



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 01:19 PM UTC

PDB ID : 7VQO / pdb_00007vqo
EMDB ID : EMD-32091
Title : Cryo-EM structure of Ams1 bound to the FW domain of Nbr1
Authors : Zhang, J.; Ye, K.
Deposited on : 2021-10-20
Resolution : 2.19 Å(reported)
Based on initial model : 6LZ1

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

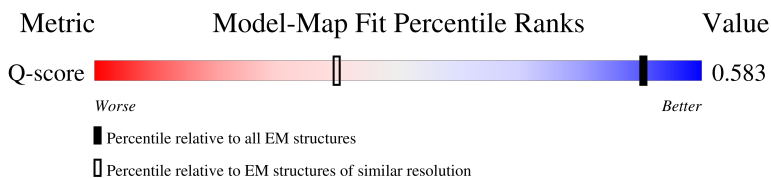
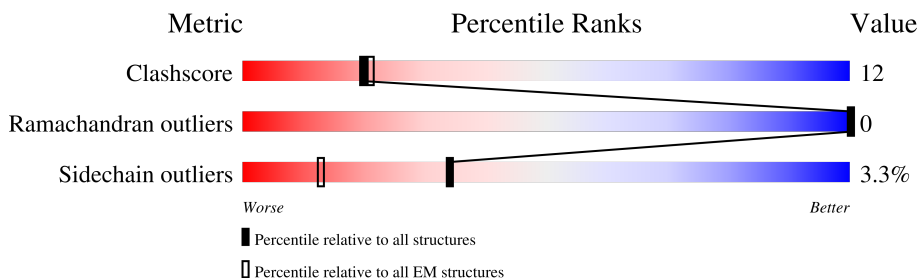
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.19 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	2745 (1.70 - 2.69)

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	1616	53% 19% • 27%
1	B	1616	53% 19% • 27%
1	C	1616	53% 19% • 27%
1	D	1616	53% 19% • 27%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 38640 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 Ams1, Nbr1 and malE fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1180	Total	C	N	O	S	0	0
			9487	6039	1666	1743	39		
1	B	1180	Total	C	N	O	S	0	0
			9487	6039	1666	1743	39		
1	C	1180	Total	C	N	O	S	0	0
			9487	6039	1666	1743	39		
1	D	1180	Total	C	N	O	S	0	0
			9487	6039	1666	1743	39		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1080	GLY	-	linker	UNP G0SGP6
A	1081	GLY	-	linker	UNP G0SGP6
A	1082	GLY	-	linker	UNP G0SGP6
A	1083	GLY	-	linker	UNP G0SGP6
A	1084	SER	-	linker	UNP G0SGP6
A	1085	GLY	-	linker	UNP G0SGP6
A	1086	GLY	-	linker	UNP G0SGP6
A	1087	GLY	-	linker	UNP G0SGP6
A	1088	PHE	-	linker	UNP G0SGP6
A	1089	LYS	-	linker	UNP G0SGP6
A	1090	LYS	-	linker	UNP G0SGP6
A	1091	ALA	-	linker	UNP G0SGP6
A	1092	SER	-	linker	UNP G0SGP6
A	1093	SER	-	linker	UNP G0SGP6
A	1094	SER	-	linker	UNP G0SGP6
A	1095	ASP	-	linker	UNP G0SGP6
A	1096	ASN	-	linker	UNP G0SGP6
A	1097	LYS	-	linker	UNP G0SGP6
A	1098	GLU	-	linker	UNP G0SGP6
A	1099	GLN	-	linker	UNP G0SGP6
A	1100	GLY	-	linker	UNP G0SGP6
A	1101	GLY	-	linker	UNP G0SGP6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1102	GLY	-	linker	UNP G0SGP6
A	1103	GLY	-	linker	UNP G0SGP6
A	1104	SER	-	linker	UNP G0SGP6
A	1105	GLY	-	linker	UNP G0SGP6
A	1106	GLY	-	linker	UNP G0SGP6
A	1107	GLY	-	linker	UNP G0SGP6
A	1108	SER	-	linker	UNP G0SGP6
A	1109	GLY	-	linker	UNP G0SGP6
B	1080	GLY	-	linker	UNP G0SGP6
B	1081	GLY	-	linker	UNP G0SGP6
B	1082	GLY	-	linker	UNP G0SGP6
B	1083	GLY	-	linker	UNP G0SGP6
B	1084	SER	-	linker	UNP G0SGP6
B	1085	GLY	-	linker	UNP G0SGP6
B	1086	GLY	-	linker	UNP G0SGP6
B	1087	GLY	-	linker	UNP G0SGP6
B	1088	PHE	-	linker	UNP G0SGP6
B	1089	LYS	-	linker	UNP G0SGP6
B	1090	LYS	-	linker	UNP G0SGP6
B	1091	ALA	-	linker	UNP G0SGP6
B	1092	SER	-	linker	UNP G0SGP6
B	1093	SER	-	linker	UNP G0SGP6
B	1094	SER	-	linker	UNP G0SGP6
B	1095	ASP	-	linker	UNP G0SGP6
B	1096	ASN	-	linker	UNP G0SGP6
B	1097	LYS	-	linker	UNP G0SGP6
B	1098	GLU	-	linker	UNP G0SGP6
B	1099	GLN	-	linker	UNP G0SGP6
B	1100	GLY	-	linker	UNP G0SGP6
B	1101	GLY	-	linker	UNP G0SGP6
B	1102	GLY	-	linker	UNP G0SGP6
B	1103	GLY	-	linker	UNP G0SGP6
B	1104	SER	-	linker	UNP G0SGP6
B	1105	GLY	-	linker	UNP G0SGP6
B	1106	GLY	-	linker	UNP G0SGP6
B	1107	GLY	-	linker	UNP G0SGP6
B	1108	SER	-	linker	UNP G0SGP6
B	1109	GLY	-	linker	UNP G0SGP6
C	1080	GLY	-	linker	UNP G0SGP6
C	1081	GLY	-	linker	UNP G0SGP6
C	1082	GLY	-	linker	UNP G0SGP6
C	1083	GLY	-	linker	UNP G0SGP6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1084	SER	-	linker	UNP G0SGP6
C	1085	GLY	-	linker	UNP G0SGP6
C	1086	GLY	-	linker	UNP G0SGP6
C	1087	GLY	-	linker	UNP G0SGP6
C	1088	PHE	-	linker	UNP G0SGP6
C	1089	LYS	-	linker	UNP G0SGP6
C	1090	LYS	-	linker	UNP G0SGP6
C	1091	ALA	-	linker	UNP G0SGP6
C	1092	SER	-	linker	UNP G0SGP6
C	1093	SER	-	linker	UNP G0SGP6
C	1094	SER	-	linker	UNP G0SGP6
C	1095	ASP	-	linker	UNP G0SGP6
C	1096	ASN	-	linker	UNP G0SGP6
C	1097	LYS	-	linker	UNP G0SGP6
C	1098	GLU	-	linker	UNP G0SGP6
C	1099	GLN	-	linker	UNP G0SGP6
C	1100	GLY	-	linker	UNP G0SGP6
C	1101	GLY	-	linker	UNP G0SGP6
C	1102	GLY	-	linker	UNP G0SGP6
C	1103	GLY	-	linker	UNP G0SGP6
C	1104	SER	-	linker	UNP G0SGP6
C	1105	GLY	-	linker	UNP G0SGP6
C	1106	GLY	-	linker	UNP G0SGP6
C	1107	GLY	-	linker	UNP G0SGP6
C	1108	SER	-	linker	UNP G0SGP6
C	1109	GLY	-	linker	UNP G0SGP6
D	1080	GLY	-	linker	UNP G0SGP6
D	1081	GLY	-	linker	UNP G0SGP6
D	1082	GLY	-	linker	UNP G0SGP6
D	1083	GLY	-	linker	UNP G0SGP6
D	1084	SER	-	linker	UNP G0SGP6
D	1085	GLY	-	linker	UNP G0SGP6
D	1086	GLY	-	linker	UNP G0SGP6
D	1087	GLY	-	linker	UNP G0SGP6
D	1088	PHE	-	linker	UNP G0SGP6
D	1089	LYS	-	linker	UNP G0SGP6
D	1090	LYS	-	linker	UNP G0SGP6
D	1091	ALA	-	linker	UNP G0SGP6
D	1092	SER	-	linker	UNP G0SGP6
D	1093	SER	-	linker	UNP G0SGP6
D	1094	SER	-	linker	UNP G0SGP6
D	1095	ASP	-	linker	UNP G0SGP6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1096	ASN	-	linker	UNP G0SGP6
D	1097	LYS	-	linker	UNP G0SGP6
D	1098	GLU	-	linker	UNP G0SGP6
D	1099	GLN	-	linker	UNP G0SGP6
D	1100	GLY	-	linker	UNP G0SGP6
D	1101	GLY	-	linker	UNP G0SGP6
D	1102	GLY	-	linker	UNP G0SGP6
D	1103	GLY	-	linker	UNP G0SGP6
D	1104	SER	-	linker	UNP G0SGP6
D	1105	GLY	-	linker	UNP G0SGP6
D	1106	GLY	-	linker	UNP G0SGP6
D	1107	GLY	-	linker	UNP G0SGP6
D	1108	SER	-	linker	UNP G0SGP6
D	1109	GLY	-	linker	UNP G0SGP6

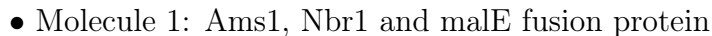
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total 1	Zn 1	0
2	B	1	Total 1	Zn 1	0
2	C	1	Total 1	Zn 1	0
2	D	1	Total 1	Zn 1	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		AltConf
3	A	167	Total 167	O 167	0
3	B	174	Total 174	O 174	0
3	C	173	Total 173	O 173	0
3	D	174	Total 174	O 174	0



[illegible]

TRP	LEU	GLY	LEU	ASN	GLY	PRO	P1228	G1234	G1160	SER	Q944	G819	L710	E599
TYR	GLU	THR	ASP	GLY	ASP	ASP	K1229	C1161	C1161	GLY	L947	A820	V713	E800
ALA	ASN	ALA	LYS	LYS	LYS	LYS	G1230	S1162	V1163	GLY	R953	E821	N722	M604
ARG	LEU	MET	LEU	ILE	GLU	GLU	G1235	K1164	F1165	PHE	R963	E822	S723	L609
THR	LEU	ILE	GLU	TYR	LYS	LYS	H1236	F1165	F1166	LYS	T962	E824	T724	L609
ALA	THR	ASN	PHE	PRO	LYS	LYS	R1237	V1166	G1167	ALA	R963	L725	Q724	H614
VAL	ASP	TYR	GLN	ILE	PRO	GLN	L1238	G1167	G1167	SER	Y965	L726	R726	L725
ALA	GLY	PRO	VAL	ALA	VAL	VAL	C1239	M1171	M1171	SER	Y965	L727	V727	L617
GLU	ALA	ALA	VAL	GLU	ALA	ALA	D1240	R1172	R1172	ASP	V974	H728	H728	L617
VAL	ALA	ALA	ALA	GLU	ALA	ALA	V1241	R1173	R1173	ASN	T839	V729	V729	S620
SER	VAL	SER	THR	LEU	THR	THR	V1242	A1174	A1174	LYS	T839	E730	E730	M624
ASN	ASN	ASN	GLY	LEU	GLY	GLY	E1244	ASP	ASP	GLN	K844	K731	K731	M624
ASN	GLY	GLY	GLY	LEU	GLY	GLY	K1245	SER	SER	GLU	V845	G732	G732	S629
THR	THR	THR	ASP	ILE	ILE	ILE	PRO	ALA	ALA	GLY	E846	S736	S736	S629
ASP	PRO	ASP	PRO	TYR	PRO	PRO	LYS	HIS	HIS	GLY	E847	L737	L737	V647
GLU	LEU	LYS	ILE	ASN	ILE	ILE	SER	PRO	PRO	GLY	F847	A742	A742	L653
ALA	GLY	VAL	ILE	LYS	ILE	ILE	ARG	ALA	ALA	GLY	P848	N743	N743	E654
LEU	ALA	ASN	ILE	LEU	LEU	LEU	SER	ALA	ALA	GLY	V849	E744	E744	E654
LYS	ALA	TYR	TRP	LEU	TRP	TRP	LYS	SER	SER	GLY	D850	E745	E745	L657
ASP	ALA	GLY	ILE	PRO	ILE	ILE	ILE	GLY	GLY	GLY	N853	I747	I747	L657
GLN	LEU	VAL	HIS	ASN	HIS	HIS	GLU	VAL	VAL	GLY	E1002	T854	T854	M660
THR	VAL	THR	ASP	PRO	ASP	ASP	GLU	VAL	VAL	GLY	D1003	E855	E855	S661
LEU	VAL	LEU	ARG	PRO	PHE	PHE	GLY	GLY	GLY	GLY	V1004	E859	E859	T662
GLU	PRO	PRO	GLY	PRO	GLY	GLY	LEU	SER	SER	GLY	S1005	I747	I747	T663
GLY	GLY	THR	GLY	THR	GLY	GLY	VAL	CYS	CYS	VAL	R1006	I864	I864	M664
THR	GLY	THR	ILE	GLU	TYR	TYR	THR	GLY	GLY	VAL	Q1015	R867	R867	T665
LEU	GLY	GLY	ALA	GLU	ALA	ALA	ILE	SER	SER	GLY	S1016	V882	V882	L668
ALA	ILE	GLY	GLN	ILE	ILE	ILE	ILE	VAL	VAL	GLY	R1020	D760	D760	M669
LYS	THR	THR	ASN	ASN	ASN	ASN	GLY	CYS	CYS	PRO	R1030	K762	K762	T670
PRO	PRO	PRO	GLY	GLY	GLY	GLY	ASP	ASP	ASP	SER	G1031	H885	H885	T670
ARG	LEU	LEU	LEU	LEU	LEU	LEU	LYS	ARG	ARG	ALA	V1034	R886	R886	M673
ILE	ASP	ASP	LEU	ASP	LEU	LEU	GLY	A1197	A1197	GLU	T1035	W887	W887	E677
ALA	ASP	PHE	ALA	GLY	ALA	ALA	TYR	V1198	V1198	GLU	V1046	L890	L890	K680
ALA	PHE	GLY	GLY	ASN	GLY	GLY	TRP	Q1199	Q1199	GLY	L1047	S891	S891	I681
VAL	ILE	ILE	ILE	ASN	GLY	GLY	ILE	P1200	P1200	GLY	E1049	E892	E892	S882
THR	GLY	GLY	THR	GLY	THR	THR	ALA	G1201	G1201	LYS	D1050	M914	M914	E883
VAL	VAL	VAL	VAL	LYS	VAL	VAL	LEU	E1202	E1202	LEU	D1051	R915	R915	K684
LEU	LEU	LEU	LEU	LYS	LEU	LEU	ALA	T1207	T1207	ALA	E1058	L918	L918	E885
ASN	ASN	ASN	ASN	GLY	LYS	LYS	GLY	L1210	L1210	GLY	L1048	L919	L919	T692
ALA	ALA	ALA	ALA	MET	LYS	LYS	VAL	R1211	R1211	GLY	L1048	R920	R920	K697
GLY	ILE	ILE	ILE	THR	LYS	LYS	GLY	T1212	T1212	LYS	D1051	K923	K923	K700
ALA	ALA	ALA	ALA	MET	GLY	GLY	ALA	P1213	P1213	PHE	E1058	V805	V805	L701
ALA	ALA	ALA	ALA	ALA	LYS	LYS	LEU	A1216	A1216	LYS	R1061	S806	S806	E702
SER	SER	SER	SER	PHE	LYS	LYS	GLY	C1217	C1217	ASP	E1065	D807	D807	T703
PRO	PRO	PRO	PRO	TYR	ASP	ASP	ASP	R1218	R1218	THR	E1065	K808	K808	T704
ASN	ASN	ASN	ASN	LEU	THR	THR	THR	V1219	V1219	GLY	E1065	I811	I811	K705
ILE	ILE	ILE	ILE	GLN	PHE	PHE	PHE	T1220	T1220	ILE	R1075	L817	L817	P706
LYS	LYS	LYS	LYS	GLU	THR	THR	THR	S1221	S1221	LYS	T1079	M931	M931	L707
PRO	PRO	PRO	PRO	PRO	ASP	ASP	VAL	H1222	H1222	VAL	GLY	H935	H935	P706
GLN	GLU	GLU	GLU	TYR	ALA	ALA	THR	W1223	W1223	GLY	GLY	I936	I936	P706
MET	LEU	LEU	LEU	PHE	VAL	VAL	GLY	R1224	R1224	GLY	GLY	L817	L817	L707
ALA	ALA	ALA	ALA	THR	ARG	ARG	GLU	G1153	G1153	GLY	GLY	M918	M918	L707
PHE	PHE	PHE	TYR	PRO	TYR	TYR	HIS	T1227	T1227	GLY	GLY			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	692409	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)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	70.628	Depositor
Minimum map value	-38.771	Depositor
Average map value	0.052	Depositor
Map value standard deviation	2.444	Depositor
Recommended contour level	10	Depositor
Map size ($\text{\AA}$)	332.8, 332.8, 332.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.04, 1.04, 1.04	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: ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.37	0/9750	0.44	1/13244 (0.0%)
1	B	0.37	0/9750	0.44	1/13244 (0.0%)
1	C	0.37	0/9750	0.44	1/13244 (0.0%)
1	D	0.37	0/9750	0.44	1/13244 (0.0%)
All	All	0.37	0/39000	0.44	4/52976 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1004	VAL	N-CA-C	-7.56	105.94	113.20
1	C	1004	VAL	N-CA-C	-7.54	105.96	113.20
1	B	1004	VAL	N-CA-C	-7.53	105.97	113.20
1	A	1004	VAL	N-CA-C	-7.52	105.98	113.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	9487	0	9246	237	0
1	B	9487	0	9246	239	0
1	C	9487	0	9246	235	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	9487	0	9246	236	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	167	0	0	18	0
3	B	174	0	0	20	0
3	C	173	0	0	19	0
3	D	174	0	0	21	0
All	All	38640	0	36984	931	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 12.

All (931) 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:B:1161:CYS:H	1:B:1228:PRO:HD3	1.44	0.83
1:A:1161:CYS:H	1:A:1228:PRO:HD3	1.44	0.83
1:D:1161:CYS:H	1:D:1228:PRO:HD3	1.44	0.83
1:C:1161:CYS:H	1:C:1228:PRO:HD3	1.44	0.82
1:B:742:ALA:HB2	1:B:944:GLN:HE21	1.44	0.82
1:A:742:ALA:HB2	1:A:944:GLN:HE21	1.44	0.82
1:C:754:ASN:O	1:C:754:ASN:ND2	2.13	0.82
1:D:754:ASN:O	1:D:754:ASN:ND2	2.13	0.82
1:C:329:CYS:HG	1:C:335:TYR:HH	1.27	0.82
1:C:742:ALA:HB2	1:C:944:GLN:HE21	1.44	0.82
1:D:742:ALA:HB2	1:D:944:GLN:HE21	1.44	0.81
1:D:986:SER:HB2	1:D:1031:GLY:HA2	1.64	0.80
1:C:986:SER:HB2	1:C:1031:GLY:HA2	1.64	0.80
1:A:754:ASN:O	1:A:754:ASN:ND2	2.13	0.80
1:B:754:ASN:ND2	1:B:754:ASN:O	2.13	0.80
1:A:986:SER:HB2	1:A:1031:GLY:HA2	1.64	0.79
1:B:986:SER:HB2	1:B:1031:GLY:HA2	1.64	0.79
1:D:677:GLU:OE1	1:D:962:THR:CG2	2.30	0.79
1:D:329:CYS:HG	1:D:335:TYR:HH	1.30	0.78
1:A:703:THR:HG22	1:A:704:THR:H	1.50	0.76
1:B:703:THR:HG22	1:B:704:THR:H	1.50	0.76
1:D:703:THR:HG22	1:D:704:THR:H	1.50	0.75
1:C:703:THR:HG22	1:C:704:THR:H	1.50	0.75
1:C:761:ASP:OD2	1:C:920:ARG:NH1	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:761:ASP:OD2	1:D:920:ARG:NH1	2.21	0.74
1:B:761:ASP:OD2	1:B:920:ARG:NH1	2.21	0.74
1:A:761:ASP:OD2	1:A:920:ARG:NH1	2.21	0.73
1:C:380:ARG:NH2	1:C:581:GLU:OE2	2.21	0.73
1:D:380:ARG:NH2	1:D:581:GLU:OE2	2.21	0.73
1:A:380:ARG:NH2	1:A:581:GLU:OE2	2.21	0.72
1:B:380:ARG:NH2	1:B:581:GLU:OE2	2.21	0.72
1:B:416:CYS:SG	3:B:1961:HOH:O	2.48	0.72
1:B:728:HIS:HB2	1:B:736:SER:HB3	1.72	0.71
1:A:728:HIS:HB2	1:A:736:SER:HB3	1.72	0.71
1:A:416:CYS:SG	3:A:1954:HOH:O	2.48	0.71
1:D:728:HIS:HB2	1:D:736:SER:HB3	1.72	0.71
1:C:728:HIS:HB2	1:C:736:SER:HB3	1.72	0.71
1:D:416:CYS:SG	3:D:1960:HOH:O	2.48	0.70
1:A:436:ARG:HH21	1:A:436:ARG:HG3	1.56	0.70
1:B:436:ARG:HG3	1:B:436:ARG:HH21	1.56	0.70
1:B:125:HIS:ND1	3:B:1808:HOH:O	2.24	0.70
1:C:125:HIS:ND1	3:C:1809:HOH:O	2.25	0.70
1:C:416:CYS:SG	3:C:1959:HOH:O	2.49	0.70
1:D:436:ARG:HH21	1:D:436:ARG:HG3	1.56	0.70
1:D:125:HIS:ND1	3:D:1809:HOH:O	2.25	0.70
1:C:436:ARG:HH21	1:C:436:ARG:HG3	1.56	0.69
1:A:1199:GLN:N	1:A:1202:GLU:OE2	2.25	0.69
1:B:1199:GLN:N	1:B:1202:GLU:OE2	2.25	0.69
1:B:329:CYS:SG	1:B:335:TYR:OH	2.50	0.69
1:C:1127:VAL:HB	1:C:1148:VAL:HG23	1.75	0.69
1:D:1127:VAL:HB	1:D:1148:VAL:HG23	1.75	0.69
1:A:329:CYS:SG	1:A:335:TYR:OH	2.50	0.69
1:C:980:VAL:HG22	1:C:1035:THR:HG22	1.76	0.68
1:D:980:VAL:HG22	1:D:1035:THR:HG22	1.76	0.68
1:C:1199:GLN:N	1:C:1202:GLU:OE2	2.25	0.68
1:D:1199:GLN:N	1:D:1202:GLU:OE2	2.26	0.68
1:B:1218:ARG:NE	3:B:1815:HOH:O	2.27	0.68
1:A:1127:VAL:HB	1:A:1148:VAL:HG23	1.75	0.68
1:B:1127:VAL:HB	1:B:1148:VAL:HG23	1.75	0.68
1:D:1218:ARG:NE	3:D:1814:HOH:O	2.27	0.68
1:A:1218:ARG:NE	3:A:1812:HOH:O	2.27	0.67
1:C:53:MET:SD	3:C:1861:HOH:O	2.52	0.67
1:A:53:MET:SD	3:A:1856:HOH:O	2.52	0.67
1:C:578:ARG:NH1	1:C:670:THR:O	2.28	0.67
1:D:578:ARG:NH1	1:D:670:THR:O	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:ARG:NH1	1:A:670:THR:O	2.28	0.67
1:A:980:VAL:HG22	1:A:1035:THR:HG22	1.76	0.67
1:B:980:VAL:HG22	1:B:1035:THR:HG22	1.76	0.67
1:B:53:MET:SD	3:B:1859:HOH:O	2.53	0.66
1:B:578:ARG:NH1	1:B:670:THR:O	2.28	0.66
1:A:110:LEU:O	1:A:165:GLU:HA	1.96	0.66
1:B:110:LEU:O	1:B:165:GLU:HA	1.96	0.66
1:B:1197:ALA:N	3:B:1817:HOH:O	2.29	0.66
1:D:1130:THR:HG1	1:D:1146:THR:HG1	1.44	0.66
1:B:707:LEU:HD23	1:B:819:GLY:HA2	1.77	0.65
1:A:707:LEU:HD23	1:A:819:GLY:HA2	1.77	0.65
1:A:1197:ALA:N	3:A:1816:HOH:O	2.29	0.65
1:C:1197:ALA:N	3:C:1819:HOH:O	2.29	0.65
1:D:707:LEU:HD23	1:D:819:GLY:HA2	1.77	0.65
1:C:707:LEU:HD23	1:C:819:GLY:HA2	1.77	0.65
1:D:1197:ALA:N	3:D:1817:HOH:O	2.29	0.65
1:A:9:LYS:N	1:A:9:LYS:HE2	2.12	0.65
1:B:9:LYS:HE2	1:B:9:LYS:N	2.12	0.65
1:C:707:LEU:HD11	1:C:817:LEU:HB3	1.78	0.65
1:B:705:LYS:N	1:B:705:LYS:HE2	2.12	0.65
1:A:705:LYS:HE2	1:A:705:LYS:N	2.12	0.64
1:D:707:LEU:HD11	1:D:817:LEU:HB3	1.78	0.64
1:A:583:LEU:HD11	1:A:668:LEU:HD21	1.79	0.64
1:A:707:LEU:HD11	1:A:817:LEU:HB3	1.78	0.64
1:C:705:LYS:N	1:C:705:LYS:HE2	2.12	0.64
1:D:110:LEU:O	1:D:165:GLU:HA	1.96	0.64
1:D:705:LYS:HE2	1:D:705:LYS:N	2.12	0.64
1:B:707:LEU:HD11	1:B:817:LEU:HB3	1.78	0.64
1:B:583:LEU:HD11	1:B:668:LEU:HD21	1.79	0.64
1:C:110:LEU:O	1:C:165:GLU:HA	1.96	0.64
1:C:9:LYS:N	1:C:9:LYS:HE2	2.12	0.64
1:C:700:LYS:O	1:C:700:LYS:NZ	2.31	0.64
1:D:9:LYS:HE2	1:D:9:LYS:N	2.12	0.64
1:D:700:LYS:O	1:D:700:LYS:NZ	2.31	0.64
1:C:583:LEU:HD11	1:C:668:LEU:HD21	1.79	0.63
1:D:68:TRP:HB3	1:D:88:PHE:HB3	1.79	0.63
1:C:68:TRP:HB3	1:C:88:PHE:HB3	1.80	0.63
1:D:583:LEU:HD11	1:D:668:LEU:HD21	1.79	0.63
1:A:68:TRP:HB3	1:A:88:PHE:HB3	1.79	0.63
1:B:68:TRP:HB3	1:B:88:PHE:HB3	1.80	0.63
1:B:175:ASN:HA	1:B:180:ASN:HD21	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:677:GLU:OE1	1:D:962:THR:HG23	1.96	0.63
1:A:175:ASN:HA	1:A:180:ASN:HD21	1.63	0.62
1:A:2:GLY:N	3:A:1819:HOH:O	2.32	0.62
1:B:329:CYS:HG	1:B:335:TYR:HH	1.41	0.62
1:A:550:GLU:OE1	1:A:867:ARG:NH2	2.28	0.62
1:B:550:GLU:OE1	1:B:867:ARG:NH2	2.28	0.62
1:B:1122:LEU:N	3:B:1821:HOH:O	2.32	0.62
1:C:677:GLU:OE1	1:C:962:THR:HG23	2.00	0.62
1:A:1122:LEU:N	3:A:1822:HOH:O	2.33	0.62
1:A:743:ASN:O	1:B:1030:ARG:NH2	2.31	0.61
1:A:700:LYS:O	1:A:700:LYS:NZ	2.31	0.61
1:D:1122:LEU:N	3:D:1824:HOH:O	2.33	0.61
1:B:700:LYS:O	1:B:700:LYS:NZ	2.31	0.61
1:C:175:ASN:ND2	3:C:1824:HOH:O	2.33	0.61
1:A:1030:ARG:NH2	1:B:743:ASN:O	2.32	0.61
1:B:216:ASP:OD1	1:B:510:ARG:NE	2.28	0.61
1:B:484:ASP:OD1	1:B:536:ARG:NH2	2.34	0.61
1:C:216:ASP:OD1	1:C:510:ARG:NE	2.28	0.61
1:D:216:ASP:OD1	1:D:510:ARG:NE	2.28	0.61
1:D:371:ASN:O	1:D:885:HIS:NE2	2.32	0.61
1:A:216:ASP:OD1	1:A:510:ARG:NE	2.28	0.60
1:A:484:ASP:OD1	1:A:536:ARG:NH2	2.34	0.60
1:C:484:ASP:OD1	1:C:536:ARG:NH2	2.34	0.60
1:D:484:ASP:OD1	1:D:536:ARG:NH2	2.34	0.60
1:B:371:ASN:O	1:B:885:HIS:NE2	2.32	0.60
1:C:371:ASN:O	1:C:885:HIS:NE2	2.32	0.60
1:A:371:ASN:O	1:A:885:HIS:NE2	2.32	0.60
1:C:165:GLU:O	1:C:165:GLU:HG3	2.01	0.60
1:A:244:ILE:HD11	1:A:263:ALA:HB2	1.84	0.60
1:A:165:GLU:O	1:A:165:GLU:HG3	2.01	0.60
1:B:165:GLU:HG3	1:B:165:GLU:O	2.01	0.60
1:B:244:ILE:HD11	1:B:263:ALA:HB2	1.84	0.60
1:A:924:ALA:HB3	1:A:925:PRO:HD3	1.84	0.60
1:B:924:ALA:HB3	1:B:925:PRO:HD3	1.84	0.60
1:D:165:GLU:O	1:D:165:GLU:HG3	2.01	0.60
1:C:1030:ARG:NH2	1:D:743:ASN:O	2.32	0.59
1:D:244:ILE:HD11	1:D:263:ALA:HB2	1.84	0.59
1:C:244:ILE:HD11	1:C:263:ALA:HB2	1.84	0.59
1:C:1130:THR:OG1	1:C:1146:THR:OG1	2.20	0.59
1:C:743:ASN:O	1:D:1030:ARG:NH2	2.31	0.59
1:C:924:ALA:HB3	1:C:925:PRO:HD3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:600:GLU:O	1:C:604:MET:HG3	2.02	0.59
1:D:600:GLU:O	1:D:604:MET:HG3	2.02	0.59
1:D:924:ALA:HB3	1:D:925:PRO:HD3	1.84	0.59
1:D:1213:PRO:HG3	1:D:1219:VAL:HG11	1.85	0.59
1:C:1213:PRO:HG3	1:C:1219:VAL:HG11	1.85	0.59
1:A:744:ARG:NH2	1:A:892:GLU:OE2	2.35	0.59
1:B:744:ARG:NH2	1:B:892:GLU:OE2	2.35	0.59
1:A:1213:PRO:HG3	1:A:1219:VAL:HG11	1.85	0.59
1:B:539:ARG:HD2	1:B:1218:ARG:O	2.03	0.59
1:B:1213:PRO:HG3	1:B:1219:VAL:HG11	1.85	0.59
1:A:539:ARG:HD2	1:A:1218:ARG:O	2.03	0.59
1:C:821:VAL:HG23	1:C:824:GLU:HB2	1.85	0.58
1:D:821:VAL:HG23	1:D:824:GLU:HB2	1.85	0.58
1:A:1160:GLY:H	1:A:1228:PRO:HG3	1.67	0.58
1:B:1160:GLY:H	1:B:1228:PRO:HG3	1.67	0.58
1:C:682:SER:O	1:C:685:GLU:N	2.34	0.58
1:C:1160:GLY:H	1:C:1228:PRO:HG3	1.67	0.58
1:D:53:MET:SD	3:D:1866:HOH:O	2.57	0.58
1:A:1224:ARG:NH1	1:A:1234:GLY:O	2.36	0.58
1:B:600:GLU:O	1:B:604:MET:HG3	2.02	0.58
1:B:1130:THR:OG1	1:B:1146:THR:OG1	2.20	0.58
1:A:600:GLU:O	1:A:604:MET:HG3	2.02	0.58
1:A:680:LYS:HZ2	1:A:683:GLU:HG2	1.67	0.58
1:B:1224:ARG:NH1	1:B:1234:GLY:O	2.36	0.58
1:C:744:ARG:HD3	1:C:895:TYR:CD2	2.39	0.58
1:C:1224:ARG:NH1	1:C:1234:GLY:O	2.36	0.58
1:D:682:SER:O	1:D:685:GLU:N	2.34	0.58
1:D:744:ARG:HD3	1:D:895:TYR:CD2	2.39	0.58
1:D:1160:GLY:H	1:D:1228:PRO:HG3	1.67	0.58
1:A:357:ARG:NE	3:A:1821:HOH:O	2.32	0.58
1:C:550:GLU:OE1	1:C:867:ARG:NH2	2.28	0.58
1:D:1224:ARG:NH1	1:D:1234:GLY:O	2.36	0.58
1:A:329:CYS:HG	1:A:335:TYR:HH	1.42	0.58
1:B:357:ARG:NE	3:B:1820:HOH:O	2.31	0.58
1:B:744:ARG:HD3	1:B:895:TYR:CD2	2.39	0.58
1:C:578:ARG:NH2	1:C:993:ASP:O	2.37	0.58
1:D:550:GLU:OE1	1:D:867:ARG:NH2	2.28	0.58
1:D:578:ARG:NH2	1:D:993:ASP:O	2.37	0.58
1:D:677:GLU:OE1	1:D:962:THR:HG21	2.03	0.58
1:B:821:VAL:HG23	1:B:824:GLU:HB2	1.85	0.58
1:A:744:ARG:HD3	1:A:895:TYR:CD2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:821:VAL:HG23	1:A:824:GLU:HB2	1.85	0.57
1:D:1030:ARG:HG3	1:D:1030:ARG:HH11	1.69	0.57
1:B:677:GLU:OE1	1:B:962:THR:HG23	2.05	0.57
1:C:1030:ARG:HG3	1:C:1030:ARG:HH11	1.69	0.57
1:D:329:CYS:SG	1:D:335:TYR:OH	2.50	0.57
1:B:1030:ARG:HG3	1:B:1030:ARG:HH11	1.69	0.57
1:A:1030:ARG:HG3	1:A:1030:ARG:HH11	1.69	0.57
1:D:1130:THR:OG1	1:D:1146:THR:OG1	2.20	0.57
1:B:369:ASP:OD1	1:B:371:ASN:N	2.36	0.57
1:B:162:ASP:OD2	1:B:162:ASP:N	2.37	0.57
1:A:369:ASP:OD1	1:A:371:ASN:N	2.36	0.57
1:C:329:CYS:SG	1:C:335:TYR:OH	2.50	0.57
1:A:162:ASP:N	1:A:162:ASP:OD2	2.37	0.57
1:C:539:ARG:HD2	1:C:1218:ARG:O	2.03	0.57
1:D:1020:ARG:NH2	3:D:1835:HOH:O	2.38	0.57
1:C:744:ARG:NH2	1:C:892:GLU:OE2	2.35	0.57
1:D:175:ASN:ND2	3:D:1832:HOH:O	2.37	0.57
1:D:369:ASP:OD1	1:D:371:ASN:N	2.36	0.57
1:D:539:ARG:HD2	1:D:1218:ARG:O	2.03	0.57
1:C:369:ASP:OD1	1:C:371:ASN:N	2.36	0.56
1:D:744:ARG:NH2	1:D:892:GLU:OE2	2.35	0.56
1:D:297:TRP:HE1	1:D:769:TRP:HZ2	1.53	0.56
1:C:297:TRP:HE1	1:C:769:TRP:HZ2	1.53	0.56
1:C:571:ARG:NH2	1:C:885:HIS:O	2.38	0.56
1:D:571:ARG:NH2	1:D:885:HIS:O	2.38	0.56
1:A:578:ARG:NH2	1:A:993:ASP:O	2.37	0.56
1:B:578:ARG:NH2	1:B:993:ASP:O	2.37	0.56
1:B:175:ASN:ND2	3:B:1835:HOH:O	2.38	0.56
1:A:571:ARG:NH2	1:A:885:HIS:O	2.38	0.56
1:C:753:ALA:HA	1:C:848:PRO:HD2	1.87	0.56
1:C:1020:ARG:NH2	3:C:1830:HOH:O	2.39	0.56
1:A:753:ALA:HA	1:A:848:PRO:HD2	1.87	0.56
1:B:571:ARG:NH2	1:B:885:HIS:O	2.38	0.56
1:B:753:ALA:HA	1:B:848:PRO:HD2	1.87	0.56
1:D:753:ALA:HA	1:D:848:PRO:HD2	1.86	0.56
1:A:297:TRP:HE1	1:A:769:TRP:HZ2	1.53	0.55
1:B:297:TRP:HE1	1:B:769:TRP:HZ2	1.53	0.55
1:D:162:ASP:OD2	1:D:162:ASP:N	2.37	0.55
1:C:225:ARG:NH2	3:C:1836:HOH:O	2.39	0.55
1:B:225:ARG:NH2	3:B:1834:HOH:O	2.38	0.55
1:C:8:VAL:C	1:C:9:LYS:HE2	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:VAL:C	1:D:9:LYS:HE2	2.32	0.55
1:A:8:VAL:C	1:A:9:LYS:HE2	2.32	0.55
1:C:162:ASP:OD2	1:C:162:ASP:N	2.37	0.55
1:D:1015:GLN:NE2	3:D:1823:HOH:O	2.32	0.55
1:A:673:TRP:CD2	1:A:953:ARG:HD3	2.42	0.55
1:B:8:VAL:C	1:B:9:LYS:HE2	2.32	0.55
1:B:673:TRP:CD2	1:B:953:ARG:HD3	2.42	0.55
1:C:1015:GLN:NE2	3:C:1822:HOH:O	2.31	0.55
1:C:1218:ARG:HG3	1:C:1242:VAL:HG22	1.88	0.55
1:D:1218:ARG:HG3	1:D:1242:VAL:HG22	1.88	0.55
1:A:682:SER:O	1:A:685:GLU:N	2.34	0.55
1:B:682:SER:O	1:B:685:GLU:N	2.34	0.55
1:D:225:ARG:NH2	3:D:1837:HOH:O	2.39	0.55
1:A:1219:VAL:HG23	1:A:1241:VAL:HG23	1.89	0.55
1:C:680:LYS:HZ2	1:C:683:GLU:HG2	1.72	0.55
1:A:225:ARG:NH2	3:A:1828:HOH:O	2.38	0.55
1:B:1219:VAL:HG23	1:B:1241:VAL:HG23	1.89	0.55
1:B:1129:ASP:OD1	1:B:1129:ASP:N	2.38	0.54
1:A:1129:ASP:OD1	1:A:1129:ASP:N	2.39	0.54
1:A:99:PRO:O	1:A:102:THR:OG1	2.25	0.54
1:A:1218:ARG:HG3	1:A:1242:VAL:HG22	1.88	0.54
1:B:99:PRO:O	1:B:102:THR:OG1	2.25	0.54
1:C:703:THR:HG22	1:C:704:THR:HG22	1.89	0.54
1:D:703:THR:HG22	1:D:704:THR:HG22	1.89	0.54
1:C:673:TRP:CD2	1:C:953:ARG:HD3	2.42	0.54
1:B:1218:ARG:HG3	1:B:1242:VAL:HG22	1.88	0.54
1:C:91:THR:OG1	1:C:92:ASN:N	2.41	0.54
1:D:91:THR:OG1	1:D:92:ASN:N	2.41	0.54
1:D:673:TRP:CD2	1:D:953:ARG:HD3	2.42	0.54
1:C:1129:ASP:OD1	1:C:1129:ASP:N	2.39	0.54
1:A:241:CYS:O	1:A:245:ILE:HG12	2.07	0.54
1:C:677:GLU:OE1	1:C:962:THR:CG2	2.56	0.54
1:B:91:THR:OG1	1:B:92:ASN:N	2.41	0.54
1:B:1020:ARG:NH2	3:B:1831:HOH:O	2.40	0.54
1:D:1129:ASP:N	1:D:1129:ASP:OD1	2.38	0.54
1:A:91:THR:OG1	1:A:92:ASN:N	2.41	0.54
1:B:241:CYS:O	1:B:245:ILE:HG12	2.07	0.54
1:C:241:CYS:O	1:C:245:ILE:HG12	2.07	0.54
1:D:241:CYS:O	1:D:245:ILE:HG12	2.07	0.54
1:C:418:LEU:O	1:C:1046:ASN:HB2	2.08	0.53
1:D:418:LEU:O	1:D:1046:ASN:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:LEU:O	1:A:1046:ASN:HB2	2.08	0.53
1:B:418:LEU:O	1:B:1046:ASN:HB2	2.08	0.53
1:B:703:THR:HG22	1:B:704:THR:HG22	1.89	0.53
1:A:106:PHE:HE1	1:A:172:MET:HE3	1.74	0.53
1:B:106:PHE:HE1	1:B:172:MET:HE3	1.74	0.53
1:A:703:THR:HG22	1:A:704:THR:HG22	1.89	0.53
1:C:1219:VAL:HG23	1:C:1241:VAL:HG23	1.89	0.53
1:D:274:PRO:HG2	1:D:1230:GLY:HA3	1.91	0.53
1:D:1219:VAL:HG23	1:D:1241:VAL:HG23	1.89	0.53
1:B:1015:GLN:NE2	3:B:1822:HOH:O	2.32	0.53
1:C:274:PRO:HG2	1:C:1230:GLY:HA3	1.91	0.53
1:B:274:PRO:HG2	1:B:1230:GLY:HA3	1.91	0.53
1:B:680:LYS:HZ2	1:B:683:GLU:HG2	1.73	0.53
1:A:274:PRO:HG2	1:A:1230:GLY:HA3	1.91	0.53
1:A:1020:ARG:NH2	3:A:1833:HOH:O	2.42	0.53
1:B:822:GLU:OE2	1:B:822:GLU:N	2.38	0.53
1:C:352:LYS:NZ	3:C:1832:HOH:O	2.38	0.53
1:C:736:SER:OG	1:C:745:GLU:OE2	2.25	0.52
1:A:600:GLU:N	1:A:600:GLU:OE2	2.42	0.52
1:B:600:GLU:OE2	1:B:600:GLU:N	2.42	0.52
1:B:703:THR:HG22	1:B:704:THR:N	2.23	0.52
1:C:831:GLN:NE2	3:C:1838:HOH:O	2.42	0.52
1:D:357:ARG:NE	3:D:1822:HOH:O	2.30	0.52
1:D:736:SER:OG	1:D:745:GLU:OE2	2.25	0.52
1:A:703:THR:HG22	1:A:704:THR:N	2.23	0.52
1:A:822:GLU:OE2	1:A:822:GLU:N	2.38	0.52
1:B:831:GLN:NE2	3:B:1843:HOH:O	2.42	0.52
1:C:106:PHE:HE1	1:C:172:MET:HE3	1.74	0.52
1:A:34:ASP:OD1	1:A:225:ARG:NH1	2.43	0.52
1:A:754:ASN:HD22	1:A:754:ASN:C	2.15	0.52
1:B:34:ASP:OD1	1:B:225:ARG:NH1	2.43	0.52
1:A:243:GLU:HG2	1:A:262:ILE:HD13	1.92	0.52
1:B:680:LYS:NZ	1:B:683:GLU:HG2	2.25	0.52
1:D:106:PHE:HE1	1:D:172:MET:HE3	1.74	0.52
1:D:131:GLU:OE2	1:D:175:ASN:ND2	2.34	0.52
1:B:243:GLU:HG2	1:B:262:ILE:HD13	1.92	0.52
1:B:754:ASN:HD22	1:B:754:ASN:C	2.15	0.52
1:C:131:GLU:OE2	1:C:175:ASN:ND2	2.34	0.52
1:C:357:ARG:NE	3:C:1821:HOH:O	2.31	0.52
1:C:493:LYS:NZ	3:C:1839:HOH:O	2.43	0.52
1:C:66:GLN:HG3	1:C:109:VAL:HB	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:GLN:HG3	1:D:109:VAL:HB	1.92	0.52
1:D:600:GLU:N	1:D:600:GLU:OE2	2.42	0.52
1:D:822:GLU:OE2	1:D:822:GLU:N	2.38	0.52
1:D:400:PHE:HB2	1:D:421:MET:HE3	1.92	0.52
1:D:867:ARG:HD3	1:D:882:VAL:HG11	1.92	0.52
1:C:400:PHE:HB2	1:C:421:MET:HE3	1.92	0.51
1:C:600:GLU:OE2	1:C:600:GLU:N	2.42	0.51
1:C:867:ARG:HD3	1:C:882:VAL:HG11	1.92	0.51
1:D:831:GLN:NE2	3:D:1843:HOH:O	2.43	0.51
1:B:400:PHE:HB2	1:B:421:MET:HE3	1.92	0.51
1:C:103:THR:HB	1:C:306:ARG:HH12	1.76	0.51
1:C:1165:PHE:HB2	1:C:1223:TRP:CZ3	2.45	0.51
1:D:243:GLU:HG2	1:D:262:ILE:HD13	1.92	0.51
1:D:1165:PHE:HB2	1:D:1223:TRP:CZ3	2.45	0.51
1:A:103:THR:HB	1:A:306:ARG:HH12	1.76	0.51
1:A:831:GLN:NE2	3:A:1834:HOH:O	2.43	0.51
1:C:99:PRO:O	1:C:102:THR:OG1	2.25	0.51
1:C:822:GLU:OE2	1:C:822:GLU:N	2.38	0.51
1:D:103:THR:HB	1:D:306:ARG:HH12	1.76	0.51
1:D:680:LYS:NZ	1:D:683:GLU:HG2	2.25	0.51
1:B:131:GLU:OE2	1:B:175:ASN:ND2	2.34	0.51
1:C:243:GLU:HG2	1:C:262:ILE:HD13	1.92	0.51
1:C:680:LYS:NZ	1:C:683:GLU:HG2	2.25	0.51
1:D:34:ASP:OD1	1:D:225:ARG:NH1	2.43	0.51
1:A:400:PHE:HB2	1:A:421:MET:HE3	1.92	0.51
1:B:103:THR:HB	1:B:306:ARG:HH12	1.76	0.51
1:C:436:ARG:HG3	1:C:436:ARG:NH2	2.23	0.51
1:D:99:PRO:O	1:D:102:THR:OG1	2.25	0.51
1:D:436:ARG:HG3	1:D:436:ARG:NH2	2.23	0.51
1:D:493:LYS:NZ	3:D:1844:HOH:O	2.44	0.51
1:A:131:GLU:OE2	1:A:175:ASN:ND2	2.34	0.51
1:A:436:ARG:HG3	1:A:436:ARG:NH2	2.23	0.51
1:A:680:LYS:NZ	1:A:683:GLU:HG2	2.25	0.51
1:B:1216:ALA:HA	1:B:1243:VAL:HB	1.93	0.51
1:C:34:ASP:OD1	1:C:225:ARG:NH1	2.43	0.51
1:C:802:ARG:HB3	1:C:802:ARG:HH11	1.76	0.51
1:A:1216:ALA:HA	1:A:1243:VAL:HB	1.93	0.51
1:B:436:ARG:HG3	1:B:436:ARG:NH2	2.23	0.51
1:B:742:ALA:O	1:B:744:ARG:N	2.44	0.51
1:A:867:ARG:HD3	1:A:882:VAL:HG11	1.92	0.51
1:C:380:ARG:NH2	1:C:996:LYS:HD3	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:380:ARG:NH2	1:D:996:LYS:HD3	2.26	0.51
1:D:802:ARG:HH11	1:D:802:ARG:HB3	1.76	0.51
1:A:66:GLN:HG3	1:A:109:VAL:HB	1.92	0.50
1:A:742:ALA:O	1:A:744:ARG:N	2.44	0.50
1:B:66:GLN:HG3	1:B:109:VAL:HB	1.92	0.50
1:B:867:ARG:HD3	1:B:882:VAL:HG11	1.92	0.50
1:A:654:GLU:HB3	1:A:965:TYR:HB3	1.94	0.50
1:A:380:ARG:NH2	1:A:996:LYS:HD3	2.26	0.50
1:B:654:GLU:HB3	1:B:965:TYR:HB3	1.94	0.50
1:A:682:SER:O	1:A:684:LYS:N	2.44	0.50
1:A:1165:PHE:HB2	1:A:1223:TRP:CZ3	2.45	0.50
1:B:1165:PHE:HB2	1:B:1223:TRP:CZ3	2.45	0.50
1:D:682:SER:O	1:D:684:LYS:N	2.44	0.50
1:B:380:ARG:NH2	1:B:996:LYS:HD3	2.26	0.50
1:B:846:GLU:HG2	1:B:915:ARG:HG3	1.93	0.50
1:C:682:SER:O	1:C:684:LYS:N	2.44	0.50
1:B:682:SER:O	1:B:684:LYS:N	2.44	0.50
1:C:722:ASN:OD1	1:C:723:SER:N	2.44	0.50
1:D:722:ASN:OD1	1:D:723:SER:N	2.44	0.50
1:A:846:GLU:HG2	1:A:915:ARG:HG3	1.93	0.50
1:A:754:ASN:ND2	1:A:754:ASN:C	2.70	0.50
1:B:754:ASN:ND2	1:B:754:ASN:C	2.70	0.49
1:B:759:PHE:CE2	1:B:844:LYS:HD2	2.47	0.49
1:A:759:PHE:CE2	1:A:844:LYS:HD2	2.47	0.49
1:B:662:THR:O	1:B:662:THR:OG1	2.30	0.49
1:A:123:GLU:OE1	1:A:206:ILE:HG13	2.12	0.49
1:B:123:GLU:OE1	1:B:206:ILE:HG13	2.12	0.49
1:C:742:ALA:O	1:C:744:ARG:N	2.44	0.49
1:D:742:ALA:O	1:D:744:ARG:N	2.44	0.49
1:B:352:LYS:NZ	3:B:1837:HOH:O	2.39	0.49
1:D:654:GLU:HB3	1:D:965:TYR:HB3	1.94	0.49
1:D:730:GLU:O	1:D:732:GLY:N	2.45	0.49
1:D:1212:THR:HG22	1:D:1213:PRO:HD2	1.94	0.49
1:A:101:TRP:O	3:A:1801:HOH:O	2.20	0.49
1:B:802:ARG:HH11	1:B:802:ARG:HB3	1.76	0.49
1:C:730:GLU:O	1:C:732:GLY:N	2.45	0.49
1:A:802:ARG:HH11	1:A:802:ARG:HB3	1.76	0.49
1:C:361:ILE:HD11	1:C:401:TRP:CE3	2.48	0.49
1:C:759:PHE:CE2	1:C:844:LYS:HD2	2.47	0.49
1:D:361:ILE:HD11	1:D:401:TRP:CE3	2.48	0.49
1:D:1216:ALA:HA	1:D:1243:VAL:HB	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:838:GLU:O	1:A:931:MET:HE1	2.13	0.49
1:C:654:GLU:HB3	1:C:965:TYR:HB3	1.94	0.49
1:C:1212:THR:HG22	1:C:1213:PRO:HD2	1.94	0.49
1:C:1216:ALA:HA	1:C:1243:VAL:HB	1.93	0.49
1:D:759:PHE:CE2	1:D:844:LYS:HD2	2.47	0.49
1:B:838:GLU:O	1:B:931:MET:HE1	2.13	0.49
1:C:62:GLU:N	1:C:63:PRO:HD2	2.28	0.49
1:D:62:GLU:N	1:D:63:PRO:HD2	2.28	0.49
1:C:123:GLU:OE1	1:C:206:ILE:HG13	2.12	0.49
1:C:512:ARG:HG3	1:C:524:VAL:O	2.13	0.49
1:C:681:ILE:O	1:C:681:ILE:HD12	2.13	0.49
1:C:697:LYS:HB3	1:C:974:VAL:HG11	1.95	0.49
1:C:838:GLU:O	1:C:931:MET:HE1	2.13	0.49
1:D:512:ARG:HG3	1:D:524:VAL:O	2.13	0.49
1:D:807:ASP:O	1:D:808:LYS:HG2	2.13	0.49
1:D:838:GLU:O	1:D:931:MET:HE1	2.13	0.49
1:B:807:ASP:O	1:B:808:LYS:HG2	2.13	0.48
1:B:839:THR:HG23	1:B:923:LYS:HE3	1.95	0.48
1:C:807:ASP:O	1:C:808:LYS:HG2	2.13	0.48
1:D:681:ILE:HD12	1:D:681:ILE:O	2.13	0.48
1:D:697:LYS:HB3	1:D:974:VAL:HG11	1.95	0.48
1:D:846:GLU:HG2	1:D:915:ARG:HG3	1.93	0.48
1:A:493:LYS:NZ	3:A:1836:HOH:O	2.43	0.48
1:A:807:ASP:O	1:A:808:LYS:HG2	2.13	0.48
1:B:443:ASN:OD1	1:D:16:TYR:OH	2.30	0.48
1:C:846:GLU:HG2	1:C:915:ARG:HG3	1.93	0.48
1:D:101:TRP:O	3:D:1801:HOH:O	2.20	0.48
1:D:123:GLU:OE1	1:D:206:ILE:HG13	2.12	0.48
1:D:662:THR:O	1:D:662:THR:OG1	2.30	0.48
1:A:697:LYS:HB3	1:A:974:VAL:HG11	1.95	0.48
1:D:703:THR:HG22	1:D:704:THR:N	2.23	0.48
1:A:381:GLN:HG2	1:A:609:LEU:HD22	1.95	0.48
1:A:839:THR:HG23	1:A:923:LYS:HE3	1.96	0.48
1:B:528:SER:OG	1:B:529:SER:N	2.47	0.48
1:B:697:LYS:HB3	1:B:974:VAL:HG11	1.95	0.48
1:C:101:TRP:O	3:C:1801:HOH:O	2.20	0.48
1:C:222:ASP:HB3	1:C:468:PHE:HB3	1.95	0.48
1:C:703:THR:HG22	1:C:704:THR:N	2.23	0.48
1:D:222:ASP:HB3	1:D:468:PHE:HB3	1.95	0.48
1:A:528:SER:OG	1:A:529:SER:N	2.47	0.48
1:B:62:GLU:N	1:B:63:PRO:HD2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:ILE:HD11	1:B:401:TRP:CE3	2.48	0.48
1:B:381:GLN:HG2	1:B:609:LEU:HD22	1.95	0.48
1:D:381:GLN:HG2	1:D:609:LEU:HD22	1.95	0.48
1:A:62:GLU:N	1:A:63:PRO:HD2	2.28	0.48
1:A:222:ASP:HB3	1:A:468:PHE:HB3	1.95	0.48
1:B:1212:THR:HG22	1:B:1213:PRO:HD2	1.94	0.48
1:C:381:GLN:HG2	1:C:609:LEU:HD22	1.95	0.48
1:B:222:ASP:HB3	1:B:468:PHE:HB3	1.95	0.48
1:D:162:ASP:O	1:D:164:LYS:N	2.45	0.48
1:A:361:ILE:HD11	1:A:401:TRP:CE3	2.48	0.48
1:A:512:ARG:HG3	1:A:524:VAL:O	2.13	0.48
1:A:1212:THR:HG22	1:A:1213:PRO:HD2	1.94	0.48
1:B:996:LYS:NZ	1:B:1049:GLU:OE2	2.46	0.48
1:A:996:LYS:NZ	1:A:1049:GLU:OE2	2.46	0.48
1:A:1130:THR:OG1	1:A:1146:THR:OG1	2.20	0.48
1:D:424:PHE:CE2	1:D:426:THR:CG2	2.96	0.48
1:A:443:ASN:OD1	1:C:16:TYR:OH	2.30	0.48
1:B:512:ARG:HG3	1:B:524:VAL:O	2.13	0.48
1:C:162:ASP:O	1:C:164:LYS:N	2.45	0.48
1:C:300:PRO:HG3	1:C:624:MET:HE2	1.96	0.48
1:D:754:ASN:ND2	1:D:754:ASN:C	2.70	0.48
1:A:802:ARG:HB3	1:A:802:ARG:NH1	2.29	0.47
1:B:424:PHE:CE2	1:B:426:THR:CG2	2.96	0.47
1:B:668:LEU:HD12	1:B:668:LEU:HA	1.71	0.47
1:D:300:PRO:HG3	1:D:624:MET:HE2	1.96	0.47
1:A:681:ILE:O	1:A:681:ILE:HD12	2.13	0.47
1:B:681:ILE:HD12	1:B:681:ILE:O	2.13	0.47
1:B:802:ARG:HB3	1:B:802:ARG:NH1	2.29	0.47
1:B:1172:GLY:N	3:B:1832:HOH:O	2.46	0.47
1:C:291:CYS:HB3	1:C:327:PHE:HZ	1.80	0.47
1:C:424:PHE:CE2	1:C:426:THR:CG2	2.96	0.47
1:C:463:THR:O	1:C:463:THR:OG1	2.27	0.47
1:D:367:GLU:OE2	1:D:403:PRO:HD2	2.15	0.47
1:A:668:LEU:HD12	1:A:668:LEU:HA	1.71	0.47
1:C:367:GLU:OE2	1:C:403:PRO:HD2	2.15	0.47
1:D:291:CYS:HB3	1:D:327:PHE:HZ	1.80	0.47
1:D:1172:GLY:N	3:D:1834:HOH:O	2.47	0.47
1:A:424:PHE:CE2	1:A:426:THR:CG2	2.97	0.47
1:A:722:ASN:OD1	1:A:723:SER:N	2.44	0.47
1:B:231:SER:OG	1:B:233:GLU:OE2	2.31	0.47
1:D:463:THR:O	1:D:463:THR:OG1	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:SER:OG	1:A:233:GLU:OE2	2.31	0.47
1:A:367:GLU:OE2	1:A:403:PRO:HD2	2.15	0.47
1:B:367:GLU:OE2	1:B:403:PRO:HD2	2.15	0.47
1:B:722:ASN:OD1	1:B:723:SER:N	2.44	0.47
1:B:1030:ARG:HG3	1:B:1030:ARG:NH1	2.29	0.47
1:C:528:SER:OG	1:C:529:SER:N	2.47	0.47
1:C:766:TRP:HB3	1:C:769:TRP:CE3	2.50	0.47
1:C:839:THR:HG23	1:C:923:LYS:HE3	1.96	0.47
1:D:766:TRP:HB3	1:D:769:TRP:CE3	2.50	0.47
1:D:839:THR:HG23	1:D:923:LYS:HE3	1.95	0.47
1:A:1030:ARG:HG3	1:A:1030:ARG:NH1	2.29	0.47
1:B:730:GLU:O	1:B:732:GLY:N	2.45	0.47
1:C:802:ARG:HB3	1:C:802:ARG:NH1	2.29	0.47
1:D:528:SER:OG	1:D:529:SER:N	2.47	0.47
1:D:802:ARG:HB3	1:D:802:ARG:NH1	2.29	0.47
1:A:890:LEU:HB2	1:A:914:MET:HE3	1.97	0.47
1:B:890:LEU:HB2	1:B:914:MET:HE3	1.97	0.47
1:A:730:GLU:O	1:A:732:GLY:N	2.45	0.47
1:C:620:SER:HB2	1:C:769:TRP:CE2	2.50	0.47
1:D:220:LEU:HB3	1:D:241:CYS:SG	2.55	0.47
1:A:220:LEU:HB3	1:A:241:CYS:SG	2.55	0.46
1:A:300:PRO:HG3	1:A:624:MET:HE2	1.96	0.46
1:A:1030:ARG:NE	1:A:1065:GLU:OE1	2.35	0.46
1:B:220:LEU:HB3	1:B:241:CYS:SG	2.55	0.46
1:B:1030:ARG:NE	1:B:1065:GLU:OE1	2.35	0.46
1:D:620:SER:HB2	1:D:769:TRP:CE2	2.50	0.46
1:A:291:CYS:HB3	1:A:327:PHE:HZ	1.80	0.46
1:A:448:ASP:C	1:A:448:ASP:OD1	2.58	0.46
1:A:620:SER:HB2	1:A:769:TRP:CE2	2.50	0.46
1:B:448:ASP:OD1	1:B:448:ASP:C	2.58	0.46
1:B:620:SER:HB2	1:B:769:TRP:CE2	2.50	0.46
1:C:220:LEU:HB3	1:C:241:CYS:SG	2.56	0.46
1:C:763:PRO:HG2	1:C:767:GLN:HA	1.97	0.46
1:C:996:LYS:NZ	1:C:1049:GLU:OE2	2.46	0.46
1:C:1172:GLY:N	3:C:1831:HOH:O	2.48	0.46
1:D:763:PRO:HG2	1:D:767:GLN:HA	1.97	0.46
1:D:996:LYS:NZ	1:D:1049:GLU:OE2	2.46	0.46
1:B:291:CYS:HB3	1:B:327:PHE:HZ	1.80	0.46
1:B:300:PRO:HG3	1:B:624:MET:HE2	1.96	0.46
1:B:493:LYS:NZ	3:B:1846:HOH:O	2.45	0.46
1:C:577:LEU:HD21	1:C:604:MET:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:668:LEU:HA	1:D:668:LEU:HD12	1.71	0.46
1:D:577:LEU:HD21	1:D:604:MET:HE2	1.97	0.46
1:A:1172:GLY:N	3:A:1830:HOH:O	2.48	0.46
1:D:890:LEU:HB2	1:D:914:MET:HE3	1.97	0.46
1:A:577:LEU:HD21	1:A:604:MET:HE2	1.97	0.46
1:B:362:GLY:HA2	1:B:401:TRP:H	1.81	0.46
1:B:766:TRP:HB3	1:B:769:TRP:CE3	2.50	0.46
1:C:19:ARG:NH1	3:C:1844:HOH:O	2.47	0.46
1:C:448:ASP:C	1:C:448:ASP:OD1	2.58	0.46
1:C:890:LEU:HB2	1:C:914:MET:HE3	1.97	0.46
1:D:448:ASP:OD1	1:D:448:ASP:C	2.58	0.46
1:A:362:GLY:HA2	1:A:401:TRP:H	1.81	0.46
1:A:662:THR:O	1:A:662:THR:OG1	2.30	0.46
1:A:736:SER:OG	1:A:745:GLU:OE2	2.25	0.46
1:A:766:TRP:HB3	1:A:769:TRP:CE3	2.50	0.46
1:C:417:ARG:HD2	1:C:417:ARG:HA	1.72	0.46
1:D:1144:GLU:OE2	1:D:1144:GLU:N	2.48	0.46
1:A:33:LYS:O	3:A:1802:HOH:O	2.20	0.46
1:B:577:LEU:HD21	1:B:604:MET:HE2	1.97	0.46
1:C:668:LEU:HD12	1:C:668:LEU:HA	1.71	0.46
1:C:1030:ARG:NE	1:C:1065:GLU:OE1	2.35	0.46
1:C:1144:GLU:N	1:C:1144:GLU:OE2	2.48	0.46
1:D:1030:ARG:NE	1:D:1065:GLU:OE1	2.35	0.46
1:A:599:GLU:OE2	1:A:1006:ARG:NH1	2.49	0.46
1:B:599:GLU:OE2	1:B:1006:ARG:NH1	2.49	0.46
1:C:436:ARG:HD3	1:C:479:LYS:HE2	1.96	0.46
1:D:436:ARG:HD3	1:D:479:LYS:HE2	1.96	0.46
1:D:599:GLU:OE2	1:D:1006:ARG:NH1	2.49	0.46
1:B:436:ARG:HD3	1:B:479:LYS:HE2	1.96	0.46
1:C:599:GLU:OE2	1:C:1006:ARG:NH1	2.49	0.46
1:D:1001:ASP:C	1:D:1003:ASP:H	2.24	0.46
1:D:1199:GLN:N	1:D:1199:GLN:CD	2.74	0.46
1:A:1143:PHE:CE1	1:A:1210:LEU:HB2	2.52	0.45
1:B:1001:ASP:C	1:B:1003:ASP:H	2.24	0.45
1:B:1143:PHE:CE1	1:B:1210:LEU:HB2	2.52	0.45
1:C:754:ASN:ND2	1:C:754:ASN:C	2.70	0.45
1:C:1199:GLN:N	1:C:1199:GLN:CD	2.74	0.45
1:A:436:ARG:HD3	1:A:479:LYS:HE2	1.96	0.45
1:A:1001:ASP:C	1:A:1003:ASP:H	2.24	0.45
1:B:954:LYS:HA	1:B:954:LYS:HD3	1.64	0.45
1:C:518:VAL:HG23	1:C:518:VAL:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1001:ASP:C	1:C:1003:ASP:H	2.24	0.45
1:D:518:VAL:HG23	1:D:518:VAL:O	2.17	0.45
1:C:430:SER:HB2	1:C:460:GLU:HG2	1.99	0.45
1:D:430:SER:HB2	1:D:460:GLU:HG2	1.99	0.45
1:B:1171:MET:HB2	1:B:1210:LEU:HD22	1.99	0.45
1:A:308:VAL:HG12	1:A:338:LEU:HD13	1.98	0.45
1:A:1171:MET:HB2	1:A:1210:LEU:HD22	1.99	0.45
1:A:1173:ARG:NH1	1:A:1173:ARG:HB3	2.32	0.45
1:B:308:VAL:HG12	1:B:338:LEU:HD13	1.98	0.45
1:B:1173:ARG:HB3	1:B:1173:ARG:NH1	2.32	0.45
1:D:417:ARG:HA	1:D:417:ARG:HD2	1.72	0.45
1:A:292:HIS:CE1	1:A:614:HIS:HE1	2.35	0.45
1:A:1051:ASP:OD2	1:A:1051:ASP:N	2.50	0.45
1:B:1051:ASP:OD2	1:B:1051:ASP:N	2.50	0.45
1:C:567:LYS:NZ	1:C:617:LEU:O	2.49	0.45
1:B:162:ASP:O	1:B:164:LYS:N	2.45	0.45
1:B:292:HIS:CE1	1:B:614:HIS:HE1	2.35	0.45
1:C:1143:PHE:CE1	1:C:1210:LEU:HB2	2.51	0.45
1:D:567:LYS:NZ	1:D:617:LEU:O	2.49	0.45
1:D:1143:PHE:CE1	1:D:1210:LEU:HB2	2.52	0.45
1:A:954:LYS:HA	1:A:954:LYS:HD3	1.64	0.45
1:B:704:THR:HA	1:B:705:LYS:HE2	1.99	0.45
1:B:1146:THR:HG22	1:B:1207:THR:OG1	2.16	0.45
1:B:1167:GLY:HA3	1:B:1222:HIS:HB2	1.98	0.45
1:C:1030:ARG:HG3	1:C:1030:ARG:NH1	2.29	0.45
1:C:1173:ARG:HB3	1:C:1173:ARG:NH1	2.32	0.45
1:D:1030:ARG:HG3	1:D:1030:ARG:NH1	2.29	0.45
1:D:1171:MET:HB2	1:D:1210:LEU:HD22	1.99	0.45
1:A:429:LEU:HD22	1:A:456:MET:HE1	1.99	0.45
1:A:430:SER:HB2	1:A:460:GLU:HG2	1.99	0.45
1:A:1034:VAL:HG22	1:A:1061:ARG:HG2	1.99	0.45
1:A:1167:GLY:HA3	1:A:1222:HIS:HB2	1.98	0.45
1:B:430:SER:HB2	1:B:460:GLU:HG2	1.99	0.45
1:B:1199:GLN:N	1:B:1199:GLN:CD	2.74	0.45
1:D:308:VAL:HG12	1:D:338:LEU:HD13	1.98	0.45
1:D:1173:ARG:NH1	1:D:1173:ARG:HB3	2.32	0.45
1:A:162:ASP:O	1:A:164:LYS:N	2.45	0.44
1:A:261:LYS:HE2	1:A:261:LYS:HB2	1.89	0.44
1:A:704:THR:HA	1:A:705:LYS:HE2	2.00	0.44
1:A:763:PRO:HG2	1:A:767:GLN:HA	1.97	0.44
1:A:1146:THR:HG22	1:A:1207:THR:OG1	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1199:GLN:N	1:A:1199:GLN:CD	2.74	0.44
1:B:429:LEU:HD22	1:B:456:MET:HE1	2.00	0.44
1:B:677:GLU:OE1	1:B:962:THR:CG2	2.65	0.44
1:B:1034:VAL:HG22	1:B:1061:ARG:HG2	1.99	0.44
1:C:784:SER:HG	1:C:804:LYS:H	1.57	0.44
1:C:1146:THR:HG22	1:C:1207:THR:OG1	2.16	0.44
1:C:1171:MET:HB2	1:C:1210:LEU:HD22	1.99	0.44
1:D:1146:THR:HG22	1:D:1207:THR:OG1	2.16	0.44
1:A:379:VAL:HG13	1:A:1047:LEU:HD13	1.99	0.44
1:B:178:PHE:HE2	1:B:495:ASP:HB2	1.82	0.44
1:B:379:VAL:HG13	1:B:1047:LEU:HD13	1.99	0.44
1:B:763:PRO:HG2	1:B:767:GLN:HA	1.97	0.44
1:C:292:HIS:CE1	1:C:614:HIS:HE1	2.35	0.44
1:C:308:VAL:HG12	1:C:338:LEU:HD13	1.98	0.44
1:C:357:ARG:NH1	3:C:1832:HOH:O	2.50	0.44
1:C:362:GLY:HA2	1:C:401:TRP:H	1.81	0.44
1:C:1051:ASP:OD2	1:C:1051:ASP:N	2.50	0.44
1:D:292:HIS:CE1	1:D:614:HIS:HE1	2.35	0.44
1:D:1051:ASP:OD2	1:D:1051:ASP:N	2.50	0.44
1:A:178:PHE:HE2	1:A:495:ASP:HB2	1.83	0.44
1:B:518:VAL:HG23	1:B:518:VAL:O	2.17	0.44
1:C:379:VAL:HG13	1:C:1047:LEU:HD13	1.99	0.44
1:C:429:LEU:HD22	1:C:456:MET:HE1	1.99	0.44
1:D:379:VAL:HG13	1:D:1047:LEU:HD13	1.99	0.44
1:A:15:ASP:OD1	1:A:15:ASP:N	2.46	0.44
1:A:518:VAL:O	1:A:518:VAL:HG23	2.17	0.44
1:A:1139:PRO:HA	1:A:1243:VAL:CG1	2.48	0.44
1:B:15:ASP:OD1	1:B:15:ASP:N	2.46	0.44
1:B:1139:PRO:HA	1:B:1243:VAL:CG1	2.48	0.44
1:D:357:ARG:NH1	3:D:1836:HOH:O	2.50	0.44
1:D:362:GLY:HA2	1:D:401:TRP:H	1.81	0.44
1:D:429:LEU:HD22	1:D:456:MET:HE1	2.00	0.44
1:D:295:SER:O	1:D:304:THR:OG1	2.29	0.44
1:C:177:MET:HE3	1:C:177:MET:HA	1.99	0.44
1:C:1221:SER:O	1:C:1238:TRP:HA	2.17	0.44
1:D:177:MET:HA	1:D:177:MET:HE3	1.99	0.44
1:D:231:SER:OG	1:D:233:GLU:OE2	2.31	0.44
1:A:219:ILE:HG13	1:A:510:ARG:HB2	2.00	0.44
1:A:361:ILE:HG12	3:A:1809:HOH:O	2.18	0.44
1:B:219:ILE:HG13	1:B:510:ARG:HB2	2.00	0.44
1:B:413:PRO:HB2	1:B:446:ALA:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1139:PRO:HA	1:C:1243:VAL:CG1	2.48	0.44
1:C:1167:GLY:HA3	1:C:1222:HIS:HB2	1.98	0.44
1:D:1139:PRO:HA	1:D:1243:VAL:CG1	2.48	0.44
1:D:1167:GLY:HA3	1:D:1222:HIS:HB2	1.98	0.44
1:A:177:MET:HE3	1:A:177:MET:HA	1.98	0.44
1:A:1144:GLU:OE2	1:A:1144:GLU:N	2.48	0.44
1:A:1221:SER:O	1:A:1238:TRP:HA	2.17	0.44
1:C:704:THR:HA	1:C:705:LYS:HE2	1.99	0.44
1:C:782:LEU:HD13	1:C:805:VAL:HG22	2.00	0.44
1:D:704:THR:HA	1:D:705:LYS:HE2	1.99	0.44
1:D:782:LEU:HD13	1:D:805:VAL:HG22	2.00	0.44
1:D:1221:SER:O	1:D:1238:TRP:HA	2.17	0.44
1:A:413:PRO:HB2	1:A:446:ALA:HB2	2.00	0.44
1:B:1144:GLU:OE2	1:B:1144:GLU:N	2.48	0.44
1:C:178:PHE:HE2	1:C:495:ASP:HB2	1.82	0.44
1:C:295:SER:O	1:C:304:THR:OG1	2.29	0.44
1:D:178:PHE:HE2	1:D:495:ASP:HB2	1.82	0.44
1:A:782:LEU:HD13	1:A:805:VAL:HG22	2.00	0.43
1:A:1220:ILE:HG13	3:A:1812:HOH:O	2.17	0.43
1:B:782:LEU:HD13	1:B:805:VAL:HG22	2.00	0.43
1:B:1221:SER:O	1:B:1238:TRP:HA	2.17	0.43
1:C:231:SER:OG	1:C:233:GLU:OE2	2.31	0.43
1:C:1034:VAL:HG22	1:C:1061:ARG:HG2	1.99	0.43
1:C:1153:GLY:O	1:C:1200:PRO:HB3	2.18	0.43
1:B:361:ILE:HG12	3:B:1811:HOH:O	2.18	0.43
1:C:292:HIS:HE1	1:C:614:HIS:HE1	1.65	0.43
1:D:292:HIS:HE1	1:D:614:HIS:HE1	1.65	0.43
1:D:1034:VAL:HG22	1:D:1061:ARG:HG2	1.99	0.43
1:D:1153:GLY:O	1:D:1200:PRO:HB3	2.18	0.43
1:B:177:MET:HE3	1:B:177:MET:HA	1.99	0.43
1:B:292:HIS:HE1	1:B:614:HIS:HE1	1.65	0.43
1:C:1001:ASP:OD1	1:C:1016:SER:N	2.49	0.43
1:D:1001:ASP:OD1	1:D:1016:SER:N	2.49	0.43
1:A:292:HIS:HE1	1:A:614:HIS:HE1	1.65	0.43
1:B:558:GLY:N	1:B:771:VAL:HG12	2.33	0.43
1:C:657:LEU:HD21	1:C:964:LEU:C	2.44	0.43
1:C:1058:GLU:OE2	1:C:1058:GLU:HA	2.19	0.43
1:A:423:ARG:HG2	1:A:534:PHE:CG	2.53	0.43
1:A:558:GLY:N	1:A:771:VAL:HG12	2.33	0.43
1:A:661:SER:O	1:A:663:THR:HG22	2.18	0.43
1:A:748:PRO:HG3	1:A:850:ASP:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:ARG:NH1	3:B:1837:HOH:O	2.51	0.43
1:B:423:ARG:HG2	1:B:534:PHE:CG	2.53	0.43
1:B:661:SER:O	1:B:663:THR:HG22	2.18	0.43
1:B:748:PRO:HG3	1:B:850:ASP:HB2	2.01	0.43
1:C:222:ASP:OD2	3:C:1802:HOH:O	2.21	0.43
1:C:318:LEU:HD23	1:C:318:LEU:HA	1.78	0.43
1:C:1139:PRO:HG3	1:C:1245:LYS:HA	2.00	0.43
1:D:5:THR:C	1:D:7:ASP:H	2.27	0.43
1:D:657:LEU:HD21	1:D:964:LEU:C	2.44	0.43
1:D:1058:GLU:OE2	1:D:1058:GLU:HA	2.19	0.43
1:A:657:LEU:HD21	1:A:964:LEU:C	2.44	0.43
1:A:1058:GLU:HA	1:A:1058:GLU:OE2	2.19	0.43
1:B:401:TRP:CD1	1:B:403:PRO:HD3	2.54	0.43
1:B:657:LEU:HD21	1:B:964:LEU:C	2.44	0.43
1:B:1220:ILE:HG13	3:B:1815:HOH:O	2.18	0.43
1:C:219:ILE:HG13	1:C:510:ARG:HB2	2.00	0.43
1:C:767:GLN:HB2	1:C:924:ALA:HB2	2.01	0.43
1:C:1049:GLU:HB3	1:C:1075:ARG:NH1	2.32	0.43
1:D:1049:GLU:HB3	1:D:1075:ARG:NH1	2.32	0.43
1:A:401:TRP:CD1	1:A:403:PRO:HD3	2.54	0.43
1:A:1049:GLU:HB3	1:A:1075:ARG:NH1	2.32	0.43
1:B:5:THR:C	1:B:7:ASP:H	2.27	0.43
1:B:1049:GLU:HB3	1:B:1075:ARG:NH1	2.32	0.43
1:B:1058:GLU:OE2	1:B:1058:GLU:HA	2.19	0.43
1:C:5:THR:C	1:C:7:ASP:H	2.27	0.43
1:C:748:PRO:HG3	1:C:850:ASP:HB2	2.01	0.43
1:C:864:ILE:HD13	1:C:947:LEU:HD21	2.01	0.43
1:D:767:GLN:HB2	1:D:924:ALA:HB2	2.01	0.43
1:D:1139:PRO:HG3	1:D:1245:LYS:HA	2.00	0.43
1:A:5:THR:C	1:A:7:ASP:H	2.27	0.43
1:A:448:ASP:OD1	1:A:450:SER:N	2.37	0.43
1:A:1153:GLY:O	1:A:1200:PRO:HB3	2.18	0.43
1:B:1153:GLY:O	1:B:1200:PRO:HB3	2.18	0.43
1:D:219:ILE:HG13	1:D:510:ARG:HB2	2.00	0.43
1:D:318:LEU:HD23	1:D:318:LEU:HA	1.78	0.43
1:D:748:PRO:HG3	1:D:850:ASP:HB2	2.01	0.43
1:D:864:ILE:HD13	1:D:947:LEU:HD21	2.01	0.43
1:B:767:GLN:HB2	1:B:924:ALA:HB2	2.01	0.43
1:A:767:GLN:HB2	1:A:924:ALA:HB2	2.01	0.43
1:A:1139:PRO:HG3	1:A:1245:LYS:HA	2.00	0.43
1:B:101:TRP:O	3:B:1801:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:GLU:CD	1:C:994:THR:HG21	2.43	0.43
1:C:1133:ASP:HA	1:C:1240:ASP:HB3	2.01	0.43
1:D:423:ARG:HG2	1:D:534:PHE:CG	2.53	0.43
1:D:1133:ASP:HA	1:D:1240:ASP:HB3	2.01	0.43
1:B:598:LYS:HD2	1:B:598:LYS:HA	1.87	0.42
1:C:423:ARG:HG2	1:C:534:PHE:CG	2.53	0.42
1:C:558:GLY:N	1:C:771:VAL:HG12	2.33	0.42
1:D:376:GLU:CD	1:D:994:THR:HG21	2.43	0.42
1:D:558:GLY:N	1:D:771:VAL:HG12	2.33	0.42
1:D:1220:ILE:HG13	3:D:1814:HOH:O	2.18	0.42
1:B:1139:PRO:HG3	1:B:1245:LYS:HA	2.00	0.42
1:C:106:PHE:CE1	1:C:172:MET:HE3	2.53	0.42
1:C:413:PRO:HB2	1:C:446:ALA:HB2	2.00	0.42
1:D:106:PHE:CE1	1:D:172:MET:HE3	2.53	0.42
1:A:418:LEU:HB3	1:A:1047:LEU:HG	2.01	0.42
1:A:811:ILE:HG12	1:A:834:VAL:HG13	2.01	0.42
1:B:16:TYR:OH	1:D:443:ASN:OD1	2.30	0.42
1:D:413:PRO:HB2	1:D:446:ALA:HB2	2.00	0.42
1:D:661:SER:O	1:D:663:THR:HG22	2.19	0.42
1:A:376:GLU:CD	1:A:994:THR:HG21	2.43	0.42
1:B:418:LEU:HB3	1:B:1047:LEU:HG	2.01	0.42
1:C:312:TRP:CE3	1:C:338:LEU:HD22	2.55	0.42
1:C:661:SER:O	1:C:663:THR:HG22	2.18	0.42
1:C:811:ILE:HG12	1:C:834:VAL:HG13	2.02	0.42
1:D:227:PHE:HD2	1:D:227:PHE:HA	1.73	0.42
1:D:811:ILE:HG12	1:D:834:VAL:HG13	2.02	0.42
1:B:87:GLN:OE1	3:B:1803:HOH:O	2.22	0.42
1:B:376:GLU:CD	1:B:994:THR:HG21	2.43	0.42
1:B:811:ILE:HG12	1:B:834:VAL:HG13	2.02	0.42
1:C:859:GLU:HB2	1:C:887:TRP:CE2	2.54	0.42
1:D:312:TRP:CE3	1:D:338:LEU:HD22	2.55	0.42
1:A:106:PHE:CE1	1:A:172:MET:HE3	2.53	0.42
1:A:864:ILE:HD13	1:A:947:LEU:HD21	2.00	0.42
1:A:1133:ASP:HA	1:A:1240:ASP:HB3	2.01	0.42
1:B:859:GLU:HB2	1:B:887:TRP:CE2	2.55	0.42
1:C:227:PHE:HD2	1:C:227:PHE:HA	1.72	0.42
1:C:824:GLU:OE1	1:C:954:LYS:NZ	2.32	0.42
1:D:50:LEU:HD12	1:D:50:LEU:HA	1.88	0.42
1:D:424:PHE:CE2	1:D:426:THR:HG21	2.54	0.42
1:A:583:LEU:HD23	1:A:583:LEU:HA	1.87	0.42
1:A:859:GLU:HB2	1:A:887:TRP:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:PHE:CE1	1:B:172:MET:HE3	2.53	0.42
1:C:50:LEU:HD12	1:C:50:LEU:HA	1.88	0.42
1:C:361:ILE:HG12	3:C:1811:HOH:O	2.18	0.42
1:C:859:GLU:OE1	1:C:886:ARG:NH2	2.53	0.42
1:D:401:TRP:CD1	1:D:403:PRO:HD3	2.54	0.42
1:D:859:GLU:HB2	1:D:887:TRP:CE2	2.55	0.42
1:D:859:GLU:OE1	1:D:886:ARG:NH2	2.53	0.42
1:A:16:TYR:OH	1:C:443:ASN:OD1	2.30	0.42
1:A:423:ARG:HG2	1:A:534:PHE:CD1	2.55	0.42
1:B:424:PHE:CE2	1:B:426:THR:HG21	2.54	0.42
1:B:624:MET:H	1:B:624:MET:HG3	1.60	0.42
1:B:1133:ASP:HA	1:B:1240:ASP:HB3	2.01	0.42
1:C:424:PHE:CE2	1:C:426:THR:HG21	2.54	0.42
1:D:87:GLN:OE1	3:D:1802:HOH:O	2.22	0.42
1:D:352:LYS:NZ	3:D:1836:HOH:O	2.39	0.42
1:B:50:LEU:HD12	1:B:50:LEU:HA	1.88	0.42
1:B:423:ARG:HG2	1:B:534:PHE:CD1	2.55	0.42
1:B:864:ILE:HD13	1:B:947:LEU:HD21	2.01	0.42
1:C:369:ASP:HA	1:C:405:THR:HG23	2.02	0.42
1:C:401:TRP:CD1	1:C:403:PRO:HD3	2.54	0.42
1:C:423:ARG:HG2	1:C:534:PHE:CD1	2.55	0.42
1:C:727:VAL:HG22	1:C:737:LEU:HD13	2.02	0.42
1:C:742:ALA:O	1:C:744:ARG:HG2	2.20	0.42
1:D:727:VAL:HG22	1:D:737:LEU:HD13	2.02	0.42
1:D:742:ALA:O	1:D:744:ARG:HG2	2.20	0.42
1:A:50:LEU:HD12	1:A:50:LEU:HA	1.88	0.41
1:A:376:GLU:O	1:A:380:ARG:HG2	2.20	0.41
1:B:859:GLU:OE1	1:B:886:ARG:HB2	2.21	0.41
1:C:475:MET:HE2	1:C:475:MET:HB2	1.77	0.41
1:D:361:ILE:HG12	3:D:1810:HOH:O	2.18	0.41
1:D:423:ARG:HG2	1:D:534:PHE:CD1	2.55	0.41
1:D:508:LEU:HD23	1:D:508:LEU:HA	1.93	0.41
1:D:767:GLN:HB2	1:D:924:ALA:CB	2.50	0.41
1:A:859:GLU:OE1	1:A:886:ARG:HB2	2.21	0.41
1:A:1129:ASP:OD2	1:C:2:GLY:HA3	2.20	0.41
1:B:376:GLU:O	1:B:380:ARG:HG2	2.20	0.41
1:B:583:LEU:HD23	1:B:583:LEU:HA	1.87	0.41
1:C:767:GLN:HB2	1:C:924:ALA:CB	2.50	0.41
1:C:918:LEU:HD22	1:C:936:ILE:HG21	2.02	0.41
1:D:369:ASP:HA	1:D:405:THR:HG23	2.02	0.41
1:D:475:MET:HE2	1:D:475:MET:HB2	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:918:LEU:HD22	1:D:936:ILE:HG21	2.02	0.41
1:A:318:LEU:HD23	1:A:318:LEU:HA	1.78	0.41
1:A:624:MET:H	1:A:624:MET:HG3	1.60	0.41
1:A:707:LEU:HD12	1:A:797:VAL:HG22	2.02	0.41
1:A:1001:ASP:OD1	1:A:1016:SER:N	2.49	0.41
1:B:707:LEU:HD12	1:B:797:VAL:HG22	2.02	0.41
1:B:1001:ASP:OD1	1:B:1016:SER:N	2.49	0.41
1:C:418:LEU:HB3	1:C:1047:LEU:HG	2.01	0.41
1:C:742:ALA:HB3	1:C:895:TYR:HE2	1.85	0.41
1:D:418:LEU:HB3	1:D:1047:LEU:HG	2.01	0.41
1:A:312:TRP:CE3	1:A:338:LEU:HD22	2.55	0.41
1:A:424:PHE:CE2	1:A:426:THR:HG21	2.55	0.41
1:A:859:GLU:OE1	1:A:886:ARG:NH2	2.53	0.41
1:B:312:TRP:CE3	1:B:338:LEU:HD22	2.55	0.41
1:B:859:GLU:OE1	1:B:886:ARG:NH2	2.53	0.41
1:C:1227:THR:C	1:C:1229:LYS:H	2.29	0.41
1:D:742:ALA:HB3	1:D:895:TYR:HE2	1.85	0.41
1:D:1227:THR:C	1:D:1229:LYS:H	2.29	0.41
1:B:318:LEU:HD23	1:B:318:LEU:HA	1.78	0.41
1:B:1236:ARG:NH2	1:D:4:GLU:OE2	2.54	0.41
1:C:303:GLU:OE1	3:C:1803:HOH:O	2.22	0.41
1:C:859:GLU:OE1	1:C:886:ARG:HB2	2.20	0.41
1:D:164:LYS:HA	1:D:164:LYS:HD2	1.93	0.41
1:A:2:GLY:HA3	1:C:1129:ASP:OD2	2.21	0.41
1:A:539:ARG:CZ	1:A:1220:ILE:HB	2.51	0.41
1:A:722:ASN:HB3	1:A:725:LEU:H	1.86	0.41
1:B:4:GLU:OE2	1:D:1236:ARG:NH2	2.54	0.41
1:B:539:ARG:CZ	1:B:1220:ILE:HB	2.51	0.41
1:B:722:ASN:HB3	1:B:725:LEU:H	1.86	0.41
1:C:157:PRO:C	1:C:159:SER:H	2.29	0.41
1:C:508:LEU:HD23	1:C:508:LEU:HA	1.93	0.41
1:D:157:PRO:C	1:D:159:SER:H	2.29	0.41
1:D:424:PHE:CE2	1:D:426:THR:HG22	2.55	0.41
1:D:660:MET:HG3	1:D:665:THR:HG21	2.03	0.41
1:A:742:ALA:HB3	1:A:895:TYR:HE2	1.85	0.41
1:B:2:GLY:HA3	1:D:1129:ASP:OD2	2.21	0.41
1:B:227:PHE:HD2	1:B:227:PHE:HA	1.73	0.41
1:B:424:PHE:CE2	1:B:426:THR:HG22	2.55	0.41
1:B:475:MET:HE2	1:B:475:MET:HB2	1.77	0.41
1:C:194:LYS:HZ2	1:C:194:LYS:HG2	1.76	0.41
1:C:315:GLN:HG3	1:C:327:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:660:MET:HG3	1:C:665:THR:HG21	2.03	0.41
1:C:817:LEU:HD12	1:C:817:LEU:HA	1.88	0.41
1:D:315:GLN:HG3	1:D:327:PHE:CE1	2.56	0.41
1:D:859:GLU:OE1	1:D:886:ARG:HB2	2.21	0.41
1:A:475:MET:HE2	1:A:475:MET:HB2	1.77	0.41
1:A:1227:THR:C	1:A:1229:LYS:H	2.29	0.41
1:B:742:ALA:HB3	1:B:895:TYR:HE2	1.85	0.41
1:D:352:LYS:HA	1:D:352:LYS:HD3	1.86	0.41
1:D:370:THR:OG1	1:D:408:TYR:HA	2.21	0.41
1:D:707:LEU:HD12	1:D:797:VAL:HG22	2.02	0.41
1:A:4:GLU:OE2	1:C:1236:ARG:NH2	2.54	0.41
1:A:369:ASP:HA	1:A:405:THR:HG23	2.02	0.41
1:A:678:LEU:HD23	1:A:678:LEU:HA	1.93	0.41
1:A:681:ILE:HD12	1:A:681:ILE:C	2.46	0.41
1:A:853:ASN:ND2	1:A:855:GLU:HG3	2.36	0.41
1:B:678:LEU:HD23	1:B:678:LEU:HA	1.93	0.41
1:B:681:ILE:HD12	1:B:681:ILE:C	2.46	0.41
1:B:853:ASN:ND2	1:B:855:GLU:HG3	2.36	0.41
1:B:1129:ASP:OD2	1:D:2:GLY:HA3	2.21	0.41
1:B:1227:THR:C	1:B:1229:LYS:H	2.29	0.41
1:C:352:LYS:HA	1:C:352:LYS:HD3	1.86	0.41
1:C:370:THR:OG1	1:C:408:TYR:HA	2.21	0.41
1:C:424:PHE:CE2	1:C:426:THR:HG22	2.55	0.41
1:C:707:LEU:HD12	1:C:797:VAL:HG22	2.02	0.41
1:C:853:ASN:ND2	1:C:855:GLU:HG3	2.36	0.41
1:C:1199:GLN:CD	1:C:1199:GLN:H	2.29	0.41
1:D:376:GLU:O	1:D:380:ARG:HG2	2.20	0.41
1:D:1199:GLN:CD	1:D:1199:GLN:H	2.29	0.41
1:A:227:PHE:HD2	1:A:227:PHE:HA	1.72	0.41
1:A:417:ARG:HA	1:A:417:ARG:HD2	1.72	0.41
1:A:424:PHE:CE2	1:A:426:THR:HG22	2.56	0.41
1:A:855:GLU:OE2	1:A:866:ARG:HG2	2.21	0.41
1:B:369:ASP:HA	1:B:405:THR:HG23	2.02	0.41
1:B:855:GLU:OE2	1:B:866:ARG:HG2	2.21	0.41
1:C:376:GLU:O	1:C:380:ARG:HG2	2.20	0.41
1:C:423:ARG:HG2	1:C:534:PHE:HB3	2.02	0.41
1:D:303:GLU:OE1	3:D:1803:HOH:O	2.22	0.41
1:D:853:ASN:ND2	1:D:855:GLU:HG3	2.36	0.41
1:A:157:PRO:C	1:A:159:SER:H	2.29	0.40
1:B:157:PRO:C	1:B:159:SER:H	2.29	0.40
1:C:681:ILE:HD12	1:C:681:ILE:C	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:423:ARG:HG2	1:D:534:PHE:HB3	2.02	0.40
1:D:681:ILE:HD12	1:D:681:ILE:C	2.46	0.40
1:A:579:ASP:OD1	1:A:579:ASP:C	2.65	0.40
1:A:660:MET:HG3	1:A:665:THR:HG21	2.03	0.40
1:A:662:THR:N	3:A:1849:HOH:O	2.54	0.40
1:B:370:THR:OG1	1:B:408:TYR:HA	2.21	0.40
1:B:579:ASP:OD1	1:B:579:ASP:C	2.64	0.40
1:B:660:MET:HG3	1:B:665:THR:HG21	2.03	0.40
1:D:747:ILE:HD12	1:D:753:ALA:HB2	2.04	0.40
1:A:81:GLU:HA	1:A:81:GLU:OE2	2.21	0.40
1:A:457:PRO:HA	1:A:458:PRO:HD3	1.97	0.40
1:A:567:LYS:NZ	1:A:617:LEU:O	2.49	0.40
1:A:1236:ARG:NH2	1:C:4:GLU:OE2	2.54	0.40
1:B:81:GLU:HA	1:B:81:GLU:OE2	2.21	0.40
1:B:423:ARG:HG2	1:B:534:PHE:HB3	2.02	0.40
1:B:918:LEU:HD22	1:B:936:ILE:HG21	2.02	0.40
1:C:747:ILE:HD12	1:C:753:ALA:HB2	2.04	0.40
1:D:81:GLU:HA	1:D:81:GLU:OE2	2.21	0.40
1:A:315:GLN:HG3	1:A:327:PHE:CE1	2.56	0.40
1:A:370:THR:OG1	1:A:408:TYR:HA	2.21	0.40
1:A:681:ILE:HG22	1:A:964:LEU:HD13	2.02	0.40
1:A:727:VAL:HG22	1:A:737:LEU:HD13	2.02	0.40
1:B:417:ARG:HA	1:B:417:ARG:HD2	1.72	0.40
1:B:1199:GLN:CD	1:B:1199:GLN:H	2.29	0.40
1:C:81:GLU:HA	1:C:81:GLU:OE2	2.21	0.40
1:C:722:ASN:HB3	1:C:725:LEU:H	1.86	0.40
1:D:133:LEU:HD13	1:D:310:ARG:HA	2.03	0.40
1:D:722:ASN:HB3	1:D:725:LEU:H	1.86	0.40
1:A:303:GLU:OE1	3:A:1804:HOH:O	2.22	0.40
1:A:423:ARG:HG2	1:A:534:PHE:HB3	2.02	0.40
1:A:747:ILE:HD12	1:A:753:ALA:HB2	2.04	0.40
1:A:767:GLN:HB2	1:A:924:ALA:CB	2.50	0.40
1:A:918:LEU:HD22	1:A:936:ILE:HG21	2.02	0.40
1:A:1128:ARG:HG2	1:A:1148:VAL:CG2	2.52	0.40
1:A:1216:ALA:HB2	1:A:1245:LYS:HB2	2.04	0.40
1:B:315:GLN:HG3	1:B:327:PHE:CE1	2.56	0.40
1:B:457:PRO:HA	1:B:458:PRO:HD3	1.97	0.40
1:B:567:LYS:NZ	1:B:617:LEU:O	2.49	0.40
1:B:727:VAL:HG22	1:B:737:LEU:HD13	2.02	0.40
1:B:747:ILE:HD12	1:B:753:ALA:HB2	2.04	0.40
1:B:767:GLN:HB2	1:B:924:ALA:CB	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1128:ARG:HG2	1:B:1148:VAL:CG2	2.52	0.40
1:B:1216:ALA:HB2	1:B:1245:LYS:HB2	2.04	0.40
1:C:133:LEU:HD13	1:C:310:ARG:HA	2.03	0.40
1:C:681:ILE:HG22	1:C:964:LEU:HD13	2.02	0.40
1:D:681:ILE:HG22	1:D:964:LEU:HD13	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1174/1616 (73%)	1066 (91%)	108 (9%)	0	100	100
1	B	1174/1616 (73%)	1065 (91%)	109 (9%)	0	100	100
1	C	1174/1616 (73%)	1064 (91%)	110 (9%)	0	100	100
1	D	1174/1616 (73%)	1065 (91%)	109 (9%)	0	100	100
All	All	4696/6464 (73%)	4260 (91%)	436 (9%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	1023/1368 (75%)	990 (97%)	33 (3%)	34	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	1023/1368 (75%)	990 (97%)	33 (3%)	34	47
1	C	1023/1368 (75%)	989 (97%)	34 (3%)	33	45
1	D	1023/1368 (75%)	990 (97%)	33 (3%)	34	47
All	All	4092/5472 (75%)	3959 (97%)	133 (3%)	34	45

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	VAL
1	A	29	SER
1	A	53	MET
1	A	67	LEU
1	A	100	SER
1	A	103	THR
1	A	158	ASP
1	A	167	THR
1	A	426	THR
1	A	463	THR
1	A	472	LYS
1	A	495	ASP
1	A	559	THR
1	A	629	SER
1	A	647	VAL
1	A	665	THR
1	A	680	LYS
1	A	692	THR
1	A	704	THR
1	A	710	LEU
1	A	754	ASN
1	A	807	ASP
1	A	935	HIS
1	A	974	VAL
1	A	1058	GLU
1	A	1123	GLU
1	A	1130	THR
1	A	1142	LEU
1	A	1163	VAL
1	A	1174	VAL
1	A	1199	GLN
1	A	1212	THR
1	A	1241	VAL

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Mol	Chain	Res	Type
1	B	24	VAL
1	B	29	SER
1	B	53	MET
1	B	67	LEU
1	B	100	SER
1	B	103	THR
1	B	158	ASP
1	B	167	THR
1	B	426	THR
1	B	463	THR
1	B	472	LYS
1	B	495	ASP
1	B	559	THR
1	B	629	SER
1	B	647	VAL
1	B	665	THR
1	B	680	LYS
1	B	692	THR
1	B	704	THR
1	B	710	LEU
1	B	754	ASN
1	B	807	ASP
1	B	935	HIS
1	B	974	VAL
1	B	1058	GLU
1	B	1123	GLU
1	B	1130	THR
1	B	1142	LEU
1	B	1163	VAL
1	B	1174	VAL
1	B	1199	GLN
1	B	1212	THR
1	B	1241	VAL
1	C	24	VAL
1	C	29	SER
1	C	53	MET
1	C	67	LEU
1	C	100	SER
1	C	103	THR
1	C	158	ASP
1	C	167	THR
1	C	426	THR

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Mol	Chain	Res	Type
1	C	463	THR
1	C	472	LYS
1	C	495	ASP
1	C	559	THR
1	C	629	SER
1	C	647	VAL
1	C	665	THR
1	C	680	LYS
1	C	692	THR
1	C	704	THR
1	C	710	LEU
1	C	735	THR
1	C	754	ASN
1	C	807	ASP
1	C	935	HIS
1	C	974	VAL
1	C	1058	GLU
1	C	1123	GLU
1	C	1130	THR
1	C	1142	LEU
1	C	1163	VAL
1	C	1174	VAL
1	C	1199	GLN
1	C	1212	THR
1	C	1241	VAL
1	D	24	VAL
1	D	29	SER
1	D	53	MET
1	D	67	LEU
1	D	100	SER
1	D	103	THR
1	D	158	ASP
1	D	167	THR
1	D	426	THR
1	D	463	THR
1	D	472	LYS
1	D	495	ASP
1	D	559	THR
1	D	629	SER
1	D	647	VAL
1	D	665	THR
1	D	680	LYS

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Mol	Chain	Res	Type
1	D	692	THR
1	D	704	THR
1	D	710	LEU
1	D	754	ASN
1	D	807	ASP
1	D	935	HIS
1	D	974	VAL
1	D	1058	GLU
1	D	1123	GLU
1	D	1130	THR
1	D	1142	LEU
1	D	1163	VAL
1	D	1174	VAL
1	D	1199	GLN
1	D	1212	THR
1	D	1241	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	ASN
1	A	92	ASN
1	A	143	GLN
1	A	166	HIS
1	A	180	ASN
1	A	290	HIS
1	A	477	GLN
1	A	755	GLN
1	A	944	GLN
1	A	1235	HIS
1	B	86	ASN
1	B	143	GLN
1	B	166	HIS
1	B	180	ASN
1	B	290	HIS
1	B	477	GLN
1	B	755	GLN
1	B	944	GLN
1	B	1235	HIS
1	C	86	ASN
1	C	92	ASN
1	C	143	GLN

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Mol	Chain	Res	Type
1	C	166	HIS
1	C	290	HIS
1	C	590	GLN
1	C	755	GLN
1	C	825	GLN
1	C	944	GLN
1	C	1235	HIS
1	D	86	ASN
1	D	92	ASN
1	D	143	GLN
1	D	166	HIS
1	D	290	HIS
1	D	755	GLN
1	D	825	GLN
1	D	944	GLN
1	D	1235	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 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

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-32091. 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

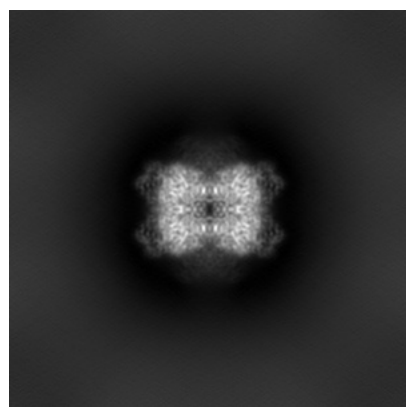


Y

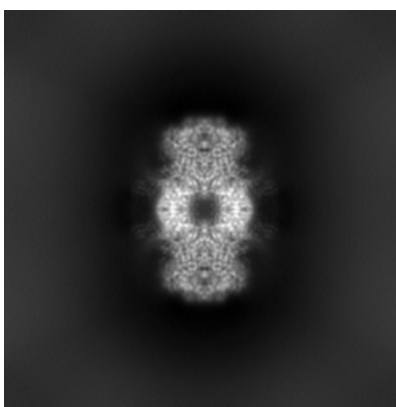


Z

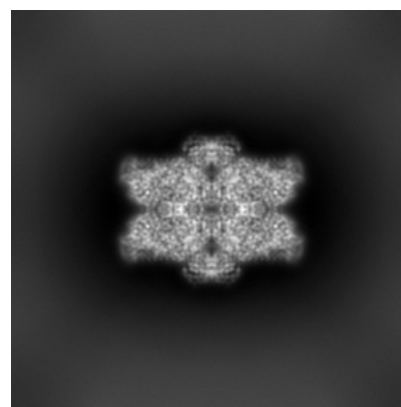
6.1.2 Raw map



X



Y



Z

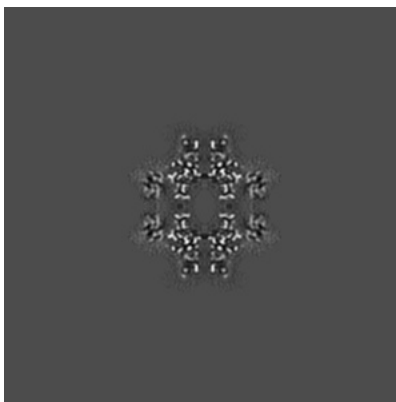
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

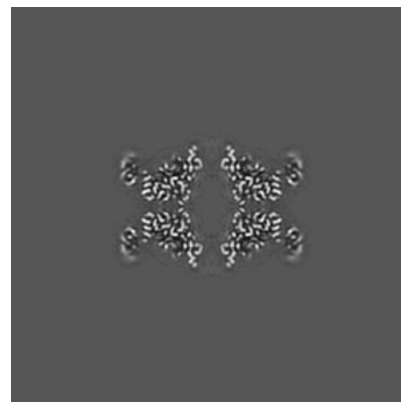
6.2.1 Primary map



X Index: 160

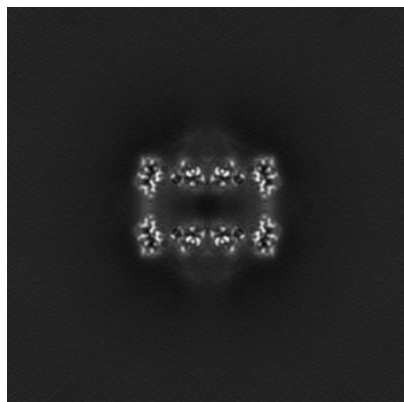


Y Index: 160

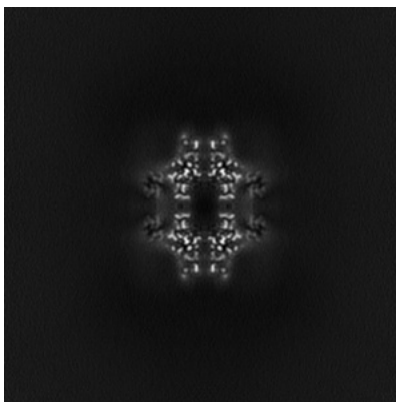


Z Index: 160

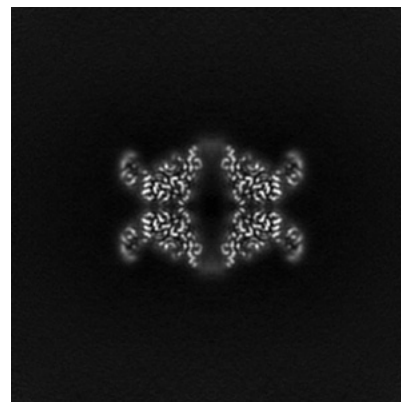
6.2.2 Raw map



X Index: 160



Y Index: 160

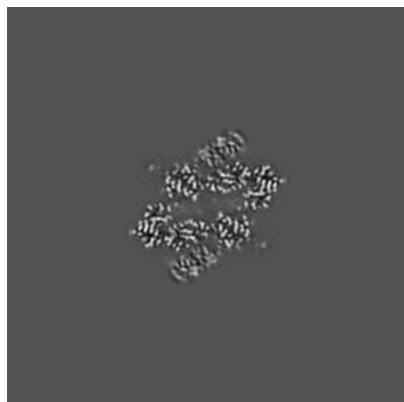


Z Index: 160

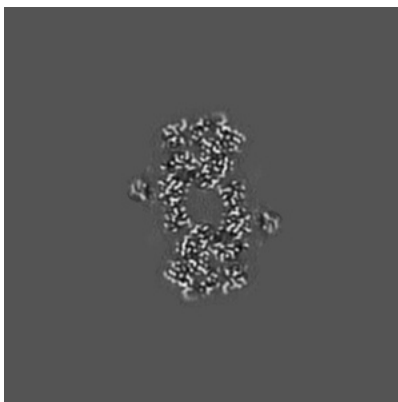
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

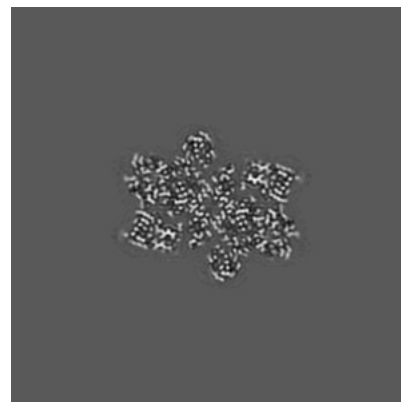
6.3.1 Primary map



X Index: 173

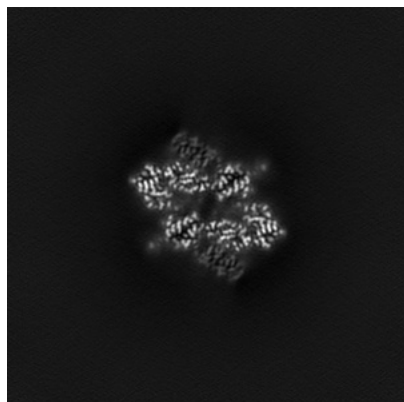


Y Index: 138

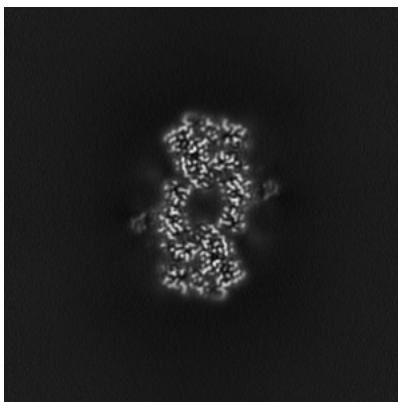


Z Index: 143

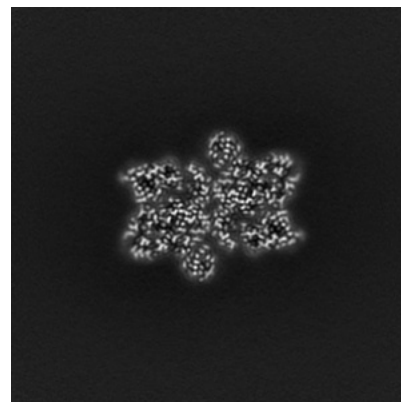
6.3.2 Raw map



X Index: 147



Y Index: 182

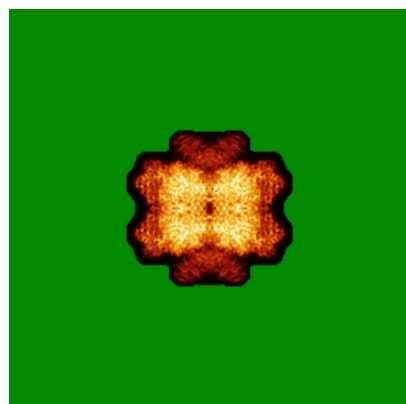


Z Index: 176

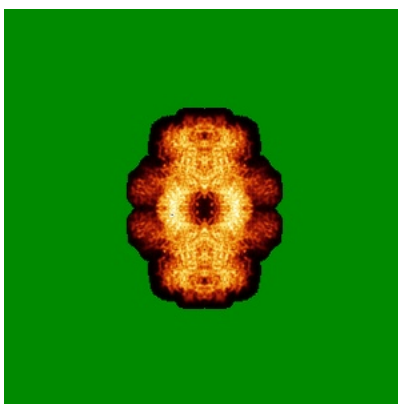
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

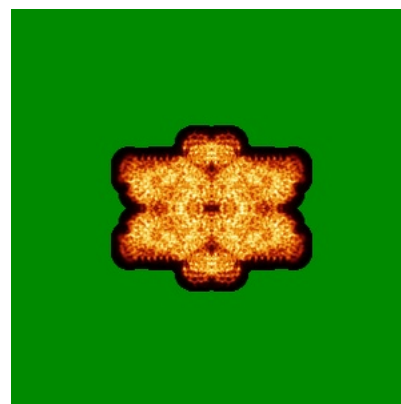
6.4.1 Primary map



X

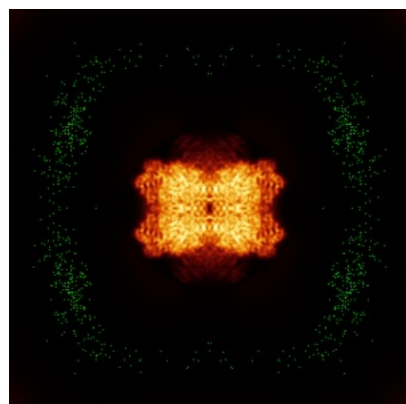


Y

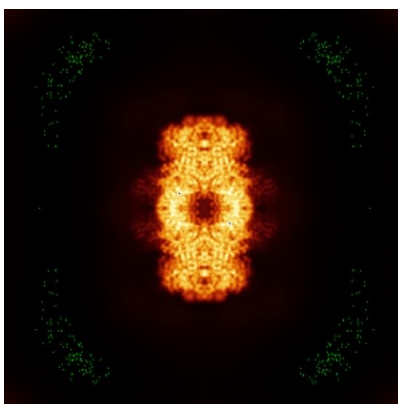


Z

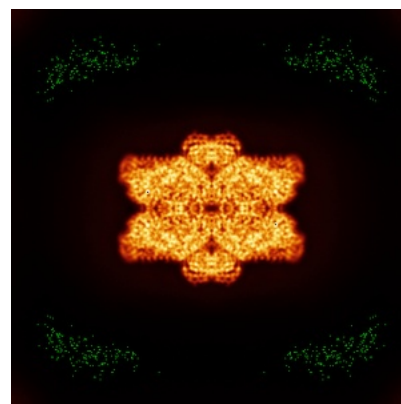
6.4.2 Raw map



X



Y

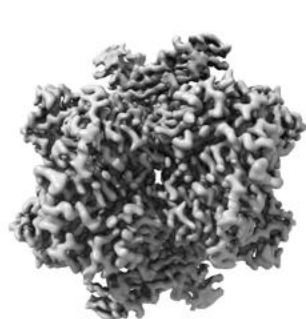


Z

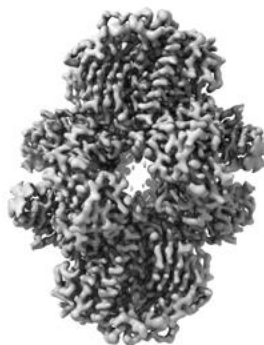
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



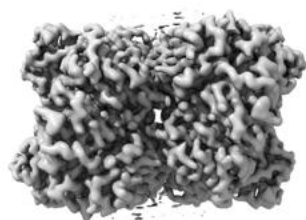
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 10.0. 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



X



Y



Z

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.

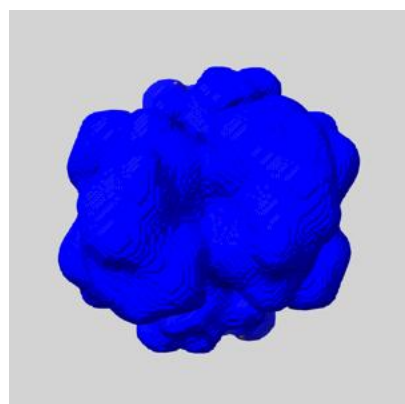
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

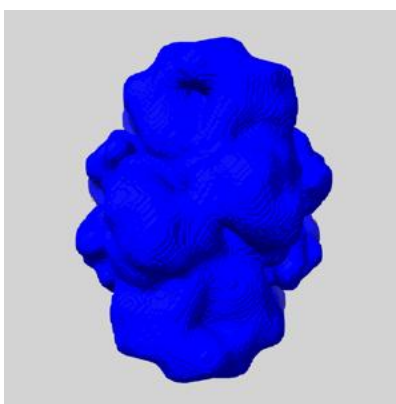
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

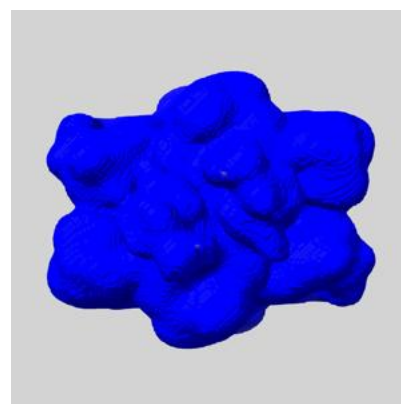
6.6.1 emd_32091_msk_1.map [i](#)



X



Y

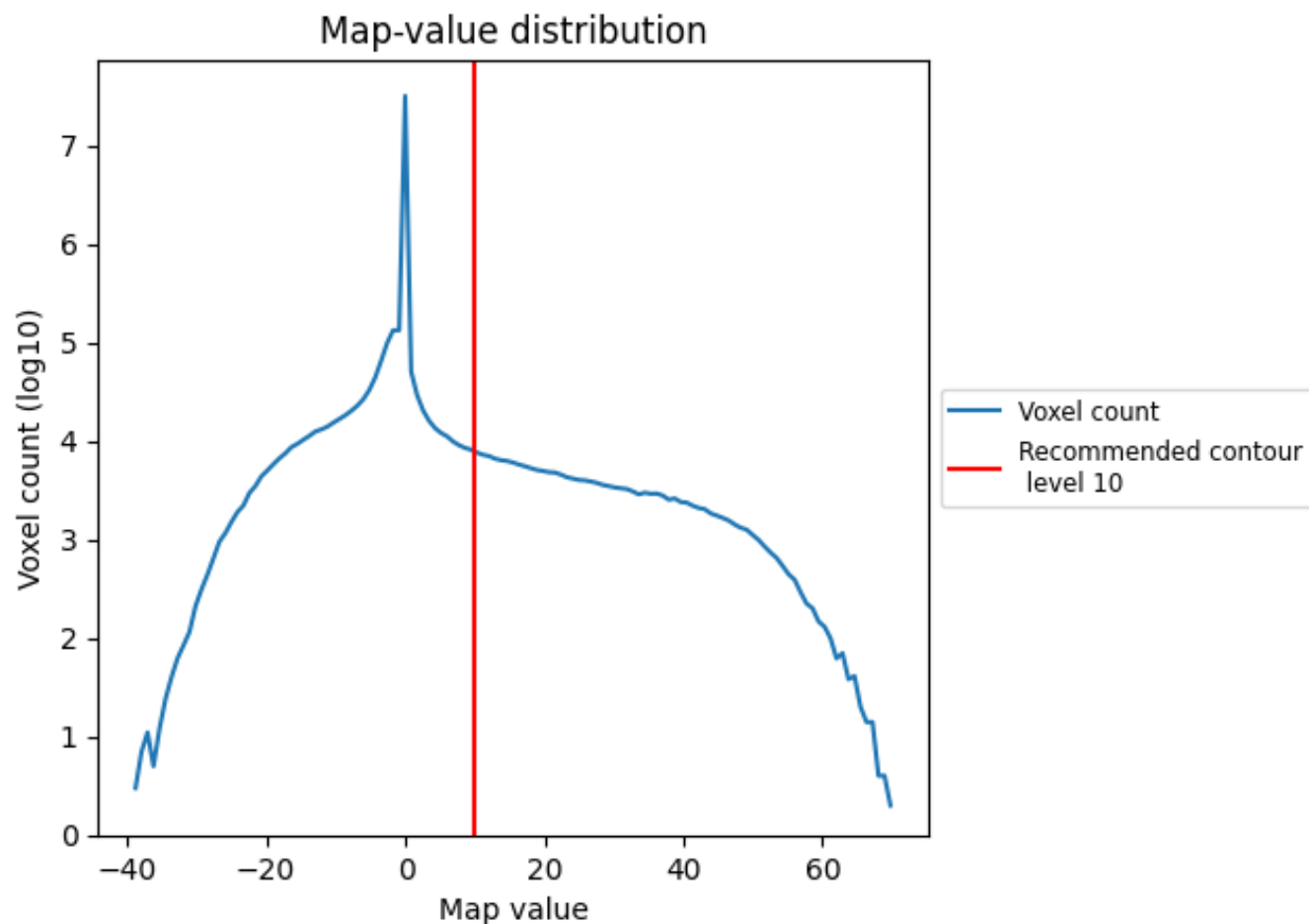


Z

7 Map analysis [i](#)

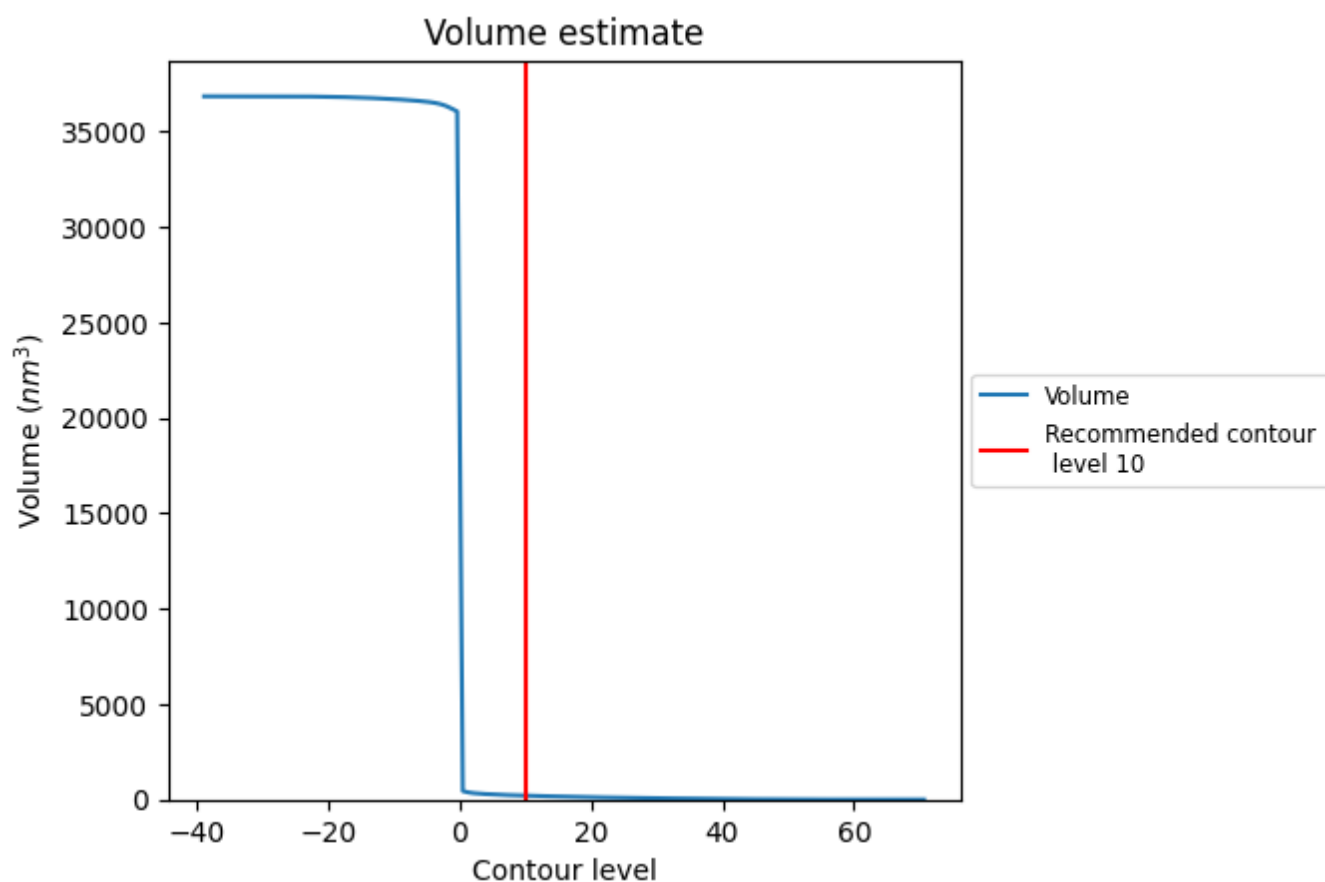
This section contains the results of statistical analysis of the map.

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.

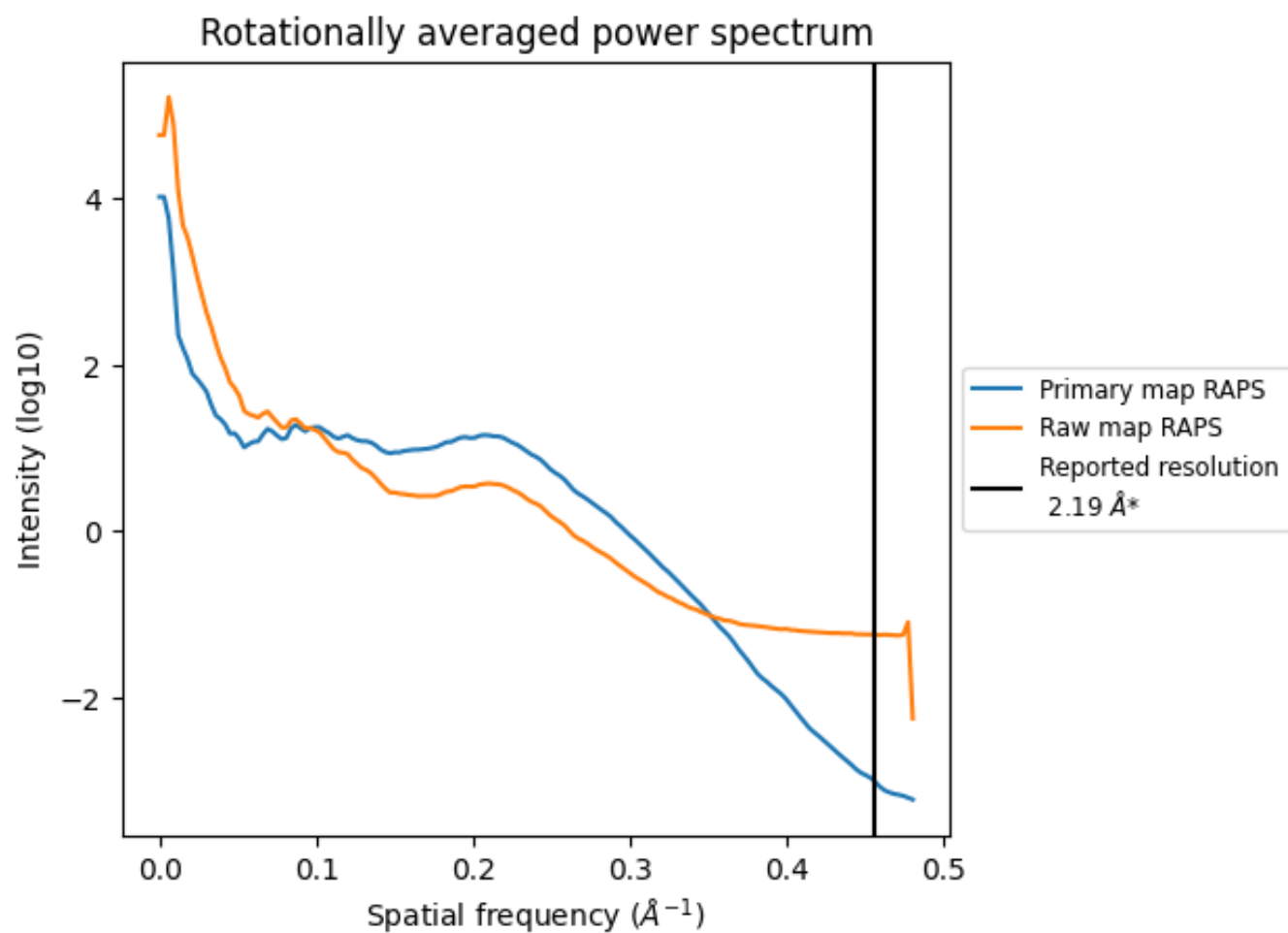
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 206 nm^3 ; this corresponds to an approximate mass of 186 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 [i](#)

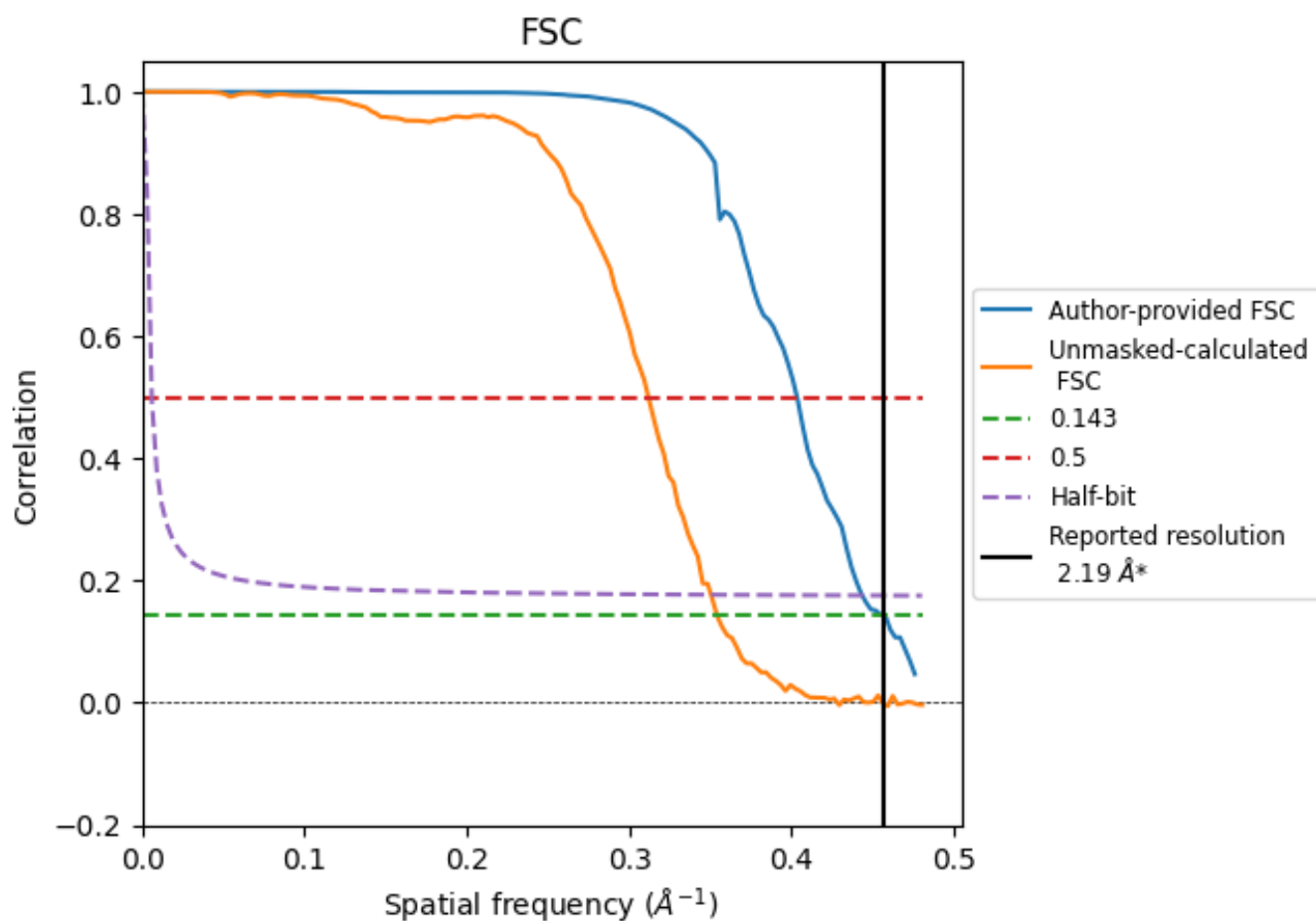


*Reported resolution corresponds to spatial frequency of 0.457 Å⁻¹

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 0.457 Å⁻¹

8.2 Resolution estimates [i](#)

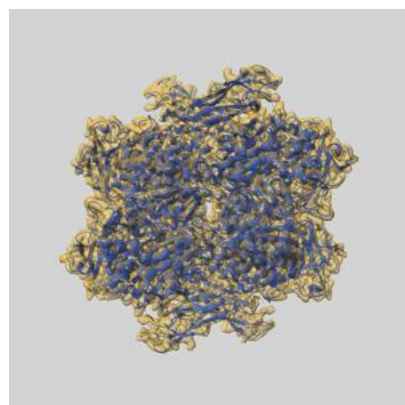
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.19	-	-
Author-provided FSC curve	2.19	2.48	2.25
Unmasked-calculated*	2.82	3.20	2.85

*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 2.82 differs from the reported value 2.19 by more than 10 %

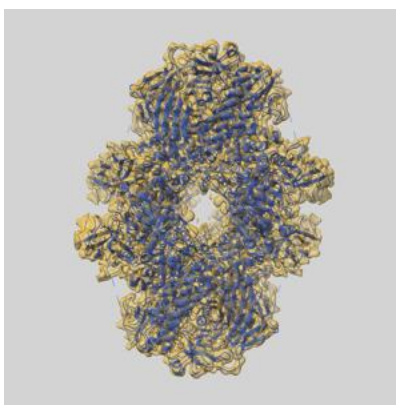
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32091 and PDB model 7VQO. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

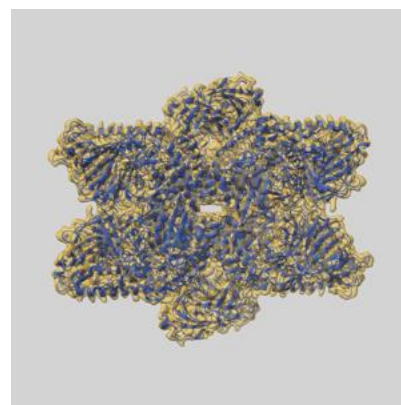
9.1 Map-model overlay [i](#)



X



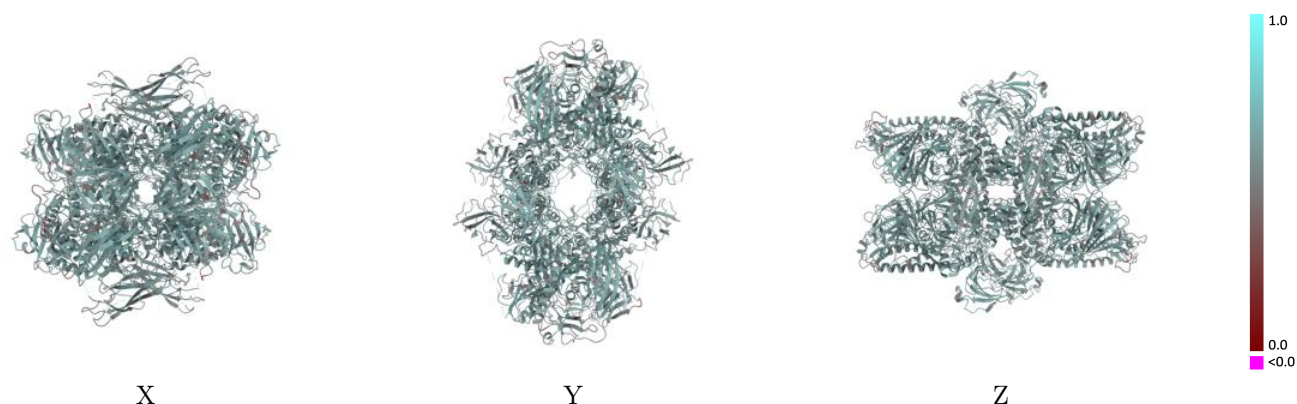
Y



Z

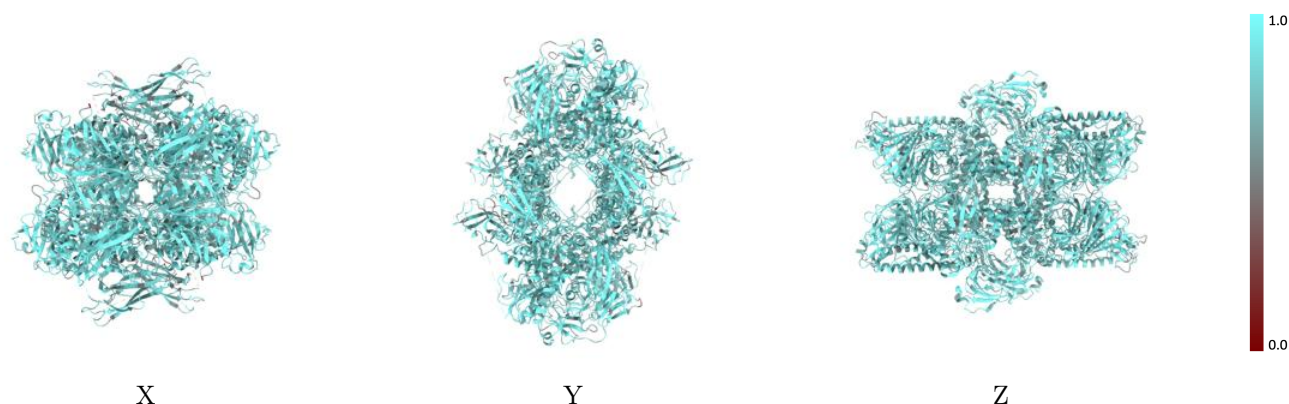
The images above show the 3D surface view of the map at the recommended contour level 10.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



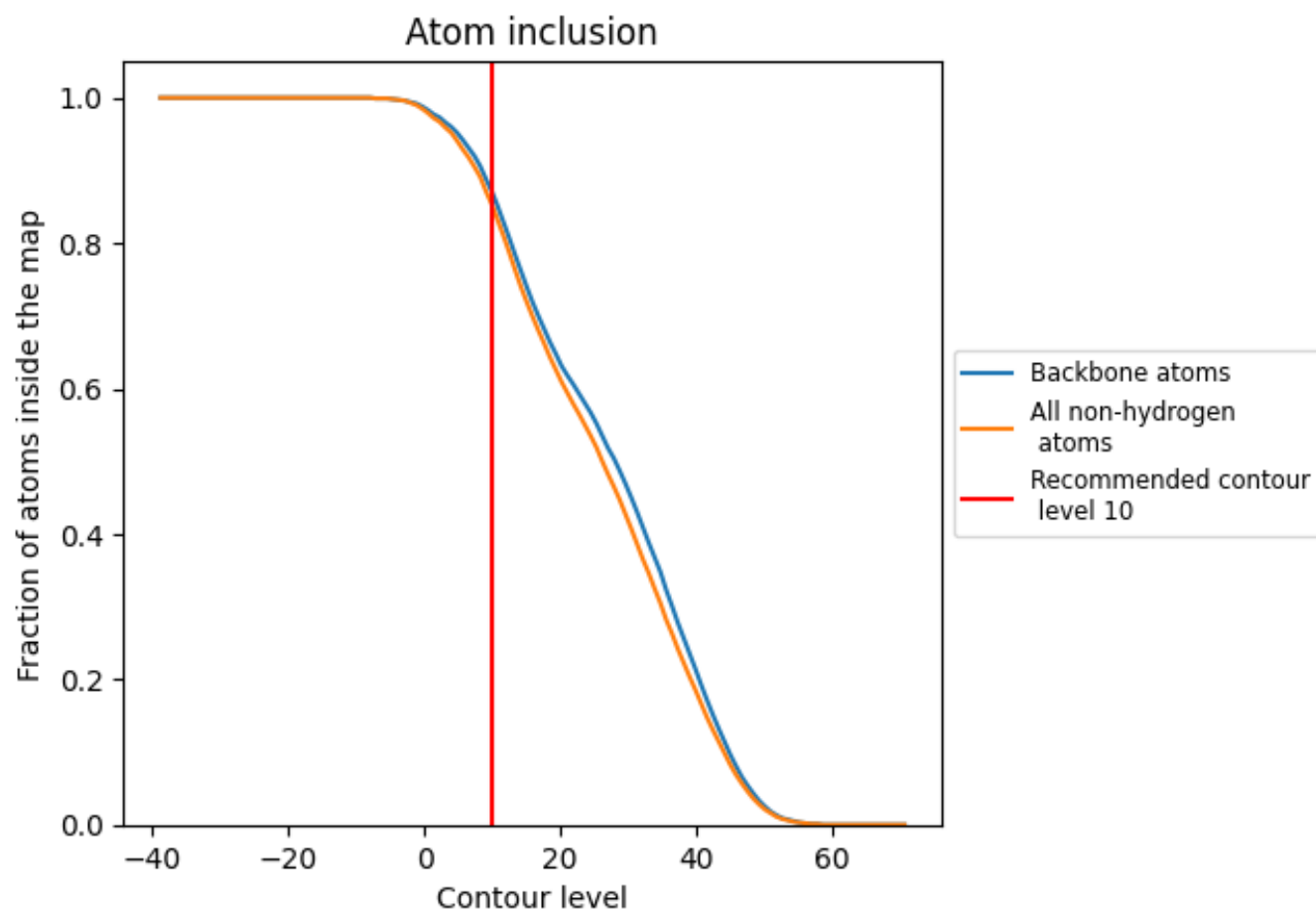
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (10).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 85% 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 (10) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8520	0.5830
A	0.8550	0.5840
B	0.8580	0.5840
C	0.8540	0.5830
D	0.8580	0.5830

