD2	1.97	0.47
1:D:367:ASN:OD1	1:D:371:LEU:N	2.36	0.47
1:A:215:ASP:O	1:A:219:ARG:HG2	2.14	0.47
1:A:230:PRO:HB2	1:A:238:GLY:HA2	1.95	0.47
1:A:499:PRO:O	1:A:501:PRO:HD3	2.14	0.47
1:B:295:THR:O	1:B:297:GLN:NE2	2.38	0.47
1:C:183:GLU:HA	1:C:186:ARG:HD3	1.96	0.47
1:A:671:LEU:O	1:A:675:LYS:HG2	2.14	0.47
1:C:463:TRP:HA	1:C:467:GLY:HA3	1.97	0.47
1:D:230:PRO:HB2	1:D:238:GLY:HA2	1.96	0.47
1:B:183:GLU:HA	1:B:186:ARG:HD3	1.97	0.47
1:B:637:ASN:HB2	1:B:638:PRO:HD3	1.96	0.47
1:C:236:TYR:HE1	1:C:272:PHE:CG	2.33	0.47
1:C:671:LEU:O	1:C:675:LYS:HG2	2.14	0.47
1:A:318:ASP:OD1	1:A:321:GLY:N	2.48	0.47
1:A:597:LYS:HB3	1:C:616:ARG:HH11	1.80	0.47
1:A:642:MET:HB3	1:A:692:PRO:HD2	1.97	0.47
1:B:230:PRO:HB2	1:B:238:GLY:HA2	1.96	0.47
1:B:236:TYR:HE1	1:B:272:PHE:CG	2.33	0.47
1:C:230:PRO:HB2	1:C:238:GLY:HA2	1.96	0.47
1:D:183:GLU:HA	1:D:186:ARG:HD3	1.97	0.47
1:D:236:TYR:HE1	1:D:272:PHE:CG	2.33	0.47
1:D:642:MET:HB3	1:D:692:PRO:HD2	1.97	0.47
1:B:337:GLU:OE1	1:D:785:TRP:HB2	2.14	0.47
1:C:315:ARG:HH22	1:C:362:LEU:HD13	1.79	0.47
1:D:488:THR:HG22	1:D:510:ARG:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:PRO:O	1:C:175:THR:OG1	2.26	0.47
1:D:215:ASP:O	1:D:219:ARG:HG2	2.14	0.47
1:A:236:TYR:HE1	1:A:272:PHE:CG	2.33	0.47
1:A:558:VAL:O	1:A:562:VAL:HG23	2.15	0.47
1:B:215:ASP:O	1:B:219:ARG:HG2	2.14	0.47
1:B:318:ASP:OD1	1:B:321:GLY:N	2.48	0.47
1:C:488:THR:HG22	1:C:510:ARG:HA	1.96	0.47
1:D:463:TRP:HA	1:D:467:GLY:HA3	1.97	0.47
1:C:318:ASP:OD1	1:C:321:GLY:N	2.48	0.46
1:C:580:PHE:CE1	1:D:698:LEU:HD11	2.49	0.46
1:C:637:ASN:HB2	1:C:638:PRO:HD3	1.96	0.46
1:D:195:LEU:HB2	1:D:226:PHE:CE2	2.50	0.46
1:D:558:VAL:O	1:D:562:VAL:HG23	2.15	0.46
1:A:332:ALA:O	1:A:382:LYS:NZ	2.48	0.46
1:B:594:ARG:NE	1:B:736:GLN:HE22	2.13	0.46
1:B:700:VAL:O	1:B:704:ILE:HG12	2.15	0.46
1:A:243:HIS:NE2	1:A:266:ALA:HB3	2.31	0.46
1:A:700:VAL:O	1:A:704:ILE:HG12	2.15	0.46
1:D:637:ASN:HB2	1:D:638:PRO:HD3	1.96	0.46
1:C:195:LEU:HB2	1:C:226:PHE:CE2	2.50	0.46
1:C:243:HIS:NE2	1:C:266:ALA:HB3	2.30	0.46
1:C:315:ARG:NH2	1:C:362:LEU:HD13	2.30	0.46
1:A:566:LEU:HB3	1:A:574:TYR:HB3	1.98	0.46
1:B:566:LEU:HB3	1:B:574:TYR:HB3	1.98	0.46
1:C:329:VAL:HG13	1:C:385:ILE:HG21	1.98	0.46
1:D:243:HIS:NE2	1:D:266:ALA:HB3	2.31	0.46
1:D:315:ARG:NH2	1:D:362:LEU:HD13	2.30	0.46
1:A:463:TRP:HA	1:A:467:GLY:HA3	1.97	0.46
1:B:664:GLU:HA	1:B:669:PHE:HZ	1.81	0.46
1:D:318:ASP:OD1	1:D:321:GLY:N	2.48	0.46
1:B:243:HIS:NE2	1:B:266:ALA:HB3	2.31	0.46
1:B:369:ASP:HB2	1:B:371:LEU:HG	1.98	0.46
1:B:637:ASN:HB2	1:B:638:PRO:CD	2.46	0.46
1:B:736:GLN:O	1:B:740:THR:OG1	2.24	0.46
1:C:369:ASP:HB2	1:C:371:LEU:HG	1.98	0.46
1:C:558:VAL:O	1:C:562:VAL:HG23	2.15	0.46
1:D:329:VAL:HG13	1:D:385:ILE:HG21	1.98	0.46
1:A:315:ARG:NH2	1:A:362:LEU:HD13	2.30	0.46
1:A:643:LYS:HG2	1:A:661:ARG:NH2	2.31	0.46
1:A:664:GLU:HA	1:A:669:PHE:HZ	1.81	0.46
1:B:642:MET:HB3	1:B:692:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:643:LYS:HG2	1:D:661:ARG:NH2	2.31	0.46
1:D:664:GLU:HA	1:D:669:PHE:HZ	1.81	0.46
1:A:195:LEU:HB2	1:A:226:PHE:CE2	2.50	0.46
1:A:369:ASP:HB2	1:A:371:LEU:HG	1.98	0.46
1:B:315:ARG:NH2	1:B:362:LEU:HD13	2.30	0.46
1:B:463:TRP:HA	1:B:467:GLY:HA3	1.97	0.46
1:D:369:ASP:HB2	1:D:371:LEU:HG	1.98	0.46
1:A:329:VAL:HG13	1:A:385:ILE:HG21	1.98	0.46
1:B:195:LEU:HB2	1:B:226:PHE:CE2	2.50	0.46
1:D:333:ASP:OD2	1:D:334:ASN:N	2.36	0.46
1:D:594:ARG:NE	1:D:736:GLN:HE22	2.13	0.46
1:C:566:LEU:HB3	1:C:574:TYR:HB3	1.98	0.45
1:C:700:VAL:O	1:C:704:ILE:HG12	2.15	0.45
1:A:295:THR:O	1:A:297:GLN:NE2	2.38	0.45
1:A:594:ARG:NE	1:A:736:GLN:HE22	2.14	0.45
1:A:627:GLY:O	1:A:630:SER:OG	2.26	0.45
1:A:637:ASN:HB2	1:A:638:PRO:CD	2.46	0.45
1:B:329:VAL:HG13	1:B:385:ILE:HG21	1.98	0.45
1:C:637:ASN:HB2	1:C:638:PRO:CD	2.46	0.45
1:A:637:ASN:HB2	1:A:638:PRO:HD3	1.96	0.45
1:B:558:VAL:O	1:B:562:VAL:HG23	2.16	0.45
1:D:637:ASN:HB2	1:D:638:PRO:CD	2.46	0.45
1:A:494:LEU:HD22	1:C:637:ASN:HD21	1.81	0.45
1:B:638:PRO:O	1:B:639:CYS:HB2	2.17	0.45
1:B:643:LYS:HG2	1:B:661:ARG:NH2	2.31	0.45
1:C:148:VAL:HG13	1:C:172:PHE:CD2	2.52	0.45
1:C:223:MET:O	1:C:227:ILE:HG12	2.17	0.45
1:D:321:GLY:O	1:D:367:ASN:HA	2.17	0.45
1:A:638:PRO:O	1:A:639:CYS:HB2	2.17	0.45
1:C:643:LYS:H	1:C:661:ARG:HH22	1.65	0.45
1:D:148:VAL:HG13	1:D:172:PHE:CD2	2.52	0.45
1:D:332:ALA:O	1:D:382:LYS:NZ	2.48	0.45
1:D:566:LEU:HB3	1:D:574:TYR:HB3	1.98	0.45
1:D:700:VAL:O	1:D:704:ILE:HG12	2.15	0.45
1:B:627:GLY:O	1:B:630:SER:OG	2.26	0.45
1:C:494:LEU:HD13	1:D:636:LEU:HD21	1.99	0.45
1:C:594:ARG:NE	1:C:736:GLN:HE22	2.14	0.45
1:C:625:MET:HE2	1:C:625:MET:HB2	1.93	0.45
1:C:643:LYS:HG2	1:C:661:ARG:NH2	2.31	0.45
1:D:469:VAL:O	1:D:473:ILE:HG12	2.17	0.45
1:A:148:VAL:HG13	1:A:172:PHE:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:420:ASP:OD2	1:D:775:ARG:NE	2.30	0.45
1:D:643:LYS:H	1:D:661:ARG:HH22	1.65	0.45
1:B:148:VAL:HG13	1:B:172:PHE:CD2	2.52	0.45
1:B:469:VAL:O	1:B:473:ILE:HG12	2.17	0.45
1:C:591:TYR:HE1	1:C:594:ARG:NH2	2.15	0.45
1:C:628:TYR:CZ	1:C:632:LEU:HD21	2.52	0.45
1:D:223:MET:O	1:D:227:ILE:HG12	2.17	0.45
1:D:379:LYS:HE3	1:D:379:LYS:HB2	1.84	0.45
1:A:591:TYR:HE1	1:A:594:ARG:NH2	2.15	0.44
1:B:321:GLY:O	1:B:367:ASN:HA	2.17	0.44
1:C:664:GLU:HA	1:C:669:PHE:HZ	1.81	0.44
1:D:193:THR:HG22	1:D:194:CYS:N	2.29	0.44
1:A:180:LEU:HD23	1:A:226:PHE:CE1	2.53	0.44
1:A:326:HIS:CD2	1:A:326:HIS:H	2.35	0.44
1:A:736:GLN:O	1:A:740:THR:OG1	2.24	0.44
1:B:628:TYR:CZ	1:B:632:LEU:HD21	2.52	0.44
1:D:628:TYR:CZ	1:D:632:LEU:HD21	2.52	0.44
1:D:638:PRO:O	1:D:639:CYS:HB2	2.17	0.44
1:A:625:MET:HE2	1:A:625:MET:HB2	1.93	0.44
1:B:326:HIS:CD2	1:B:326:HIS:H	2.35	0.44
1:C:180:LEU:HD23	1:C:226:PHE:CE1	2.53	0.44
1:A:469:VAL:O	1:A:473:ILE:HG12	2.17	0.44
1:D:591:TYR:HE1	1:D:594:ARG:NH2	2.15	0.44
1:A:496:GLY:N	1:C:637:ASN:HB3	2.28	0.44
1:A:628:TYR:CZ	1:A:632:LEU:HD21	2.52	0.44
1:B:643:LYS:H	1:B:661:ARG:HH22	1.65	0.44
1:A:571:ILE:HG22	1:A:572:GLU:H	1.83	0.44
1:A:643:LYS:H	1:A:661:ARG:HH22	1.65	0.44
1:A:717:LEU:HG	1:A:718:MET:HE2	2.00	0.44
1:B:332:ALA:O	1:B:382:LYS:NZ	2.48	0.44
1:B:606:ILE:HA	1:B:609:ILE:HG22	2.00	0.44
1:C:717:LEU:HG	1:C:718:MET:HE2	2.00	0.44
1:D:326:HIS:CD2	1:D:326:HIS:H	2.35	0.44
1:A:195:LEU:HB2	1:A:226:PHE:HE2	1.83	0.44
1:B:281:TYR:CD1	1:D:409:TRP:HH2	2.36	0.44
1:D:195:LEU:HB2	1:D:226:PHE:HE2	1.83	0.44
1:D:428:GLY:N	1:D:435:GLU:OE2	2.28	0.44
1:D:571:ILE:HG22	1:D:572:GLU:H	1.83	0.44
1:D:717:LEU:O	1:D:720:GLU:HG3	2.18	0.44
1:A:186:ARG:HG2	1:A:193:THR:HA	2.00	0.44
1:A:606:ILE:HA	1:A:609:ILE:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:257:LEU:HD23	1:C:257:LEU:HA	1.86	0.44
1:C:420:ASP:OD2	1:C:775:ARG:NE	2.30	0.44
1:C:717:LEU:O	1:C:720:GLU:HG3	2.18	0.44
1:D:171:PRO:O	1:D:175:THR:OG1	2.26	0.44
1:D:485:PHE:CD2	1:D:582:LEU:HD13	2.53	0.44
1:D:774:ARG:CZ	1:D:776:TRP:HE1	2.31	0.44
1:A:698:LEU:HD11	1:B:580:PHE:HE1	1.82	0.44
1:B:195:LEU:HB2	1:B:226:PHE:HE2	1.83	0.44
1:B:223:MET:O	1:B:227:ILE:HG12	2.17	0.44
1:B:420:ASP:HA	1:B:777:CYS:SG	2.58	0.44
1:B:597:LYS:HA	1:B:597:LYS:HD3	1.84	0.44
1:B:774:ARG:CZ	1:B:776:TRP:HE1	2.31	0.44
1:C:469:VAL:O	1:C:473:ILE:HG12	2.17	0.44
1:C:485:PHE:CD2	1:C:582:LEU:HD13	2.53	0.44
1:C:774:ARG:CZ	1:C:776:TRP:HE1	2.31	0.44
1:A:223:MET:O	1:A:227:ILE:HG12	2.17	0.43
1:A:321:GLY:O	1:A:367:ASN:HA	2.17	0.43
1:B:233:ASP:OD1	1:B:235:TYR:N	2.51	0.43
1:B:434:LEU:HA	1:B:437:LEU:HD12	2.00	0.43
1:C:321:GLY:O	1:C:367:ASN:HA	2.17	0.43
1:C:386:PHE:HA	1:C:389:ILE:HG22	1.99	0.43
1:C:638:PRO:O	1:C:639:CYS:HB2	2.17	0.43
1:D:420:ASP:HA	1:D:777:CYS:SG	2.58	0.43
1:A:709:LEU:O	1:A:713:MET:N	2.38	0.43
1:B:771:THR:HB	1:B:772:PRO:HD3	2.00	0.43
1:C:734:LYS:O	1:C:737:TRP:HB2	2.18	0.43
1:D:606:ILE:HA	1:D:609:ILE:HG22	2.00	0.43
1:A:717:LEU:O	1:A:720:GLU:HG3	2.18	0.43
1:B:698:LEU:HD11	1:D:580:PHE:HE1	1.83	0.43
1:C:250:CYS:O	1:C:254:VAL:HG23	2.18	0.43
1:C:367:ASN:OD1	1:C:371:LEU:N	2.36	0.43
1:C:420:ASP:HA	1:C:777:CYS:SG	2.58	0.43
1:D:180:LEU:HD23	1:D:226:PHE:CE1	2.53	0.43
1:A:386:PHE:HA	1:A:389:ILE:HG22	1.99	0.43
1:A:420:ASP:HA	1:A:777:CYS:SG	2.58	0.43
1:B:180:LEU:HD23	1:B:226:PHE:CE1	2.53	0.43
1:B:386:PHE:HA	1:B:389:ILE:HG22	1.99	0.43
1:C:714:LEU:O	1:C:718:MET:HG2	2.18	0.43
1:D:202:LEU:HD23	1:D:202:LEU:HA	1.86	0.43
1:D:271:ARG:HA	1:D:274:GLN:HG2	2.01	0.43
1:D:625:MET:HE2	1:D:625:MET:HB2	1.93	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:LYS:HE3	1:A:379:LYS:HB2	1.84	0.43
1:A:734:LYS:O	1:A:737:TRP:HB2	2.18	0.43
1:C:195:LEU:HB2	1:C:226:PHE:HE2	1.83	0.43
1:C:233:ASP:OD1	1:C:235:TYR:N	2.51	0.43
1:C:709:LEU:O	1:C:713:MET:N	2.38	0.43
1:D:226:PHE:HD2	1:D:227:ILE:HD13	1.84	0.43
1:D:386:PHE:HA	1:D:389:ILE:HG22	1.99	0.43
1:D:734:LYS:O	1:D:737:TRP:HB2	2.18	0.43
1:D:771:THR:HB	1:D:772:PRO:CD	2.48	0.43
1:A:420:ASP:OD2	1:A:775:ARG:NE	2.30	0.43
1:A:498:PRO:HB3	1:A:575:LEU:HD23	2.01	0.43
1:A:629:ALA:O	1:A:633:VAL:HG13	2.18	0.43
1:A:714:LEU:O	1:A:718:MET:HG2	2.18	0.43
1:B:557:SER:O	1:B:561:ILE:HG12	2.19	0.43
1:B:714:LEU:O	1:B:718:MET:HG2	2.18	0.43
1:B:734:LYS:O	1:B:737:TRP:HB2	2.18	0.43
1:C:379:LYS:HE3	1:C:379:LYS:HB2	1.84	0.43
1:C:571:ILE:HG22	1:C:572:GLU:H	1.83	0.43
1:C:736:GLN:O	1:C:740:THR:OG1	2.24	0.43
1:B:250:CYS:O	1:B:254:VAL:HG23	2.19	0.43
1:B:631:ALA:HB1	1:D:579:VAL:CG2	2.45	0.43
1:B:717:LEU:O	1:B:720:GLU:HG3	2.18	0.43
1:C:226:PHE:HD2	1:C:227:ILE:HD13	1.83	0.43
1:C:326:HIS:CD2	1:C:326:HIS:H	2.35	0.43
1:C:393:GLU:OE1	1:C:393:GLU:N	2.52	0.43
1:D:771:THR:HB	1:D:772:PRO:HD3	2.00	0.43
1:A:233:ASP:OD1	1:A:235:TYR:N	2.52	0.43
1:A:250:CYS:O	1:A:254:VAL:HG23	2.19	0.43
1:B:271:ARG:HA	1:B:274:GLN:HG2	2.01	0.43
1:B:571:ILE:HG22	1:B:572:GLU:H	1.83	0.43
1:B:591:TYR:HE1	1:B:594:ARG:NH2	2.15	0.43
1:C:474:ASN:HD22	1:C:474:ASN:HA	1.57	0.43
1:C:606:ILE:HA	1:C:609:ILE:HG22	2.00	0.43
1:D:393:GLU:N	1:D:393:GLU:OE1	2.52	0.43
1:D:498:PRO:HB3	1:D:575:LEU:HD23	2.01	0.43
1:A:271:ARG:HA	1:A:274:GLN:HG2	2.01	0.43
1:A:434:LEU:HA	1:A:437:LEU:HD12	2.00	0.43
1:B:186:ARG:HG2	1:B:193:THR:HA	2.00	0.43
1:B:771:THR:HB	1:B:772:PRO:CD	2.48	0.43
1:C:170:LEU:HD23	1:C:170:LEU:H	1.84	0.43
1:C:271:ARG:HA	1:C:274:GLN:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:PHE:CD2	1:A:582:LEU:HD13	2.53	0.43
1:B:393:GLU:N	1:B:393:GLU:OE1	2.52	0.43
1:C:353:CYS:SG	1:C:362:LEU:HB2	2.59	0.43
1:D:717:LEU:HG	1:D:718:MET:HE2	2.00	0.43
1:A:168:GLY:C	1:A:171:PRO:HD2	2.44	0.42
1:B:170:LEU:H	1:B:170:LEU:HD23	1.84	0.42
1:C:434:LEU:HA	1:C:437:LEU:HD12	2.00	0.42
1:D:186:ARG:HG2	1:D:193:THR:HA	2.00	0.42
1:D:474:ASN:HD22	1:D:474:ASN:HA	1.57	0.42
1:D:497:THR:O	1:D:497:THR:OG1	2.36	0.42
1:D:629:ALA:O	1:D:633:VAL:HG13	2.18	0.42
1:B:717:LEU:HG	1:B:718:MET:HE2	2.00	0.42
1:C:584:LEU:HA	1:C:587:MET:HE3	2.01	0.42
1:C:597:LYS:HA	1:C:597:LYS:HD3	1.84	0.42
1:D:250:CYS:O	1:D:254:VAL:HG23	2.19	0.42
1:B:226:PHE:HD2	1:B:227:ILE:HD13	1.83	0.42
1:C:438:VAL:HG13	1:C:439:TYR:N	2.34	0.42
1:B:168:GLY:C	1:B:171:PRO:HD2	2.44	0.42
1:D:353:CYS:SG	1:D:362:LEU:HB2	2.59	0.42
1:D:557:SER:O	1:D:561:ILE:HG12	2.19	0.42
1:A:438:VAL:HG13	1:A:439:TYR:N	2.34	0.42
1:A:597:LYS:HD3	1:A:597:LYS:HA	1.83	0.42
1:B:751:PHE:O	1:B:753:ARG:NH2	2.53	0.42
1:C:597:LYS:HB3	1:D:616:ARG:HH11	1.83	0.42
1:D:148:VAL:HG13	1:D:172:PHE:CE2	2.55	0.42
1:D:233:ASP:OD1	1:D:235:TYR:N	2.51	0.42
1:A:393:GLU:OE1	1:A:393:GLU:N	2.52	0.42
1:A:453:GLU:H	1:A:453:GLU:HG3	1.68	0.42
1:A:697:ILE:O	1:A:701:THR:HG22	2.20	0.42
1:A:751:PHE:O	1:A:753:ARG:NH2	2.53	0.42
1:A:774:ARG:CZ	1:A:776:TRP:HE1	2.31	0.42
1:B:584:LEU:HA	1:B:587:MET:HE3	2.01	0.42
1:B:697:ILE:O	1:B:701:THR:HG22	2.20	0.42
1:C:629:ALA:O	1:C:633:VAL:HG13	2.18	0.42
1:C:751:PHE:O	1:C:753:ARG:NH2	2.53	0.42
1:A:226:PHE:HD2	1:A:227:ILE:HD13	1.83	0.42
1:A:557:SER:O	1:A:561:ILE:HG12	2.19	0.42
1:A:584:LEU:HA	1:A:587:MET:HE3	2.01	0.42
1:B:730:LYS:O	1:B:734:LYS:HG2	2.19	0.42
1:C:148:VAL:HG13	1:C:172:PHE:CE2	2.55	0.42
1:C:730:LYS:O	1:C:734:LYS:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:584:LEU:HA	1:D:587:MET:HE3	2.01	0.42
1:D:661:ARG:NE	1:D:662:ASP:H	2.18	0.42
1:D:730:LYS:O	1:D:734:LYS:HG2	2.19	0.42
1:A:353:CYS:SG	1:A:362:LEU:HB2	2.59	0.42
1:B:148:VAL:HG13	1:B:172:PHE:CE2	2.55	0.42
1:C:168:GLY:C	1:C:171:PRO:HD2	2.44	0.42
1:D:170:LEU:H	1:D:170:LEU:HD23	1.84	0.42
1:C:498:PRO:HB3	1:C:575:LEU:HD23	2.01	0.42
1:C:557:SER:O	1:C:561:ILE:HG12	2.19	0.42
1:C:571:ILE:HG22	1:C:572:GLU:N	2.35	0.42
1:B:193:THR:HG22	1:B:194:CYS:N	2.29	0.42
1:B:629:ALA:O	1:B:633:VAL:HG13	2.18	0.42
1:C:186:ARG:HG2	1:C:193:THR:HA	2.00	0.42
1:C:215:ASP:O	1:C:218:GLU:HG3	2.20	0.42
1:D:168:GLY:C	1:D:171:PRO:HD2	2.44	0.42
1:D:367:ASN:ND2	1:D:369:ASP:H	2.18	0.42
1:D:387:GLN:HG2	1:D:391:ARG:NH1	2.35	0.42
1:B:353:CYS:SG	1:B:362:LEU:HB2	2.59	0.41
1:B:387:GLN:HG2	1:B:391:ARG:NH1	2.35	0.41
1:B:485:PHE:CD2	1:B:582:LEU:HD13	2.53	0.41
1:C:332:ALA:O	1:C:382:LYS:NZ	2.48	0.41
1:D:434:LEU:HA	1:D:437:LEU:HD12	2.00	0.41
1:D:714:LEU:O	1:D:718:MET:HG2	2.18	0.41
1:A:148:VAL:HG13	1:A:172:PHE:CE2	2.55	0.41
1:D:441:SER:O	1:D:446:ARG:NH1	2.53	0.41
1:A:215:ASP:O	1:A:218:GLU:HG3	2.20	0.41
1:A:583:VAL:O	1:A:587:MET:HG3	2.21	0.41
1:A:730:LYS:O	1:A:734:LYS:HG2	2.19	0.41
1:B:498:PRO:HB3	1:B:575:LEU:HD23	2.01	0.41
1:C:367:ASN:ND2	1:C:369:ASP:H	2.18	0.41
1:C:497:THR:O	1:C:497:THR:OG1	2.36	0.41
1:D:571:ILE:HG22	1:D:572:GLU:N	2.35	0.41
1:D:612:LYS:HB3	1:D:616:ARG:HH12	1.84	0.41
1:A:257:LEU:HD23	1:A:257:LEU:HA	1.86	0.41
1:A:328:LEU:HD11	1:A:342:VAL:HG23	2.02	0.41
1:A:612:LYS:HB3	1:A:616:ARG:HH12	1.84	0.41
1:A:762:VAL:HG22	1:A:766:LYS:HD3	2.02	0.41
1:B:219:ARG:HA	1:B:219:ARG:HD3	1.82	0.41
1:B:438:VAL:HG13	1:B:439:TYR:N	2.35	0.41
1:B:441:SER:O	1:B:446:ARG:NH1	2.53	0.41
1:C:583:VAL:O	1:C:587:MET:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:697:ILE:O	1:D:701:THR:HG22	2.20	0.41
1:A:170:LEU:HD23	1:A:170:LEU:H	1.84	0.41
1:A:387:GLN:HG2	1:A:391:ARG:NH1	2.35	0.41
1:A:394:VAL:HG11	1:A:399:THR:O	2.21	0.41
1:C:762:VAL:HG22	1:C:766:LYS:HD3	2.02	0.41
1:D:438:VAL:HG13	1:D:439:TYR:N	2.34	0.41
1:D:762:VAL:C	1:D:764:VAL:H	2.29	0.41
1:A:318:ASP:CG	1:A:320:ARG:H	2.29	0.41
1:A:458:LEU:HD12	1:A:458:LEU:HA	1.95	0.41
1:A:571:ILE:HG22	1:A:572:GLU:N	2.35	0.41
1:B:612:LYS:HB3	1:B:616:ARG:HH12	1.84	0.41
1:C:612:LYS:HB3	1:C:616:ARG:HH12	1.84	0.41
1:D:632:LEU:HD22	1:D:695:PHE:CE1	2.56	0.41
1:D:751:PHE:O	1:D:753:ARG:NH2	2.53	0.41
1:A:321:GLY:HA3	1:A:368:ASN:H	1.86	0.41
1:A:389:ILE:HD12	1:A:392:ARG:HE	1.86	0.41
1:A:760:GLU:OE1	1:A:764:VAL:HB	2.21	0.41
1:B:213:LEU:HD12	1:B:213:LEU:HA	1.92	0.41
1:B:218:GLU:C	1:B:221:GLY:H	2.29	0.41
1:B:321:GLY:HA3	1:B:368:ASN:N	2.36	0.41
1:B:328:LEU:HD11	1:B:342:VAL:HG23	2.02	0.41
1:B:367:ASN:ND2	1:B:369:ASP:H	2.18	0.41
1:B:632:LEU:HD22	1:B:695:PHE:CE1	2.56	0.41
1:C:394:VAL:HG11	1:C:399:THR:O	2.21	0.41
1:C:697:ILE:O	1:C:701:THR:HG22	2.20	0.41
1:D:321:GLY:HA3	1:D:368:ASN:H	1.86	0.41
1:A:381:GLY:HA3	1:A:443:ILE:HG21	2.03	0.41
1:A:474:ASN:HD22	1:A:474:ASN:HA	1.57	0.41
1:B:257:LEU:HD23	1:B:257:LEU:HA	1.86	0.41
1:B:381:GLY:HA3	1:B:443:ILE:HG21	2.03	0.41
1:C:193:THR:HG22	1:C:194:CYS:N	2.29	0.41
1:D:291:LEU:O	1:D:295:THR:OG1	2.22	0.41
1:D:321:GLY:HA3	1:D:368:ASN:N	2.36	0.41
1:D:394:VAL:HG11	1:D:399:THR:O	2.21	0.41
1:A:495:GLU:N	1:C:637:ASN:OD1	2.53	0.41
1:B:179:ARG:NH2	1:B:222:ASN:HD22	2.18	0.41
1:B:227:ILE:HD12	1:B:227:ILE:HG23	1.83	0.41
1:B:583:VAL:O	1:B:587:MET:HG3	2.21	0.41
1:B:661:ARG:NE	1:B:662:ASP:H	2.18	0.41
1:B:711:LEU:O	1:B:715:ILE:HG13	2.21	0.41
1:B:760:GLU:OE1	1:B:764:VAL:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:ARG:NH2	1:C:222:ASN:HD22	2.18	0.41
1:C:387:GLN:HG2	1:C:391:ARG:NH1	2.35	0.41
1:C:441:SER:O	1:C:446:ARG:NH1	2.53	0.41
1:D:173:LEU:HA	1:D:178:LYS:HB2	2.03	0.41
1:D:328:LEU:HD11	1:D:342:VAL:HG23	2.02	0.41
1:D:389:ILE:HD12	1:D:392:ARG:HE	1.86	0.41
1:D:760:GLU:OE1	1:D:764:VAL:HB	2.21	0.41
1:A:218:GLU:C	1:A:221:GLY:H	2.29	0.41
1:A:636:LEU:HD21	1:B:494:LEU:HD13	2.03	0.41
1:B:321:GLY:HA3	1:B:368:ASN:H	1.86	0.41
1:B:571:ILE:HG22	1:B:572:GLU:N	2.35	0.41
1:C:632:LEU:HD22	1:C:695:PHE:CE1	2.56	0.41
1:D:583:VAL:O	1:D:587:MET:HG3	2.21	0.41
1:D:711:LEU:O	1:D:715:ILE:HG13	2.21	0.41
1:A:176:HIS:HB3	1:A:178:LYS:HG2	2.03	0.40
1:A:179:ARG:NH2	1:A:222:ASN:HD22	2.18	0.40
1:A:211:PRO:HA	1:A:214:LEU:HD12	2.04	0.40
1:A:632:LEU:HD22	1:A:695:PHE:CE1	2.56	0.40
1:C:318:ASP:N	1:C:322:ASN:O	2.54	0.40
1:C:661:ARG:NE	1:C:662:ASP:H	2.18	0.40
1:D:762:VAL:HG22	1:D:766:LYS:HD3	2.02	0.40
1:A:367:ASN:ND2	1:A:369:ASP:H	2.18	0.40
1:B:628:TYR:CE2	1:B:632:LEU:HD21	2.57	0.40
1:C:318:ASP:CG	1:C:320:ARG:H	2.29	0.40
1:C:321:GLY:HA3	1:C:368:ASN:H	1.86	0.40
1:C:321:GLY:HA3	1:C:368:ASN:N	2.36	0.40
1:C:586:TRP:HH2	1:D:623:LEU:HD12	1.85	0.40
1:D:179:ARG:NH2	1:D:222:ASN:HD22	2.18	0.40
1:D:215:ASP:O	1:D:218:GLU:HG3	2.20	0.40
1:A:173:LEU:HA	1:A:178:LYS:HB2	2.03	0.40
1:A:785:TRP:NE1	1:C:338:ASN:OD1	2.55	0.40
1:B:211:PRO:HA	1:B:214:LEU:HD12	2.03	0.40
1:B:318:ASP:N	1:B:322:ASN:O	2.54	0.40
1:B:389:ILE:HD12	1:B:392:ARG:HE	1.86	0.40
1:B:762:VAL:HG22	1:B:766:LYS:HD3	2.02	0.40
1:C:389:ILE:HD12	1:C:392:ARG:HE	1.86	0.40
1:C:760:GLU:OE1	1:C:764:VAL:HB	2.21	0.40
1:C:762:VAL:C	1:C:764:VAL:H	2.29	0.40
1:D:176:HIS:HB3	1:D:178:LYS:HG2	2.03	0.40
1:D:257:LEU:HD23	1:D:257:LEU:HA	1.86	0.40
1:D:628:TYR:CE2	1:D:632:LEU:HD21	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:CYS:SG	1:A:693:VAL:N	2.93	0.40
1:A:762:VAL:C	1:A:764:VAL:H	2.29	0.40
1:B:514:GLU:O	1:B:518:LEU:HG	2.22	0.40
1:B:685:MET:HB2	1:D:674:PHE:CE2	2.57	0.40
1:C:514:GLU:O	1:C:518:LEU:HG	2.22	0.40
1:C:643:LYS:N	1:C:661:ARG:HH22	2.20	0.40
1:D:381:GLY:HA3	1:D:443:ILE:HG21	2.03	0.40
1:D:643:LYS:N	1:D:661:ARG:HH22	2.20	0.40
1:A:213:LEU:HD12	1:A:213:LEU:HA	1.92	0.40
1:A:421:LEU:HG	1:A:776:TRP:O	2.22	0.40
1:B:625:MET:HE2	1:B:625:MET:HB2	1.93	0.40
1:C:328:LEU:HD11	1:C:342:VAL:HG23	2.02	0.40
1:C:453:GLU:H	1:C:453:GLU:HG3	1.67	0.40
1:C:628:TYR:CE2	1:C:632:LEU:HD21	2.57	0.40
1:C:718:MET:O	1:C:722:VAL:HG13	2.22	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	606/935 (65%)	515 (85%)	89 (15%)	2 (0%)	36	71
1	B	606/935 (65%)	513 (85%)	92 (15%)	1 (0%)	43	77
1	C	606/935 (65%)	513 (85%)	92 (15%)	1 (0%)	43	77
1	D	606/935 (65%)	513 (85%)	92 (15%)	1 (0%)	43	77
All	All	2424/3740 (65%)	2054 (85%)	365 (15%)	5 (0%)	44	77

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	771	THR
1	B	771	THR
1	C	771	THR
1	D	771	THR
1	A	772	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	540/819 (66%)	529 (98%)	11 (2%)	48	66
1	B	540/819 (66%)	529 (98%)	11 (2%)	48	66
1	C	540/819 (66%)	529 (98%)	11 (2%)	48	66
1	D	540/819 (66%)	529 (98%)	11 (2%)	48	66
All	All	2160/3276 (66%)	2116 (98%)	44 (2%)	48	66

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

Mol	Chain	Res	Type
1	A	335	THR
1	A	414	VAL
1	A	474	ASN
1	A	483	VAL
1	A	605	MET
1	A	614	LEU
1	A	634	SER
1	A	645	CYS
1	A	683	LEU
1	A	687	SER
1	A	713	MET
1	B	335	THR
1	B	414	VAL
1	B	474	ASN
1	B	483	VAL
1	B	605	MET
1	B	614	LEU

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Mol	Chain	Res	Type
1	B	634	SER
1	B	645	CYS
1	B	683	LEU
1	B	687	SER
1	B	713	MET
1	C	335	THR
1	C	414	VAL
1	C	474	ASN
1	C	483	VAL
1	C	605	MET
1	C	614	LEU
1	C	634	SER
1	C	645	CYS
1	C	683	LEU
1	C	687	SER
1	C	713	MET
1	D	335	THR
1	D	414	VAL
1	D	474	ASN
1	D	483	VAL
1	D	605	MET
1	D	614	LEU
1	D	634	SER
1	D	645	CYS
1	D	683	LEU
1	D	687	SER
1	D	713	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	296	ASN
1	A	326	HIS
1	A	334	ASN
1	A	447	HIS
1	A	474	ASN
1	A	731	HIS
1	B	326	HIS
1	B	334	ASN
1	B	474	ASN
1	B	731	HIS
1	C	326	HIS

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Mol	Chain	Res	Type
1	C	334	ASN
1	C	447	HIS
1	C	474	ASN
1	C	731	HIS
1	D	326	HIS
1	D	334	ASN
1	D	447	HIS
1	D	474	ASN
1	D	731	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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

There are no chain breaks in this entry.

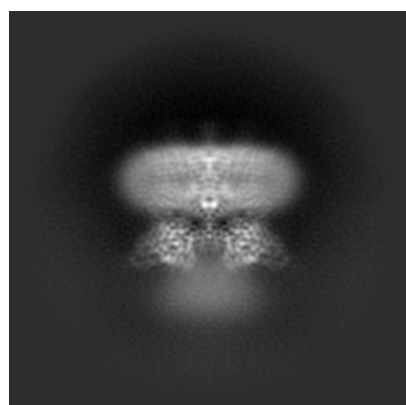
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11690. These allow visual inspection of the internal detail of the map and identification of artifacts.

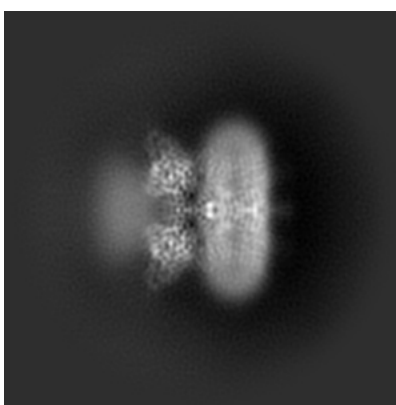
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

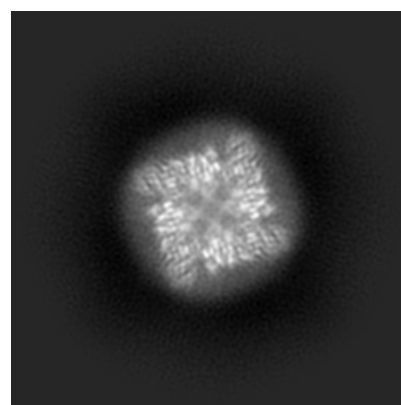
6.1.1 Primary map



X



Y

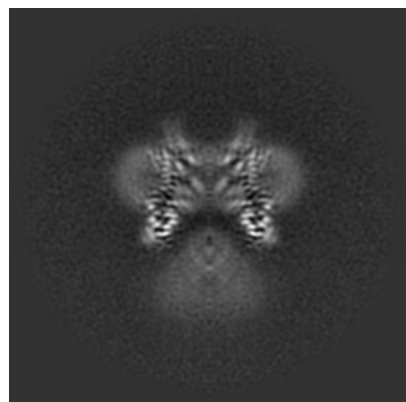


Z

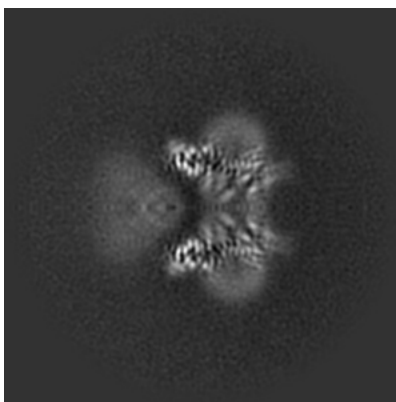
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

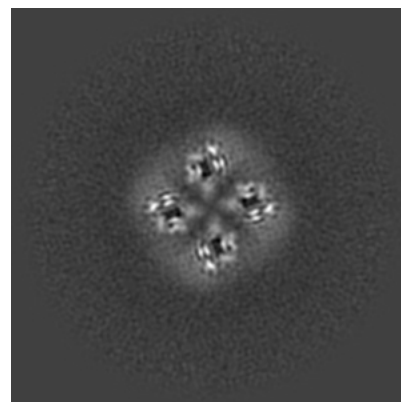
6.2.1 Primary map



X Index: 256



Y Index: 256

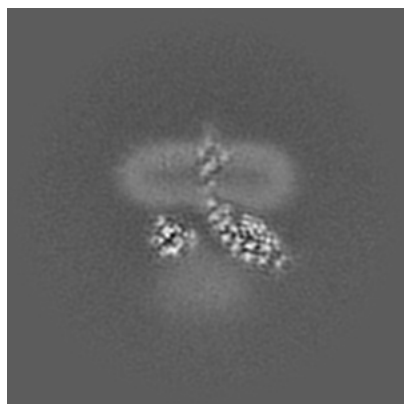


Z Index: 256

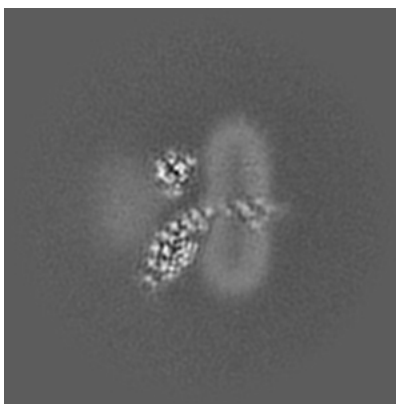
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

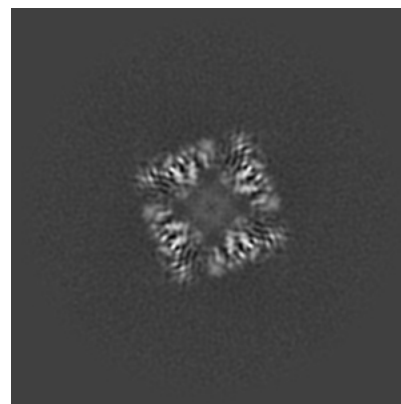
6.3.1 Primary map



X Index: 293



Y Index: 293

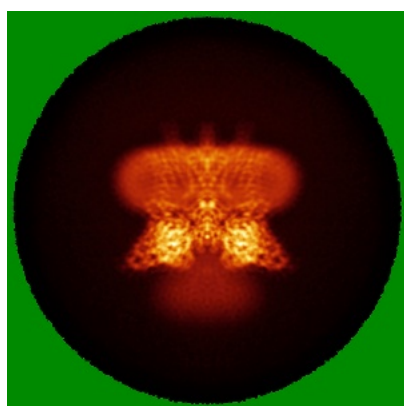


Z Index: 214

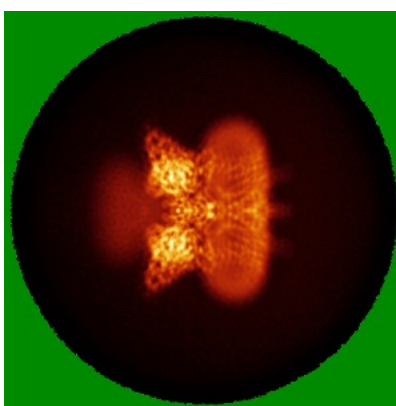
The images above show the largest variance slices of the map in three orthogonal directions.

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

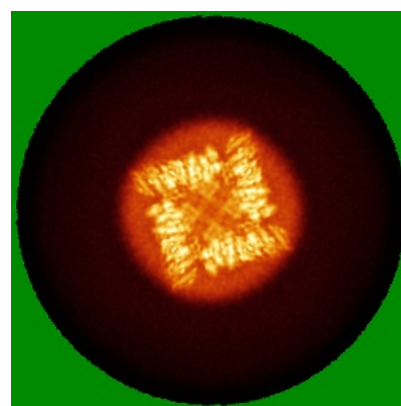
6.4.1 Primary map



X



Y

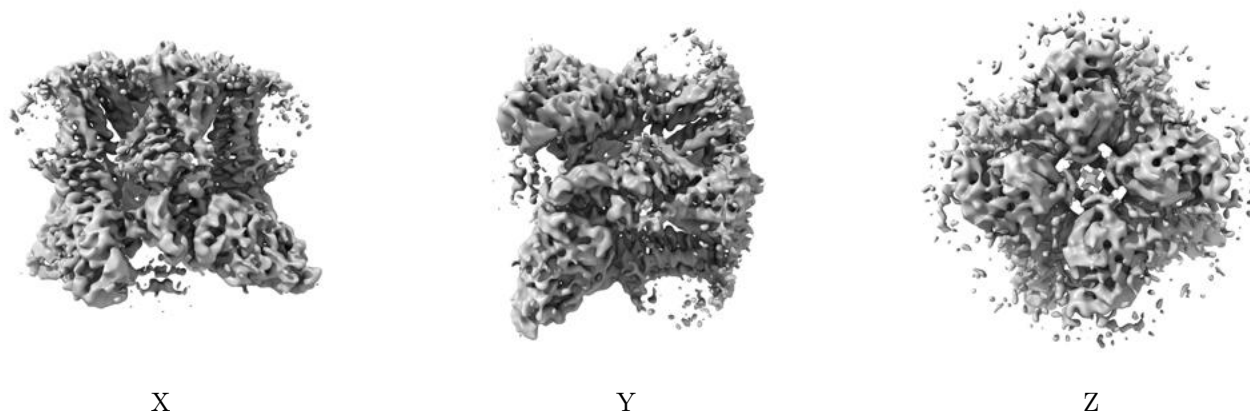


Z

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 0.148. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

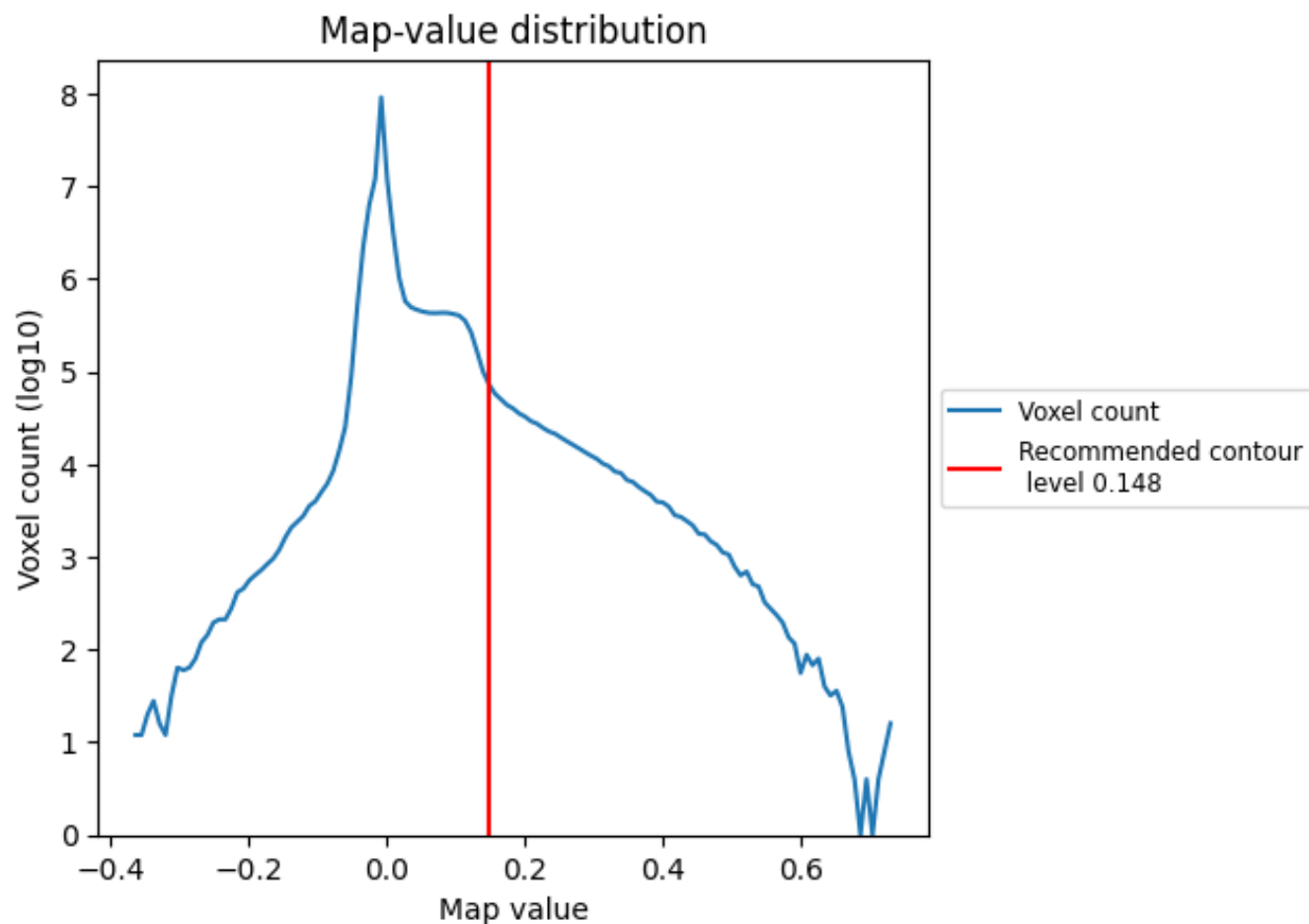
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

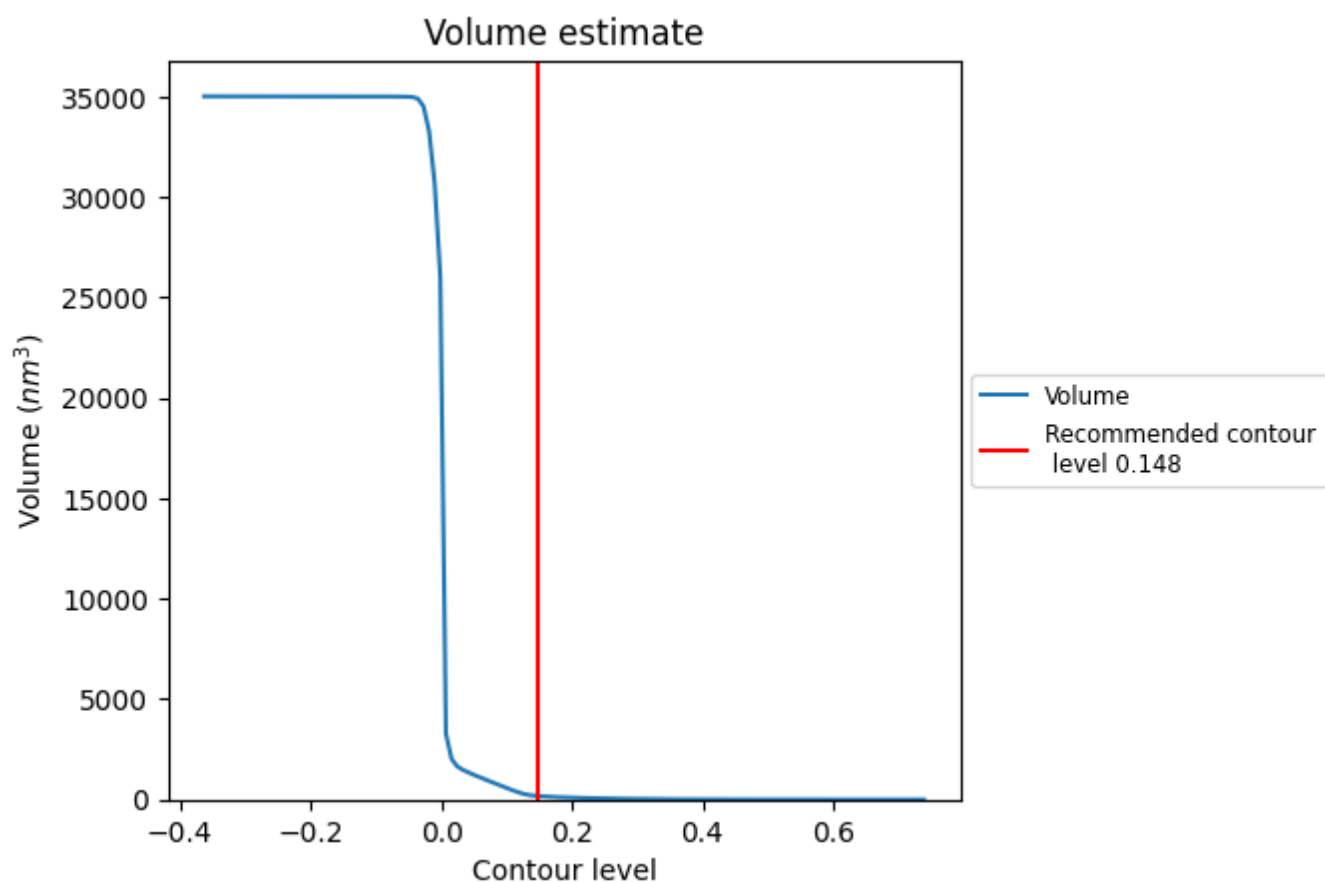
This section contains the results of statistical analysis of the map.

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.

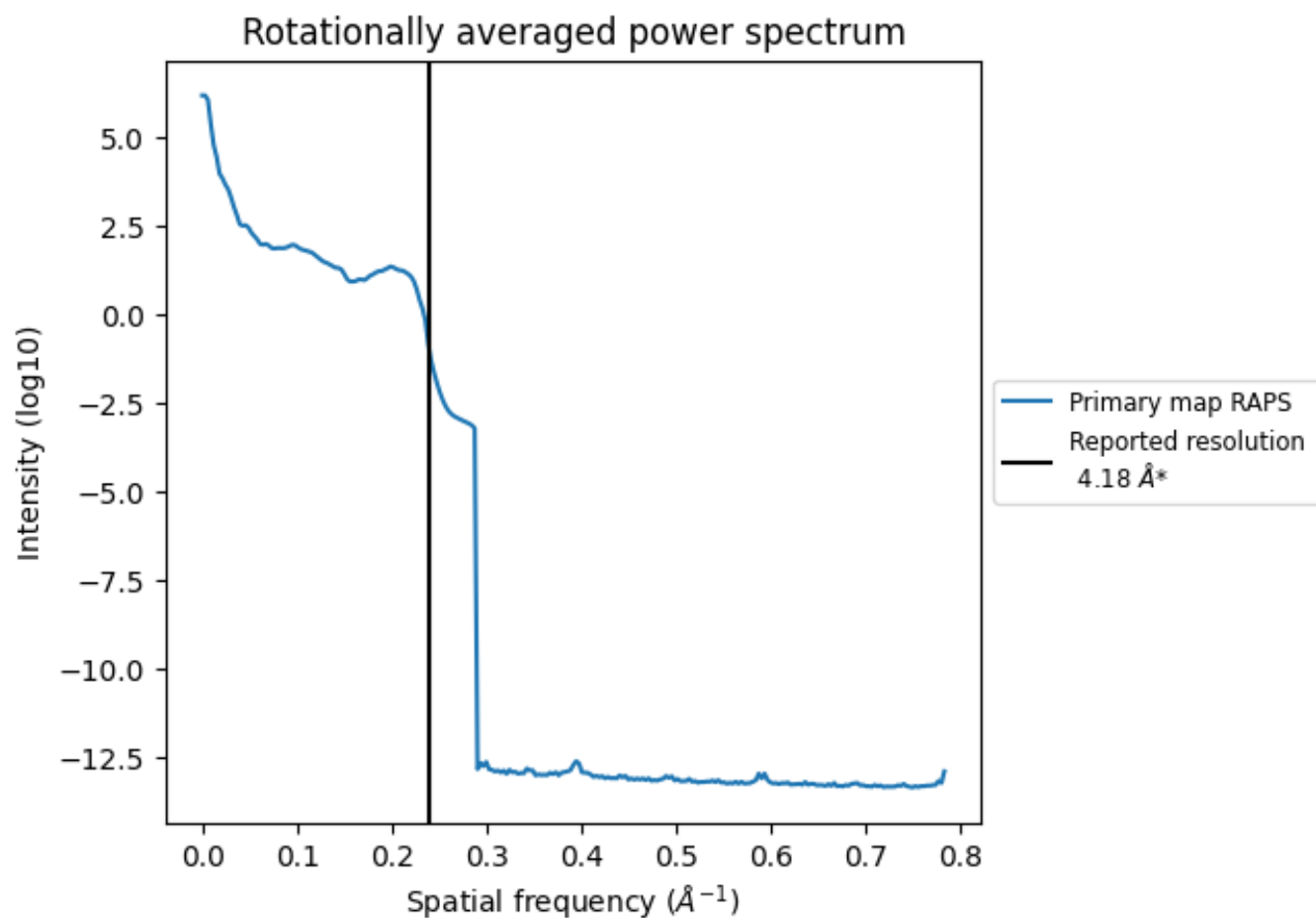
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 176 nm³; this corresponds to an approximate mass of 159 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 0.239 Å⁻¹

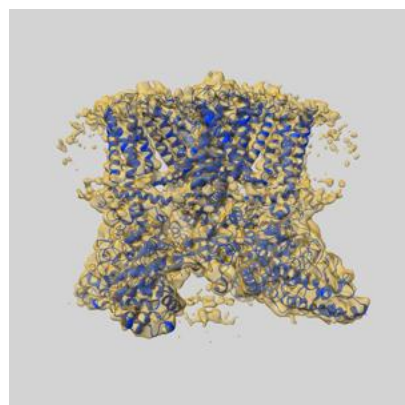
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

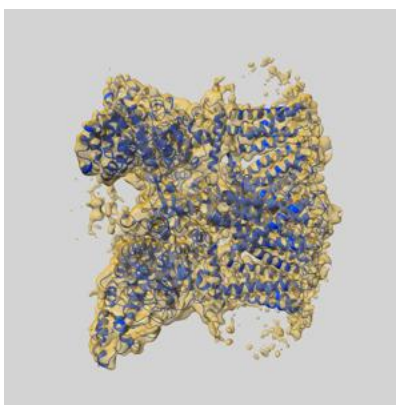
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11690 and PDB model 7AA5. Per-residue inclusion information can be found in section [3](#) on page [10](#).

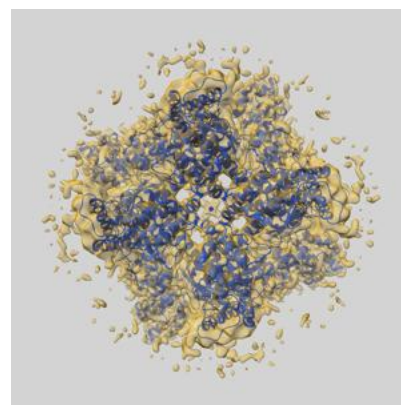
9.1 Map-model overlay [i](#)



X



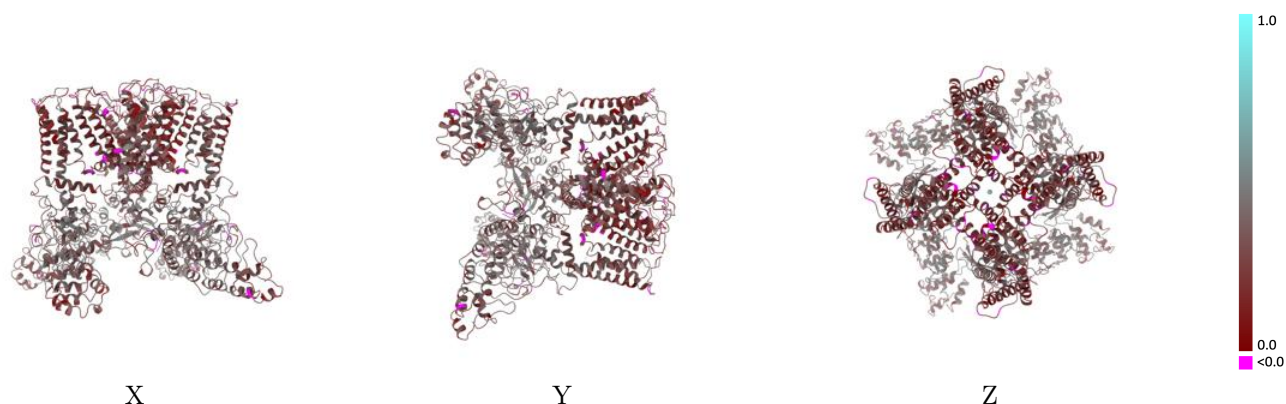
Y



Z

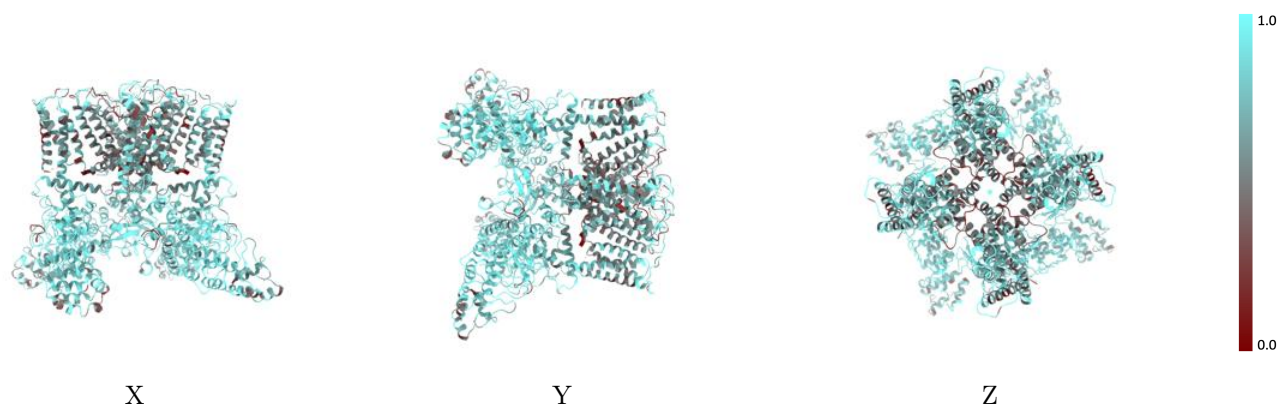
The images above show the 3D surface view of the map at the recommended contour level 0.148 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



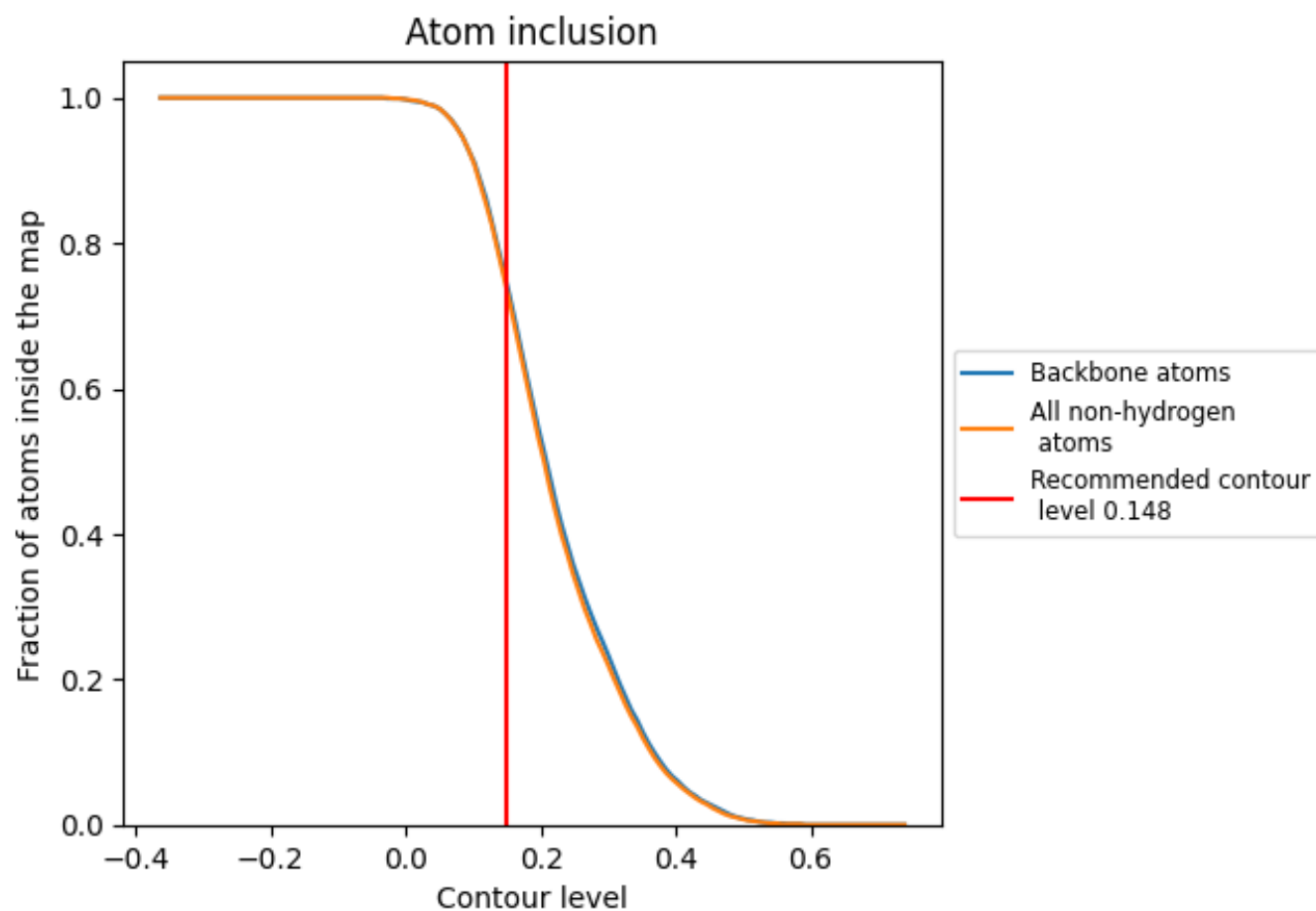
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.148).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 74% 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 (0.148) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7430	0.3250
A	0.7540	0.3270
B	0.7420	0.3220
C	0.7530	0.3270
D	0.7510	0.3260

