



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 11:06 PM UTC

PDB ID : 6JPQ / pdb_00006jpq
EMDB ID : EMD-9870
Title : CryoEM structure of Abo1 hexamer - ADP complex
Authors : Cho, C.; Jang, J.; Song, J.J.
Deposited on : 2019-03-27
Resolution : 4.44 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:

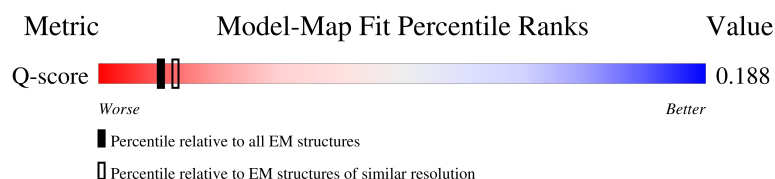
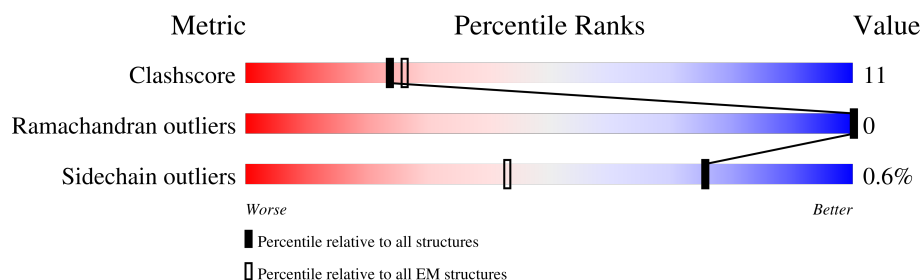
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.44 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	3025 (3.95 - 4.94)

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	1198	 5% 35% 13% 52%
1	B	1198	 5% 35% 13% 52%
1	C	1198	 5% 34% 14% 52%
1	D	1198	 5% 35% 13% 52%

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Mol	Chain	Length	Quality of chain
1	E	1198	 34% 14% 52%
1	F	1198	 5% 35% 13% 52%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 27768 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 Uncharacterized AAA domain-containing protein C31G5.19.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	577	Total	C	N	O	S	0	0
			4628	2963	789	854	22		
1	B	577	Total	C	N	O	S	0	0
			4628	2963	789	854	22		
1	C	577	Total	C	N	O	S	0	0
			4628	2963	789	854	22		
1	D	577	Total	C	N	O	S	0	0
			4628	2963	789	854	22		
1	E	577	Total	C	N	O	S	0	0
			4628	2963	789	854	22		
1	F	577	Total	C	N	O	S	0	0
			4628	2963	789	854	22		

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP O14114
A	-6	ALA	-	expression tag	UNP O14114
A	-5	MET	-	expression tag	UNP O14114
A	-4	GLY	-	expression tag	UNP O14114
A	-3	SER	-	expression tag	UNP O14114
A	-2	GLY	-	expression tag	UNP O14114
A	-1	ILE	-	expression tag	UNP O14114
A	0	GLN	-	expression tag	UNP O14114
B	-7	GLY	-	expression tag	UNP O14114
B	-6	ALA	-	expression tag	UNP O14114
B	-5	MET	-	expression tag	UNP O14114
B	-4	GLY	-	expression tag	UNP O14114
B	-3	SER	-	expression tag	UNP O14114
B	-2	GLY	-	expression tag	UNP O14114
B	-1	ILE	-	expression tag	UNP O14114
B	0	GLN	-	expression tag	UNP O14114
C	-7	GLY	-	expression tag	UNP O14114
C	-6	ALA	-	expression tag	UNP O14114

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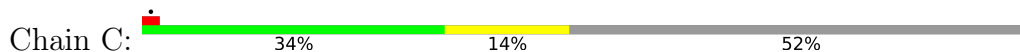
Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	MET	-	expression tag	UNP O14114
C	-4	GLY	-	expression tag	UNP O14114
C	-3	SER	-	expression tag	UNP O14114
C	-2	GLY	-	expression tag	UNP O14114
C	-1	ILE	-	expression tag	UNP O14114
C	0	GLN	-	expression tag	UNP O14114
D	-7	GLY	-	expression tag	UNP O14114
D	-6	ALA	-	expression tag	UNP O14114
D	-5	MET	-	expression tag	UNP O14114
D	-4	GLY	-	expression tag	UNP O14114
D	-3	SER	-	expression tag	UNP O14114
D	-2	GLY	-	expression tag	UNP O14114
D	-1	ILE	-	expression tag	UNP O14114
D	0	GLN	-	expression tag	UNP O14114
E	-7	GLY	-	expression tag	UNP O14114
E	-6	ALA	-	expression tag	UNP O14114
E	-5	MET	-	expression tag	UNP O14114
E	-4	GLY	-	expression tag	UNP O14114
E	-3	SER	-	expression tag	UNP O14114
E	-2	GLY	-	expression tag	UNP O14114
E	-1	ILE	-	expression tag	UNP O14114
E	0	GLN	-	expression tag	UNP O14114
F	-7	GLY	-	expression tag	UNP O14114
F	-6	ALA	-	expression tag	UNP O14114
F	-5	MET	-	expression tag	UNP O14114
F	-4	GLY	-	expression tag	UNP O14114
F	-3	SER	-	expression tag	UNP O14114
F	-2	GLY	-	expression tag	UNP O14114
F	-1	ILE	-	expression tag	UNP O14114
F	0	GLN	-	expression tag	UNP O14114

- Molecule 1: Uncharacterized AAA domain-containing protein C31G5.19

VAL	L769	L671	D518	D431	R336	PRO	SER	ARG	GLU	GLY
ASP	P770	P519	F519	R432	K337	ALA	GLN	SER	ASP	ALA
PRO		D520	D520	R432	K337	ASN	SER	GLN	GLU	GLU
THR	P773	P672	P520	E433	K337	SER	GLY	PRO	GLY	GLY
GLY		P673	L549	L438	L342	GLY	GLN	LYS	ASP	GLY
GLY		P674	N550	L438	S343	GLY	GLN	TVR	GLY	GLY
HIS		L678		L438	S343	PRO	SER	LYS	ASP	ILE
PRO		P679		P439	K344	PRO	ARG	PRO	TRP	GLN
PRO		P680		D440	K345	ASP	SER	GLY	GLU	GLY
TVR		T681		R444	V346	PHE	ARG	THR	GLU	LYS
ARG		T682		R445	V347	GLY	LYS	THR	GLU	GLY
SER		A682		K445	G347	ARG	THR	ARG	GLU	GLU
ARG		L683		T448	E348	ILE	HIS	SER	HIS	ALA
GLN		T684		T448	A349	GLU	GLU	THR	GLU	ALA
LYS		P685		R451	E350	GLU	GLU	ARG	PRO	GLU
ILE		T685		R451	R351	LYS	LEU	LEU	LYS	HIS
THR		F686		R456	L356	SER	ALA	ARG	ALA	ALA
LEU		S687		P460	Q364	ASP	ILE	ASN	LYS	GLY
LYS		S688		D456	P365	LEU	THR	ARG	ARG	SER
GLN		P689		P460	P365	ALA	LYS	THR	ARG	SER
THR		L690		L463	S366	ASP	THR	ARG	ARG	ALA
VAL		L693		C464	S366	SER	LYS	ARG	ALA	ALA
ASP		D694		S465	I367	ASP	LEU	GLN	TYR	ASP
ASP		F695		S465	I367	ASP	LEU	GLN	ASN	GLU
VAL		S696		S471	I373	P256	GLN	GLU	THR	THR
ASP		P697		R471	I373	P257	GLN	GLU	ARG	GLN
LYS		D698		K472	L376	L257	GLN	GLU	SER	GLU
GLN		P708		D478	L376	C258	VAL	GLU	ASN	LEU
LYS		L712		R480	A377	V259	SER	GLU	GLU	SER
ILE		L712		R481	P378	D260	SER	GLU	PRO	PRO
PHE		L712		R481	A378	S261	PHE	GLU	PHE	VAL
MET		R717		L482	V379	S262	MET	GLU	SER	VAL
ALA		E718		L482	V379	L263	GLU	HIS	SER	SER
LEU		P634		E485	R380	S262	PRO	GLU	ASP	ASP
LEU		D635		E485	S382	L263	ILE	PRO	GLY	SER
LEU		P636		E485	K383	F295	ASP	ILE	ASP	ASP
LEU		S722		E485	Q384	Q298	LEU	LEU	GLU	GLU
GLY		K723		E485	Q384	Q298	GLY	GLU	PHE	PRO
GLY		S724		L488	Q386	R301	SER	THR	VAL	ASN
SER		D724		L488	Q386	R301	SER	ARG	VAL	ALA
LEU		S725		M489	I387	L304	GLU	SER	GLU	LYS
ARG		T733		S490	H388	F305	SER	ILE	GLU	LYS
ALA		R734		T491	H388	H306	ASP	ARG	SER	ARG
ARG		D735		R492	A389	G307	ASN	TYR	SER	ARG
THR		T736		R493	V392	THR	THR	SER	LEU	ARG
TRP		S736		T494	V392	G310	VAL	VAL	GLU	SER
ASP		I737		Y495	G401	G310	ILE	PRO	ASP	GLN
ASN		P741		P496	M402	K313	LYS	LEU	GLU	SER
CYS		L744		E648	M402	K313	LYS	ALA	LEU	MET
LYS		L744		S650	R405	M316	LYS	PHE	LEU	SER
LYS		L744		T651	R405	A317	SER	PRO	SER	ILE
PRO		L744		Y499	Q407	R318	ALA	PRO	ASP	ALA
THR		L747		B500	Y408	A319	LYS	VAL	GLU	LYS
PRO		L747		K503	Y408	A319	THR	ASP		

R1130	P1133	L1134	L1137	S1141	T1142	T1143	D1148	L1151	H1152	S1155	K1165	R1170	D1175	E1178	T1186	ASN	ALA	LEU	GLN
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- Molecule 1: Uncharacterized AAA domain-containing protein C31G5.19



GLU	CYS	THR	T684	D440	P572	T684	T685	R336	PRO	SER	ARG	GLU	GLY	ALA	GLY
HIS	TYR	LEU	F686	R444	E575	S687	S688	D340	ASN	SER	SER	GLN	LYS	ASP	ASP
GLU	PHE	THR	T689	I448	V576	T690	T691	C341	GLY	ASN	VAL	LYS	PRO	GLY	GLY
VAL	ASP	LYS	L690	H451	Y578	L691	L692	L342	PRO	SER	LYS	TVR	GLY	ASP	GLY
ASP	ASP	GLN	D693	Y588	Y588	D694	D695	S343	PRO	ARG	PRO	LYS	TRP	TRP	GLN
ASP	VAL	ALA	L696	Q589	Q589	Q590	Q591	K344	ASP	SER	THR	GLY	GLU	GLU	LYS
VAL	VAL	MET	F695	D456	Q590	F696	F697	W345	PHE	ARG	GLY	ARG	GLU	GLU	LYS
LYS	LYS	ARG	S696	R691	R691	S697	S698	V346	ARG	THR	ARG	ARG	GLU	GLU	GLY
GLN	LEU	LEU	D697	P460	L592	Q698	Q699	G347	ILE	HIS	SER	HIS	HIS	ALA	ALA
ILE	GLY	LEU	Q698	E593	E593	L699	L700	E348	ARG	THR	THR	LYS	LYS	SER	SER
LYS	SER	ASN	L700	L463	T594	F595	F596	A349	GLU	GLU	ARG	PRO	PRO	GLU	HIS
ASP	ASP	LEU	S707	S465	E596	E597	E598	E350	SER	ALA	ARG	ALA	ALA	ALA	GLY
GLN	GLN	LYS	S707	T597	T597	L598	L599	R351	ASP	ILE	ASN	LYS	LYS	GLY	GLY
LYS	LYS	ILE	P708	S471	L598	R599	I600	L356	LEU	THR	ARG	ARG	ARG	ARG	GLY
PHE	PHE	LYS	L712	K472	R599	I600	I601	Q364	ALA	LYS	ARG	ARG	ARG	ALA	ALA
SER	SER	LEU	S713	G473	G473	G474	G475	P365	ASP	LEU	SER	TYR	TYR	ASP	ASP
MET	MET	ALA	R717	G475	P603	R717	R718	E372	ASP	ARG	ASP	THR	THR	THR	THR
LEU	SER	LEU	E718	D478	R610	S722	S723	I373	P256	GLN	GLU	GLU	GLU	SER	GLU
GLU	GLU	GLY	S722	L479	F634	S723	S724	D374	L257	VAL	GLU	ASN	ASN	LEU	LEU
ILE	ILE	LEU	S725	R480	F634	S726	S727	G375	G258	SER	SER	GLU	GLU	GLU	GLU
GLU	GLU	ARG	S725	D635	M636	S726	S727	L376	V259	GLU	PHE	GLU	PHE	VAL	PRO
LYS	LYS	ALA	T733	L482	M636	T733	T734	A377	S261	MET	GLU	SER	SER	SER	SER
ARG	ARG	TYR	R734	E485	Q645	R734	R735	R380	L278	PRO	HIS	GLU	GLU	ASP	ASP
THR	THR	TYR	S735	S646	S646	S736	S737	S381	L278	TYR	ARG	GLY	GLY	SER	SER
ASP	ASP	LYS	I737	L488	I647	E648	E649	S382	Q258	ILE	PRO	ASP	ASP	ASP	ASP
ASN	ASN	PHE	T741	S490	T649	S490	S491	K383	R301	SER	LEU	GLU	GLU	GLU	GLU
CYS	CYS	LYS	F741	S650	S650	S651	S652	Q384	R301	SER	ARG	PRO	PRO	MET	PRO
TYR	TYR	LYS	I744	K492	I651	I651	I652	E385	L304	GLY	GLU	PHE	GLU	PRO	PRO
CYS	CYS	PRO	I744	R493	I652	I653	I654	R386	F305	SER	THR	VAL	VAL	ASN	ASN
THR	THR	LEU	L747	P496	E657	E658	E659	I387	H306	SER	ARG	THR	THR	GLY	GLY
PRO	PRO	ILE	L747	Q497	E658	E659	E660	H388	G307	GLU	ARG	GLU	GLU	LYS	LYS
LYS	LYS	ASP	S761	Q497	E659	E660	E661	A389	P308	SER	ILE	SER	SER	ARG	ARG
GLN	GLN	PHE	S761	R500	R659	R660	R661	V392	G310	ASN	ASP	TYR	ALA	ARG	ARG
PHE	PHE	ASN	P756	R500	H661	H662	H663	S393	G310	ASN	ASN	TYR	ALA	ARG	ARG
VAL	VAL	ASP	P756	R500	H661	H662	H663	V392	G310	ASN	ASN	TYR	ALA	ARG	



ILE	GLY	THR	GLU	LYS
GLU	LYS	ASN	ARG	ARG
ASN	SER	SER	MET	THR
ILE	PRO	LEU	ALA	TRP
GLU	VAL	MET	LEU	ASP
GLN	GLY	GLU	ARG	ASN
GLU	VAL	ASP	GLU	CYS
VAL	PRO	VAL	ALA	TYR
VAL	SER	GLY	GLU	CYS
PHE	GLU	PRO	ARG	THR
PRO	ALA	GLU	ARG	PRO
ASP	ALA	ASN	LYS	LYS
LEU	LEU	VAL	LEU	GLN
VAL	ARG	ASP	ARG	PHE
PHE	VAL	MET	HIS	VAL
ASP	SER	ASP	GLY	HIS
E1128	THR	ILE	LYS	ASP
D1129	ASP	GLU	LEU	ILE
R1130	VAL	ASP	GLN	LYS
	SER	ASN	LEU	LYS
P1133	THR	GLU	HIS	ILE
L1134	ASN	ILE	LEU	ILE
K1135	ILE	PHE	ASP	ARG
Q1136	SER	THR	GLU	ASP
L1137	SER	ASN	THR	ALA
L1138	ASN	GLN	LYS	LEU
I1139	GLY	SER	ALA	GLN
D1140	ARG	THR	ASP	LEU
S1141	ALA	MET	GLU	GLU
T1142	ASP	SER	GLN	ASP
T1143	ILE	VAL	PHE	SER
	PRO	PRO	THR	GLU
D1148	VAL	SER	THR	THR
	ASP	MET	GLU	ILE
L1151	THR	LYS	LYS	ILE
H1152	LEU	VAL	PRO	ARG
	ILE	GLU	SER	ALA
S1155	THR	ASN	VAL	GLN
	SER	GLU	ASP	GLU
K1165	PRO	GLU	GLU	MET
	ALA	SER	SER	TYR
R1170	ASP	PRO	ILE	ALA
	VAL	LYS	THR	ASN
D1175	PRO	PRO	GLU	VAL
	ASN	ASP	VAL	LEU
E1178	ASN	GLU	LEU	LEU
	ALA	TYR	ASP	GLY
I1186	PRO	ILE	ALA	VAL
ASN	THR	ASP	ILE	GLU
ALA	ASP	GLN	LYS	ASP
LEU	ALA	LYS	ASP	MET
GLN	HIS	ASP	GLY	GLU
	ASN	LYS	PRO	ASP
	ILE	VAL	PRO	ASP
	THR	GLN	VAL	PHE
	SER	SER	LEU	GLN
	ALA	PRO	ALA	SER
	ASP	LEU	ASP	GLN
	GLY	THR	THR	ARG
	HIS	ASN	CYS	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	53582	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 ($e^-/\text{\AA}^2$)	1.02	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	10.447	Depositor
Minimum map value	-5.122	Depositor
Average map value	-0.034	Depositor
Map value standard deviation	0.576	Depositor
Recommended contour level	1.4	Depositor
Map size (Å)	335.0, 335.0, 335.0	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.31	0/4734	0.67	0/6411
1	B	0.31	0/4734	0.67	0/6411
1	C	0.31	0/4734	0.67	0/6411
1	D	0.31	0/4734	0.67	0/6411
1	E	0.31	0/4734	0.67	0/6411
1	F	0.31	0/4734	0.67	0/6411
All	All	0.31	0/28404	0.67	0/38466

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	2
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
All	All	0	12

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	298	GLN	Peptide
1	A	751	SER	Peptide
1	B	298	GLN	Peptide

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Mol	Chain	Res	Type	Group
1	B	751	SER	Peptide
1	C	298	GLN	Peptide
1	C	751	SER	Peptide
1	D	298	GLN	Peptide
1	D	751	SER	Peptide
1	E	298	GLN	Peptide
1	E	751	SER	Peptide
1	F	298	GLN	Peptide
1	F	751	SER	Peptide

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	4628	0	4700	104	0
1	B	4628	0	4700	114	0
1	C	4628	0	4700	114	0
1	D	4628	0	4700	103	0
1	E	4628	0	4700	104	0
1	F	4628	0	4700	104	0
All	All	27768	0	28200	610	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 11.

All (610) 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:E:319:ALA:O	1:E:323:ALA:HB2	1.91	0.71
1:F:319:ALA:O	1:F:323:ALA:HB2	1.91	0.71
1:D:319:ALA:O	1:D:323:ALA:HB2	1.91	0.71
1:A:319:ALA:O	1:A:323:ALA:HB2	1.91	0.70
1:B:319:ALA:O	1:B:323:ALA:HB2	1.91	0.70
1:C:319:ALA:O	1:C:323:ALA:HB2	1.91	0.70
1:C:599:ARG:HG2	1:D:1158:TYR:HB3	1.75	0.68
1:E:438:LEU:HD21	1:E:473:GLY:HA2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:438:LEU:HD21	1:D:473:GLY:HA2	1.77	0.67
1:B:438:LEU:HD21	1:B:473:GLY:HA2	1.77	0.66
1:C:438:LEU:HD21	1:C:473:GLY:HA2	1.77	0.66
1:F:304:LEU:HB2	1:F:433:GLU:HG2	1.79	0.65
1:F:438:LEU:HD21	1:F:473:GLY:HA2	1.77	0.65
1:A:438:LEU:HD21	1:A:473:GLY:HA2	1.77	0.65
1:B:599:ARG:HE	1:C:1159:GLN:HA	1.62	0.65
1:D:304:LEU:HB2	1:D:433:GLU:HG2	1.79	0.65
1:B:304:LEU:HB2	1:B:433:GLU:HG2	1.79	0.65
1:E:304:LEU:HB2	1:E:433:GLU:HG2	1.79	0.65
1:C:304:LEU:HB2	1:C:433:GLU:HG2	1.78	0.64
1:A:304:LEU:HB2	1:A:433:GLU:HG2	1.79	0.64
1:A:307:GLY:O	1:A:415:ASN:ND2	2.32	0.63
1:F:307:GLY:O	1:F:415:ASN:ND2	2.32	0.63
1:D:307:GLY:O	1:D:415:ASN:ND2	2.31	0.63
1:B:599:ARG:O	1:C:1159:GLN:NE2	2.32	0.63
1:E:307:GLY:O	1:E:415:ASN:ND2	2.32	0.63
1:B:307:GLY:O	1:B:415:ASN:ND2	2.31	0.62
1:C:307:GLY:O	1:C:415:ASN:ND2	2.32	0.62
1:A:310:GLY:H	1:A:313:LYS:HB2	1.65	0.62
1:B:599:ARG:HG2	1:C:1158:TYR:HB3	1.82	0.61
1:C:310:GLY:H	1:C:313:LYS:HB2	1.65	0.61
1:F:663:PRO:HB3	1:F:698:GLN:HB2	1.83	0.61
1:F:405:ARG:HH11	1:F:410:ILE:HD12	1.66	0.61
1:D:405:ARG:HH11	1:D:410:ILE:HD12	1.66	0.61
1:D:310:GLY:H	1:D:313:LYS:HB2	1.65	0.61
1:F:310:GLY:H	1:F:313:LYS:HB2	1.65	0.61
1:B:663:PRO:HB3	1:B:698:GLN:HB2	1.83	0.61
1:D:663:PRO:HB3	1:D:698:GLN:HB2	1.83	0.61
1:A:405:ARG:HH11	1:A:410:ILE:HD12	1.66	0.60
1:E:405:ARG:HH11	1:E:410:ILE:HD12	1.66	0.60
1:E:663:PRO:HB3	1:E:698:GLN:HB2	1.83	0.60
1:C:663:PRO:HB3	1:C:698:GLN:HB2	1.83	0.60
1:A:492:LYS:NZ	1:A:496:PRO:O	2.35	0.60
1:E:310:GLY:H	1:E:313:LYS:HB2	1.65	0.60
1:A:456:ASP:OD1	1:A:456:ASP:N	2.34	0.60
1:D:456:ASP:OD1	1:D:456:ASP:N	2.34	0.60
1:B:310:GLY:H	1:B:313:LYS:HB2	1.65	0.59
1:B:1175:ASP:OD1	1:B:1175:ASP:N	2.35	0.59
1:A:663:PRO:HB3	1:A:698:GLN:HB2	1.83	0.59
1:F:492:LYS:NZ	1:F:496:PRO:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:440:ASP:O	1:D:472:LYS:NZ	2.36	0.59
1:A:440:ASP:O	1:A:472:LYS:NZ	2.36	0.59
1:B:440:ASP:O	1:B:472:LYS:NZ	2.36	0.59
1:B:405:ARG:HH11	1:B:410:ILE:HD12	1.66	0.59
1:C:492:LYS:NZ	1:C:496:PRO:O	2.35	0.59
1:F:1175:ASP:N	1:F:1175:ASP:OD1	2.35	0.59
1:E:594:THR:HA	1:E:598:LEU:HD13	1.85	0.59
1:C:405:ARG:HH11	1:C:410:ILE:HD12	1.66	0.59
1:C:603:PRO:HB2	1:C:700:LEU:HA	1.85	0.59
1:D:603:PRO:HB2	1:D:700:LEU:HA	1.85	0.59
1:B:594:THR:HA	1:B:598:LEU:HD13	1.85	0.59
1:D:492:LYS:NZ	1:D:496:PRO:O	2.35	0.59
1:D:1175:ASP:N	1:D:1175:ASP:OD1	2.35	0.59
1:A:337:LYS:O	1:F:393:SER:OG	2.20	0.58
1:B:603:PRO:HB2	1:B:700:LEU:HA	1.85	0.58
1:C:456:ASP:OD1	1:C:456:ASP:N	2.34	0.58
1:F:440:ASP:O	1:F:472:LYS:NZ	2.36	0.58
1:E:456:ASP:OD1	1:E:456:ASP:N	2.34	0.58
1:E:734:ARG:HH22	1:E:1143:THR:HA	1.69	0.58
1:B:492:LYS:NZ	1:B:496:PRO:O	2.35	0.58
1:E:440:ASP:O	1:E:472:LYS:NZ	2.36	0.58
1:A:594:THR:HA	1:A:598:LEU:HD13	1.85	0.58
1:B:734:ARG:HH22	1:B:1143:THR:HA	1.69	0.58
1:D:734:ARG:HH22	1:D:1143:THR:HA	1.69	0.58
1:C:440:ASP:O	1:C:472:LYS:NZ	2.36	0.58
1:F:734:ARG:HH22	1:F:1143:THR:HA	1.69	0.58
1:B:380:ARG:HH21	1:C:375:GLY:HA3	1.68	0.57
1:F:603:PRO:HB2	1:F:700:LEU:HA	1.85	0.57
1:C:594:THR:HA	1:C:598:LEU:HD13	1.85	0.57
1:C:734:ARG:HH22	1:C:1143:THR:HA	1.68	0.57
1:A:603:PRO:HB2	1:A:700:LEU:HA	1.85	0.57
1:E:603:PRO:HB2	1:E:700:LEU:HA	1.85	0.57
1:A:1175:ASP:N	1:A:1175:ASP:OD1	2.35	0.57
1:D:594:THR:HA	1:D:598:LEU:HD13	1.85	0.57
1:F:456:ASP:N	1:F:456:ASP:OD1	2.34	0.57
1:F:594:THR:HA	1:F:598:LEU:HD13	1.85	0.56
1:A:734:ARG:HH22	1:A:1143:THR:HA	1.69	0.56
1:B:456:ASP:OD1	1:B:456:ASP:N	2.34	0.56
1:B:325:SER:O	1:B:329:LYS:NZ	2.38	0.56
1:A:393:SER:OG	1:B:337:LYS:O	2.19	0.56
1:C:325:SER:O	1:C:329:LYS:NZ	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:331:VAL:HA	1:E:365:PRO:HB2	1.88	0.56
1:E:1175:ASP:OD1	1:E:1175:ASP:N	2.35	0.56
1:C:1137:LEU:O	1:C:1141:SER:OG	2.24	0.55
1:D:331:VAL:HA	1:D:365:PRO:HB2	1.88	0.55
1:D:1137:LEU:O	1:D:1141:SER:OG	2.24	0.55
1:E:492:LYS:NZ	1:E:496:PRO:O	2.35	0.55
1:A:325:SER:O	1:A:329:LYS:NZ	2.38	0.55
1:F:331:VAL:HA	1:F:365:PRO:HB2	1.88	0.55
1:F:1137:LEU:O	1:F:1141:SER:OG	2.24	0.55
1:A:1137:LEU:O	1:A:1141:SER:OG	2.24	0.55
1:E:1137:LEU:O	1:E:1141:SER:OG	2.24	0.55
1:C:1175:ASP:OD1	1:C:1175:ASP:N	2.35	0.55
1:B:331:VAL:HA	1:B:365:PRO:HB2	1.88	0.54
1:A:331:VAL:HA	1:A:365:PRO:HB2	1.88	0.54
1:B:1137:LEU:O	1:B:1141:SER:OG	2.24	0.54
1:F:444:ARG:NH1	1:F:471:SER:O	2.41	0.54
1:C:331:VAL:HA	1:C:365:PRO:HB2	1.88	0.54
1:C:444:ARG:NH1	1:C:471:SER:O	2.41	0.54
1:E:444:ARG:NH1	1:E:471:SER:O	2.41	0.54
1:A:636:MET:SD	1:A:636:MET:N	2.80	0.54
1:B:444:ARG:NH1	1:B:471:SER:O	2.41	0.54
1:B:636:MET:SD	1:B:636:MET:N	2.80	0.54
1:C:636:MET:SD	1:C:636:MET:N	2.80	0.54
1:C:751:SER:OG	1:C:1165:LYS:O	2.26	0.53
1:B:751:SER:OG	1:B:1165:LYS:O	2.26	0.53
1:D:751:SER:OG	1:D:1165:LYS:O	2.26	0.53
1:A:444:ARG:NH1	1:A:471:SER:O	2.41	0.53
1:B:506:GLN:HE21	1:B:770:PRO:HG2	1.74	0.53
1:D:444:ARG:NH1	1:D:471:SER:O	2.41	0.53
1:E:451:HIS:CG	1:E:480:ARG:HE	2.26	0.53
1:A:451:HIS:CG	1:A:480:ARG:HE	2.26	0.53
1:D:294:ARG:NH1	1:E:509:PRO:O	2.41	0.53
1:F:451:HIS:CG	1:F:480:ARG:HE	2.26	0.53
1:A:681:THR:O	1:A:685:THR:OG1	2.25	0.53
1:C:506:GLN:HE21	1:C:770:PRO:HG2	1.74	0.53
1:A:751:SER:OG	1:A:1165:LYS:O	2.26	0.53
1:D:451:HIS:CG	1:D:480:ARG:HE	2.26	0.53
1:D:634:PHE:HB2	1:D:668:ILE:HG12	1.91	0.53
1:E:751:SER:OG	1:E:1165:LYS:O	2.26	0.53
1:C:451:HIS:CG	1:C:480:ARG:HE	2.26	0.53
1:C:634:PHE:HB2	1:C:668:ILE:HG12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:733:THR:HG23	1:C:736:SER:H	1.75	0.53
1:D:506:GLN:HE21	1:D:770:PRO:HG2	1.74	0.53
1:B:451:HIS:CG	1:B:480:ARG:HE	2.26	0.52
1:F:751:SER:HB3	1:F:1170:ARG:HH22	1.74	0.52
1:E:506:GLN:HE21	1:E:770:PRO:HG2	1.74	0.52
1:A:751:SER:HB3	1:A:1170:ARG:HH22	1.74	0.52
1:D:325:SER:O	1:D:329:LYS:NZ	2.38	0.52
1:D:636:MET:N	1:D:636:MET:SD	2.80	0.52
1:D:751:SER:HB3	1:D:1170:ARG:HH22	1.74	0.52
1:E:634:PHE:HB2	1:E:668:ILE:HG12	1.91	0.52
1:E:751:SER:HB3	1:E:1170:ARG:HH22	1.74	0.52
1:F:588:TYR:HA	1:F:591:ARG:HD2	1.92	0.52
1:F:751:SER:OG	1:F:1165:LYS:O	2.26	0.52
1:C:751:SER:HB3	1:C:1170:ARG:HH22	1.74	0.52
1:B:751:SER:HB3	1:B:1170:ARG:HH22	1.74	0.52
1:D:733:THR:HG23	1:D:736:SER:H	1.75	0.52
1:F:733:THR:HG23	1:F:736:SER:H	1.74	0.52
1:A:506:GLN:HE21	1:A:770:PRO:HG2	1.74	0.52
1:A:588:TYR:HA	1:A:591:ARG:HD2	1.92	0.52
1:B:380:ARG:HH12	1:C:372:GLU:HG2	1.74	0.52
1:A:733:THR:HG23	1:A:736:SER:H	1.75	0.52
1:B:588:TYR:HA	1:B:591:ARG:HD2	1.92	0.52
1:D:588:TYR:HA	1:D:591:ARG:HD2	1.92	0.51
1:A:671:ILE:HA	1:A:674:TRP:HB3	1.92	0.51
1:B:634:PHE:HB2	1:B:668:ILE:HG12	1.91	0.51
1:B:1148:ASP:O	1:B:1152:HIS:ND1	2.42	0.51
1:A:497:GLN:HB3	1:A:769:LEU:HD12	1.93	0.51
1:A:634:PHE:HB2	1:A:668:ILE:HG12	1.91	0.51
1:B:590:GLN:HA	1:B:593:GLU:HB2	1.91	0.51
1:E:671:ILE:HA	1:E:674:TRP:HB3	1.92	0.51
1:F:345:TRP:HB2	1:F:348:GLU:HB2	1.93	0.51
1:B:671:ILE:HA	1:B:674:TRP:HB3	1.92	0.51
1:B:733:THR:HG23	1:B:736:SER:H	1.75	0.51
1:C:671:ILE:HA	1:C:674:TRP:HB3	1.93	0.51
1:E:497:GLN:HB3	1:E:769:LEU:HD12	1.93	0.51
1:F:590:GLN:HA	1:F:593:GLU:HB2	1.91	0.51
1:B:345:TRP:HB2	1:B:348:GLU:HB2	1.93	0.51
1:C:590:GLN:HA	1:C:593:GLU:HB2	1.91	0.51
1:A:590:GLN:HA	1:A:593:GLU:HB2	1.91	0.51
1:E:590:GLN:HA	1:E:593:GLU:HB2	1.91	0.51
1:F:634:PHE:HB2	1:F:668:ILE:HG12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:345:TRP:HB2	1:D:348:GLU:HB2	1.93	0.51
1:D:590:GLN:HA	1:D:593:GLU:HB2	1.91	0.51
1:E:588:TYR:HA	1:E:591:ARG:HD2	1.92	0.51
1:F:681:THR:O	1:F:685:THR:OG1	2.25	0.51
1:E:610:ARG:HA	1:E:708:PRO:HD3	1.93	0.51
1:B:610:ARG:HA	1:B:708:PRO:HD3	1.93	0.51
1:D:497:GLN:HB3	1:D:769:LEU:HD12	1.93	0.51
1:E:733:THR:HG23	1:E:736:SER:H	1.74	0.51
1:E:1148:ASP:O	1:E:1152:HIS:ND1	2.42	0.51
1:A:338:GLY:HA3	1:F:380:ARG:HH22	1.76	0.50
1:A:610:ARG:HA	1:A:708:PRO:HD3	1.93	0.50
1:A:328:ASN:HB3	1:B:504:ARG:HH11	1.77	0.50
1:C:588:TYR:HA	1:C:591:ARG:HD2	1.92	0.50
1:F:497:GLN:HB3	1:F:769:LEU:HD12	1.93	0.50
1:F:506:GLN:HE21	1:F:770:PRO:HG2	1.74	0.50
1:F:685:THR:O	1:F:688:SER:OG	2.26	0.50
1:C:685:THR:O	1:C:688:SER:OG	2.26	0.50
1:D:671:ILE:HA	1:D:674:TRP:HB3	1.92	0.50
1:A:680:LEU:HA	1:A:683:ILE:HB	1.93	0.50
1:B:645:GLN:NE2	1:B:650:SER:OG	2.44	0.50
1:C:497:GLN:HB3	1:C:769:LEU:HD12	1.93	0.50
1:A:1148:ASP:O	1:A:1152:HIS:ND1	2.42	0.50
1:B:497:GLN:HB3	1:B:769:LEU:HD12	1.93	0.50
1:C:610:ARG:HA	1:C:708:PRO:HD3	1.93	0.50
1:E:345:TRP:HB2	1:E:348:GLU:HB2	1.93	0.50
1:F:671:ILE:HA	1:F:674:TRP:HB3	1.92	0.50
1:A:345:TRP:HB2	1:A:348:GLU:HB2	1.93	0.50
1:C:345:TRP:HB2	1:C:348:GLU:HB2	1.93	0.50
1:C:680:LEU:HA	1:C:683:ILE:HB	1.93	0.50
1:B:680:LEU:HA	1:B:683:ILE:HB	1.93	0.50
1:F:680:LEU:HA	1:F:683:ILE:HB	1.93	0.50
1:A:645:GLN:NE2	1:A:650:SER:OG	2.44	0.49
1:E:583:GLU:O	1:F:515:LYS:NZ	2.33	0.49
1:D:599:ARG:HG2	1:E:1158:TYR:HB3	1.93	0.49
1:D:610:ARG:HA	1:D:708:PRO:HD3	1.93	0.49
1:E:636:MET:SD	1:E:636:MET:N	2.80	0.49
1:B:364:GLN:HA	1:B:407:GLN:HE21	1.77	0.49
1:A:364:GLN:HA	1:A:407:GLN:HE21	1.77	0.49
1:C:681:THR:O	1:C:685:THR:OG1	2.26	0.49
1:E:373:ILE:HD13	1:E:376:LEU:HD12	1.95	0.49
1:E:1148:ASP:OD1	1:E:1148:ASP:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:ILE:HD13	1:A:376:LEU:HD12	1.95	0.49
1:C:364:GLN:HA	1:C:407:GLN:HE21	1.78	0.49
1:D:364:GLN:HA	1:D:407:GLN:HE21	1.78	0.49
1:D:482:LEU:HA	1:D:485:GLU:HG2	1.95	0.49
1:D:680:LEU:HA	1:D:683:ILE:HB	1.93	0.49
1:F:694:ASP:OD2	1:F:696:SER:OG	2.29	0.49
1:C:482:LEU:HA	1:C:485:GLU:HG2	1.95	0.49
1:D:600:ILE:HD13	1:D:698:GLN:HG3	1.95	0.49
1:F:610:ARG:HA	1:F:708:PRO:HD3	1.93	0.49
1:A:647:ILE:HD13	1:A:678:LEU:HD11	1.95	0.49
1:B:319:ALA:O	1:B:323:ALA:CB	2.59	0.49
1:C:600:ILE:HD13	1:C:698:GLN:HG3	1.95	0.49
1:F:373:ILE:HD13	1:F:376:LEU:HD12	1.95	0.49
1:F:636:MET:SD	1:F:636:MET:N	2.80	0.49
1:C:319:ALA:O	1:C:323:ALA:CB	2.59	0.49
1:A:319:ALA:O	1:A:323:ALA:CB	2.59	0.48
1:A:377:ALA:HB1	1:A:392:VAL:HG22	1.95	0.48
1:B:685:THR:O	1:B:688:SER:OG	2.26	0.48
1:B:1148:ASP:OD1	1:B:1148:ASP:N	2.46	0.48
1:F:1148:ASP:N	1:F:1148:ASP:OD1	2.46	0.48
1:B:600:ILE:HD13	1:B:698:GLN:HG3	1.95	0.48
1:E:319:ALA:O	1:E:323:ALA:CB	2.59	0.48
1:E:647:ILE:HD13	1:E:678:LEU:HD11	1.95	0.48
1:F:645:GLN:NE2	1:F:650:SER:OG	2.44	0.48
1:B:377:ALA:HB1	1:B:392:VAL:HG22	1.95	0.48
1:B:482:LEU:HA	1:B:485:GLU:HG2	1.95	0.48
1:E:482:LEU:HA	1:E:485:GLU:HG2	1.95	0.48
1:E:680:LEU:HA	1:E:683:ILE:HB	1.93	0.48
1:C:599:ARG:HE	1:D:1159:GLN:HA	1.78	0.48
1:C:647:ILE:HD13	1:C:678:LEU:HD11	1.95	0.48
1:D:377:ALA:HB1	1:D:392:VAL:HG22	1.96	0.48
1:D:645:GLN:NE2	1:D:650:SER:OG	2.44	0.48
1:F:647:ILE:HD13	1:F:678:LEU:HD11	1.95	0.48
1:A:600:ILE:HD13	1:A:698:GLN:HG3	1.95	0.48
1:D:647:ILE:HD13	1:D:678:LEU:HD11	1.95	0.48
1:E:645:GLN:NE2	1:E:650:SER:OG	2.44	0.48
1:F:364:GLN:HA	1:F:407:GLN:HE21	1.78	0.48
1:F:687:SER:HA	1:F:690:LEU:HD12	1.96	0.48
1:B:386:GLN:HG2	1:C:388:HIS:CE1	2.49	0.48
1:C:377:ALA:HB1	1:C:392:VAL:HG22	1.95	0.48
1:F:377:ALA:HB1	1:F:392:VAL:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:ASN:O	1:A:493:ARG:CB	2.62	0.48
1:B:426:ARG:HH22	1:C:309:PRO:HG2	1.79	0.48
1:B:723:LYS:HE3	1:C:1186:ILE:HD12	1.96	0.48
1:E:364:GLN:HA	1:E:407:GLN:HE21	1.78	0.48
1:F:489:ASN:O	1:F:493:ARG:CB	2.62	0.48
1:B:373:ILE:HD13	1:B:376:LEU:HD12	1.95	0.48
1:D:1148:ASP:O	1:D:1152:HIS:ND1	2.42	0.48
1:E:489:ASN:O	1:E:493:ARG:CB	2.62	0.48
1:F:319:ALA:O	1:F:323:ALA:CB	2.59	0.48
1:A:482:LEU:HA	1:A:485:GLU:HG2	1.95	0.48
1:C:373:ILE:HD13	1:C:376:LEU:HD12	1.95	0.48
1:B:647:ILE:HD13	1:B:678:LEU:HD11	1.95	0.48
1:D:319:ALA:O	1:D:323:ALA:CB	2.59	0.48
1:D:489:ASN:O	1:D:493:ARG:HB2	2.14	0.48
1:D:373:ILE:HD13	1:D:376:LEU:HD12	1.95	0.47
1:E:685:THR:O	1:E:688:SER:OG	2.26	0.47
1:D:687:SER:HA	1:D:690:LEU:HD12	1.96	0.47
1:A:489:ASN:O	1:A:493:ARG:HB2	2.14	0.47
1:C:489:ASN:O	1:C:493:ARG:CB	2.62	0.47
1:E:687:SER:HA	1:E:690:LEU:HD12	1.96	0.47
1:A:685:THR:O	1:A:688:SER:OG	2.26	0.47
1:A:687:SER:HA	1:A:690:LEU:HD12	1.96	0.47
1:B:295:PHE:HB3	1:C:455:TRP:HE1	1.79	0.47
1:C:489:ASN:O	1:C:493:ARG:HB2	2.14	0.47
1:C:645:GLN:NE2	1:C:650:SER:OG	2.44	0.47
1:D:648:GLU:HA	1:D:651:ILE:HD12	1.97	0.47
1:E:600:ILE:HD13	1:E:698:GLN:HG3	1.95	0.47
1:F:600:ILE:HD13	1:F:698:GLN:HG3	1.95	0.47
1:C:648:GLU:HA	1:C:651:ILE:HD12	1.97	0.47
1:D:489:ASN:O	1:D:493:ARG:CB	2.62	0.47
1:E:751:SER:H	1:E:1170:ARG:HH22	1.63	0.47
1:F:482:LEU:HA	1:F:485:GLU:HG2	1.95	0.47
1:C:550:ASN:HA	1:C:553:PHE:HB3	1.96	0.47
1:C:694:ASP:OD2	1:C:696:SER:OG	2.29	0.47
1:D:1148:ASP:OD1	1:D:1148:ASP:N	2.46	0.47
1:E:648:GLU:HA	1:E:651:ILE:HD12	1.97	0.47
1:A:550:ASN:HA	1:A:553:PHE:HB3	1.96	0.47
1:B:694:ASP:OD2	1:B:696:SER:OG	2.29	0.47
1:D:685:THR:O	1:D:688:SER:OG	2.26	0.47
1:E:489:ASN:O	1:E:493:ARG:HB2	2.14	0.47
1:A:577:MET:O	1:B:764:ARG:N	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1152:HIS:O	1:A:1155:SER:OG	2.33	0.47
1:D:751:SER:H	1:D:1170:ARG:HH22	1.63	0.47
1:A:496:PRO:HB3	1:A:764:ARG:HH11	1.80	0.47
1:A:648:GLU:HA	1:A:651:ILE:HD12	1.97	0.47
1:C:496:PRO:HB3	1:C:764:ARG:HH11	1.80	0.47
1:D:1152:HIS:O	1:D:1155:SER:OG	2.33	0.47
1:F:329:LYS:HA	1:F:330:LYS:HA	1.70	0.47
1:A:445:LYS:HA	1:A:448:ILE:HG22	1.97	0.47
1:A:694:ASP:OD2	1:A:696:SER:OG	2.29	0.47
1:B:489:ASN:O	1:B:493:ARG:CB	2.62	0.47
1:B:550:ASN:HA	1:B:553:PHE:HB3	1.96	0.47
1:B:648:GLU:HA	1:B:651:ILE:HD12	1.97	0.47
1:C:1148:ASP:OD1	1:C:1148:ASP:N	2.46	0.47
1:F:751:SER:H	1:F:1170:ARG:HH22	1.63	0.47
1:B:687:SER:HA	1:B:690:LEU:HD12	1.96	0.46
1:C:1152:HIS:O	1:C:1155:SER:OG	2.33	0.46
1:E:445:LYS:HA	1:E:448:ILE:HG22	1.97	0.46
1:B:489:ASN:O	1:B:493:ARG:HB2	2.14	0.46
1:D:550:ASN:HA	1:D:553:PHE:HB3	1.96	0.46
1:F:496:PRO:HB3	1:F:764:ARG:HH11	1.80	0.46
1:D:445:LYS:HA	1:D:448:ILE:HG22	1.97	0.46
1:D:490:SER:OG	1:D:518:ASP:OD2	2.30	0.46
1:D:496:PRO:HB3	1:D:764:ARG:HH11	1.80	0.46
1:F:325:SER:O	1:F:329:LYS:NZ	2.38	0.46
1:F:657:GLU:O	1:F:661:HIS:ND1	2.42	0.46
1:A:1148:ASP:N	1:A:1148:ASP:OD1	2.46	0.46
1:D:672:ASP:OD2	1:D:707:SER:N	2.49	0.46
1:E:550:ASN:HA	1:E:553:PHE:HB3	1.96	0.46
1:F:489:ASN:O	1:F:493:ARG:HB2	2.14	0.46
1:F:1152:HIS:O	1:F:1155:SER:OG	2.33	0.46
1:F:672:ASP:OD2	1:F:707:SER:N	2.49	0.46
1:A:751:SER:H	1:A:1170:ARG:HH22	1.63	0.46
1:B:1152:HIS:O	1:B:1155:SER:OG	2.33	0.46
1:B:556:ILE:O	1:B:560:LEU:HB2	2.16	0.46
1:D:556:ILE:O	1:D:560:LEU:HB2	2.16	0.46
1:E:377:ALA:HB1	1:E:392:VAL:HG22	1.96	0.46
1:F:550:ASN:HA	1:F:553:PHE:HB3	1.96	0.46
1:F:648:GLU:HA	1:F:651:ILE:HD12	1.97	0.46
1:C:445:LYS:HA	1:C:448:ILE:HG22	1.97	0.46
1:E:744:ILE:HA	1:E:747:LEU:HB2	1.98	0.46
1:A:517:LYS:HA	1:A:520:VAL:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:ILE:O	1:A:560:LEU:HB2	2.16	0.46
1:B:1134:LEU:HD11	1:B:1178:GLU:HB3	1.98	0.46
1:C:672:ASP:OD2	1:C:707:SER:N	2.48	0.46
1:E:325:SER:O	1:E:329:LYS:NZ	2.38	0.46
1:F:744:ILE:HA	1:F:747:LEU:HB2	1.98	0.46
1:B:596:GLU:HA	1:B:599:ARG:HD3	1.98	0.45
1:B:657:GLU:O	1:B:661:HIS:ND1	2.42	0.45
1:B:744:ILE:HA	1:B:747:LEU:HB2	1.98	0.45
1:B:751:SER:H	1:B:1170:ARG:HH22	1.63	0.45
1:D:517:LYS:HA	1:D:520:VAL:HG12	1.98	0.45
1:D:694:ASP:OD2	1:D:696:SER:OG	2.29	0.45
1:D:744:ILE:HA	1:D:747:LEU:HB2	1.98	0.45
1:D:1134:LEU:HD11	1:D:1178:GLU:HB3	1.98	0.45
1:F:445:LYS:HA	1:F:448:ILE:HG22	1.97	0.45
1:A:734:ARG:HA	1:A:737:ILE:HD12	1.99	0.45
1:B:496:PRO:HB3	1:B:764:ARG:HH11	1.80	0.45
1:C:556:ILE:O	1:C:560:LEU:HB2	2.16	0.45
1:C:671:ILE:HG23	1:C:674:TRP:HE3	1.82	0.45
1:C:687:SER:HA	1:C:690:LEU:HD12	1.96	0.45
1:E:556:ILE:O	1:E:560:LEU:HB2	2.16	0.45
1:F:517:LYS:HA	1:F:520:VAL:HG12	1.99	0.45
1:C:734:ARG:HA	1:C:737:ILE:HD12	1.99	0.45
1:E:496:PRO:HB3	1:E:764:ARG:HH11	1.80	0.45
1:F:556:ILE:O	1:F:560:LEU:HB2	2.16	0.45
1:A:1134:LEU:HD11	1:A:1178:GLU:HB3	1.98	0.45
1:B:517:LYS:HA	1:B:520:VAL:HG12	1.98	0.45
1:C:553:PHE:HA	1:C:556:ILE:HD12	1.98	0.45
1:C:1134:LEU:HD11	1:C:1178:GLU:HB3	1.98	0.45
1:E:517:LYS:HA	1:E:520:VAL:HG12	1.98	0.45
1:E:553:PHE:HA	1:E:556:ILE:HD12	1.98	0.45
1:E:694:ASP:OD2	1:E:696:SER:OG	2.29	0.45
1:C:517:LYS:HA	1:C:520:VAL:HG12	1.98	0.45
1:C:751:SER:H	1:C:1170:ARG:HH22	1.63	0.45
1:E:1152:HIS:O	1:E:1155:SER:OG	2.33	0.45
1:F:596:GLU:HA	1:F:599:ARG:HD3	1.98	0.45
1:F:1134:LEU:HD11	1:F:1178:GLU:HB3	1.98	0.45
1:D:596:GLU:HA	1:D:599:ARG:HD3	1.99	0.45
1:E:671:ILE:HG23	1:E:674:TRP:HE3	1.82	0.45
1:B:445:LYS:HA	1:B:448:ILE:HG22	1.97	0.45
1:B:734:ARG:HA	1:B:737:ILE:HD12	1.99	0.45
1:C:659:ARG:HH11	1:C:693:LEU:HD22	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:PHE:HA	1:A:556:ILE:HD12	1.98	0.45
1:A:672:ASP:OD2	1:A:707:SER:N	2.49	0.45
1:B:488:LEU:HA	1:B:491:ILE:HD12	1.99	0.45
1:C:657:GLU:O	1:C:661:HIS:ND1	2.42	0.45
1:C:744:ILE:HA	1:C:747:LEU:HB2	1.98	0.45
1:D:553:PHE:HA	1:D:556:ILE:HD12	1.98	0.45
1:E:596:GLU:HA	1:E:599:ARG:HD3	1.98	0.45
1:A:488:LEU:HA	1:A:491:ILE:HD12	1.99	0.45
1:D:671:ILE:HG23	1:D:674:TRP:HE3	1.82	0.45
1:D:1138:LEU:O	1:D:1142:THR:OG1	2.31	0.45
1:E:672:ASP:OD2	1:E:707:SER:N	2.49	0.45
1:A:596:GLU:HA	1:A:599:ARG:HD3	1.98	0.45
1:A:671:ILE:HG23	1:A:674:TRP:HE3	1.82	0.44
1:E:329:LYS:HA	1:E:330:LYS:HA	1.70	0.44
1:E:488:LEU:HA	1:E:491:ILE:HD12	1.99	0.44
1:E:1134:LEU:HD11	1:E:1178:GLU:HB3	1.98	0.44
1:F:671:ILE:HG23	1:F:674:TRP:HE3	1.82	0.44
1:C:488:LEU:HA	1:C:491:ILE:HD12	1.99	0.44
1:E:659:ARG:HH11	1:E:693:LEU:HD22	1.82	0.44
1:E:1138:LEU:O	1:E:1142:THR:OG1	2.31	0.44
1:A:744:ILE:HA	1:A:747:LEU:HB2	1.98	0.44
1:B:295:PHE:O	1:C:455:TRP:NE1	2.50	0.44
1:B:671:ILE:HG23	1:B:674:TRP:HE3	1.82	0.44
1:D:734:ARG:HA	1:D:737:ILE:HD12	1.99	0.44
1:F:733:THR:O	1:F:736:SER:OG	2.35	0.44
1:B:553:PHE:HA	1:B:556:ILE:HD12	1.98	0.44
1:B:672:ASP:OD2	1:B:707:SER:N	2.48	0.44
1:E:734:ARG:HA	1:E:737:ILE:HD12	1.99	0.44
1:F:659:ARG:HH11	1:F:693:LEU:HD22	1.82	0.44
1:F:734:ARG:HA	1:F:737:ILE:HD12	1.99	0.44
1:A:336:ARG:HD2	1:A:356:LEU:HD11	1.99	0.44
1:D:659:ARG:HH11	1:D:693:LEU:HD22	1.82	0.44
1:F:336:ARG:HD2	1:F:356:LEU:HD11	1.99	0.44
1:F:553:PHE:HA	1:F:556:ILE:HD12	1.98	0.44
1:B:316:MET:HA	1:B:319:ALA:HB3	2.00	0.44
1:B:659:ARG:HH11	1:B:693:LEU:HD22	1.82	0.44
1:C:741:PHE:HD1	1:C:744:ILE:HD11	1.83	0.44
1:F:488:LEU:HA	1:F:491:ILE:HD12	1.99	0.44
1:B:336:ARG:HD2	1:B:356:LEU:HD11	2.00	0.44
1:C:596:GLU:HA	1:C:599:ARG:HD3	1.98	0.44
1:C:1148:ASP:O	1:C:1152:HIS:ND1	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:657:GLU:O	1:D:661:HIS:ND1	2.42	0.44
1:D:712:LEU:H	1:D:717:ARG:NH2	2.16	0.44
1:F:380:ARG:HG3	1:F:389:ALA:HA	2.00	0.44
1:D:316:MET:HA	1:D:319:ALA:HB3	2.00	0.43
1:D:488:LEU:HA	1:D:491:ILE:HD12	1.99	0.43
1:E:465:SER:O	1:E:465:SER:OG	2.35	0.43
1:A:659:ARG:HH11	1:A:693:LEU:HD22	1.82	0.43
1:B:386:GLN:HG2	1:C:388:HIS:HE1	1.82	0.43
1:B:712:LEU:H	1:B:717:ARG:NH2	2.16	0.43
1:C:336:ARG:HD2	1:C:356:LEU:HD11	2.00	0.43
1:E:741:PHE:HD1	1:E:744:ILE:HD11	1.83	0.43
1:F:316:MET:HA	1:F:319:ALA:HB3	2.00	0.43
1:A:279:LYS:HZ1	1:B:499:TYR:HB2	1.82	0.43
1:E:342:LEU:HD13	1:E:349:ALA:HB1	2.01	0.43
1:E:380:ARG:HG3	1:E:389:ALA:HA	2.00	0.43
1:A:733:THR:O	1:A:736:SER:OG	2.35	0.43
1:B:342:LEU:HD13	1:B:349:ALA:HB1	2.01	0.43
1:B:595:PHE:HE2	1:C:756:PRO:HD2	1.83	0.43
1:A:257:LEU:HB3	1:F:298:GLN:O	2.17	0.43
1:A:712:LEU:H	1:A:717:ARG:NH2	2.16	0.43
1:C:577:MET:HG3	1:D:763:ARG:HE	1.84	0.43
1:C:712:LEU:H	1:C:717:ARG:NH2	2.16	0.43
1:C:1138:LEU:O	1:C:1142:THR:OG1	2.31	0.43
1:D:336:ARG:HD2	1:D:356:LEU:HD11	1.99	0.43
1:D:741:PHE:HD1	1:D:744:ILE:HD11	1.83	0.43
1:E:712:LEU:H	1:E:717:ARG:NH2	2.16	0.43
1:F:741:PHE:HD1	1:F:744:ILE:HD11	1.83	0.43
1:A:316:MET:HA	1:A:319:ALA:HB3	2.00	0.43
1:A:380:ARG:HG3	1:A:389:ALA:HA	2.00	0.43
1:C:342:LEU:HD13	1:C:349:ALA:HB1	2.01	0.43
1:C:595:PHE:HE2	1:D:756:PRO:HD2	1.83	0.43
1:E:336:ARG:HD2	1:E:356:LEU:HD11	1.99	0.43
1:E:499:TYR:HD2	1:E:500:ARG:HE	1.66	0.43
1:D:421:ASP:OD1	1:D:421:ASP:N	2.52	0.43
1:D:499:TYR:HD2	1:D:500:ARG:HE	1.66	0.43
1:F:712:LEU:H	1:F:717:ARG:NH2	2.16	0.43
1:F:1148:ASP:O	1:F:1152:HIS:ND1	2.42	0.43
1:E:421:ASP:OD1	1:E:421:ASP:N	2.52	0.43
1:A:421:ASP:OD1	1:A:421:ASP:N	2.52	0.42
1:C:305:PHE:HB2	1:C:413:ALA:HA	2.01	0.42
1:C:499:TYR:HD2	1:C:500:ARG:HE	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:305:PHE:HB2	1:E:413:ALA:HA	2.01	0.42
1:F:489:ASN:ND2	1:F:518:ASP:HA	2.34	0.42
1:A:555:ASP:O	1:A:559:THR:OG1	2.34	0.42
1:B:380:ARG:HG3	1:B:389:ALA:HA	2.00	0.42
1:B:421:ASP:OD1	1:B:421:ASP:N	2.52	0.42
1:B:681:THR:O	1:B:685:THR:OG1	2.25	0.42
1:B:741:PHE:HD1	1:B:744:ILE:HD11	1.83	0.42
1:B:1148:ASP:HA	1:B:1151:LEU:HD12	2.01	0.42
1:E:733:THR:O	1:E:736:SER:OG	2.35	0.42
1:A:722:SER:HB3	1:A:725:SER:HB3	2.02	0.42
1:B:722:SER:HB3	1:B:725:SER:HB3	2.02	0.42
1:C:316:MET:HA	1:C:319:ALA:HB3	2.00	0.42
1:D:380:ARG:HG3	1:D:389:ALA:HA	2.00	0.42
1:D:489:ASN:ND2	1:D:518:ASP:HA	2.34	0.42
1:E:722:SER:HB3	1:E:725:SER:HB3	2.02	0.42
1:A:499:TYR:HD2	1:A:500:ARG:HE	1.66	0.42
1:B:489:ASN:ND2	1:B:518:ASP:HA	2.34	0.42
1:D:342:LEU:HD13	1:D:349:ALA:HB1	2.01	0.42
1:E:316:MET:HA	1:E:319:ALA:HB3	2.00	0.42
1:F:722:SER:HB3	1:F:725:SER:HB3	2.02	0.42
1:A:577:MET:HG3	1:B:763:ARG:HE	1.82	0.42
1:B:499:TYR:HD2	1:B:500:ARG:HE	1.66	0.42
1:B:734:ARG:HD3	1:B:737:ILE:HD12	2.02	0.42
1:C:490:SER:OG	1:C:518:ASP:OD2	2.30	0.42
1:D:681:THR:O	1:D:685:THR:OG1	2.25	0.42
1:E:734:ARG:HD3	1:E:737:ILE:HD12	2.02	0.42
1:F:530:SER:O	1:F:534:SER:OG	2.36	0.42
1:A:460:PRO:HD2	1:A:463:LEU:HD21	2.02	0.42
1:A:489:ASN:ND2	1:A:518:ASP:HA	2.34	0.42
1:B:460:PRO:HD2	1:B:463:LEU:HD21	2.02	0.42
1:C:307:GLY:O	1:C:313:LYS:NZ	2.46	0.42
1:C:380:ARG:HG3	1:C:389:ALA:HA	2.00	0.42
1:D:734:ARG:HD3	1:D:737:ILE:HD12	2.02	0.42
1:E:489:ASN:ND2	1:E:518:ASP:HA	2.34	0.42
1:E:1139:ILE:HD12	1:E:1139:ILE:HA	1.96	0.42
1:A:741:PHE:HD1	1:A:744:ILE:HD11	1.83	0.42
1:A:1148:ASP:HA	1:A:1151:LEU:HD12	2.01	0.42
1:B:329:LYS:HA	1:B:330:LYS:HA	1.70	0.42
1:D:460:PRO:HD2	1:D:463:LEU:HD21	2.02	0.42
1:D:1148:ASP:HA	1:D:1151:LEU:HD12	2.01	0.42
1:B:475:GLY:N	1:B:478:ASP:OD1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1148:ASP:HA	1:C:1151:LEU:HD12	2.01	0.42
1:D:256:PRO:HB2	1:D:257:LEU:H	1.72	0.42
1:F:301:ARG:H	1:F:405:ARG:NH2	2.18	0.42
1:F:342:LEU:HD13	1:F:349:ALA:HB1	2.01	0.42
1:F:1138:LEU:O	1:F:1142:THR:OG1	2.31	0.42
1:F:1148:ASP:HA	1:F:1151:LEU:HD12	2.01	0.42
1:E:475:GLY:N	1:E:478:ASP:OD1	2.53	0.42
1:E:1148:ASP:HA	1:E:1151:LEU:HD12	2.01	0.42
1:F:499:TYR:HD2	1:F:500:ARG:HE	1.66	0.42
1:F:734:ARG:HD3	1:F:737:ILE:HD12	2.02	0.42
1:A:305:PHE:HB2	1:A:413:ALA:HA	2.01	0.42
1:A:475:GLY:N	1:A:478:ASP:OD1	2.53	0.42
1:B:733:THR:O	1:B:736:SER:OG	2.35	0.42
1:F:305:PHE:HB2	1:F:413:ALA:HA	2.01	0.42
1:F:367:ILE:HG22	1:F:409:ILE:HB	2.02	0.42
1:F:460:PRO:HD2	1:F:463:LEU:HD21	2.02	0.42
1:A:278:LEU:HD22	1:A:320:LEU:HD21	2.02	0.41
1:A:342:LEU:HD13	1:A:349:ALA:HB1	2.01	0.41
1:B:348:GLU:HA	1:B:351:ARG:HG2	2.02	0.41
1:B:367:ILE:HG22	1:B:409:ILE:HB	2.02	0.41
1:C:301:ARG:H	1:C:405:ARG:NH2	2.18	0.41
1:C:380:ARG:NH1	1:D:372:GLU:HG2	2.35	0.41
1:C:489:ASN:ND2	1:C:518:ASP:HA	2.34	0.41
1:E:256:PRO:HB2	1:E:257:LEU:H	1.72	0.41
1:B:301:ARG:H	1:B:405:ARG:NH2	2.18	0.41
1:B:465:SER:O	1:B:465:SER:OG	2.35	0.41
1:B:751:SER:H	1:B:1170:ARG:NH2	2.18	0.41
1:D:475:GLY:N	1:D:478:ASP:OD1	2.53	0.41
1:D:549:LEU:O	1:D:553:PHE:HB2	2.20	0.41
1:E:460:PRO:HD2	1:E:463:LEU:HD21	2.02	0.41
1:B:549:LEU:O	1:B:553:PHE:HB2	2.20	0.41
1:C:734:ARG:HD3	1:C:737:ILE:HD12	2.02	0.41
1:F:490:SER:OG	1:F:518:ASP:OD2	2.30	0.41
1:F:1139:ILE:HD12	1:F:1139:ILE:HA	1.96	0.41
1:A:579:ASP:OD1	1:B:762:LYS:HG3	2.21	0.41
1:A:751:SER:H	1:A:1170:ARG:NH2	2.18	0.41
1:C:348:GLU:HA	1:C:351:ARG:HG2	2.02	0.41
1:D:1130:ARG:HA	1:D:1133:PRO:HD2	2.02	0.41
1:E:301:ARG:H	1:E:405:ARG:NH2	2.18	0.41
1:A:549:LEU:O	1:A:553:PHE:HB2	2.20	0.41
1:A:1130:ARG:HA	1:A:1133:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1130:ARG:HA	1:B:1133:PRO:HD2	2.02	0.41
1:C:278:LEU:HD22	1:C:320:LEU:HD21	2.02	0.41
1:C:460:PRO:HD2	1:C:463:LEU:HD21	2.02	0.41
1:C:578:TYR:CD1	1:D:761:ARG:HG3	2.55	0.41
1:C:1130:ARG:HA	1:C:1133:PRO:HD2	2.02	0.41
1:D:305:PHE:HB2	1:D:413:ALA:HA	2.02	0.41
1:E:278:LEU:HD22	1:E:320:LEU:HD21	2.02	0.41
1:E:318:ARG:O	1:E:322:ALA:HB3	2.21	0.41
1:E:445:LYS:HG3	1:E:465:SER:HB2	2.03	0.41
1:E:593:GLU:O	1:E:597:THR:OG1	2.33	0.41
1:A:572:PRO:HA	1:A:575:GLU:HB3	2.03	0.41
1:C:572:PRO:HA	1:C:575:GLU:HB3	2.03	0.41
1:D:301:ARG:H	1:D:405:ARG:NH2	2.18	0.41
1:D:318:ARG:O	1:D:322:ALA:HB3	2.20	0.41
1:E:751:SER:H	1:E:1170:ARG:NH2	2.18	0.41
1:F:348:GLU:HA	1:F:351:ARG:HG2	2.02	0.41
1:A:318:ARG:O	1:A:322:ALA:HB3	2.21	0.41
1:D:751:SER:H	1:D:1170:ARG:NH2	2.18	0.41
1:E:348:GLU:HA	1:E:351:ARG:HG2	2.02	0.41
1:E:367:ILE:HG22	1:E:409:ILE:HB	2.02	0.41
1:E:549:LEU:O	1:E:553:PHE:HB2	2.20	0.41
1:E:681:THR:O	1:E:685:THR:OG1	2.25	0.41
1:F:307:GLY:O	1:F:313:LYS:NZ	2.46	0.41
1:A:348:GLU:HA	1:A:351:ARG:HG2	2.02	0.41
1:C:445:LYS:HG3	1:C:465:SER:HB2	2.03	0.41
1:D:348:GLU:HA	1:D:351:ARG:HG2	2.02	0.41
1:F:318:ARG:O	1:F:322:ALA:HB3	2.21	0.41
1:F:475:GLY:N	1:F:478:ASP:OD1	2.53	0.41
1:F:549:LEU:O	1:F:553:PHE:HB2	2.20	0.41
1:F:1130:ARG:HA	1:F:1133:PRO:HD2	2.02	0.41
1:A:268:VAL:HB	1:A:315:LEU:HB3	2.03	0.41
1:A:764:ARG:HB2	1:F:579:ASP:HB3	2.02	0.41
1:B:445:LYS:HG3	1:B:465:SER:HB2	2.03	0.41
1:B:572:PRO:HA	1:B:575:GLU:HB3	2.03	0.41
1:C:475:GLY:N	1:C:478:ASP:OD1	2.53	0.41
1:C:549:LEU:O	1:C:553:PHE:HB2	2.20	0.41
1:D:278:LEU:HD22	1:D:320:LEU:HD21	2.02	0.41
1:D:318:ARG:HE	1:D:322:ALA:HB2	1.86	0.41
1:D:722:SER:HB3	1:D:725:SER:HB3	2.02	0.41
1:E:393:SER:HA	1:E:396:LEU:HD12	2.03	0.41
1:F:268:VAL:HB	1:F:315:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:421:ASP:OD1	1:F:421:ASP:N	2.52	0.41
1:F:751:SER:H	1:F:1170:ARG:NH2	2.18	0.41
1:A:301:ARG:H	1:A:405:ARG:NH2	2.18	0.41
1:A:393:SER:HA	1:A:396:LEU:HD12	2.03	0.41
1:A:445:LYS:HG3	1:A:465:SER:HB2	2.03	0.41
1:B:345:TRP:CZ3	1:C:344:LYS:HB3	2.55	0.41
1:C:393:SER:HA	1:C:396:LEU:HD12	2.03	0.41
1:C:722:SER:HB3	1:C:725:SER:HB3	2.02	0.41
1:D:445:LYS:HG3	1:D:465:SER:HB2	2.03	0.41
1:E:657:GLU:O	1:E:661:HIS:ND1	2.42	0.41
1:F:1135:LYS:HD2	1:F:1138:LEU:HD11	2.03	0.41
1:B:305:PHE:HB2	1:B:413:ALA:HA	2.01	0.40
1:B:494:THR:HG22	1:B:513:LYS:HD2	2.04	0.40
1:C:577:MET:HE2	1:D:763:ARG:HH21	1.85	0.40
1:E:494:THR:HG22	1:E:513:LYS:HD2	2.03	0.40
1:A:734:ARG:HD3	1:A:737:ILE:HD12	2.02	0.40
1:E:318:ARG:HE	1:E:322:ALA:HB2	1.86	0.40
1:E:635:ASP:O	1:E:638:THR:OG1	2.29	0.40
1:F:278:LEU:HD22	1:F:320:LEU:HD21	2.02	0.40
1:A:367:ILE:HG22	1:A:409:ILE:HB	2.02	0.40
1:B:318:ARG:O	1:B:322:ALA:HB3	2.21	0.40
1:C:318:ARG:O	1:C:322:ALA:HB3	2.21	0.40
1:C:751:SER:H	1:C:1170:ARG:NH2	2.18	0.40
1:C:1135:LYS:HD2	1:C:1138:LEU:HD11	2.04	0.40
1:E:398:LEU:HD23	1:E:398:LEU:HA	1.97	0.40
1:B:490:SER:OG	1:B:518:ASP:OD2	2.30	0.40
1:D:367:ILE:HG22	1:D:409:ILE:HB	2.02	0.40
1:F:572:PRO:HA	1:F:575:GLU:HB3	2.03	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	573/1198 (48%)	521 (91%)	52 (9%)	0	100	100
1	B	573/1198 (48%)	521 (91%)	52 (9%)	0	100	100
1	C	573/1198 (48%)	521 (91%)	52 (9%)	0	100	100
1	D	573/1198 (48%)	521 (91%)	52 (9%)	0	100	100
1	E	573/1198 (48%)	521 (91%)	52 (9%)	0	100	100
1	F	573/1198 (48%)	521 (91%)	52 (9%)	0	100	100
All	All	3438/7188 (48%)	3126 (91%)	312 (9%)	0	100	100

There are no Ramachandran outliers to report.

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	516/1086 (48%)	513 (99%)	3 (1%)	78	80
1	B	522/1086 (48%)	519 (99%)	3 (1%)	78	80
1	C	522/1086 (48%)	519 (99%)	3 (1%)	78	80
1	D	522/1086 (48%)	519 (99%)	3 (1%)	78	80
1	E	515/1086 (47%)	512 (99%)	3 (1%)	78	80
1	F	522/1086 (48%)	519 (99%)	3 (1%)	78	80
All	All	3119/6516 (48%)	3101 (99%)	18 (1%)	76	80

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	456	ASP
1	A	652	ILE
1	A	718	GLU
1	B	456	ASP
1	B	652	ILE
1	B	718	GLU
1	C	456	ASP

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Mol	Chain	Res	Type
1	C	652	ILE
1	C	718	GLU
1	D	456	ASP
1	D	652	ILE
1	D	718	GLU
1	E	456	ASP
1	E	652	ILE
1	E	718	GLU
1	F	456	ASP
1	F	652	ILE
1	F	718	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	273	ASN
1	A	276	ASN
1	A	298	GLN
1	A	306	HIS
1	A	328	ASN
1	A	384	GLN
1	A	386	GLN
1	A	415	ASN
1	A	497	GLN
1	A	506	GLN
1	A	645	GLN
1	A	653	HIS
1	A	676	ASN
1	A	730	GLN
1	A	742	GLN
1	A	1136	GLN
1	A	1163	ASN
1	A	1171	ASN
1	B	273	ASN
1	B	306	HIS
1	B	328	ASN
1	B	384	GLN
1	B	386	GLN
1	B	415	ASN
1	B	497	GLN
1	B	506	GLN
1	B	645	GLN

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Mol	Chain	Res	Type
1	B	653	HIS
1	B	676	ASN
1	B	730	GLN
1	B	742	GLN
1	B	1136	GLN
1	B	1163	ASN
1	B	1171	ASN
1	C	273	ASN
1	C	306	HIS
1	C	328	ASN
1	C	384	GLN
1	C	386	GLN
1	C	415	ASN
1	C	497	GLN
1	C	506	GLN
1	C	645	GLN
1	C	653	HIS
1	C	676	ASN
1	C	730	GLN
1	C	742	GLN
1	C	1136	GLN
1	C	1163	ASN
1	C	1171	ASN
1	D	273	ASN
1	D	276	ASN
1	D	306	HIS
1	D	328	ASN
1	D	384	GLN
1	D	386	GLN
1	D	415	ASN
1	D	497	GLN
1	D	506	GLN
1	D	676	ASN
1	D	730	GLN
1	D	742	GLN
1	D	1136	GLN
1	D	1163	ASN
1	D	1171	ASN
1	E	273	ASN
1	E	276	ASN
1	E	306	HIS
1	E	328	ASN

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Mol	Chain	Res	Type
1	E	384	GLN
1	E	386	GLN
1	E	415	ASN
1	E	497	GLN
1	E	506	GLN
1	E	589	GLN
1	E	645	GLN
1	E	653	HIS
1	E	676	ASN
1	E	730	GLN
1	E	742	GLN
1	E	1136	GLN
1	E	1163	ASN
1	E	1171	ASN
1	F	273	ASN
1	F	276	ASN
1	F	306	HIS
1	F	328	ASN
1	F	384	GLN
1	F	386	GLN
1	F	415	ASN
1	F	497	GLN
1	F	506	GLN
1	F	589	GLN
1	F	645	GLN
1	F	653	HIS
1	F	676	ASN
1	F	730	GLN
1	F	742	GLN
1	F	1136	GLN
1	F	1163	ASN
1	F	1171	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

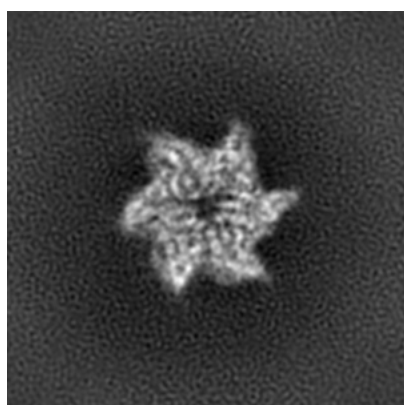
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9870. These allow visual inspection of the internal detail of the map and identification of artifacts.

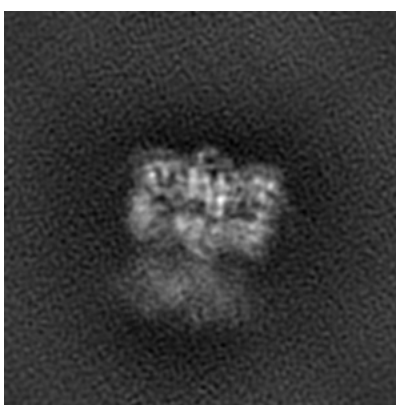
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

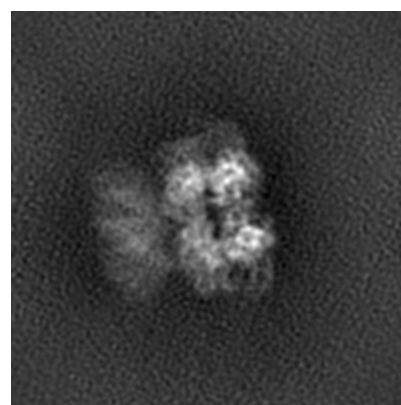
6.1.1 Primary map



X



Y

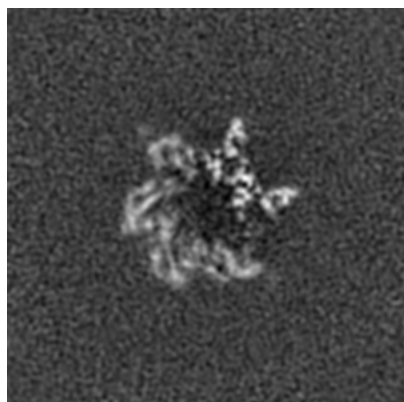


Z

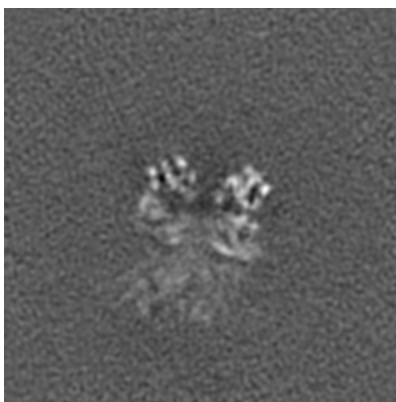
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 125



Y Index: 125

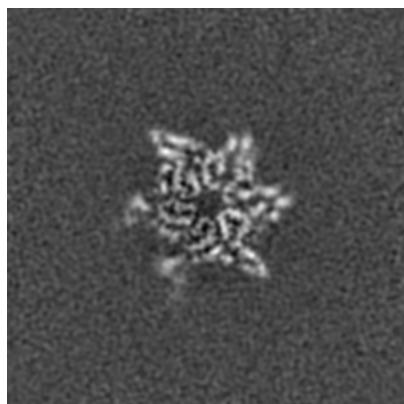


Z Index: 125

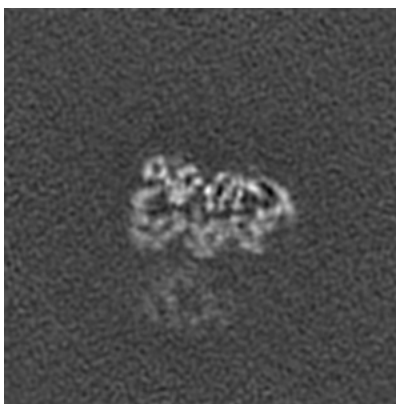
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 141



Y Index: 144

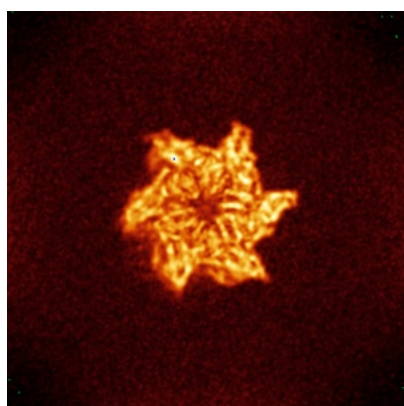


Z Index: 135

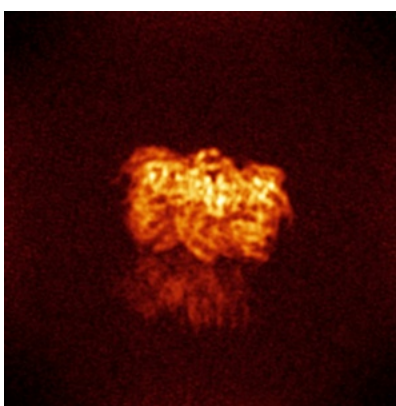
The images above show the largest variance slices of the map in three orthogonal directions.

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

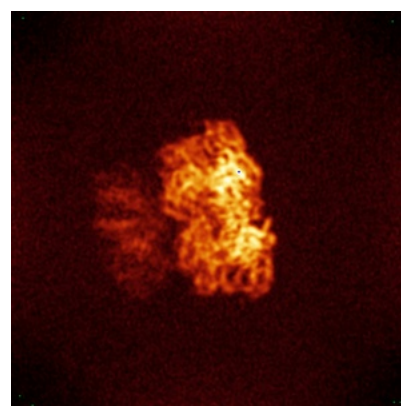
6.4.1 Primary map



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

This section was not generated.

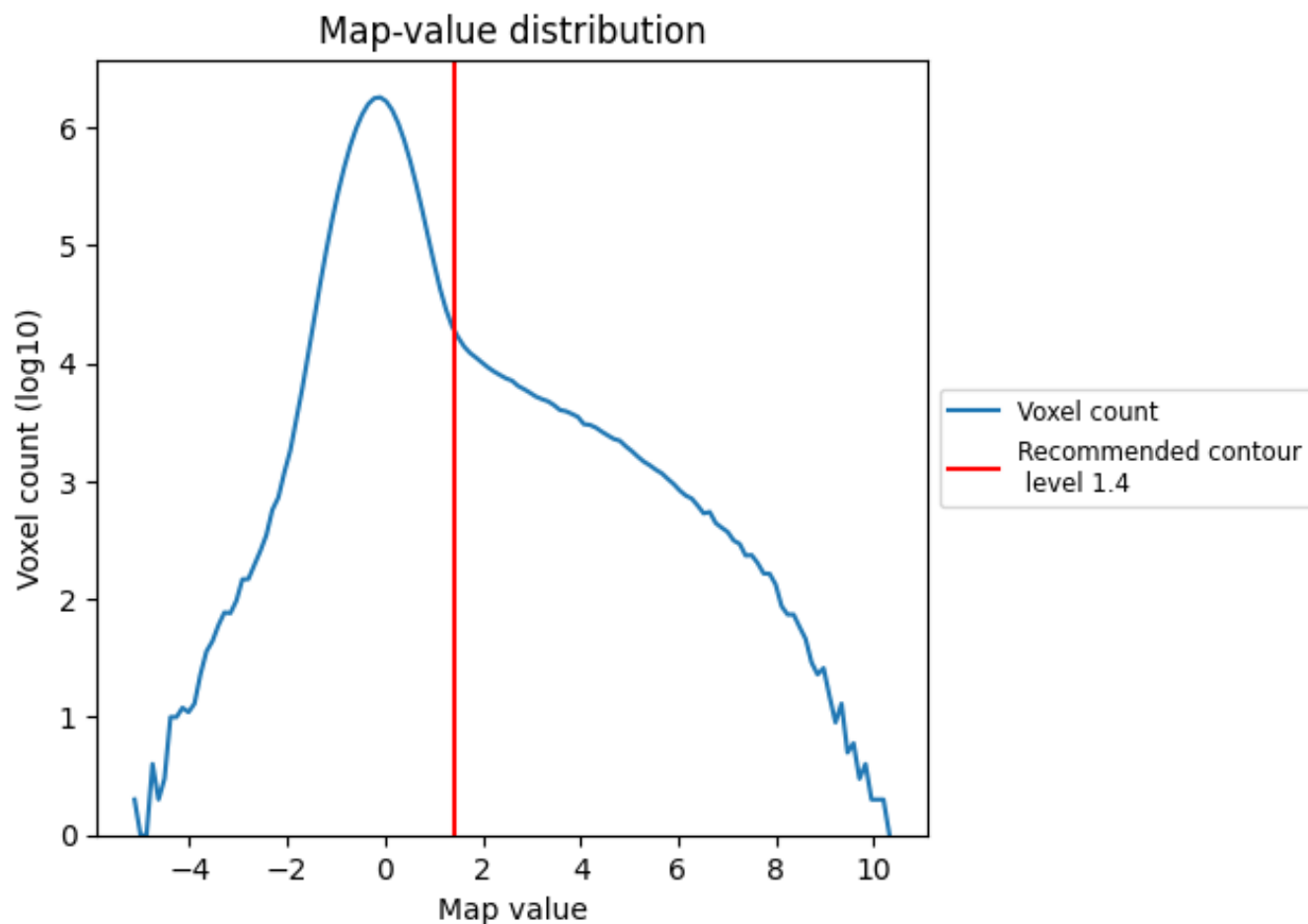
6.6 Mask visualisation

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

7 Map analysis [i](#)

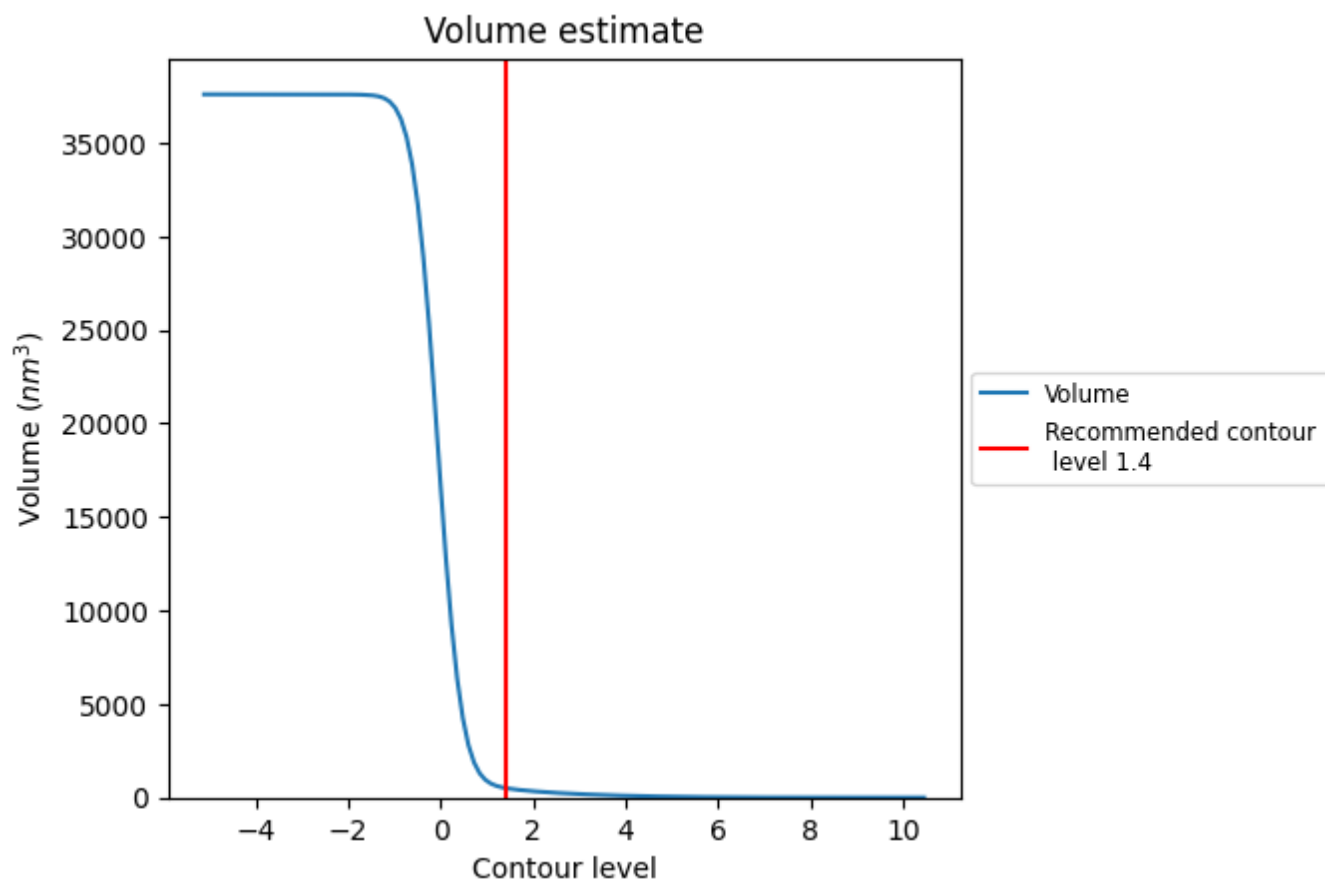
This section contains the results of statistical analysis of the map.

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.

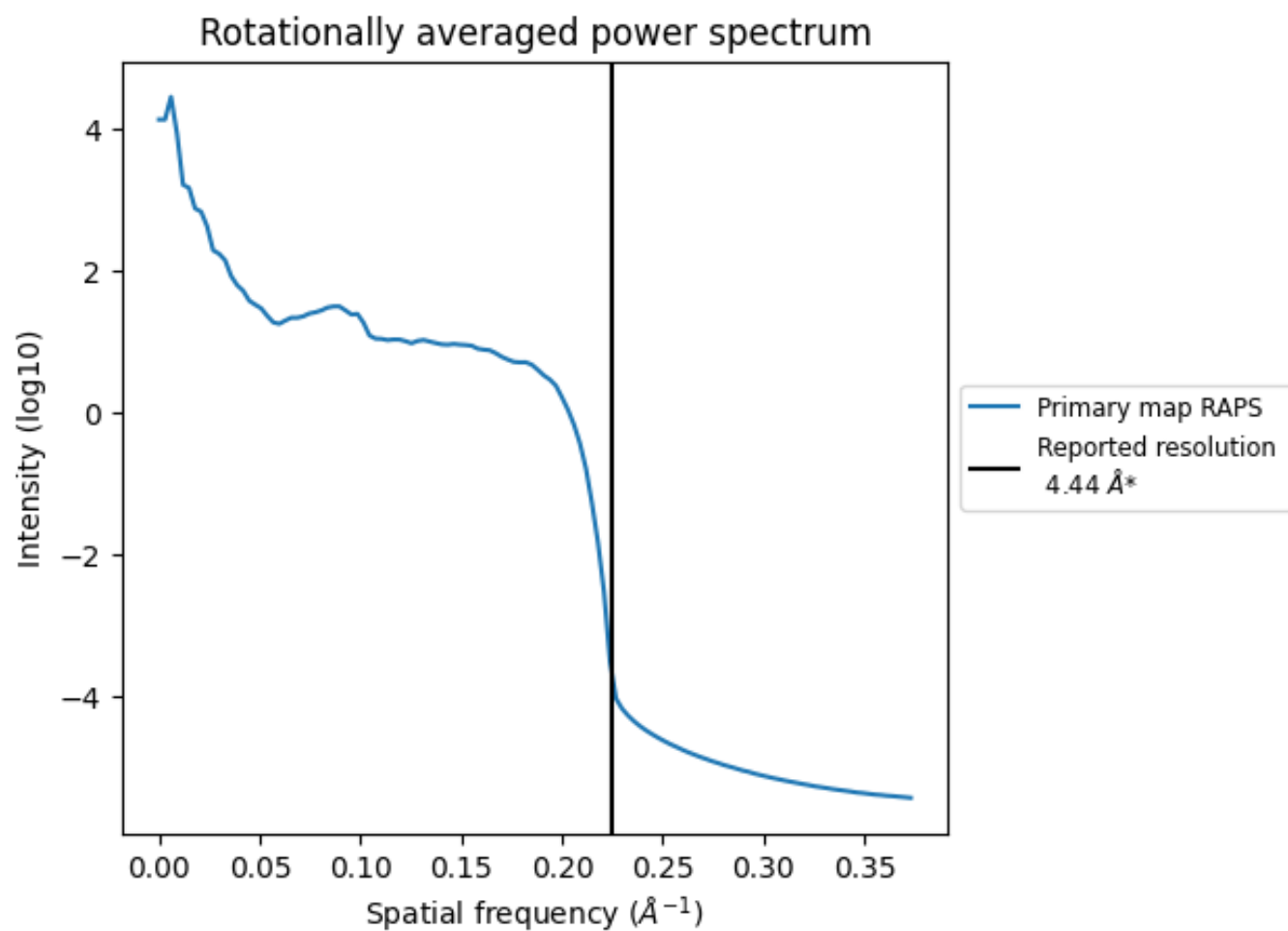
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 510 nm³; this corresponds to an approximate mass of 460 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 0.225 $\text{\AA}^{-1}$

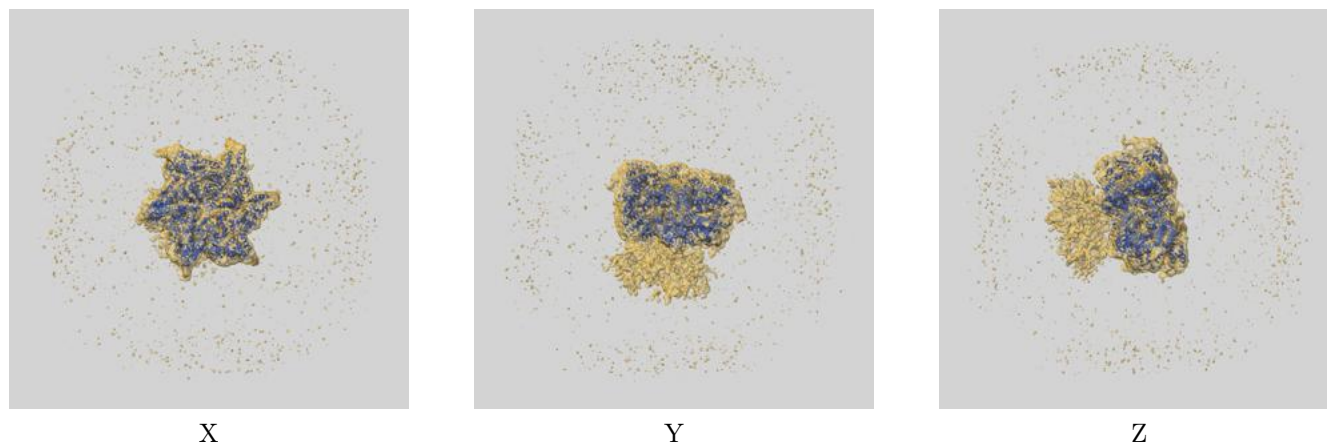
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

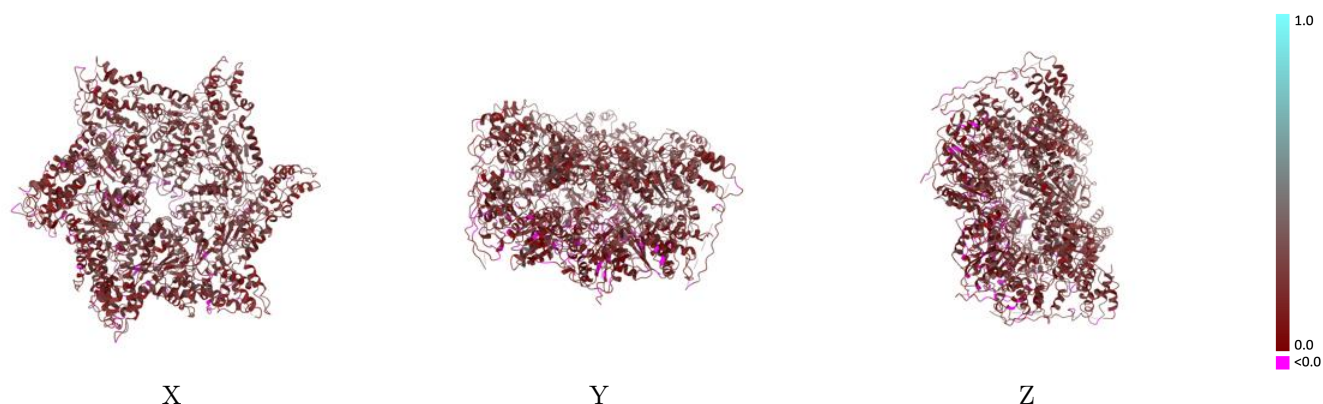
This section contains information regarding the fit between EMDB map EMD-9870 and PDB model 6JPQ. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



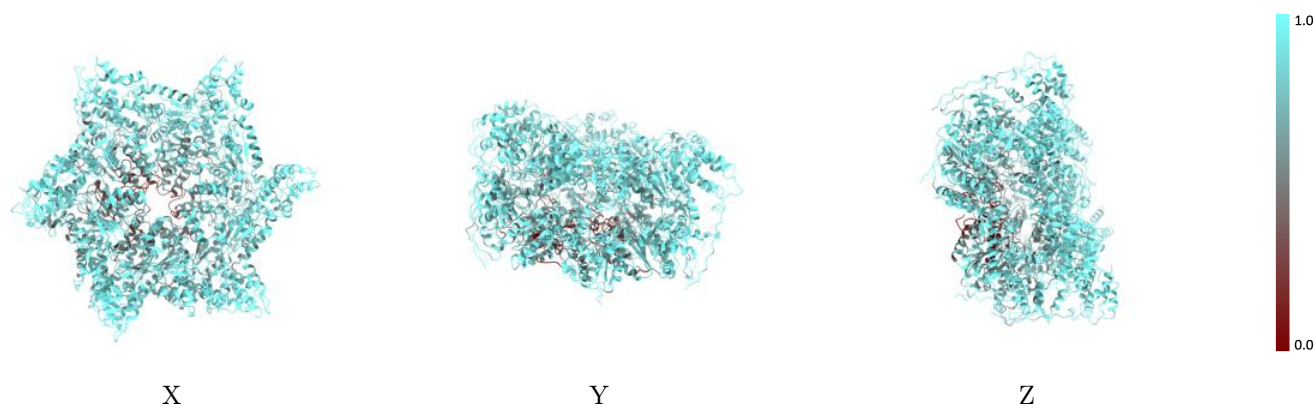
The images above show the 3D surface view of the map at the recommended contour level 1.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



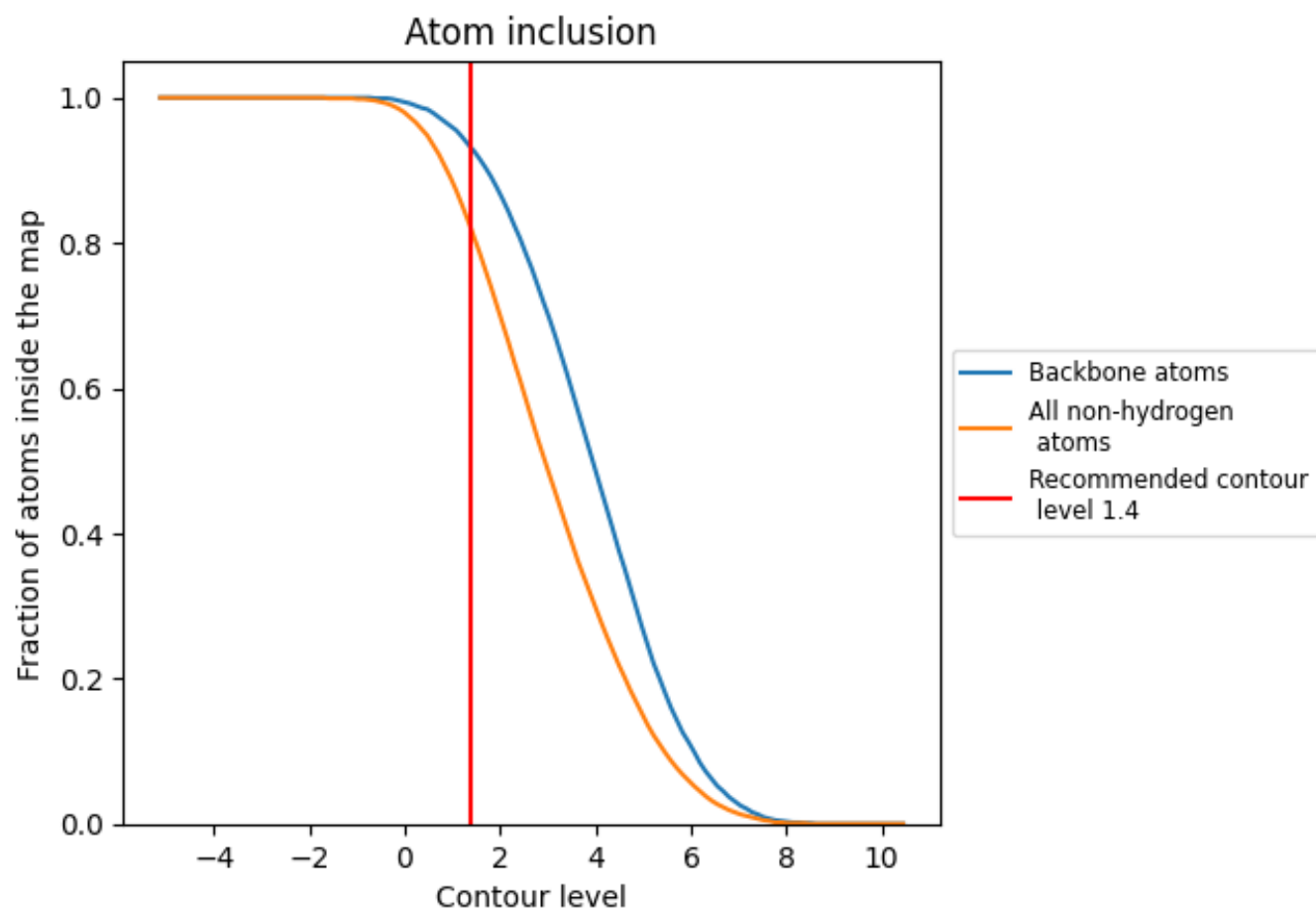
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 82% 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 (1.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8180	0.1880
A	0.7740	0.1790
B	0.8510	0.2030
C	0.8630	0.1970
D	0.8230	0.1890
E	0.8060	0.1850
F	0.7890	0.1770

1.0

0.0

<0.0