



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 09:27 AM UTC

PDB ID : 7ALW / pdb_00007alw
EMDB ID : EMD-11820
Title : Nonameric cytoplasmic domain of SctV from Yersinia enterocolitica
Authors : Kuhlen, L.; Johnson, S.
Deposited on : 2020-10-07
Resolution : 3.70 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:

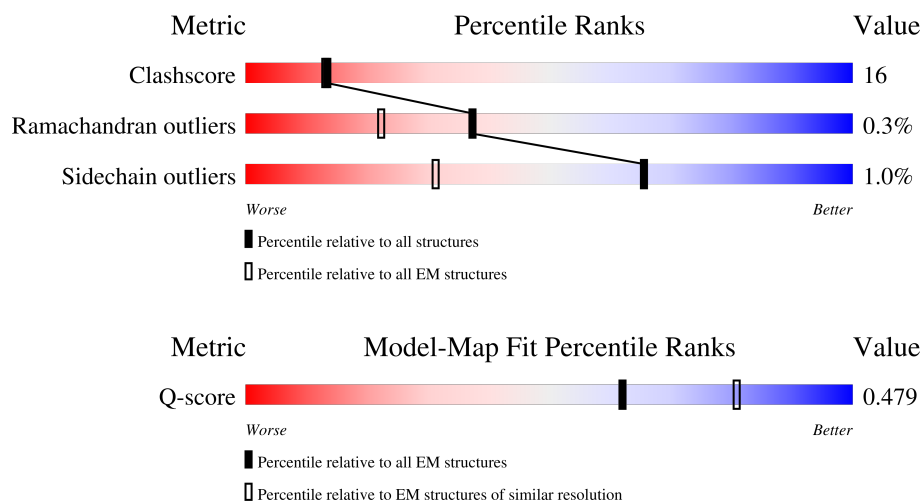
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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.



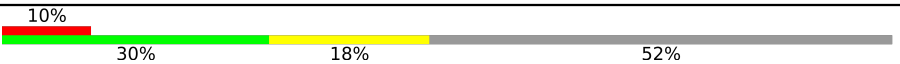
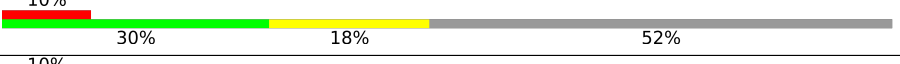
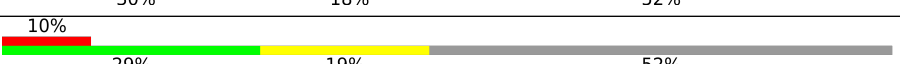
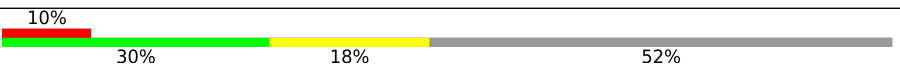
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

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	710	10% 29% 19% 52%
1	B	710	10% 30% 18% 52%
1	C	710	10% 30% 18% 52%
1	D	710	10% 30% 18% 52%

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Mol	Chain	Length	Quality of chain
1	E	710	
1	F	710	
1	G	710	
1	H	710	
1	I	710	
1	J	710	
1	K	710	
1	L	710	
1	M	710	
1	N	710	
1	O	710	
1	P	710	
1	Q	710	
1	R	710	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 50148 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 Low calcium response protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	344	Total	C	N	O	S	0	0
			2786	1776	469	532	9		
1	B	344	Total	C	N	O	S	0	0
			2786	1776	469	532	9		
1	C	344	Total	C	N	O	S	0	0
			2786	1776	469	532	9		
1	D	344	Total	C	N	O	S	0	0
			2786	1776	469	532	9		
1	E	344	Total	C	N	O	S	0	0
			2786	1776	469	532	9		
1	F	344	Total	C	N	O	S	0	0
			2786	1776	469	532	9		
1	G	344	Total	C	N	O	S	0	0
			2786	1776	469	532	9		
1	H	344	Total	C	N	O	S	0	0
			2786	1776	469	532	9		
1	I	344	Total	C	N	O	S	0	0
			2786	1776	469	532	9		
1	J	344	Total	C	N	O	S	0	0
			2786	1776	469	532	9		
1	K	344	Total	C	N	O	S	0	0
			2786	1776	469	532	9		
1	L	344	Total	C	N	O	S	0	0
			2786	1776	469	532	9		
1	M	344	Total	C	N	O	S	0	0
			2786	1776	469	532	9		
1	N	344	Total	C	N	O	S	0	0
			2786	1776	469	532	9		
1	O	344	Total	C	N	O	S	0	0
			2786	1776	469	532	9		
1	P	344	Total	C	N	O	S	0	0
			2786	1776	469	532	9		
1	Q	344	Total	C	N	O	S	0	0
			2786	1776	469	532	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	344	Total	C	N	O	S	0	0
			2786	1776	469	532	9		

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	ILE	LEU	conflict	UNP Q51875
A	705	GLU	-	expression tag	UNP Q51875
A	706	ASN	-	expression tag	UNP Q51875
A	707	LEU	-	expression tag	UNP Q51875
A	708	TYR	-	expression tag	UNP Q51875
A	709	PHE	-	expression tag	UNP Q51875
A	710	GLN	-	expression tag	UNP Q51875
B	38	ILE	LEU	conflict	UNP Q51875
B	705	GLU	-	expression tag	UNP Q51875
B	706	ASN	-	expression tag	UNP Q51875
B	707	LEU	-	expression tag	UNP Q51875
B	708	TYR	-	expression tag	UNP Q51875
B	709	PHE	-	expression tag	UNP Q51875
B	710	GLN	-	expression tag	UNP Q51875
C	38	ILE	LEU	conflict	UNP Q51875
C	705	GLU	-	expression tag	UNP Q51875
C	706	ASN	-	expression tag	UNP Q51875
C	707	LEU	-	expression tag	UNP Q51875
C	708	TYR	-	expression tag	UNP Q51875
C	709	PHE	-	expression tag	UNP Q51875
C	710	GLN	-	expression tag	UNP Q51875
D	38	ILE	LEU	conflict	UNP Q51875
D	705	GLU	-	expression tag	UNP Q51875
D	706	ASN	-	expression tag	UNP Q51875
D	707	LEU	-	expression tag	UNP Q51875
D	708	TYR	-	expression tag	UNP Q51875
D	709	PHE	-	expression tag	UNP Q51875
D	710	GLN	-	expression tag	UNP Q51875
E	38	ILE	LEU	conflict	UNP Q51875
E	705	GLU	-	expression tag	UNP Q51875
E	706	ASN	-	expression tag	UNP Q51875
E	707	LEU	-	expression tag	UNP Q51875
E	708	TYR	-	expression tag	UNP Q51875
E	709	PHE	-	expression tag	UNP Q51875
E	710	GLN	-	expression tag	UNP Q51875
F	38	ILE	LEU	conflict	UNP Q51875

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Chain	Residue	Modelled	Actual	Comment	Reference
F	705	GLU	-	expression tag	UNP Q51875
F	706	ASN	-	expression tag	UNP Q51875
F	707	LEU	-	expression tag	UNP Q51875
F	708	TYR	-	expression tag	UNP Q51875
F	709	PHE	-	expression tag	UNP Q51875
F	710	GLN	-	expression tag	UNP Q51875
G	38	ILE	LEU	conflict	UNP Q51875
G	705	GLU	-	expression tag	UNP Q51875
G	706	ASN	-	expression tag	UNP Q51875
G	707	LEU	-	expression tag	UNP Q51875
G	708	TYR	-	expression tag	UNP Q51875
G	709	PHE	-	expression tag	UNP Q51875
G	710	GLN	-	expression tag	UNP Q51875
H	38	ILE	LEU	conflict	UNP Q51875
H	705	GLU	-	expression tag	UNP Q51875
H	706	ASN	-	expression tag	UNP Q51875
H	707	LEU	-	expression tag	UNP Q51875
H	708	TYR	-	expression tag	UNP Q51875
H	709	PHE	-	expression tag	UNP Q51875
H	710	GLN	-	expression tag	UNP Q51875
I	38	ILE	LEU	conflict	UNP Q51875
I	705	GLU	-	expression tag	UNP Q51875
I	706	ASN	-	expression tag	UNP Q51875
I	707	LEU	-	expression tag	UNP Q51875
I	708	TYR	-	expression tag	UNP Q51875
I	709	PHE	-	expression tag	UNP Q51875
I	710	GLN	-	expression tag	UNP Q51875
J	38	ILE	LEU	conflict	UNP Q51875
J	705	GLU	-	expression tag	UNP Q51875
J	706	ASN	-	expression tag	UNP Q51875
J	707	LEU	-	expression tag	UNP Q51875
J	708	TYR	-	expression tag	UNP Q51875
J	709	PHE	-	expression tag	UNP Q51875
J	710	GLN	-	expression tag	UNP Q51875
K	38	ILE	LEU	conflict	UNP Q51875
K	705	GLU	-	expression tag	UNP Q51875
K	706	ASN	-	expression tag	UNP Q51875
K	707	LEU	-	expression tag	UNP Q51875
K	708	TYR	-	expression tag	UNP Q51875
K	709	PHE	-	expression tag	UNP Q51875
K	710	GLN	-	expression tag	UNP Q51875
L	38	ILE	LEU	conflict	UNP Q51875

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Chain	Residue	Modelled	Actual	Comment	Reference
L	705	GLU	-	expression tag	UNP Q51875
L	706	ASN	-	expression tag	UNP Q51875
L	707	LEU	-	expression tag	UNP Q51875
L	708	TYR	-	expression tag	UNP Q51875
L	709	PHE	-	expression tag	UNP Q51875
L	710	GLN	-	expression tag	UNP Q51875
M	38	ILE	LEU	conflict	UNP Q51875
M	705	GLU	-	expression tag	UNP Q51875
M	706	ASN	-	expression tag	UNP Q51875
M	707	LEU	-	expression tag	UNP Q51875
M	708	TYR	-	expression tag	UNP Q51875
M	709	PHE	-	expression tag	UNP Q51875
M	710	GLN	-	expression tag	UNP Q51875
N	38	ILE	LEU	conflict	UNP Q51875
N	705	GLU	-	expression tag	UNP Q51875
N	706	ASN	-	expression tag	UNP Q51875
N	707	LEU	-	expression tag	UNP Q51875
N	708	TYR	-	expression tag	UNP Q51875
N	709	PHE	-	expression tag	UNP Q51875
N	710	GLN	-	expression tag	UNP Q51875
O	38	ILE	LEU	conflict	UNP Q51875
O	705	GLU	-	expression tag	UNP Q51875
O	706	ASN	-	expression tag	UNP Q51875
O	707	LEU	-	expression tag	UNP Q51875
O	708	TYR	-	expression tag	UNP Q51875
O	709	PHE	-	expression tag	UNP Q51875
O	710	GLN	-	expression tag	UNP Q51875
P	38	ILE	LEU	conflict	UNP Q51875
P	705	GLU	-	expression tag	UNP Q51875
P	706	ASN	-	expression tag	UNP Q51875
P	707	LEU	-	expression tag	UNP Q51875
P	708	TYR	-	expression tag	UNP Q51875
P	709	PHE	-	expression tag	UNP Q51875
P	710	GLN	-	expression tag	UNP Q51875
Q	38	ILE	LEU	conflict	UNP Q51875
Q	705	GLU	-	expression tag	UNP Q51875
Q	706	ASN	-	expression tag	UNP Q51875
Q	707	LEU	-	expression tag	UNP Q51875
Q	708	TYR	-	expression tag	UNP Q51875
Q	709	PHE	-	expression tag	UNP Q51875
Q	710	GLN	-	expression tag	UNP Q51875
R	38	ILE	LEU	conflict	UNP Q51875

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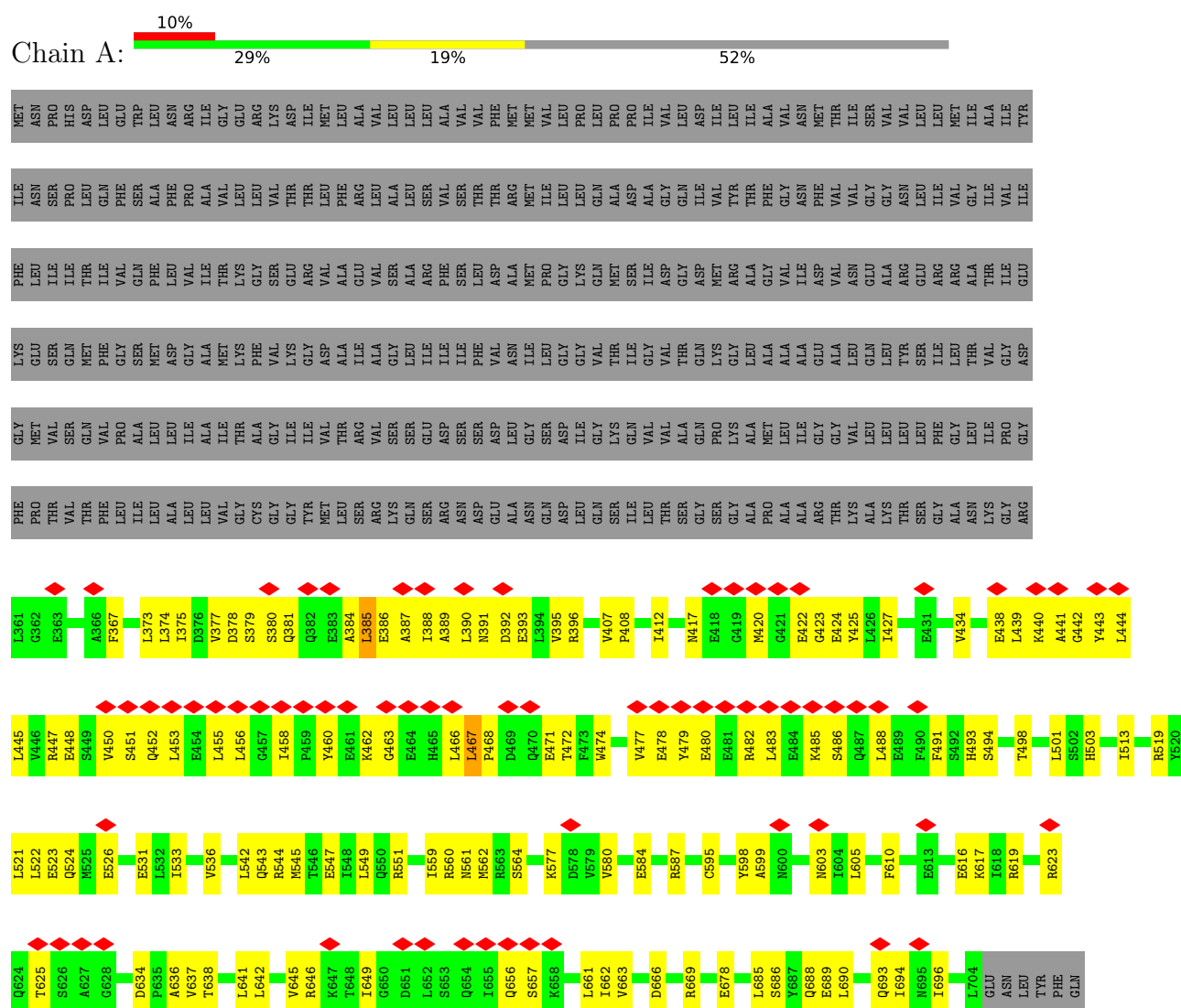
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Chain	Residue	Modelled	Actual	Comment	Reference
R	705	GLU	-	expression tag	UNP Q51875
R	706	ASN	-	expression tag	UNP Q51875
R	707	LEU	-	expression tag	UNP Q51875
R	708	TYR	-	expression tag	UNP Q51875
R	709	PHE	-	expression tag	UNP Q51875
R	710	GLN	-	expression tag	UNP Q51875

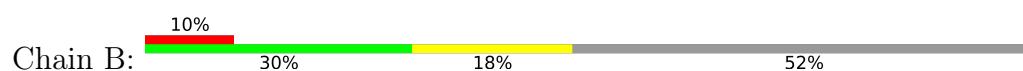
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

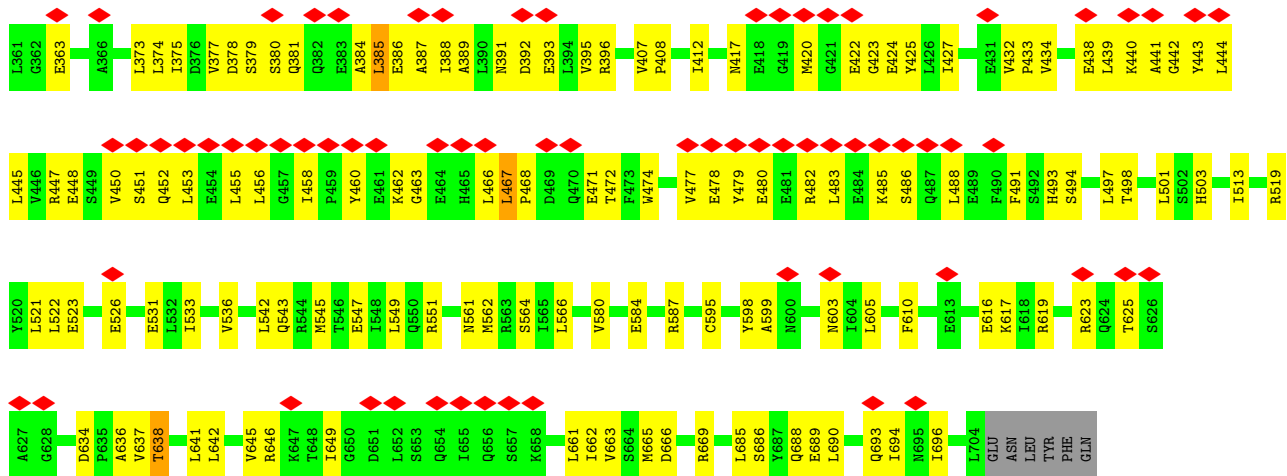
• Molecule 1: Low calcium response protein



• Molecule 1: Low calcium response protein

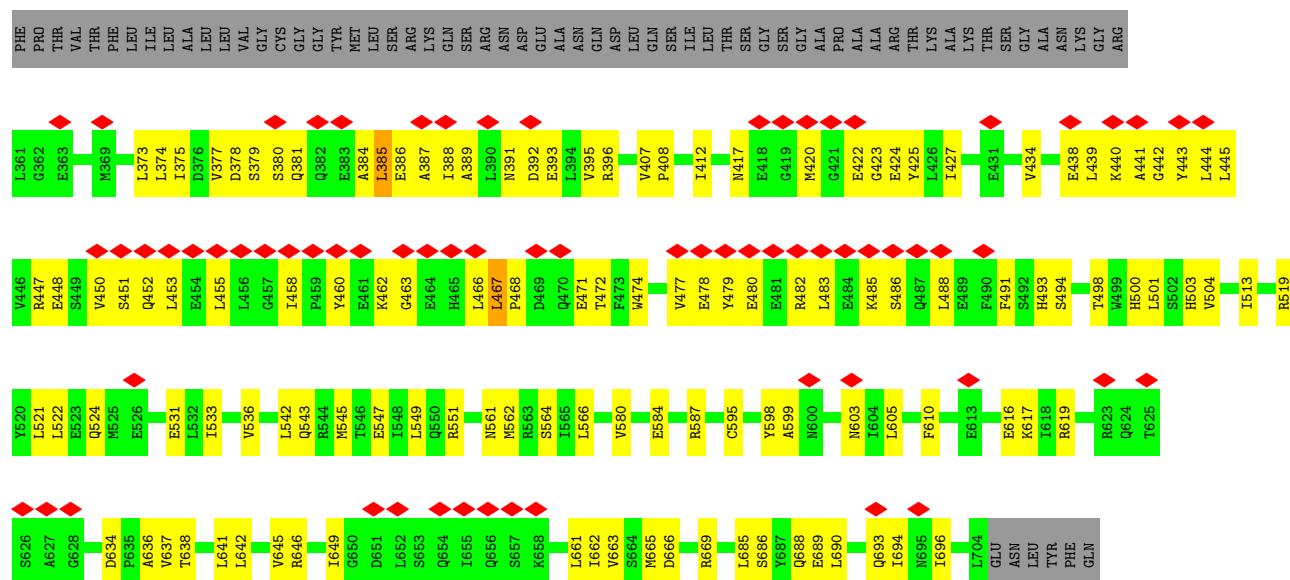




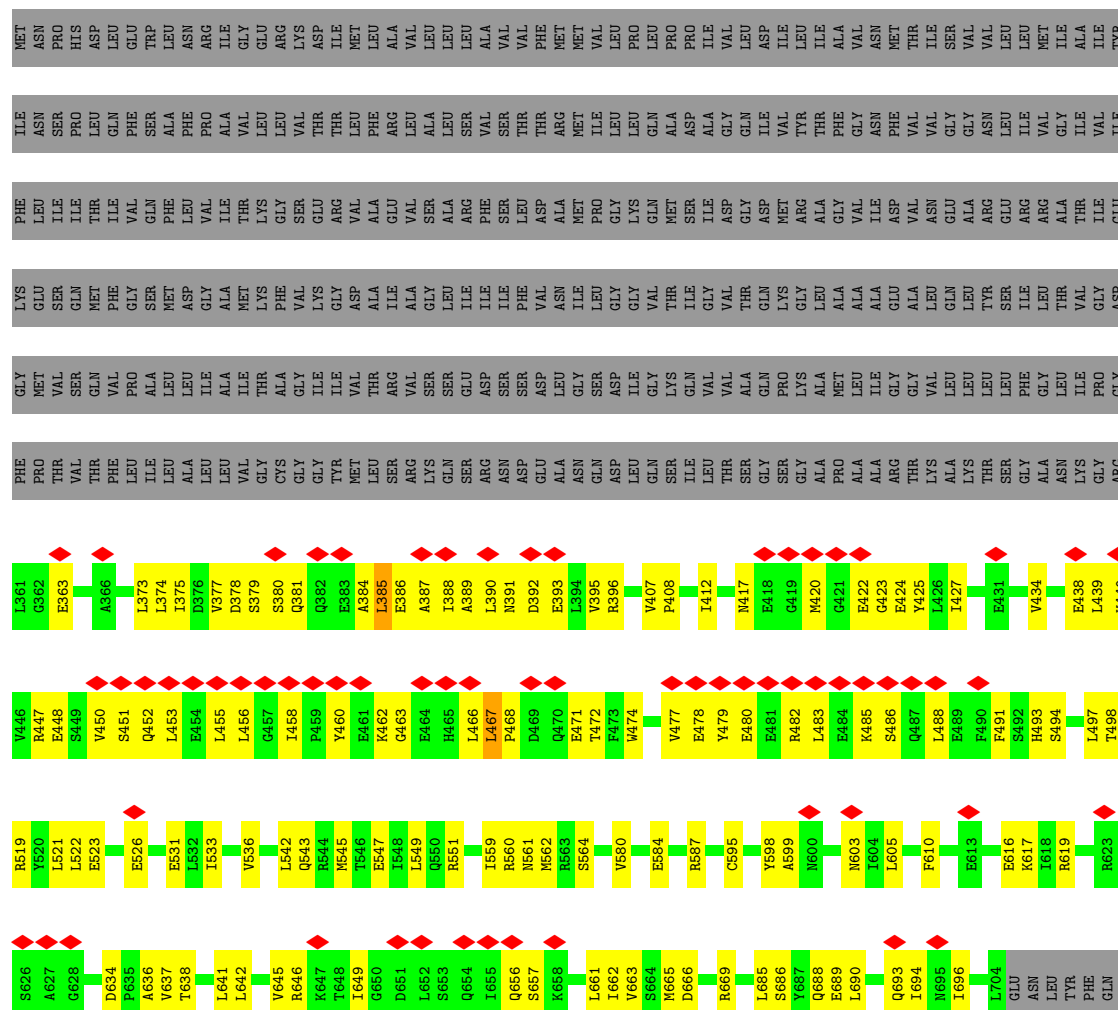
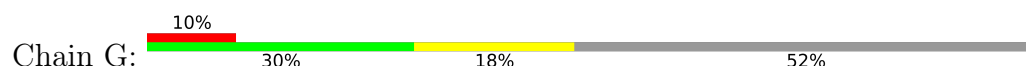


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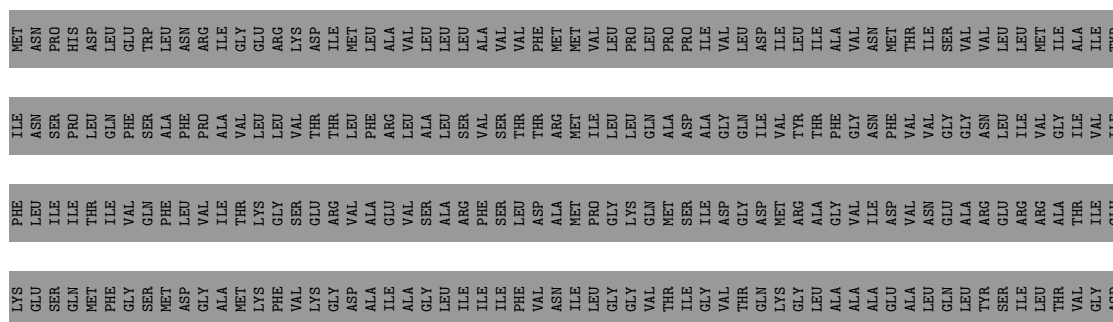
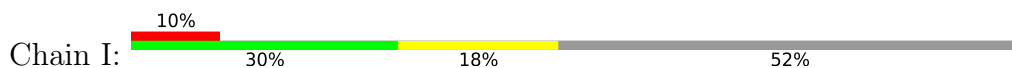
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MET	GLU	LEU	ASN	ASN	ASN
VAL	SER	ILE	SER	PRO	TRP
SER	GLN	ILE	PRO	HIS	ASP
GLN	MET	THR	LEU	ASP	LEU
VAL	PHE	ILE	GLN	LEU	GLU
PRO	GLY	VAL	PHE	GLU	ASP
ALA	SER	GLN	SER	THR	TRP
LEU	MET	PHE	ALA	LEU	ALA
LEU	ASP	LEU	PHE	ASN	ASN
ILE	GLY	VAL	PRO	ARG	ARG
ALA	ALA	ILE	ALA	ILE	ILE
ILE	MET	THR	VAL	GLY	GLY
THR	LYS	LYS	LEU	GLU	ARG
ARG	PHE	GLY	LEU	LEU	GLU
ILE	VAL	GLY	VAL	LYS	ASP
VAL	LYS	GLU	THR	ASP	ILE
GLY	ASP	ARG	THR	ILE	MET
THR	ALA	VAL	PHE	LEU	LEU
THR	ILE	ALA	ARG	ALA	ALA
ARG	ILE	GLU	THR	VAL	VAL
VAL	ALA	VAL	LEU	ALA	ALA
SER	GLY	SER	ALA	LEU	LEU
SER	LEU	ALA	LEU	LEU	LEU
GLU	ILE	ARG	SER	LEU	LEU
ASP	ILE	PHE	VAL	ALA	ALA
SER	ILE	SER	SER	VAL	VAL
SER	PHE	LEU	THR	THR	PHE
ASP	VAL	ASP	THR	ARG	MET
LEU	ASN	ALA	ARG	MET	MET
GLY	ILE	MET	MET	MET	VAL
ASP	LEU	PRO	ILE	VAL	LEU
ASP	GLY	GLY	LEU	LEU	LEU
ILE	GLY	LYS	LEU	PRO	LEU
GLY	VAL	GLN	GLN	GLN	LEU
LYS	THR	MET	ALA	PRO	PRO
ILE	ILE	SER	ASP	PRO	PRO
VAL	GLY	ILE	ALA	ILE	ILE
VAL	VAL	ASP	GLY	VAL	VAL
ALA	THR	GLY	ILE	VAL	VAL
GLN	GLN	ASP	GLN	ASN	ASN
PRO	LYS	MET	VAL	THR	MET
LYS	GLY	ARG	TYR	ILE	ILE
LEU	LEU	ALA	THR	ILE	ILE
MET	ALA	GLY	PHE	ALA	ALA
ILE	ALA	ILE	ASN	VAL	VAL
ILE	ALA	THR	ASN	THR	THR
GLY	GLU	ASP	PHE	MET	MET
GLY	ALA	VAL	VAL	THR	THR
VAL	LEU	GLN	GLY	VAL	VAL
LEU	LEU	ARG	ASN	VAL	VAL
LEU	TYR	ALA	GLY	VAL	VAL
PHE	SER	GLU	LEU	LEU	LEU
ILE	ILE	ARG	ILE	LEU	LEU
GLY	LEU	ARG	VAL	VAL	VAL
LEU	THR	ALA	GLY	ILE	ILE
ILE	VAL	THR	ILE	THR	ALA
PRO	GLY	ILE	THR	THR	THR
VAL	ASP	THR	VAL	THR	THR

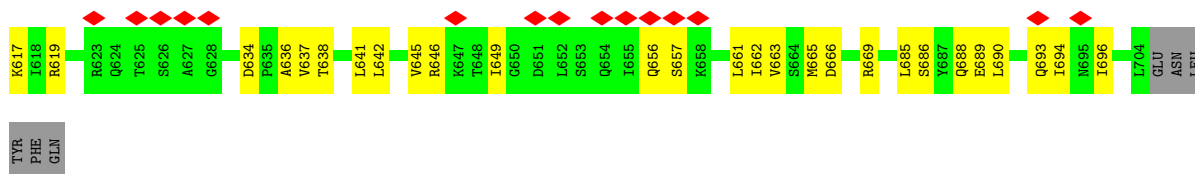


• Molecule 1: Low calcium response protein

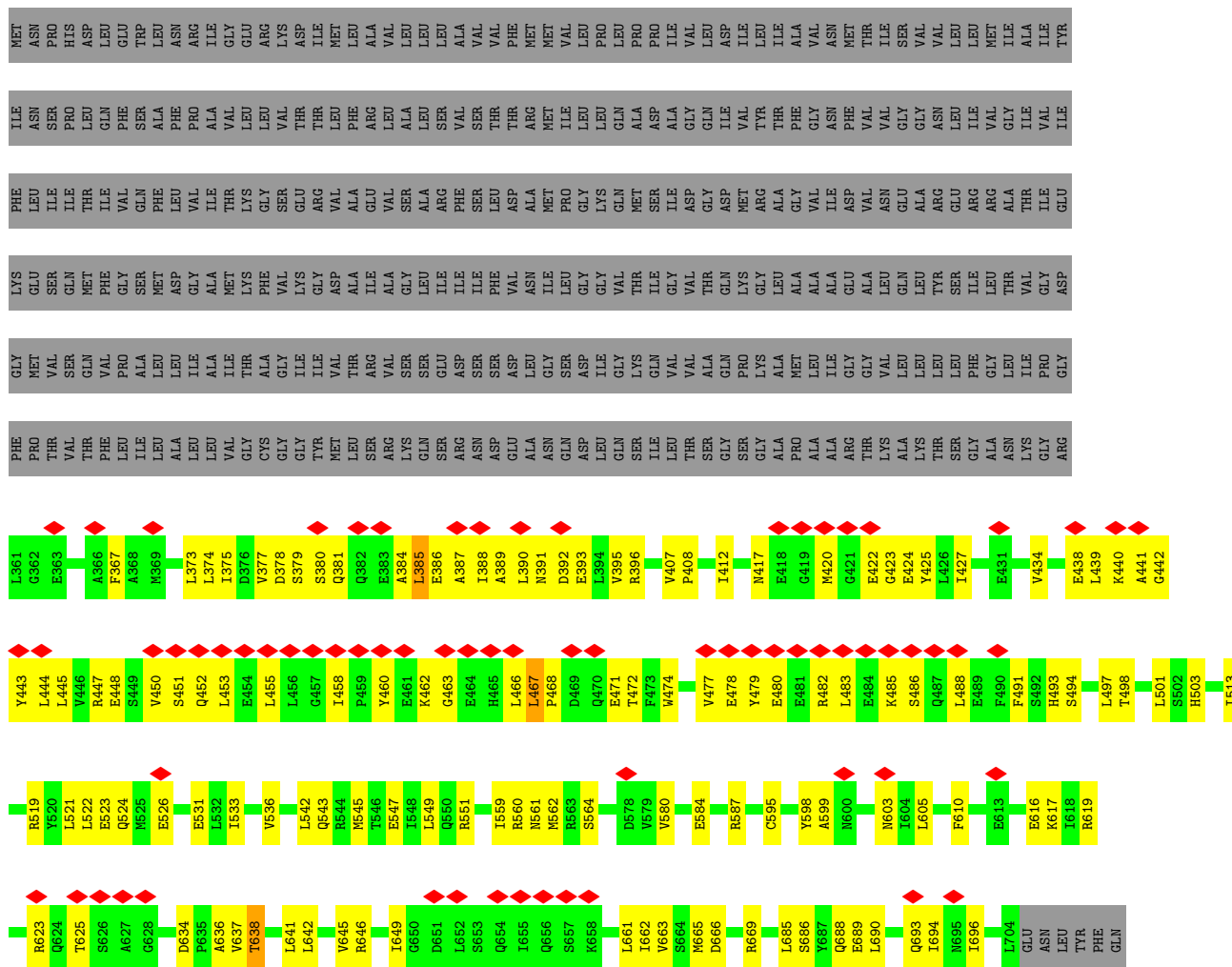
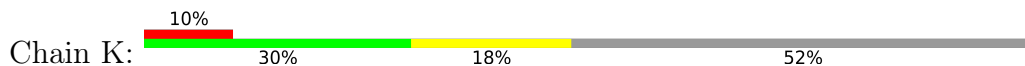


Chain H:

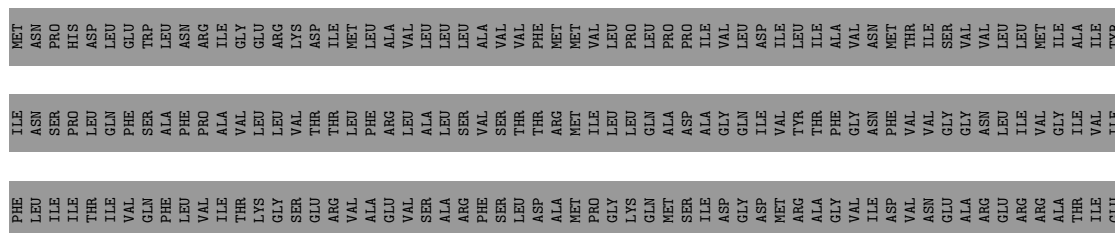
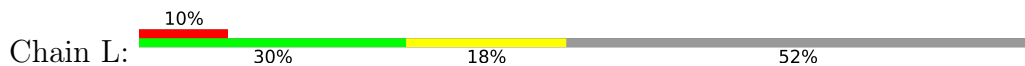




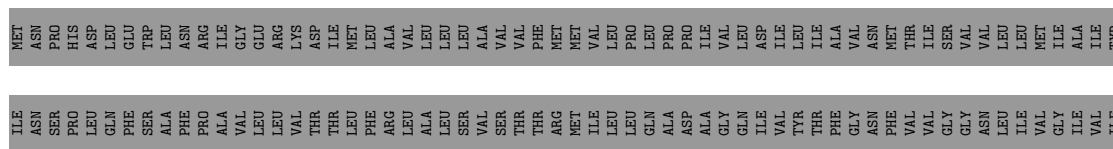
• Molecule 1: Low calcium response protein

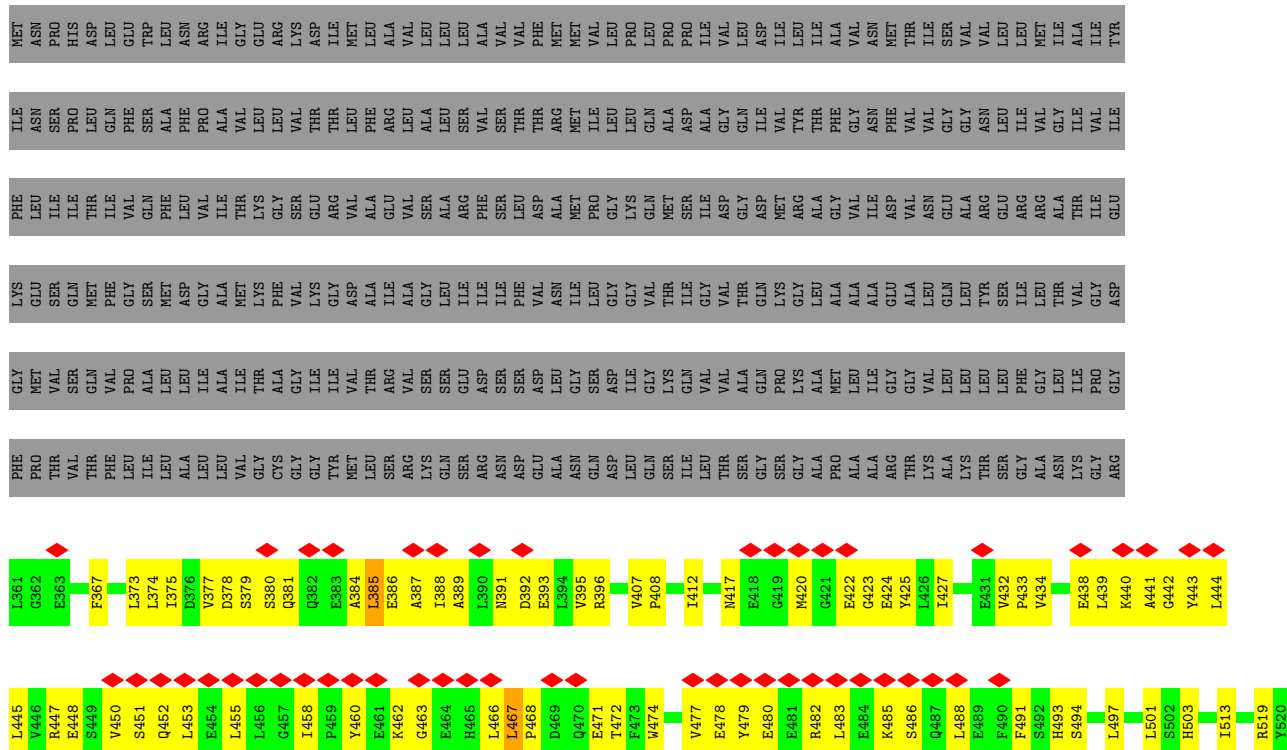


• Molecule 1: Low calcium response protein











L361	G362	E363	L373	L374	L375	D376	V377	D378	S379	S380	Q381	Q382	E383	A384	L385	E386	A387	I388	A389	L390	N391	D392	E393	L394	V395	R396	V407	P408	I412	N417	E418	G419	M420	G421	E422	G423	E424	Y425	L426	I427	E431	V434	E438	L439	K440	A441	G442	Y443	L444	L445	V446	R447			
E448	S449	V450	S451	Q452	L453	E454	L455	L456	Q457	I458	P459	Y460	E461	K462	Q463	E464	H465	L466	L467	P468	D469	Q470	E471	T472	F473	W474	Y477	E478	Y479	E480	E481	R482	L483	E484	K485	S486	Q487	L488	E489	F490	F491	S492	H493	S494	T498	W499	H500	L501	S502	H503	V504	I513	R519	Y520	L521
L522	E523	Q524	M525	E526	E531	L532	I533	V536	L542	Q543	R544	M545	T546	E547	I548	L549	Q550	R551	N561	M562	R563	S564	I565	L566	K577	V580	E584	R587	C595	Y598	A599	N600	N603	I604	L605	F610	E613	E616	K617	I618	R619	R623	Q624	T625											
S626	A627	G628	D634	P635	A636	V637	T638	L641	L642	V645	R646	I649	G650	D651	L652	S653	Q654	I655	Q656	S657	K658	L661	I662	M665	D666	R669	L685	S686	Y687	Q688	E689	L690	Q693	I694	N695	T696	L704	GLU	ASN	LEU	TYR	PHE	GLN												
ILE	ASN	SER	LEU	GLN	PHE	GLN	PHE	ALA	ALA	PRO	VAL	THR	GLY	GLY	THR	LEU	PHE	ARG	ALA	LEU	SER	VAL	VAL	SER	THR	ILE	PRO	GLY	ASP	GLN	ALA	ASP	GLN	THR	VAL	GLY	GLY	ASN	GLY	LEU	ASN	GLY	VAL	GLY	ILE	VAL	ILE	VAL	ILE	ILE					
PHE	LEU	ILE	THR	THR	ILE	VAL	VAL	GLY	ALA	SER	ILE	PHE	LEU	LEU	ALA	ILE	THR	LYS	LYS	PHE	GLY	VAL	GLY	THR	GLY	ARG	VAL	ALA	VAL	VAL	ARG	LEU	ALA	LEU	GLY	ASN	GLY	ARG	GLY	ILE	ARG	ALA	THR	ILE	VAL	GLY	ILE	VAL	GLU						
LYS	GLU	SER	GLN	MET	PHE	GLY	ALA	SER	MET	LEU	ALA	ALA	THR	LYS	PHE	GLY	VAL	GLY	THR	ASP	VAL	ALA	ILE	PHE	ILE	LEU	GLY	ASP	GLY	THR	ILE	ASP	GLN	THR	GLN	LYS	LYS	GLY	LEU	ALA	ALA	ILE	ASP	GLY	VAL	ASN	GLY	THR	VAL	PRO	GLY	ASP			
GLY	MET	VAL	SER	GLN	VAL	VAL	PRO	ALA	ALA	LEU	ILE	THR	THR	GLY	ALA	GLY	TYR	ILE	VAL	THR	ARG	VAL	THR	ARG	ASN	ASP	GLU	ALA	LEU	ASN	GLY	SER	ILE	LEU	ASP	ILE	GLY	VAL	LEU	LEU	LEU	LEU	THR	LEU	LEU	PHE	GLY	ILE	LEU	THR	ILE	PRO	GLY	GLY	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D9	Depositor
Number of particles used	15913	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 ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.047	Depositor
Minimum map value	-0.025	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0112	Depositor
Map size ($\text{\AA}$)	420.864, 420.864, 420.864	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.822, 0.822, 0.822	Depositor

5 Model quality

5.1 Standard geometry

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	0.43	0/2834	0.56	0/3833
1	B	0.43	0/2834	0.56	0/3833
1	C	0.43	0/2834	0.56	0/3833
1	D	0.43	0/2834	0.56	0/3833
1	E	0.43	0/2834	0.56	0/3833
1	F	0.43	0/2834	0.56	0/3833
1	G	0.43	0/2834	0.56	0/3833
1	H	0.43	0/2834	0.56	0/3833
1	I	0.43	0/2834	0.56	0/3833
1	J	0.43	0/2834	0.56	0/3833
1	K	0.43	0/2834	0.56	0/3833
1	L	0.43	0/2834	0.56	0/3833
1	M	0.43	0/2834	0.56	0/3833
1	N	0.43	0/2834	0.56	0/3833
1	O	0.43	0/2834	0.56	0/3833
1	P	0.43	0/2834	0.56	0/3833
1	Q	0.43	0/2834	0.56	0/3833
1	R	0.43	0/2834	0.56	0/3833
All	All	0.43	0/51012	0.56	0/68994

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	4
1	B	0	4
1	C	0	4
1	D	0	4
1	E	0	4
1	F	0	4
1	G	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	4
1	I	0	4
1	J	0	4
1	K	0	4
1	L	0	4
1	M	0	4
1	N	0	4
1	O	0	4
1	P	0	4
1	Q	0	4
1	R	0	4
All	All	0	72

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (72) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	385	LEU	Peptide
1	A	388	ILE	Peptide
1	A	458	ILE	Peptide
1	A	467	LEU	Peptide
1	B	385	LEU	Peptide
1	B	388	ILE	Peptide
1	B	458	ILE	Peptide
1	B	467	LEU	Peptide
1	C	385	LEU	Peptide
1	C	388	ILE	Peptide
1	C	458	ILE	Peptide
1	C	467	LEU	Peptide
1	D	385	LEU	Peptide
1	D	388	ILE	Peptide
1	D	458	ILE	Peptide
1	D	467	LEU	Peptide
1	E	385	LEU	Peptide
1	E	388	ILE	Peptide
1	E	458	ILE	Peptide
1	E	467	LEU	Peptide
1	F	385	LEU	Peptide
1	F	388	ILE	Peptide

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Mol	Chain	Res	Type	Group
1	F	458	ILE	Peptide
1	F	467	LEU	Peptide
1	G	385	LEU	Peptide
1	G	388	ILE	Peptide
1	G	458	ILE	Peptide
1	G	467	LEU	Peptide
1	H	385	LEU	Peptide
1	H	388	ILE	Peptide
1	H	458	ILE	Peptide
1	H	467	LEU	Peptide
1	I	385	LEU	Peptide
1	I	388	ILE	Peptide
1	I	458	ILE	Peptide
1	I	467	LEU	Peptide
1	J	385	LEU	Peptide
1	J	388	ILE	Peptide
1	J	458	ILE	Peptide
1	J	467	LEU	Peptide
1	K	385	LEU	Peptide
1	K	388	ILE	Peptide
1	K	458	ILE	Peptide
1	K	467	LEU	Peptide
1	L	385	LEU	Peptide
1	L	388	ILE	Peptide
1	L	458	ILE	Peptide
1	L	467	LEU	Peptide
1	M	385	LEU	Peptide
1	M	388	ILE	Peptide
1	M	458	ILE	Peptide
1	M	467	LEU	Peptide
1	N	385	LEU	Peptide
1	N	388	ILE	Peptide
1	N	458	ILE	Peptide
1	N	467	LEU	Peptide
1	O	385	LEU	Peptide
1	O	388	ILE	Peptide
1	O	458	ILE	Peptide
1	O	467	LEU	Peptide
1	P	385	LEU	Peptide
1	P	388	ILE	Peptide
1	P	458	ILE	Peptide
1	P	467	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	Q	385	LEU	Peptide
1	Q	388	ILE	Peptide
1	Q	458	ILE	Peptide
1	Q	467	LEU	Peptide
1	R	385	LEU	Peptide
1	R	388	ILE	Peptide
1	R	458	ILE	Peptide
1	R	467	LEU	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2786	0	2799	93	0
1	B	2786	0	2799	91	0
1	C	2786	0	2799	91	0
1	D	2786	0	2799	92	0
1	E	2786	0	2799	92	0
1	F	2786	0	2799	85	0
1	G	2786	0	2799	95	0
1	H	2786	0	2799	93	0
1	I	2786	0	2799	92	0
1	J	2786	0	2799	96	0
1	K	2786	0	2799	94	0
1	L	2786	0	2799	92	0
1	M	2786	0	2799	95	0
1	N	2786	0	2799	90	0
1	O	2786	0	2799	93	0
1	P	2786	0	2799	91	0
1	Q	2786	0	2799	92	0
1	R	2786	0	2799	90	0
All	All	50148	0	50382	1621	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 16.

All (1621) 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:F:385:LEU:O	1:F:387:ALA:N	2.15	0.80
1:R:385:LEU:O	1:R:387:ALA:N	2.15	0.80
1:E:385:LEU:O	1:E:387:ALA:N	2.15	0.80
1:Q:385:LEU:O	1:Q:387:ALA:N	2.15	0.80
1:G:385:LEU:O	1:G:387:ALA:N	2.15	0.80
1:J:385:LEU:O	1:J:387:ALA:N	2.15	0.80
1:D:385:LEU:O	1:D:387:ALA:N	2.15	0.79
1:P:385:LEU:O	1:P:387:ALA:N	2.15	0.79
1:H:385:LEU:O	1:H:387:ALA:N	2.15	0.79
1:K:385:LEU:O	1:K:387:ALA:N	2.15	0.79
1:A:385:LEU:O	1:A:387:ALA:N	2.15	0.79
1:M:385:LEU:O	1:M:387:ALA:N	2.15	0.79
1:O:385:LEU:O	1:O:387:ALA:N	2.15	0.79
1:C:385:LEU:O	1:C:387:ALA:N	2.15	0.79
1:I:385:LEU:O	1:I:387:ALA:N	2.15	0.78
1:L:385:LEU:O	1:L:387:ALA:N	2.15	0.78
1:B:385:LEU:O	1:B:387:ALA:N	2.15	0.78
1:N:385:LEU:O	1:N:387:ALA:N	2.15	0.78
1:G:519:ARG:HG2	1:H:531:GLU:HG2	1.68	0.76
1:G:522:LEU:HD21	1:G:545:MET:HE1	1.68	0.75
1:H:522:LEU:HD21	1:H:545:MET:HE1	1.68	0.75
1:J:522:LEU:HD21	1:J:545:MET:HE1	1.69	0.75
1:N:522:LEU:HD21	1:N:545:MET:HE1	1.69	0.75
1:B:522:LEU:HD21	1:B:545:MET:HE1	1.69	0.75
1:E:522:LEU:HD21	1:E:545:MET:HE1	1.68	0.75
1:K:522:LEU:HD21	1:K:545:MET:HE1	1.69	0.75
1:Q:522:LEU:HD21	1:Q:545:MET:HE1	1.69	0.75
1:C:522:LEU:HD21	1:C:545:MET:HE1	1.68	0.75
1:D:519:ARG:HG2	1:E:531:GLU:HG2	1.69	0.75
1:I:522:LEU:HD21	1:I:545:MET:HE1	1.68	0.75
1:O:522:LEU:HD21	1:O:545:MET:HE1	1.68	0.74
1:L:522:LEU:HD21	1:L:545:MET:HE1	1.69	0.74
1:P:522:LEU:HD21	1:P:545:MET:HE1	1.68	0.74
1:A:522:LEU:HD21	1:A:545:MET:HE1	1.68	0.74
1:M:522:LEU:HD21	1:M:545:MET:HE1	1.69	0.74
1:D:522:LEU:HD21	1:D:545:MET:HE1	1.68	0.73
1:R:522:LEU:HD21	1:R:545:MET:HE1	1.68	0.73
1:J:531:GLU:HG2	1:R:519:ARG:HG2	1.71	0.73
1:F:522:LEU:HD21	1:F:545:MET:HE1	1.69	0.73
1:J:519:ARG:HG2	1:K:531:GLU:HG2	1.72	0.72
1:K:519:ARG:HG2	1:L:531:GLU:HG2	1.72	0.72
1:A:531:GLU:HG2	1:I:519:ARG:HG2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:519:ARG:HG2	1:F:531:GLU:HG2	1.72	0.72
1:L:444:LEU:HD13	1:L:477:VAL:HG11	1.72	0.72
1:M:519:ARG:HG2	1:N:531:GLU:HG2	1.72	0.72
1:A:519:ARG:HG2	1:B:531:GLU:HG2	1.72	0.71
1:H:519:ARG:HG2	1:I:531:GLU:HG2	1.72	0.71
1:I:444:LEU:HD13	1:I:477:VAL:HG11	1.72	0.71
1:L:519:ARG:HG2	1:M:531:GLU:HG2	1.72	0.71
1:F:444:LEU:HD13	1:F:477:VAL:HG11	1.72	0.71
1:R:444:LEU:HD13	1:R:477:VAL:HG11	1.72	0.71
1:H:444:LEU:HD13	1:H:477:VAL:HG11	1.72	0.71
1:N:519:ARG:HG2	1:O:531:GLU:HG2	1.72	0.71
1:K:444:LEU:HD13	1:K:477:VAL:HG11	1.72	0.71
1:P:519:ARG:HG2	1:Q:531:GLU:HG2	1.71	0.71
1:B:519:ARG:HG2	1:C:531:GLU:HG2	1.72	0.71
1:J:444:LEU:HD13	1:J:477:VAL:HG11	1.72	0.71
1:G:444:LEU:HD13	1:G:477:VAL:HG11	1.72	0.71
1:B:444:LEU:HD13	1:B:477:VAL:HG11	1.72	0.70
1:N:444:LEU:HD13	1:N:477:VAL:HG11	1.72	0.70
1:O:519:ARG:HG2	1:P:531:GLU:HG2	1.73	0.70
1:P:444:LEU:HD13	1:P:477:VAL:HG11	1.72	0.70
1:D:444:LEU:HD13	1:D:477:VAL:HG11	1.72	0.70
1:M:444:LEU:HD13	1:M:477:VAL:HG11	1.72	0.70
1:A:444:LEU:HD13	1:A:477:VAL:HG11	1.72	0.69
1:C:444:LEU:HD13	1:C:477:VAL:HG11	1.72	0.69
1:O:444:LEU:HD13	1:O:477:VAL:HG11	1.72	0.69
1:D:407:VAL:HG22	1:D:513:ILE:HD11	1.74	0.69
1:E:444:LEU:HD13	1:E:477:VAL:HG11	1.72	0.69
1:N:407:VAL:HG22	1:N:513:ILE:HD11	1.74	0.69
1:A:407:VAL:HG22	1:A:513:ILE:HD11	1.74	0.69
1:B:407:VAL:HG22	1:B:513:ILE:HD11	1.74	0.69
1:M:407:VAL:HG22	1:M:513:ILE:HD11	1.74	0.69
1:P:407:VAL:HG22	1:P:513:ILE:HD11	1.74	0.69
1:Q:444:LEU:HD13	1:Q:477:VAL:HG11	1.72	0.69
1:J:407:VAL:HG22	1:J:513:ILE:HD11	1.74	0.68
1:E:378:ASP:OD2	1:E:424:GLU:N	2.27	0.68
1:G:407:VAL:HG22	1:G:513:ILE:HD11	1.74	0.68
1:K:407:VAL:HG22	1:K:513:ILE:HD11	1.74	0.68
1:C:407:VAL:HG22	1:C:513:ILE:HD11	1.74	0.68
1:Q:378:ASP:OD2	1:Q:424:GLU:N	2.27	0.68
1:D:378:ASP:OD2	1:D:424:GLU:N	2.27	0.68
1:H:407:VAL:HG22	1:H:513:ILE:HD11	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:407:VAL:HG22	1:O:513:ILE:HD11	1.74	0.68
1:P:378:ASP:OD2	1:P:424:GLU:N	2.27	0.68
1:R:407:VAL:HG22	1:R:513:ILE:HD11	1.74	0.68
1:F:378:ASP:OD2	1:F:424:GLU:N	2.27	0.68
1:F:407:VAL:HG22	1:F:513:ILE:HD11	1.74	0.68
1:Q:519:ARG:HG2	1:R:531:GLU:HG2	1.75	0.68
1:G:688:GLN:N	1:G:688:GLN:OE1	2.28	0.67
1:J:688:GLN:N	1:J:688:GLN:OE1	2.28	0.67
1:K:447:ARG:NH2	1:K:472:THR:OG1	2.21	0.67
1:Q:407:VAL:HG22	1:Q:513:ILE:HD11	1.74	0.67
1:A:688:GLN:N	1:A:688:GLN:OE1	2.28	0.67
1:I:407:VAL:HG22	1:I:513:ILE:HD11	1.74	0.67
1:Q:447:ARG:NH2	1:Q:472:THR:OG1	2.21	0.67
1:E:688:GLN:N	1:E:688:GLN:OE1	2.28	0.67
1:L:407:VAL:HG22	1:L:513:ILE:HD11	1.74	0.67
1:L:447:ARG:NH2	1:L:472:THR:OG1	2.21	0.67
1:M:688:GLN:N	1:M:688:GLN:OE1	2.28	0.67
1:Q:688:GLN:N	1:Q:688:GLN:OE1	2.28	0.67
1:E:407:VAL:HG22	1:E:513:ILE:HD11	1.74	0.67
1:H:447:ARG:NH2	1:H:472:THR:OG1	2.21	0.67
1:H:688:GLN:N	1:H:688:GLN:OE1	2.28	0.67
1:L:688:GLN:N	1:L:688:GLN:OE1	2.28	0.67
1:E:447:ARG:NH2	1:E:472:THR:OG1	2.21	0.67
1:K:688:GLN:OE1	1:K:688:GLN:N	2.28	0.67
1:N:378:ASP:OD2	1:N:424:GLU:N	2.27	0.67
1:I:447:ARG:NH2	1:I:472:THR:OG1	2.21	0.67
1:I:688:GLN:OE1	1:I:688:GLN:N	2.28	0.67
1:P:688:GLN:OE1	1:P:688:GLN:N	2.28	0.67
1:R:688:GLN:N	1:R:688:GLN:OE1	2.28	0.67
1:B:378:ASP:OD2	1:B:424:GLU:N	2.27	0.67
1:C:688:GLN:N	1:C:688:GLN:OE1	2.28	0.67
1:D:688:GLN:OE1	1:D:688:GLN:N	2.28	0.67
1:E:599:ALA:HB2	1:E:605:LEU:HD13	1.77	0.67
1:F:688:GLN:OE1	1:F:688:GLN:N	2.28	0.67
1:M:378:ASP:OD2	1:M:424:GLU:N	2.27	0.67
1:O:688:GLN:N	1:O:688:GLN:OE1	2.28	0.67
1:Q:599:ALA:HB2	1:Q:605:LEU:HD13	1.77	0.67
1:C:599:ALA:HB2	1:C:605:LEU:HD13	1.77	0.66
1:K:478:GLU:N	1:K:478:GLU:OE1	2.28	0.66
1:O:599:ALA:HB2	1:O:605:LEU:HD13	1.77	0.66
1:R:543:GLN:NE2	1:R:547:GLU:OE1	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:599:ALA:HB2	1:R:605:LEU:HD13	1.77	0.66
1:A:378:ASP:OD2	1:A:424:GLU:N	2.27	0.66
1:F:543:GLN:NE2	1:F:547:GLU:OE1	2.28	0.66
1:F:599:ALA:HB2	1:F:605:LEU:HD13	1.77	0.66
1:H:478:GLU:N	1:H:478:GLU:OE1	2.28	0.66
1:P:599:ALA:HB2	1:P:605:LEU:HD13	1.77	0.66
1:D:599:ALA:HB2	1:D:605:LEU:HD13	1.77	0.66
1:H:378:ASP:OD2	1:H:424:GLU:N	2.27	0.66
1:H:543:GLN:NE2	1:H:547:GLU:OE1	2.28	0.66
1:K:378:ASP:OD2	1:K:424:GLU:N	2.27	0.66
1:K:543:GLN:NE2	1:K:547:GLU:OE1	2.28	0.66
1:E:543:GLN:NE2	1:E:547:GLU:OE1	2.28	0.66
1:J:447:ARG:NH2	1:J:472:THR:OG1	2.21	0.66
1:N:688:GLN:OE1	1:N:688:GLN:N	2.28	0.66
1:O:378:ASP:OD2	1:O:424:GLU:N	2.27	0.66
1:Q:543:GLN:NE2	1:Q:547:GLU:OE1	2.28	0.66
1:G:543:GLN:NE2	1:G:547:GLU:OE1	2.28	0.66
1:I:478:GLU:OE1	1:I:478:GLU:N	2.28	0.66
1:J:543:GLN:NE2	1:J:547:GLU:OE1	2.28	0.66
1:B:688:GLN:N	1:B:688:GLN:OE1	2.28	0.66
1:C:378:ASP:OD2	1:C:424:GLU:N	2.27	0.66
1:G:447:ARG:NH2	1:G:472:THR:OG1	2.21	0.66
1:J:478:GLU:N	1:J:478:GLU:OE1	2.28	0.66
1:M:447:ARG:NH2	1:M:472:THR:OG1	2.21	0.66
1:G:478:GLU:OE1	1:G:478:GLU:N	2.29	0.66
1:L:478:GLU:OE1	1:L:478:GLU:N	2.29	0.66
1:R:392:ASP:HA	1:R:395:VAL:HG12	1.78	0.66
1:B:478:GLU:OE1	1:B:478:GLU:N	2.28	0.66
1:F:392:ASP:HA	1:F:395:VAL:HG12	1.78	0.66
1:N:478:GLU:OE1	1:N:478:GLU:N	2.29	0.66
1:L:378:ASP:OD2	1:L:424:GLU:N	2.27	0.66
1:A:447:ARG:NH2	1:A:472:THR:OG1	2.21	0.65
1:B:543:GLN:NE2	1:B:547:GLU:OE1	2.28	0.65
1:B:599:ALA:HB2	1:B:605:LEU:HD13	1.77	0.65
1:C:543:GLN:NE2	1:C:547:GLU:OE1	2.28	0.65
1:J:599:ALA:HB2	1:J:605:LEU:HD13	1.77	0.65
1:O:543:GLN:NE2	1:O:547:GLU:OE1	2.28	0.65
1:G:599:ALA:HB2	1:G:605:LEU:HD13	1.77	0.65
1:I:378:ASP:OD2	1:I:424:GLU:N	2.27	0.65
1:N:543:GLN:NE2	1:N:547:GLU:OE1	2.28	0.65
1:N:599:ALA:HB2	1:N:605:LEU:HD13	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:543:GLN:NE2	1:P:547:GLU:OE1	2.28	0.65
1:C:478:GLU:OE1	1:C:478:GLU:N	2.28	0.65
1:D:543:GLN:NE2	1:D:547:GLU:OE1	2.28	0.65
1:O:478:GLU:OE1	1:O:478:GLU:N	2.28	0.65
1:H:392:ASP:HA	1:H:395:VAL:HG12	1.78	0.65
1:B:392:ASP:HA	1:B:395:VAL:HG12	1.78	0.65
1:F:445:LEU:HG	1:F:474:TRP:HB3	1.79	0.65
1:G:445:LEU:HG	1:G:474:TRP:HB3	1.79	0.65
1:J:445:LEU:HG	1:J:474:TRP:HB3	1.79	0.65
1:K:392:ASP:HA	1:K:395:VAL:HG12	1.78	0.65
1:R:445:LEU:HG	1:R:474:TRP:HB3	1.79	0.65
1:A:599:ALA:HB2	1:A:605:LEU:HD13	1.77	0.65
1:E:445:LEU:HG	1:E:474:TRP:HB3	1.79	0.65
1:I:543:GLN:NE2	1:I:547:GLU:OE1	2.28	0.65
1:L:543:GLN:NE2	1:L:547:GLU:OE1	2.28	0.65
1:M:599:ALA:HB2	1:M:605:LEU:HD13	1.77	0.65
1:N:392:ASP:HA	1:N:395:VAL:HG12	1.78	0.65
1:Q:392:ASP:HA	1:Q:395:VAL:HG12	1.78	0.65
1:Q:445:LEU:HG	1:Q:474:TRP:HB3	1.79	0.65
1:R:378:ASP:OD2	1:R:424:GLU:N	2.27	0.65
1:D:445:LEU:HG	1:D:474:TRP:HB3	1.79	0.65
1:J:392:ASP:HA	1:J:395:VAL:HG12	1.78	0.65
1:K:445:LEU:HG	1:K:474:TRP:HB3	1.79	0.65
1:A:478:GLU:N	1:A:478:GLU:OE1	2.28	0.65
1:C:445:LEU:HG	1:C:474:TRP:HB3	1.79	0.65
1:E:392:ASP:HA	1:E:395:VAL:HG12	1.78	0.65
1:G:378:ASP:OD2	1:G:424:GLU:N	2.27	0.65
1:G:392:ASP:HA	1:G:395:VAL:HG12	1.78	0.65
1:I:599:ALA:HB2	1:I:605:LEU:HD13	1.77	0.65
1:J:378:ASP:OD2	1:J:424:GLU:N	2.27	0.65
1:P:445:LEU:HG	1:P:474:TRP:HB3	1.79	0.65
1:A:543:GLN:NE2	1:A:547:GLU:OE1	2.28	0.65
1:D:392:ASP:HA	1:D:395:VAL:HG12	1.78	0.65
1:H:445:LEU:HG	1:H:474:TRP:HB3	1.79	0.65
1:O:392:ASP:HA	1:O:395:VAL:HG12	1.78	0.65
1:Q:662:ILE:HD13	1:Q:690:LEU:HD11	1.79	0.65
1:R:447:ARG:NH2	1:R:472:THR:OG1	2.21	0.65
1:E:662:ILE:HD13	1:E:690:LEU:HD11	1.79	0.64
1:K:599:ALA:HB2	1:K:605:LEU:HD13	1.77	0.64
1:L:599:ALA:HB2	1:L:605:LEU:HD13	1.77	0.64
1:M:392:ASP:HA	1:M:395:VAL:HG12	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:478:GLU:OE1	1:M:478:GLU:N	2.28	0.64
1:M:543:GLN:NE2	1:M:547:GLU:OE1	2.28	0.64
1:O:445:LEU:HG	1:O:474:TRP:HB3	1.79	0.64
1:P:392:ASP:HA	1:P:395:VAL:HG12	1.78	0.64
1:R:478:GLU:N	1:R:478:GLU:OE1	2.28	0.64
1:A:392:ASP:HA	1:A:395:VAL:HG12	1.78	0.64
1:C:392:ASP:HA	1:C:395:VAL:HG12	1.78	0.64
1:F:478:GLU:N	1:F:478:GLU:OE1	2.28	0.64
1:H:599:ALA:HB2	1:H:605:LEU:HD13	1.77	0.64
1:D:478:GLU:OE1	1:D:478:GLU:N	2.28	0.64
1:N:447:ARG:NH2	1:N:472:THR:OG1	2.21	0.64
1:P:662:ILE:HD13	1:P:690:LEU:HD11	1.79	0.64
1:D:662:ILE:HD13	1:D:690:LEU:HD11	1.79	0.64
1:P:478:GLU:OE1	1:P:478:GLU:N	2.28	0.64
1:F:447:ARG:NH2	1:F:472:THR:OG1	2.21	0.64
1:L:445:LEU:HG	1:L:474:TRP:HB3	1.79	0.64
1:B:445:LEU:HG	1:B:474:TRP:HB3	1.79	0.64
1:I:392:ASP:HA	1:I:395:VAL:HG12	1.78	0.64
1:I:445:LEU:HG	1:I:474:TRP:HB3	1.79	0.64
1:N:445:LEU:HG	1:N:474:TRP:HB3	1.79	0.64
1:B:447:ARG:NH2	1:B:472:THR:OG1	2.21	0.64
1:L:392:ASP:HA	1:L:395:VAL:HG12	1.78	0.64
1:E:478:GLU:N	1:E:478:GLU:OE1	2.28	0.64
1:F:662:ILE:HD13	1:F:690:LEU:HD11	1.79	0.64
1:O:447:ARG:NH2	1:O:472:THR:OG1	2.21	0.64
1:A:662:ILE:HD13	1:A:690:LEU:HD11	1.79	0.64
1:C:662:ILE:HD13	1:C:690:LEU:HD11	1.79	0.64
1:G:662:ILE:HD13	1:G:690:LEU:HD11	1.79	0.64
1:M:662:ILE:HD13	1:M:690:LEU:HD11	1.79	0.64
1:O:662:ILE:HD13	1:O:690:LEU:HD11	1.79	0.64
1:R:662:ILE:HD13	1:R:690:LEU:HD11	1.79	0.64
1:F:377:VAL:HG12	1:F:425:TYR:HB2	1.81	0.64
1:J:662:ILE:HD13	1:J:690:LEU:HD11	1.79	0.64
1:Q:478:GLU:OE1	1:Q:478:GLU:N	2.28	0.64
1:R:377:VAL:HG12	1:R:425:TYR:HB2	1.80	0.64
1:C:447:ARG:NH2	1:C:472:THR:OG1	2.21	0.63
1:E:377:VAL:HG12	1:E:425:TYR:HB2	1.80	0.63
1:H:662:ILE:HD13	1:H:690:LEU:HD11	1.79	0.63
1:K:662:ILE:HD13	1:K:690:LEU:HD11	1.79	0.63
1:M:445:LEU:HG	1:M:474:TRP:HB3	1.79	0.63
1:Q:377:VAL:HG12	1:Q:425:TYR:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:519:ARG:HG2	1:G:531:GLU:HG2	1.80	0.63
1:G:561:ASN:ND2	1:G:564:SER:OG	2.32	0.63
1:J:561:ASN:ND2	1:J:564:SER:OG	2.32	0.63
1:A:445:LEU:HG	1:A:474:TRP:HB3	1.79	0.63
1:E:561:ASN:ND2	1:E:564:SER:OG	2.32	0.63
1:J:377:VAL:HG12	1:J:425:TYR:HB2	1.81	0.63
1:N:377:VAL:HG12	1:N:425:TYR:HB2	1.80	0.63
1:Q:561:ASN:ND2	1:Q:564:SER:OG	2.32	0.63
1:B:377:VAL:HG12	1:B:425:TYR:HB2	1.81	0.63
1:C:561:ASN:ND2	1:C:564:SER:OG	2.32	0.63
1:G:377:VAL:HG12	1:G:425:TYR:HB2	1.81	0.63
1:B:561:ASN:ND2	1:B:564:SER:OG	2.32	0.63
1:H:561:ASN:ND2	1:H:564:SER:OG	2.32	0.63
1:K:561:ASN:ND2	1:K:564:SER:OG	2.32	0.63
1:I:377:VAL:HG12	1:I:425:TYR:HB2	1.80	0.63
1:I:561:ASN:ND2	1:I:564:SER:OG	2.32	0.63
1:L:561:ASN:ND2	1:L:564:SER:OG	2.32	0.63
1:N:561:ASN:ND2	1:N:564:SER:OG	2.32	0.63
1:O:377:VAL:HG12	1:O:425:TYR:HB2	1.81	0.63
1:O:561:ASN:ND2	1:O:564:SER:OG	2.32	0.63
1:B:662:ILE:HD13	1:B:690:LEU:HD11	1.79	0.62
1:C:377:VAL:HG12	1:C:425:TYR:HB2	1.80	0.62
1:D:377:VAL:HG12	1:D:425:TYR:HB2	1.80	0.62
1:L:377:VAL:HG12	1:L:425:TYR:HB2	1.80	0.62
1:N:662:ILE:HD13	1:N:690:LEU:HD11	1.79	0.62
1:B:412:ILE:HD13	1:B:501:LEU:HD11	1.81	0.62
1:N:412:ILE:HD13	1:N:501:LEU:HD11	1.81	0.62
1:P:377:VAL:HG12	1:P:425:TYR:HB2	1.80	0.62
1:P:447:ARG:NH2	1:P:472:THR:OG1	2.21	0.62
1:R:561:ASN:ND2	1:R:564:SER:OG	2.32	0.62
1:A:412:ILE:HD13	1:A:501:LEU:HD11	1.81	0.62
1:B:423:GLY:O	1:B:439:LEU:N	2.33	0.62
1:E:423:GLY:O	1:E:439:LEU:N	2.33	0.62
1:N:423:GLY:O	1:N:439:LEU:N	2.33	0.62
1:R:412:ILE:HD13	1:R:501:LEU:HD11	1.81	0.62
1:D:447:ARG:NH2	1:D:472:THR:OG1	2.21	0.62
1:F:412:ILE:HD13	1:F:501:LEU:HD11	1.81	0.62
1:F:561:ASN:ND2	1:F:564:SER:OG	2.32	0.62
1:H:377:VAL:HG12	1:H:425:TYR:HB2	1.80	0.62
1:M:412:ILE:HD13	1:M:501:LEU:HD11	1.81	0.62
1:O:412:ILE:HD13	1:O:501:LEU:HD11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:423:GLY:O	1:Q:439:LEU:N	2.33	0.62
1:C:412:ILE:HD13	1:C:501:LEU:HD11	1.81	0.62
1:I:412:ILE:HD13	1:I:501:LEU:HD11	1.81	0.62
1:I:662:ILE:HD13	1:I:690:LEU:HD11	1.79	0.62
1:K:377:VAL:HG12	1:K:425:TYR:HB2	1.80	0.62
1:L:412:ILE:HD13	1:L:501:LEU:HD11	1.81	0.62
1:M:561:ASN:ND2	1:M:564:SER:OG	2.32	0.62
1:D:423:GLY:O	1:D:439:LEU:N	2.33	0.62
1:D:561:ASN:ND2	1:D:564:SER:OG	2.32	0.62
1:F:455:LEU:HB3	1:F:462:LYS:HE2	1.82	0.62
1:G:686:SER:HB2	1:G:689:GLU:HG3	1.82	0.62
1:I:423:GLY:O	1:I:439:LEU:N	2.33	0.62
1:J:686:SER:HB2	1:J:689:GLU:HG3	1.82	0.62
1:O:455:LEU:HB3	1:O:462:LYS:HE2	1.82	0.62
1:P:423:GLY:O	1:P:439:LEU:N	2.33	0.62
1:A:561:ASN:ND2	1:A:564:SER:OG	2.32	0.62
1:B:455:LEU:HB3	1:B:462:LYS:HE2	1.82	0.62
1:C:455:LEU:HB3	1:C:462:LYS:HE2	1.82	0.62
1:C:519:ARG:HG2	1:D:531:GLU:HG2	1.80	0.62
1:E:686:SER:HB2	1:E:689:GLU:HG3	1.82	0.62
1:G:423:GLY:O	1:G:439:LEU:N	2.33	0.62
1:J:423:GLY:O	1:J:439:LEU:N	2.33	0.62
1:L:662:ILE:HD13	1:L:690:LEU:HD11	1.79	0.62
1:N:455:LEU:HB3	1:N:462:LYS:HE2	1.82	0.62
1:P:412:ILE:HD13	1:P:501:LEU:HD11	1.81	0.62
1:P:455:LEU:HB3	1:P:462:LYS:HE2	1.82	0.62
1:Q:686:SER:HB2	1:Q:689:GLU:HG3	1.82	0.62
1:R:455:LEU:HB3	1:R:462:LYS:HE2	1.82	0.62
1:D:412:ILE:HD13	1:D:501:LEU:HD11	1.81	0.62
1:H:455:LEU:HB3	1:H:462:LYS:HE2	1.82	0.62
1:J:412:ILE:HD13	1:J:501:LEU:HD11	1.81	0.62
1:J:455:LEU:HB3	1:J:462:LYS:HE2	1.82	0.62
1:K:455:LEU:HB3	1:K:462:LYS:HE2	1.82	0.62
1:L:423:GLY:O	1:L:439:LEU:N	2.33	0.62
1:P:561:ASN:ND2	1:P:564:SER:OG	2.32	0.62
1:A:423:GLY:O	1:A:439:LEU:N	2.33	0.61
1:D:455:LEU:HB3	1:D:462:LYS:HE2	1.82	0.61
1:G:412:ILE:HD13	1:G:501:LEU:HD11	1.81	0.61
1:G:455:LEU:HB3	1:G:462:LYS:HE2	1.82	0.61
1:L:686:SER:HB2	1:L:689:GLU:HG3	1.82	0.61
1:M:423:GLY:O	1:M:439:LEU:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:LEU:HB3	1:A:462:LYS:HE2	1.82	0.61
1:I:686:SER:HB2	1:I:689:GLU:HG3	1.82	0.61
1:M:455:LEU:HB3	1:M:462:LYS:HE2	1.82	0.61
1:P:686:SER:HB2	1:P:689:GLU:HG3	1.82	0.61
1:A:686:SER:HB2	1:A:689:GLU:HG3	1.82	0.61
1:E:455:LEU:HB3	1:E:462:LYS:HE2	1.82	0.61
1:H:412:ILE:HD13	1:H:501:LEU:HD11	1.81	0.61
1:K:412:ILE:HD13	1:K:501:LEU:HD11	1.81	0.61
1:M:686:SER:HB2	1:M:689:GLU:HG3	1.82	0.61
1:Q:455:LEU:HB3	1:Q:462:LYS:HE2	1.82	0.61
1:C:423:GLY:O	1:C:439:LEU:N	2.33	0.61
1:A:377:VAL:HG12	1:A:425:TYR:HB2	1.80	0.61
1:D:686:SER:HB2	1:D:689:GLU:HG3	1.82	0.61
1:L:455:LEU:HB3	1:L:462:LYS:HE2	1.82	0.61
1:O:423:GLY:O	1:O:439:LEU:N	2.33	0.61
1:I:455:LEU:HB3	1:I:462:LYS:HE2	1.82	0.61
1:N:686:SER:HB2	1:N:689:GLU:HG3	1.82	0.61
1:B:686:SER:HB2	1:B:689:GLU:HG3	1.82	0.61
1:M:377:VAL:HG12	1:M:425:TYR:HB2	1.80	0.61
1:B:381:GLN:NE2	1:B:422:GLU:OE2	2.34	0.61
1:K:423:GLY:O	1:K:439:LEU:N	2.33	0.61
1:M:381:GLN:NE2	1:M:422:GLU:OE2	2.34	0.61
1:Q:412:ILE:HD13	1:Q:501:LEU:HD11	1.81	0.61
1:A:381:GLN:NE2	1:A:422:GLU:OE2	2.34	0.61
1:E:412:ILE:HD13	1:E:501:LEU:HD11	1.81	0.61
1:H:423:GLY:O	1:H:439:LEU:N	2.33	0.61
1:C:686:SER:HB2	1:C:689:GLU:HG3	1.82	0.61
1:I:381:GLN:NE2	1:I:422:GLU:OE2	2.34	0.61
1:L:381:GLN:NE2	1:L:422:GLU:OE2	2.34	0.61
1:N:381:GLN:NE2	1:N:422:GLU:OE2	2.34	0.61
1:O:686:SER:HB2	1:O:689:GLU:HG3	1.82	0.61
1:C:381:GLN:NE2	1:C:422:GLU:OE2	2.34	0.60
1:K:381:GLN:NE2	1:K:422:GLU:OE2	2.34	0.60
1:O:381:GLN:NE2	1:O:422:GLU:OE2	2.34	0.60
1:H:381:GLN:NE2	1:H:422:GLU:OE2	2.34	0.60
1:H:686:SER:HB2	1:H:689:GLU:HG3	1.82	0.60
1:R:686:SER:HB2	1:R:689:GLU:HG3	1.82	0.60
1:F:423:GLY:O	1:F:439:LEU:N	2.33	0.60
1:K:686:SER:HB2	1:K:689:GLU:HG3	1.82	0.60
1:F:686:SER:HB2	1:F:689:GLU:HG3	1.82	0.60
1:G:381:GLN:NE2	1:G:422:GLU:OE2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:381:GLN:NE2	1:J:422:GLU:OE2	2.34	0.60
1:R:423:GLY:O	1:R:439:LEU:N	2.33	0.60
1:E:381:GLN:NE2	1:E:422:GLU:OE2	2.34	0.60
1:Q:381:GLN:NE2	1:Q:422:GLU:OE2	2.34	0.60
1:D:381:GLN:NE2	1:D:422:GLU:OE2	2.34	0.59
1:F:381:GLN:NE2	1:F:422:GLU:OE2	2.34	0.59
1:R:381:GLN:NE2	1:R:422:GLU:OE2	2.34	0.59
1:P:381:GLN:NE2	1:P:422:GLU:OE2	2.34	0.59
1:P:467:LEU:HG	1:P:468:PRO:HD2	1.85	0.59
1:R:467:LEU:HG	1:R:468:PRO:HD2	1.85	0.59
1:F:467:LEU:HG	1:F:468:PRO:HD2	1.85	0.58
1:G:467:LEU:HG	1:G:468:PRO:HD2	1.85	0.58
1:D:467:LEU:HG	1:D:468:PRO:HD2	1.85	0.58
1:J:467:LEU:HG	1:J:468:PRO:HD2	1.85	0.58
1:E:467:LEU:HG	1:E:468:PRO:HD2	1.85	0.58
1:Q:467:LEU:HG	1:Q:468:PRO:HD2	1.85	0.58
1:J:482:ARG:HA	1:J:485:LYS:HD2	1.86	0.58
1:K:467:LEU:HG	1:K:468:PRO:HD2	1.85	0.58
1:C:634:ASP:HB3	1:C:637:VAL:HG23	1.86	0.58
1:F:482:ARG:HA	1:F:485:LYS:HD2	1.86	0.58
1:G:482:ARG:HA	1:G:485:LYS:HD2	1.86	0.58
1:H:467:LEU:HG	1:H:468:PRO:HD2	1.85	0.58
1:R:482:ARG:HA	1:R:485:LYS:HD2	1.86	0.58
1:C:467:LEU:HG	1:C:468:PRO:HD2	1.85	0.58
1:O:634:ASP:HB3	1:O:637:VAL:HG23	1.86	0.58
1:B:451:SER:OG	1:B:471:GLU:O	2.21	0.58
1:N:451:SER:OG	1:N:471:GLU:O	2.21	0.58
1:O:467:LEU:HG	1:O:468:PRO:HD2	1.85	0.58
1:H:482:ARG:HA	1:H:485:LYS:HD2	1.85	0.58
1:K:482:ARG:HA	1:K:485:LYS:HD2	1.86	0.58
1:E:482:ARG:HA	1:E:485:LYS:HD2	1.86	0.57
1:F:441:ALA:O	1:F:493:HIS:NE2	2.37	0.57
1:Q:482:ARG:HA	1:Q:485:LYS:HD2	1.86	0.57
1:R:441:ALA:O	1:R:493:HIS:NE2	2.37	0.57
1:A:467:LEU:HG	1:A:468:PRO:HD2	1.85	0.57
1:H:634:ASP:HB3	1:H:637:VAL:HG23	1.86	0.57
1:K:634:ASP:HB3	1:K:637:VAL:HG23	1.86	0.57
1:B:482:ARG:HA	1:B:485:LYS:HD2	1.86	0.57
1:C:451:SER:OG	1:C:471:GLU:O	2.21	0.57
1:M:467:LEU:HG	1:M:468:PRO:HD2	1.85	0.57
1:E:634:ASP:HB3	1:E:637:VAL:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:482:ARG:HA	1:N:485:LYS:HD2	1.86	0.57
1:O:451:SER:OG	1:O:471:GLU:O	2.21	0.57
1:Q:634:ASP:HB3	1:Q:637:VAL:HG23	1.86	0.57
1:A:482:ARG:HA	1:A:485:LYS:HD2	1.86	0.57
1:D:441:ALA:O	1:D:493:HIS:NE2	2.37	0.57
1:J:634:ASP:HB3	1:J:637:VAL:HG23	1.86	0.57
1:D:482:ARG:HA	1:D:485:LYS:HD2	1.86	0.57
1:G:634:ASP:HB3	1:G:637:VAL:HG23	1.86	0.57
1:M:451:SER:OG	1:M:471:GLU:O	2.21	0.57
1:M:482:ARG:HA	1:M:485:LYS:HD2	1.86	0.57
1:P:441:ALA:O	1:P:493:HIS:NE2	2.37	0.57
1:P:482:ARG:HA	1:P:485:LYS:HD2	1.86	0.57
1:A:451:SER:OG	1:A:471:GLU:O	2.21	0.57
1:C:482:ARG:HA	1:C:485:LYS:HD2	1.86	0.57
1:I:467:LEU:HG	1:I:468:PRO:HD2	1.85	0.57
1:M:634:ASP:HB3	1:M:637:VAL:HG23	1.86	0.57
1:O:482:ARG:HA	1:O:485:LYS:HD2	1.86	0.57
1:A:634:ASP:HB3	1:A:637:VAL:HG23	1.86	0.57
1:L:467:LEU:HG	1:L:468:PRO:HD2	1.85	0.57
1:L:482:ARG:HA	1:L:485:LYS:HD2	1.86	0.57
1:D:451:SER:OG	1:D:471:GLU:O	2.21	0.57
1:F:533:ILE:HA	1:F:536:VAL:HG12	1.87	0.57
1:F:634:ASP:HB3	1:F:637:VAL:HG23	1.86	0.57
1:I:634:ASP:HB3	1:I:637:VAL:HG23	1.86	0.57
1:L:634:ASP:HB3	1:L:637:VAL:HG23	1.86	0.57
1:N:467:LEU:HG	1:N:468:PRO:HD2	1.85	0.57
1:P:451:SER:OG	1:P:471:GLU:O	2.21	0.57
1:B:467:LEU:HG	1:B:468:PRO:HD2	1.85	0.56
1:B:533:ILE:HA	1:B:536:VAL:HG12	1.87	0.56
1:I:441:ALA:O	1:I:493:HIS:NE2	2.37	0.56
1:L:441:ALA:O	1:L:493:HIS:NE2	2.37	0.56
1:N:533:ILE:HA	1:N:536:VAL:HG12	1.87	0.56
1:O:533:ILE:HA	1:O:536:VAL:HG12	1.87	0.56
1:R:634:ASP:HB3	1:R:637:VAL:HG23	1.86	0.56
1:B:441:ALA:O	1:B:493:HIS:NE2	2.37	0.56
1:G:441:ALA:O	1:G:493:HIS:NE2	2.37	0.56
1:I:482:ARG:HA	1:I:485:LYS:HD2	1.86	0.56
1:J:441:ALA:O	1:J:493:HIS:NE2	2.37	0.56
1:N:441:ALA:O	1:N:493:HIS:NE2	2.37	0.56
1:R:533:ILE:HA	1:R:536:VAL:HG12	1.87	0.56
1:C:533:ILE:HA	1:C:536:VAL:HG12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:666:ASP:OD1	1:D:666:ASP:N	2.39	0.56
1:E:451:SER:OG	1:E:471:GLU:O	2.21	0.56
1:P:666:ASP:OD1	1:P:666:ASP:N	2.39	0.56
1:E:666:ASP:N	1:E:666:ASP:OD1	2.39	0.56
1:N:634:ASP:HB3	1:N:637:VAL:HG23	1.86	0.56
1:P:634:ASP:HB3	1:P:637:VAL:HG23	1.86	0.56
1:B:634:ASP:HB3	1:B:637:VAL:HG23	1.86	0.56
1:J:533:ILE:HA	1:J:536:VAL:HG12	1.87	0.56
1:L:533:ILE:HA	1:L:536:VAL:HG12	1.87	0.56
1:Q:451:SER:OG	1:Q:471:GLU:O	2.21	0.56
1:Q:666:ASP:OD1	1:Q:666:ASP:N	2.39	0.56
1:B:666:ASP:OD1	1:B:666:ASP:N	2.39	0.56
1:D:634:ASP:HB3	1:D:637:VAL:HG23	1.86	0.56
1:G:533:ILE:HA	1:G:536:VAL:HG12	1.87	0.56
1:I:533:ILE:HA	1:I:536:VAL:HG12	1.88	0.56
1:N:666:ASP:OD1	1:N:666:ASP:N	2.39	0.56
1:E:441:ALA:O	1:E:493:HIS:NE2	2.37	0.56
1:H:533:ILE:HA	1:H:536:VAL:HG12	1.87	0.56
1:I:451:SER:OG	1:I:471:GLU:O	2.21	0.56
1:P:533:ILE:HA	1:P:536:VAL:HG12	1.87	0.56
1:Q:441:ALA:O	1:Q:493:HIS:NE2	2.37	0.56
1:A:533:ILE:HA	1:A:536:VAL:HG12	1.87	0.55
1:E:533:ILE:HA	1:E:536:VAL:HG12	1.87	0.55
1:F:666:ASP:OD1	1:F:666:ASP:N	2.39	0.55
1:K:533:ILE:HA	1:K:536:VAL:HG12	1.87	0.55
1:L:451:SER:OG	1:L:471:GLU:O	2.21	0.55
1:R:666:ASP:OD1	1:R:666:ASP:N	2.39	0.55
1:D:533:ILE:HA	1:D:536:VAL:HG12	1.87	0.55
1:H:451:SER:OG	1:H:471:GLU:O	2.21	0.55
1:M:533:ILE:HA	1:M:536:VAL:HG12	1.87	0.55
1:Q:533:ILE:HA	1:Q:536:VAL:HG12	1.87	0.55
1:A:666:ASP:OD1	1:A:666:ASP:N	2.39	0.55
1:K:451:SER:OG	1:K:471:GLU:O	2.21	0.55
1:M:666:ASP:N	1:M:666:ASP:OD1	2.39	0.55
1:A:441:ALA:O	1:A:493:HIS:NE2	2.37	0.55
1:G:666:ASP:OD1	1:G:666:ASP:N	2.39	0.55
1:J:666:ASP:N	1:J:666:ASP:OD1	2.39	0.55
1:F:451:SER:OG	1:F:471:GLU:O	2.21	0.55
1:M:441:ALA:O	1:M:493:HIS:NE2	2.37	0.55
1:I:666:ASP:OD1	1:I:666:ASP:N	2.39	0.55
1:L:666:ASP:OD1	1:L:666:ASP:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:451:SER:OG	1:G:471:GLU:O	2.21	0.55
1:J:451:SER:OG	1:J:471:GLU:O	2.21	0.55
1:K:666:ASP:OD1	1:K:666:ASP:N	2.39	0.55
1:H:666:ASP:N	1:H:666:ASP:OD1	2.39	0.55
1:K:381:GLN:HA	1:K:384:ALA:HB3	1.90	0.54
1:R:451:SER:OG	1:R:471:GLU:O	2.21	0.54
1:F:381:GLN:HA	1:F:384:ALA:HB3	1.90	0.54
1:H:381:GLN:HA	1:H:384:ALA:HB3	1.90	0.54
1:J:443:TYR:OH	1:J:445:LEU:HD13	2.08	0.54
1:A:443:TYR:OH	1:A:445:LEU:HD13	2.08	0.54
1:E:381:GLN:HA	1:E:384:ALA:HB3	1.90	0.54
1:G:443:TYR:OH	1:G:445:LEU:HD13	2.08	0.54
1:H:443:TYR:OH	1:H:445:LEU:HD13	2.08	0.54
1:K:443:TYR:OH	1:K:445:LEU:HD13	2.08	0.54
1:L:443:TYR:OH	1:L:445:LEU:HD13	2.08	0.54
1:M:443:TYR:OH	1:M:445:LEU:HD13	2.08	0.54
1:Q:381:GLN:HA	1:Q:384:ALA:HB3	1.90	0.54
1:I:381:GLN:HA	1:I:384:ALA:HB3	1.90	0.54
1:R:381:GLN:HA	1:R:384:ALA:HB3	1.90	0.54
1:G:617:LYS:HD2	1:G:641:LEU:HD21	1.90	0.54
1:H:441:ALA:O	1:H:493:HIS:NE2	2.37	0.54
1:H:617:LYS:HD2	1:H:641:LEU:HD21	1.90	0.54
1:I:443:TYR:OH	1:I:445:LEU:HD13	2.08	0.54
1:J:381:GLN:HA	1:J:384:ALA:HB3	1.90	0.54
1:J:617:LYS:HD2	1:J:641:LEU:HD21	1.90	0.54
1:K:617:LYS:HD2	1:K:641:LEU:HD21	1.90	0.54
1:L:381:GLN:HA	1:L:384:ALA:HB3	1.90	0.54
1:M:381:GLN:HA	1:M:384:ALA:HB3	1.90	0.54
1:N:443:TYR:OH	1:N:445:LEU:HD13	2.08	0.54
1:A:381:GLN:HA	1:A:384:ALA:HB3	1.90	0.54
1:B:443:TYR:OH	1:B:445:LEU:HD13	2.08	0.54
1:F:443:TYR:OH	1:F:445:LEU:HD13	2.08	0.54
1:G:381:GLN:HA	1:G:384:ALA:HB3	1.90	0.54
1:R:443:TYR:OH	1:R:445:LEU:HD13	2.08	0.54
1:K:441:ALA:O	1:K:493:HIS:NE2	2.37	0.54
1:C:381:GLN:HA	1:C:384:ALA:HB3	1.90	0.54
1:F:617:LYS:HD2	1:F:641:LEU:HD21	1.90	0.54
1:A:642:LEU:HG	1:A:646:ARG:HH12	1.73	0.54
1:B:381:GLN:HA	1:B:384:ALA:HB3	1.90	0.54
1:C:642:LEU:HG	1:C:646:ARG:HH12	1.73	0.54
1:D:381:GLN:HA	1:D:384:ALA:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:642:LEU:HG	1:D:646:ARG:HH12	1.73	0.54
1:L:617:LYS:HD2	1:L:641:LEU:HD21	1.90	0.54
1:M:551:ARG:HH11	1:M:669:ARG:HH12	1.56	0.54
1:M:642:LEU:HG	1:M:646:ARG:HH12	1.73	0.54
1:N:381:GLN:HA	1:N:384:ALA:HB3	1.90	0.54
1:O:381:GLN:HA	1:O:384:ALA:HB3	1.90	0.54
1:P:381:GLN:HA	1:P:384:ALA:HB3	1.90	0.54
1:P:642:LEU:HG	1:P:646:ARG:HH12	1.73	0.54
1:A:551:ARG:HH11	1:A:669:ARG:HH12	1.56	0.53
1:E:551:ARG:HH11	1:E:669:ARG:HH12	1.56	0.53
1:H:551:ARG:HH11	1:H:669:ARG:HH12	1.56	0.53
1:I:617:LYS:HD2	1:I:641:LEU:HD21	1.90	0.53
1:K:551:ARG:HH11	1:K:669:ARG:HH12	1.56	0.53
1:Q:551:ARG:HH11	1:Q:669:ARG:HH12	1.56	0.53
1:R:617:LYS:HD2	1:R:641:LEU:HD21	1.90	0.53
1:E:443:TYR:OH	1:E:445:LEU:HD13	2.08	0.53
1:G:551:ARG:HH11	1:G:669:ARG:HH12	1.56	0.53
1:J:551:ARG:HH11	1:J:669:ARG:HH12	1.56	0.53
1:O:642:LEU:HG	1:O:646:ARG:HH12	1.73	0.53
1:I:478:GLU:H	1:I:478:GLU:CD	2.17	0.53
1:O:392:ASP:O	1:O:396:ARG:NH1	2.42	0.53
1:Q:443:TYR:OH	1:Q:445:LEU:HD13	2.08	0.53
1:Q:642:LEU:HG	1:Q:646:ARG:HH12	1.73	0.53
1:B:551:ARG:HH11	1:B:669:ARG:HH12	1.56	0.53
1:E:392:ASP:O	1:E:396:ARG:NH1	2.42	0.53
1:E:393:GLU:HG2	1:E:494:SER:HB3	1.91	0.53
1:F:393:GLU:HG2	1:F:494:SER:HB3	1.91	0.53
1:K:478:GLU:H	1:K:478:GLU:CD	2.17	0.53
1:L:478:GLU:H	1:L:478:GLU:CD	2.17	0.53
1:O:443:TYR:OH	1:O:445:LEU:HD13	2.08	0.53
1:Q:392:ASP:O	1:Q:396:ARG:NH1	2.42	0.53
1:R:393:GLU:HG2	1:R:494:SER:HB3	1.91	0.53
1:C:392:ASP:O	1:C:396:ARG:NH1	2.42	0.53
1:E:642:LEU:HG	1:E:646:ARG:HH12	1.74	0.53
1:H:478:GLU:H	1:H:478:GLU:CD	2.17	0.53
1:J:393:GLU:HG2	1:J:494:SER:HB3	1.91	0.53
1:L:392:ASP:O	1:L:396:ARG:NH1	2.42	0.53
1:N:551:ARG:HH11	1:N:669:ARG:HH12	1.56	0.53
1:P:392:ASP:O	1:P:396:ARG:NH1	2.42	0.53
1:Q:393:GLU:HG2	1:Q:494:SER:HB3	1.91	0.53
1:C:443:TYR:OH	1:C:445:LEU:HD13	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:392:ASP:O	1:D:396:ARG:NH1	2.42	0.53
1:E:617:LYS:HD2	1:E:641:LEU:HD21	1.90	0.53
1:I:392:ASP:O	1:I:396:ARG:NH1	2.42	0.53
1:L:642:LEU:HG	1:L:646:ARG:HH12	1.73	0.53
1:A:392:ASP:O	1:A:396:ARG:NH1	2.42	0.53
1:C:441:ALA:O	1:C:493:HIS:NE2	2.37	0.53
1:G:393:GLU:HG2	1:G:494:SER:HB3	1.91	0.53
1:B:642:LEU:HG	1:B:646:ARG:HH12	1.74	0.53
1:D:393:GLU:HG2	1:D:494:SER:HB3	1.91	0.53
1:D:551:ARG:HH11	1:D:669:ARG:HH12	1.56	0.53
1:I:642:LEU:HG	1:I:646:ARG:HH12	1.74	0.53
1:M:392:ASP:O	1:M:396:ARG:NH1	2.42	0.53
1:M:617:LYS:HD2	1:M:641:LEU:HD21	1.90	0.53
1:P:393:GLU:HG2	1:P:494:SER:HB3	1.91	0.53
1:P:551:ARG:HH11	1:P:669:ARG:HH12	1.56	0.53
1:Q:617:LYS:HD2	1:Q:641:LEU:HD21	1.90	0.53
1:R:642:LEU:HG	1:R:646:ARG:HH12	1.73	0.53
1:A:617:LYS:HD2	1:A:641:LEU:HD21	1.90	0.53
1:F:642:LEU:HG	1:F:646:ARG:HH12	1.73	0.53
1:N:642:LEU:HG	1:N:646:ARG:HH12	1.73	0.53
1:F:392:ASP:O	1:F:396:ARG:NH1	2.42	0.53
1:G:642:LEU:HG	1:G:646:ARG:HH12	1.73	0.53
1:J:642:LEU:HG	1:J:646:ARG:HH12	1.73	0.53
1:K:642:LEU:HG	1:K:646:ARG:HH12	1.73	0.53
1:O:441:ALA:O	1:O:493:HIS:NE2	2.37	0.53
1:D:478:GLU:H	1:D:478:GLU:CD	2.17	0.52
1:O:478:GLU:H	1:O:478:GLU:CD	2.17	0.52
1:R:392:ASP:O	1:R:396:ARG:NH1	2.42	0.52
1:C:478:GLU:H	1:C:478:GLU:CD	2.17	0.52
1:D:443:TYR:OH	1:D:445:LEU:HD13	2.08	0.52
1:F:551:ARG:HH11	1:F:669:ARG:HH12	1.56	0.52
1:H:392:ASP:O	1:H:396:ARG:NH1	2.42	0.52
1:P:443:TYR:OH	1:P:445:LEU:HD13	2.08	0.52
1:P:478:GLU:H	1:P:478:GLU:CD	2.17	0.52
1:R:551:ARG:HH11	1:R:669:ARG:HH12	1.56	0.52
1:H:642:LEU:HG	1:H:646:ARG:HH12	1.73	0.52
1:K:392:ASP:O	1:K:396:ARG:NH1	2.42	0.52
1:B:392:ASP:O	1:B:396:ARG:NH1	2.42	0.52
1:C:379:SER:O	1:C:380:SER:OG	2.26	0.52
1:K:393:GLU:HG2	1:K:494:SER:HB3	1.91	0.52
1:N:519:ARG:HD3	1:N:542:LEU:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:519:ARG:HD3	1:B:542:LEU:HD11	1.92	0.52
1:C:393:GLU:HG2	1:C:494:SER:HB3	1.91	0.52
1:E:478:GLU:H	1:E:478:GLU:CD	2.17	0.52
1:H:393:GLU:HG2	1:H:494:SER:HB3	1.91	0.52
1:J:478:GLU:H	1:J:478:GLU:CD	2.17	0.52
1:L:551:ARG:HH11	1:L:669:ARG:HH12	1.56	0.52
1:N:392:ASP:O	1:N:396:ARG:NH1	2.42	0.52
1:N:617:LYS:HD2	1:N:641:LEU:HD21	1.90	0.52
1:J:392:ASP:O	1:J:396:ARG:NH1	2.42	0.52
1:O:379:SER:O	1:O:380:SER:OG	2.26	0.52
1:O:393:GLU:HG2	1:O:494:SER:HB3	1.91	0.52
1:P:617:LYS:HD2	1:P:641:LEU:HD21	1.90	0.52
1:Q:478:GLU:H	1:Q:478:GLU:CD	2.17	0.52
1:G:392:ASP:O	1:G:396:ARG:NH1	2.42	0.52
1:G:478:GLU:H	1:G:478:GLU:CD	2.17	0.52
1:H:379:SER:O	1:H:380:SER:OG	2.26	0.52
1:N:478:GLU:H	1:N:478:GLU:CD	2.17	0.52
1:O:617:LYS:HD2	1:O:641:LEU:HD21	1.90	0.52
1:A:393:GLU:HG2	1:A:494:SER:HB3	1.91	0.52
1:B:393:GLU:HG2	1:B:494:SER:HB3	1.91	0.52
1:B:617:LYS:HD2	1:B:641:LEU:HD21	1.90	0.52
1:D:617:LYS:HD2	1:D:641:LEU:HD21	1.90	0.52
1:I:551:ARG:HH11	1:I:669:ARG:HH12	1.56	0.52
1:I:645:VAL:HG13	1:I:649:ILE:HD12	1.92	0.52
1:K:645:VAL:HG13	1:K:649:ILE:HD12	1.92	0.52
1:L:645:VAL:HG13	1:L:649:ILE:HD12	1.92	0.52
1:N:393:GLU:HG2	1:N:494:SER:HB3	1.91	0.52
1:O:519:ARG:HD3	1:O:542:LEU:HD11	1.91	0.52
1:C:617:LYS:HD2	1:C:641:LEU:HD21	1.90	0.52
1:G:645:VAL:HG13	1:G:649:ILE:HD12	1.92	0.52
1:H:645:VAL:HG13	1:H:649:ILE:HD12	1.92	0.52
1:I:393:GLU:HG2	1:I:494:SER:HB3	1.91	0.52
1:J:645:VAL:HG13	1:J:649:ILE:HD12	1.92	0.52
1:M:393:GLU:HG2	1:M:494:SER:HB3	1.91	0.52
1:M:645:VAL:HG13	1:M:649:ILE:HD12	1.92	0.52
1:A:645:VAL:HG13	1:A:649:ILE:HD12	1.92	0.51
1:L:393:GLU:HG2	1:L:494:SER:HB3	1.91	0.51
1:E:645:VAL:HG13	1:E:649:ILE:HD12	1.92	0.51
1:F:478:GLU:H	1:F:478:GLU:CD	2.17	0.51
1:F:645:VAL:HG13	1:F:649:ILE:HD12	1.92	0.51
1:J:519:ARG:HD3	1:J:542:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:519:ARG:HD3	1:C:542:LEU:HD11	1.92	0.51
1:D:519:ARG:HD3	1:D:542:LEU:HD11	1.92	0.51
1:G:519:ARG:HD3	1:G:542:LEU:HD11	1.92	0.51
1:R:645:VAL:HG13	1:R:649:ILE:HD12	1.92	0.51
1:B:645:VAL:HG13	1:B:649:ILE:HD12	1.92	0.51
1:C:551:ARG:HH11	1:C:669:ARG:HH12	1.56	0.51
1:D:580:VAL:O	1:D:584:GLU:HG2	2.10	0.51
1:H:519:ARG:HD3	1:H:542:LEU:HD11	1.92	0.51
1:L:580:VAL:O	1:L:584:GLU:HG2	2.10	0.51
1:N:645:VAL:HG13	1:N:649:ILE:HD12	1.92	0.51
1:O:666:ASP:N	1:O:666:ASP:OD1	2.39	0.51
1:Q:645:VAL:HG13	1:Q:649:ILE:HD12	1.92	0.51
1:R:478:GLU:H	1:R:478:GLU:CD	2.17	0.51
1:R:519:ARG:HD3	1:R:542:LEU:HD11	1.92	0.51
1:C:580:VAL:O	1:C:584:GLU:HG2	2.10	0.51
1:C:666:ASP:N	1:C:666:ASP:OD1	2.39	0.51
1:D:645:VAL:HG13	1:D:649:ILE:HD12	1.92	0.51
1:E:519:ARG:HD3	1:E:542:LEU:HD11	1.92	0.51
1:G:580:VAL:O	1:G:584:GLU:HG2	2.10	0.51
1:H:580:VAL:O	1:H:584:GLU:HG2	2.10	0.51
1:I:580:VAL:O	1:I:584:GLU:HG2	2.10	0.51
1:J:549:LEU:HD11	1:J:562:MET:HE1	1.93	0.51
1:J:580:VAL:O	1:J:584:GLU:HG2	2.10	0.51
1:K:519:ARG:HD3	1:K:542:LEU:HD11	1.92	0.51
1:O:580:VAL:O	1:O:584:GLU:HG2	2.10	0.51
1:P:645:VAL:HG13	1:P:649:ILE:HD12	1.92	0.51
1:Q:519:ARG:HD3	1:Q:542:LEU:HD11	1.92	0.51
1:F:519:ARG:HD3	1:F:542:LEU:HD11	1.92	0.51
1:K:580:VAL:O	1:K:584:GLU:HG2	2.10	0.51
1:O:551:ARG:HH11	1:O:669:ARG:HH12	1.56	0.51
1:P:519:ARG:HD3	1:P:542:LEU:HD11	1.92	0.51
1:P:580:VAL:O	1:P:584:GLU:HG2	2.10	0.51
1:A:549:LEU:HD11	1:A:562:MET:HE1	1.93	0.51
1:B:549:LEU:HD11	1:B:562:MET:HE1	1.93	0.51
1:G:549:LEU:HD11	1:G:562:MET:HE1	1.93	0.51
1:M:549:LEU:HD11	1:M:562:MET:HE1	1.93	0.51
1:A:519:ARG:HD3	1:A:542:LEU:HD11	1.92	0.51
1:O:549:LEU:HD11	1:O:562:MET:HE1	1.93	0.51
1:C:549:LEU:HD11	1:C:562:MET:HE1	1.93	0.51
1:E:549:LEU:HD11	1:E:562:MET:HE1	1.93	0.51
1:H:549:LEU:HD11	1:H:562:MET:HE1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:549:LEU:HD11	1:Q:562:MET:HE1	1.93	0.51
1:R:580:VAL:O	1:R:584:GLU:HG2	2.10	0.51
1:F:549:LEU:HD11	1:F:562:MET:HE1	1.93	0.51
1:I:519:ARG:HD3	1:I:542:LEU:HD11	1.92	0.51
1:K:549:LEU:HD11	1:K:562:MET:HE1	1.93	0.51
1:L:519:ARG:HD3	1:L:542:LEU:HD11	1.92	0.51
1:M:519:ARG:HD3	1:M:542:LEU:HD11	1.92	0.51
1:N:549:LEU:HD11	1:N:562:MET:HE1	1.93	0.51
1:Q:580:VAL:O	1:Q:584:GLU:HG2	2.10	0.51
1:R:549:LEU:HD11	1:R:562:MET:HE1	1.93	0.51
1:C:645:VAL:HG13	1:C:649:ILE:HD12	1.92	0.50
1:D:379:SER:O	1:D:380:SER:OG	2.26	0.50
1:E:580:VAL:O	1:E:584:GLU:HG2	2.10	0.50
1:H:373:LEU:HD23	1:H:374:LEU:N	2.26	0.50
1:L:549:LEU:HD11	1:L:562:MET:HE1	1.93	0.50
1:O:645:VAL:HG13	1:O:649:ILE:HD12	1.92	0.50
1:A:580:VAL:O	1:A:584:GLU:HG2	2.10	0.50
1:C:373:LEU:HD23	1:C:374:LEU:N	2.26	0.50
1:D:373:LEU:HD23	1:D:374:LEU:N	2.26	0.50
1:F:580:VAL:O	1:F:584:GLU:HG2	2.10	0.50
1:G:373:LEU:HD23	1:G:374:LEU:N	2.26	0.50
1:I:549:LEU:HD11	1:I:562:MET:HE1	1.93	0.50
1:J:373:LEU:HD23	1:J:374:LEU:N	2.26	0.50
1:K:373:LEU:HD23	1:K:374:LEU:N	2.26	0.50
1:M:580:VAL:O	1:M:584:GLU:HG2	2.10	0.50
1:N:580:VAL:O	1:N:584:GLU:HG2	2.10	0.50
1:O:373:LEU:HD23	1:O:374:LEU:N	2.26	0.50
1:P:373:LEU:HD23	1:P:374:LEU:N	2.26	0.50
1:B:580:VAL:O	1:B:584:GLU:HG2	2.10	0.50
1:E:616:GLU:OE1	1:E:619:ARG:NH2	2.45	0.50
1:Q:616:GLU:OE1	1:Q:619:ARG:NH2	2.45	0.50
1:D:549:LEU:HD11	1:D:562:MET:HE1	1.93	0.50
1:P:379:SER:O	1:P:380:SER:OG	2.26	0.50
1:R:616:GLU:OE1	1:R:619:ARG:NH2	2.45	0.50
1:F:616:GLU:OE1	1:F:619:ARG:NH2	2.45	0.50
1:Q:595:CYS:HB2	1:Q:694:ILE:HD11	1.94	0.50
1:D:595:CYS:HB2	1:D:694:ILE:HD11	1.94	0.50
1:D:616:GLU:OE1	1:D:619:ARG:NH2	2.45	0.50
1:E:595:CYS:HB2	1:E:694:ILE:HD11	1.94	0.50
1:H:616:GLU:OE1	1:H:619:ARG:NH2	2.45	0.50
1:J:440:LYS:C	1:J:442:GLY:H	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:595:CYS:HB2	1:N:694:ILE:HD11	1.94	0.50
1:P:549:LEU:HD11	1:P:562:MET:HE1	1.93	0.50
1:E:373:LEU:HD23	1:E:374:LEU:N	2.26	0.50
1:F:595:CYS:HB2	1:F:694:ILE:HD11	1.94	0.50
1:G:440:LYS:C	1:G:442:GLY:H	2.20	0.50
1:I:595:CYS:HB2	1:I:694:ILE:HD11	1.94	0.50
1:K:616:GLU:OE1	1:K:619:ARG:NH2	2.45	0.50
1:L:373:LEU:HD23	1:L:374:LEU:N	2.26	0.50
1:M:595:CYS:HB2	1:M:694:ILE:HD11	1.94	0.50
1:P:595:CYS:HB2	1:P:694:ILE:HD11	1.94	0.50
1:Q:373:LEU:HD23	1:Q:374:LEU:N	2.26	0.50
1:R:595:CYS:HB2	1:R:694:ILE:HD11	1.94	0.50
1:B:595:CYS:HB2	1:B:694:ILE:HD11	1.94	0.50
1:C:595:CYS:HB2	1:C:694:ILE:HD11	1.94	0.50
1:H:595:CYS:HB2	1:H:694:ILE:HD11	1.94	0.50
1:I:379:SER:O	1:I:380:SER:OG	2.26	0.50
1:I:440:LYS:C	1:I:442:GLY:H	2.20	0.50
1:L:595:CYS:HB2	1:L:694:ILE:HD11	1.94	0.50
1:N:373:LEU:HD23	1:N:374:LEU:N	2.26	0.50
1:O:595:CYS:HB2	1:O:694:ILE:HD11	1.94	0.50
1:P:616:GLU:OE1	1:P:619:ARG:NH2	2.45	0.50
1:A:595:CYS:HB2	1:A:694:ILE:HD11	1.94	0.50
1:I:373:LEU:HD23	1:I:374:LEU:N	2.26	0.50
1:K:595:CYS:HB2	1:K:694:ILE:HD11	1.94	0.50
1:L:440:LYS:C	1:L:442:GLY:H	2.20	0.50
1:B:373:LEU:HD23	1:B:374:LEU:N	2.26	0.49
1:F:373:LEU:HD23	1:F:374:LEU:N	2.26	0.49
1:B:616:GLU:OE1	1:B:619:ARG:NH2	2.45	0.49
1:L:379:SER:O	1:L:380:SER:OG	2.26	0.49
1:M:373:LEU:HD23	1:M:374:LEU:N	2.26	0.49
1:N:616:GLU:OE1	1:N:619:ARG:NH2	2.45	0.49
1:J:595:CYS:HB2	1:J:694:ILE:HD11	1.94	0.49
1:L:427:ILE:O	1:L:434:VAL:HG12	2.13	0.49
1:N:427:ILE:O	1:N:434:VAL:HG12	2.13	0.49
1:R:373:LEU:HD23	1:R:374:LEU:N	2.26	0.49
1:A:373:LEU:HD23	1:A:374:LEU:N	2.26	0.49
1:B:427:ILE:O	1:B:434:VAL:HG12	2.13	0.49
1:I:427:ILE:O	1:I:434:VAL:HG12	2.13	0.49
1:I:616:GLU:OE1	1:I:619:ARG:NH2	2.45	0.49
1:J:616:GLU:OE1	1:J:619:ARG:NH2	2.45	0.49
1:B:440:LYS:C	1:B:442:GLY:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:595:CYS:HB2	1:G:694:ILE:HD11	1.94	0.49
1:J:427:ILE:O	1:J:434:VAL:HG12	2.13	0.49
1:L:440:LYS:HZ3	1:L:474:TRP:NE1	2.10	0.49
1:L:616:GLU:OE1	1:L:619:ARG:NH2	2.45	0.49
1:A:616:GLU:OE1	1:A:619:ARG:NH2	2.45	0.49
1:C:616:GLU:OE1	1:C:619:ARG:NH2	2.45	0.49
1:G:363:GLU:O	1:H:398:ARG:NH2	2.46	0.49
1:G:427:ILE:O	1:G:434:VAL:HG12	2.13	0.49
1:G:616:GLU:OE1	1:G:619:ARG:NH2	2.45	0.49
1:E:440:LYS:C	1:E:442:GLY:H	2.20	0.49
1:E:603:ASN:ND2	1:E:693:GLN:O	2.46	0.49
1:M:616:GLU:OE1	1:M:619:ARG:NH2	2.45	0.49
1:N:440:LYS:C	1:N:442:GLY:H	2.20	0.49
1:O:616:GLU:OE1	1:O:619:ARG:NH2	2.45	0.49
1:Q:603:ASN:ND2	1:Q:693:GLN:O	2.46	0.49
1:F:603:ASN:ND2	1:F:693:GLN:O	2.46	0.49
1:R:603:ASN:ND2	1:R:693:GLN:O	2.46	0.49
1:D:603:ASN:ND2	1:D:693:GLN:O	2.46	0.49
1:P:603:ASN:ND2	1:P:693:GLN:O	2.46	0.49
1:Q:440:LYS:C	1:Q:442:GLY:H	2.20	0.49
1:R:440:LYS:C	1:R:442:GLY:H	2.20	0.49
1:E:427:ILE:O	1:E:434:VAL:HG12	2.13	0.48
1:H:427:ILE:O	1:H:434:VAL:HG12	2.13	0.48
1:K:440:LYS:C	1:K:442:GLY:H	2.20	0.48
1:D:363:GLU:O	1:E:398:ARG:NH2	2.46	0.48
1:D:427:ILE:O	1:D:434:VAL:HG12	2.13	0.48
1:O:603:ASN:ND2	1:O:693:GLN:O	2.46	0.48
1:P:427:ILE:O	1:P:434:VAL:HG12	2.13	0.48
1:Q:427:ILE:O	1:Q:434:VAL:HG12	2.13	0.48
1:C:603:ASN:ND2	1:C:693:GLN:O	2.46	0.48
1:D:440:LYS:C	1:D:442:GLY:H	2.20	0.48
1:E:379:SER:O	1:E:380:SER:OG	2.26	0.48
1:F:440:LYS:C	1:F:442:GLY:H	2.20	0.48
1:I:440:LYS:HZ3	1:I:474:TRP:NE1	2.11	0.48
1:K:427:ILE:O	1:K:434:VAL:HG12	2.13	0.48
1:C:427:ILE:O	1:C:434:VAL:HG12	2.13	0.48
1:H:440:LYS:C	1:H:442:GLY:H	2.20	0.48
1:O:427:ILE:O	1:O:434:VAL:HG12	2.13	0.48
1:A:440:LYS:C	1:A:442:GLY:H	2.20	0.48
1:B:610:PHE:HE2	1:B:661:LEU:HD11	1.79	0.48
1:F:427:ILE:O	1:F:434:VAL:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:440:LYS:C	1:P:442:GLY:H	2.20	0.48
1:R:427:ILE:O	1:R:434:VAL:HG12	2.13	0.48
1:A:427:ILE:O	1:A:434:VAL:HG12	2.13	0.48
1:C:440:LYS:C	1:C:442:GLY:H	2.20	0.48
1:M:427:ILE:O	1:M:434:VAL:HG12	2.13	0.48
1:N:603:ASN:ND2	1:N:693:GLN:O	2.46	0.48
1:N:610:PHE:HE2	1:N:661:LEU:HD11	1.79	0.48
1:O:440:LYS:C	1:O:442:GLY:H	2.20	0.48
1:Q:379:SER:O	1:Q:380:SER:OG	2.26	0.48
1:B:603:ASN:ND2	1:B:693:GLN:O	2.46	0.48
1:E:610:PHE:HE2	1:E:661:LEU:HD11	1.79	0.48
1:I:603:ASN:ND2	1:I:693:GLN:O	2.46	0.48
1:L:598:TYR:CE2	1:L:685:LEU:HD21	2.49	0.48
1:M:440:LYS:C	1:M:442:GLY:H	2.20	0.48
1:M:603:ASN:ND2	1:M:693:GLN:O	2.46	0.48
1:G:440:LYS:HZ3	1:G:474:TRP:NE1	2.12	0.48
1:I:598:TYR:CE2	1:I:685:LEU:HD21	2.49	0.48
1:J:440:LYS:HZ3	1:J:474:TRP:NE1	2.12	0.48
1:L:603:ASN:ND2	1:L:693:GLN:O	2.46	0.48
1:Q:610:PHE:HE2	1:Q:661:LEU:HD11	1.79	0.48
1:A:603:ASN:ND2	1:A:693:GLN:O	2.46	0.47
1:D:598:TYR:CE2	1:D:685:LEU:HD21	2.49	0.47
1:P:598:TYR:CE2	1:P:685:LEU:HD21	2.49	0.47
1:A:598:TYR:CE2	1:A:685:LEU:HD21	2.49	0.47
1:A:610:PHE:HE2	1:A:661:LEU:HD11	1.79	0.47
1:H:598:TYR:CE2	1:H:685:LEU:HD21	2.49	0.47
1:J:610:PHE:HE2	1:J:661:LEU:HD11	1.79	0.47
1:K:598:TYR:CE2	1:K:685:LEU:HD21	2.49	0.47
1:M:598:TYR:CE2	1:M:685:LEU:HD21	2.49	0.47
1:M:610:PHE:HE2	1:M:661:LEU:HD11	1.79	0.47
1:F:598:TYR:CE2	1:F:685:LEU:HD21	2.49	0.47
1:G:610:PHE:HE2	1:G:661:LEU:HD11	1.79	0.47
1:R:440:LYS:HZ3	1:R:474:TRP:NE1	2.12	0.47
1:R:598:TYR:CE2	1:R:685:LEU:HD21	2.49	0.47
1:F:440:LYS:HZ3	1:F:474:TRP:NE1	2.12	0.47
1:F:587:ARG:NH2	1:F:689:GLU:OE1	2.47	0.47
1:H:603:ASN:ND2	1:H:693:GLN:O	2.46	0.47
1:O:610:PHE:HE2	1:O:661:LEU:HD11	1.79	0.47
1:C:598:TYR:CE2	1:C:685:LEU:HD21	2.49	0.47
1:H:610:PHE:HE2	1:H:661:LEU:HD11	1.79	0.47
1:K:603:ASN:ND2	1:K:693:GLN:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:610:PHE:HE2	1:C:661:LEU:HD11	1.79	0.47
1:K:610:PHE:HE2	1:K:661:LEU:HD11	1.79	0.47
1:O:598:TYR:CE2	1:O:685:LEU:HD21	2.49	0.47
1:R:587:ARG:NH2	1:R:689:GLU:OE1	2.47	0.47
1:A:379:SER:O	1:A:380:SER:OG	2.26	0.47
1:B:587:ARG:NH2	1:B:689:GLU:OE1	2.47	0.47
1:B:598:TYR:CE2	1:B:685:LEU:HD21	2.49	0.47
1:C:587:ARG:NH2	1:C:689:GLU:OE1	2.47	0.47
1:D:610:PHE:HE2	1:D:661:LEU:HD11	1.79	0.47
1:I:610:PHE:HE2	1:I:661:LEU:HD11	1.79	0.47
1:J:598:TYR:CE2	1:J:685:LEU:HD21	2.49	0.47
1:N:587:ARG:NH2	1:N:689:GLU:OE1	2.47	0.47
1:O:587:ARG:NH2	1:O:689:GLU:OE1	2.47	0.47
1:R:610:PHE:HE2	1:R:661:LEU:HD11	1.79	0.47
1:F:610:PHE:HE2	1:F:661:LEU:HD11	1.79	0.47
1:G:598:TYR:CE2	1:G:685:LEU:HD21	2.49	0.47
1:H:440:LYS:HZ3	1:H:474:TRP:NE1	2.12	0.47
1:L:610:PHE:HE2	1:L:661:LEU:HD11	1.79	0.47
1:N:598:TYR:CE2	1:N:685:LEU:HD21	2.49	0.47
1:P:610:PHE:HE2	1:P:661:LEU:HD11	1.79	0.47
1:Q:440:LYS:HZ3	1:Q:474:TRP:NE1	2.13	0.47
1:E:440:LYS:HZ3	1:E:474:TRP:NE1	2.13	0.47
1:K:440:LYS:HZ3	1:K:474:TRP:NE1	2.12	0.47
1:M:379:SER:O	1:M:380:SER:OG	2.26	0.47
1:M:478:GLU:H	1:M:478:GLU:CD	2.17	0.47
1:A:478:GLU:H	1:A:478:GLU:CD	2.17	0.46
1:P:440:LYS:HZ3	1:P:474:TRP:NE1	2.13	0.46
1:D:440:LYS:HZ3	1:D:474:TRP:NE1	2.13	0.46
1:G:603:ASN:ND2	1:G:693:GLN:O	2.46	0.46
1:H:587:ARG:NH2	1:H:689:GLU:OE1	2.47	0.46
1:K:587:ARG:NH2	1:K:689:GLU:OE1	2.47	0.46
1:Q:598:TYR:CE2	1:Q:685:LEU:HD21	2.49	0.46
1:E:598:TYR:CE2	1:E:685:LEU:HD21	2.49	0.46
1:H:389:ALA:C	1:H:391:ASN:H	2.24	0.46
1:J:603:ASN:ND2	1:J:693:GLN:O	2.46	0.46
1:K:389:ALA:C	1:K:391:ASN:H	2.24	0.46
1:G:379:SER:O	1:G:380:SER:OG	2.26	0.46
1:J:379:SER:O	1:J:380:SER:OG	2.26	0.46
1:J:389:ALA:C	1:J:391:ASN:H	2.24	0.46
1:J:587:ARG:NH2	1:J:689:GLU:OE1	2.47	0.46
1:D:389:ALA:C	1:D:391:ASN:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:522:LEU:HD11	1:D:545:MET:SD	2.56	0.46
1:G:389:ALA:C	1:G:391:ASN:H	2.24	0.46
1:L:522:LEU:HD11	1:L:545:MET:SD	2.56	0.46
1:P:522:LEU:HD11	1:P:545:MET:SD	2.56	0.46
1:A:440:LYS:HZ3	1:A:474:TRP:NE1	2.14	0.46
1:B:389:ALA:C	1:B:391:ASN:H	2.24	0.46
1:C:452:GLN:NE2	1:C:453:LEU:HG	2.31	0.46
1:G:587:ARG:NH2	1:G:689:GLU:OE1	2.47	0.46
1:I:522:LEU:HD11	1:I:545:MET:SD	2.56	0.46
1:B:452:GLN:NE2	1:B:453:LEU:HG	2.31	0.46
1:C:389:ALA:C	1:C:391:ASN:H	2.24	0.46
1:C:447:ARG:HE	1:C:472:THR:CG2	2.29	0.46
1:M:447:ARG:HE	1:M:472:THR:CG2	2.29	0.46
1:M:452:GLN:NE2	1:M:453:LEU:HG	2.31	0.46
1:M:587:ARG:NH2	1:M:689:GLU:OE1	2.47	0.46
1:N:389:ALA:C	1:N:391:ASN:H	2.24	0.46
1:O:389:ALA:C	1:O:391:ASN:H	2.24	0.46
1:O:439:LEU:O	1:O:439:LEU:HD12	2.16	0.46
1:O:447:ARG:HE	1:O:472:THR:CG2	2.29	0.46
1:O:452:GLN:NE2	1:O:453:LEU:HG	2.31	0.46
1:P:389:ALA:C	1:P:391:ASN:H	2.24	0.46
1:A:447:ARG:HE	1:A:472:THR:CG2	2.29	0.46
1:A:587:ARG:NH2	1:A:689:GLU:OE1	2.47	0.46
1:C:439:LEU:O	1:C:439:LEU:HD12	2.16	0.46
1:D:439:LEU:HD12	1:D:439:LEU:O	2.16	0.46
1:D:447:ARG:HE	1:D:472:THR:CG2	2.29	0.46
1:F:452:GLN:NE2	1:F:453:LEU:HG	2.31	0.46
1:I:452:GLN:NE2	1:I:453:LEU:HG	2.31	0.46
1:I:587:ARG:NH2	1:I:689:GLU:OE1	2.47	0.46
1:N:452:GLN:NE2	1:N:453:LEU:HG	2.31	0.46
1:P:439:LEU:HD12	1:P:439:LEU:O	2.16	0.46
1:A:439:LEU:HD12	1:A:439:LEU:O	2.16	0.46
1:A:452:GLN:NE2	1:A:453:LEU:HG	2.31	0.46
1:B:522:LEU:HD11	1:B:545:MET:SD	2.56	0.46
1:D:452:GLN:NE2	1:D:453:LEU:HG	2.31	0.46
1:F:379:SER:O	1:F:380:SER:OG	2.26	0.46
1:G:447:ARG:HE	1:G:472:THR:CG2	2.29	0.46
1:H:522:LEU:HD11	1:H:545:MET:SD	2.56	0.46
1:I:389:ALA:C	1:I:391:ASN:H	2.24	0.46
1:I:447:ARG:HE	1:I:472:THR:CG2	2.29	0.46
1:J:447:ARG:HE	1:J:472:THR:CG2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:452:GLN:NE2	1:L:453:LEU:HG	2.31	0.46
1:L:587:ARG:NH2	1:L:689:GLU:OE1	2.47	0.46
1:M:439:LEU:O	1:M:439:LEU:HD12	2.16	0.46
1:N:522:LEU:HD11	1:N:545:MET:SD	2.56	0.46
1:P:447:ARG:HE	1:P:472:THR:CG2	2.29	0.46
1:R:452:GLN:NE2	1:R:453:LEU:HG	2.31	0.46
1:B:439:LEU:HD12	1:B:439:LEU:O	2.16	0.45
1:D:587:ARG:NH2	1:D:689:GLU:OE1	2.47	0.45
1:K:439:LEU:HD12	1:K:439:LEU:O	2.16	0.45
1:L:389:ALA:C	1:L:391:ASN:H	2.24	0.45
1:L:447:ARG:HE	1:L:472:THR:CG2	2.29	0.45
1:N:439:LEU:HD12	1:N:439:LEU:O	2.16	0.45
1:P:452:GLN:NE2	1:P:453:LEU:HG	2.31	0.45
1:R:665:MET:HE3	1:R:665:MET:HB3	1.90	0.45
1:A:522:LEU:HD11	1:A:545:MET:SD	2.56	0.45
1:F:424:GLU:HA	1:F:438:GLU:HA	1.98	0.45
1:I:439:LEU:HD12	1:I:439:LEU:O	2.16	0.45
1:K:424:GLU:HA	1:K:438:GLU:HA	1.98	0.45
1:K:522:LEU:HD11	1:K:545:MET:SD	2.56	0.45
1:L:439:LEU:HD12	1:L:439:LEU:O	2.16	0.45
1:P:587:ARG:NH2	1:P:689:GLU:OE1	2.47	0.45
1:Q:452:GLN:NE2	1:Q:453:LEU:HG	2.31	0.45
1:Q:522:LEU:HD11	1:Q:545:MET:SD	2.56	0.45
1:R:389:ALA:C	1:R:391:ASN:H	2.24	0.45
1:R:424:GLU:HA	1:R:438:GLU:HA	1.98	0.45
1:C:424:GLU:HA	1:C:438:GLU:HA	1.98	0.45
1:E:389:ALA:C	1:E:391:ASN:H	2.24	0.45
1:E:447:ARG:HE	1:E:472:THR:CG2	2.29	0.45
1:F:389:ALA:C	1:F:391:ASN:H	2.24	0.45
1:H:424:GLU:HA	1:H:438:GLU:HA	1.98	0.45
1:H:439:LEU:O	1:H:439:LEU:HD12	2.16	0.45
1:H:452:GLN:NE2	1:H:453:LEU:HG	2.31	0.45
1:H:463:GLY:O	1:H:474:TRP:HD1	2.00	0.45
1:K:463:GLY:O	1:K:474:TRP:HD1	2.00	0.45
1:M:522:LEU:HD11	1:M:545:MET:SD	2.56	0.45
1:Q:389:ALA:C	1:Q:391:ASN:H	2.24	0.45
1:B:424:GLU:HA	1:B:438:GLU:HA	1.98	0.45
1:D:447:ARG:HE	1:D:472:THR:HG23	1.82	0.45
1:E:439:LEU:HD12	1:E:439:LEU:O	2.16	0.45
1:E:452:GLN:NE2	1:E:453:LEU:HG	2.31	0.45
1:F:665:MET:HE3	1:F:665:MET:HB3	1.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:424:GLU:HA	1:J:438:GLU:HA	1.98	0.45
1:J:452:GLN:NE2	1:J:453:LEU:HG	2.31	0.45
1:K:452:GLN:NE2	1:K:453:LEU:HG	2.31	0.45
1:N:424:GLU:HA	1:N:438:GLU:HA	1.98	0.45
1:O:424:GLU:HA	1:O:438:GLU:HA	1.98	0.45
1:P:447:ARG:HE	1:P:472:THR:HG23	1.82	0.45
1:Q:439:LEU:HD12	1:Q:439:LEU:O	2.16	0.45
1:Q:447:ARG:HE	1:Q:472:THR:CG2	2.29	0.45
1:R:379:SER:O	1:R:380:SER:OG	2.26	0.45
1:E:463:GLY:O	1:E:474:TRP:HD1	2.00	0.45
1:E:522:LEU:HD11	1:E:545:MET:SD	2.56	0.45
1:G:424:GLU:HA	1:G:438:GLU:HA	1.98	0.45
1:G:452:GLN:NE2	1:G:453:LEU:HG	2.31	0.45
1:G:463:GLY:O	1:G:474:TRP:HD1	2.00	0.45
1:J:463:GLY:O	1:J:474:TRP:HD1	2.00	0.45
1:K:447:ARG:HE	1:K:472:THR:CG2	2.29	0.45
1:Q:463:GLY:O	1:Q:474:TRP:HD1	2.00	0.45
1:B:478:GLU:H	1:B:478:GLU:CD	2.17	0.45
1:C:522:LEU:HD11	1:C:545:MET:SD	2.56	0.45
1:F:447:ARG:HE	1:F:472:THR:CG2	2.29	0.45
1:G:447:ARG:HE	1:G:472:THR:HG23	1.82	0.45
1:G:466:LEU:HD23	1:G:466:LEU:O	2.17	0.45
1:H:447:ARG:HE	1:H:472:THR:CG2	2.29	0.45
1:J:466:LEU:HD23	1:J:466:LEU:O	2.17	0.45
1:L:448:GLU:OE1	1:L:488:LEU:HB3	2.17	0.45
1:M:440:LYS:HZ3	1:M:474:TRP:NE1	2.15	0.45
1:N:440:LYS:HZ3	1:N:474:TRP:NE1	2.14	0.45
1:O:522:LEU:HD11	1:O:545:MET:SD	2.56	0.45
1:R:439:LEU:HD12	1:R:439:LEU:O	2.16	0.45
1:R:447:ARG:HE	1:R:472:THR:CG2	2.29	0.45
1:B:440:LYS:HZ3	1:B:474:TRP:NE1	2.14	0.45
1:F:439:LEU:HD12	1:F:439:LEU:O	2.16	0.45
1:G:439:LEU:HD12	1:G:439:LEU:O	2.16	0.45
1:I:448:GLU:OE1	1:I:488:LEU:HB3	2.17	0.45
1:I:463:GLY:O	1:I:474:TRP:HD1	2.00	0.45
1:J:447:ARG:HE	1:J:472:THR:HG23	1.82	0.45
1:L:447:ARG:HE	1:L:472:THR:HG23	1.82	0.45
1:L:463:GLY:O	1:L:474:TRP:HD1	2.00	0.45
1:A:424:GLU:HA	1:A:438:GLU:HA	1.98	0.45
1:A:447:ARG:HE	1:A:472:THR:HG23	1.82	0.45
1:A:466:LEU:O	1:A:466:LEU:HD23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:ARG:HE	1:B:472:THR:CG2	2.29	0.45
1:I:656:GLN:O	1:I:657:SER:OG	2.31	0.45
1:J:439:LEU:HD12	1:J:439:LEU:O	2.16	0.45
1:M:466:LEU:O	1:M:466:LEU:HD23	2.17	0.45
1:B:373:LEU:HD22	1:B:412:ILE:HG23	1.99	0.45
1:C:463:GLY:O	1:C:474:TRP:HD1	2.00	0.45
1:D:424:GLU:HA	1:D:438:GLU:HA	1.98	0.45
1:E:424:GLU:HA	1:E:438:GLU:HA	1.98	0.45
1:H:448:GLU:OE1	1:H:488:LEU:HB3	2.17	0.45
1:H:466:LEU:O	1:H:466:LEU:HD23	2.17	0.45
1:I:447:ARG:HE	1:I:472:THR:HG23	1.82	0.45
1:M:447:ARG:HE	1:M:472:THR:HG23	1.82	0.45
1:N:373:LEU:HD22	1:N:412:ILE:HG23	1.99	0.45
1:N:447:ARG:HE	1:N:472:THR:CG2	2.29	0.45
1:O:373:LEU:HD22	1:O:412:ILE:HG23	1.99	0.45
1:O:466:LEU:HD23	1:O:466:LEU:O	2.17	0.45
1:Q:447:ARG:HE	1:Q:472:THR:HG23	1.82	0.45
1:R:447:ARG:HE	1:R:472:THR:HG23	1.82	0.45
1:R:466:LEU:O	1:R:466:LEU:HD23	2.17	0.45
1:A:463:GLY:O	1:A:474:TRP:HD1	2.00	0.45
1:B:463:GLY:O	1:B:474:TRP:HD1	2.00	0.45
1:C:373:LEU:HD22	1:C:412:ILE:HG23	1.99	0.45
1:E:447:ARG:HE	1:E:472:THR:HG23	1.82	0.45
1:K:448:GLU:OE1	1:K:488:LEU:HB3	2.17	0.45
1:K:466:LEU:O	1:K:466:LEU:HD23	2.17	0.45
1:L:656:GLN:O	1:L:657:SER:OG	2.31	0.45
1:P:424:GLU:HA	1:P:438:GLU:HA	1.98	0.45
1:B:408:PRO:HG3	1:B:521:LEU:HD21	1.99	0.44
1:C:466:LEU:HD23	1:C:466:LEU:O	2.17	0.44
1:D:466:LEU:O	1:D:466:LEU:HD23	2.17	0.44
1:F:447:ARG:HE	1:F:472:THR:HG23	1.82	0.44
1:F:463:GLY:O	1:F:474:TRP:HD1	2.00	0.44
1:F:466:LEU:O	1:F:466:LEU:HD23	2.17	0.44
1:G:522:LEU:HD11	1:G:545:MET:SD	2.56	0.44
1:G:665:MET:HE3	1:G:665:MET:HB3	1.90	0.44
1:I:408:PRO:HG3	1:I:521:LEU:HD21	2.00	0.44
1:I:424:GLU:HA	1:I:438:GLU:HA	1.98	0.44
1:J:522:LEU:HD11	1:J:545:MET:SD	2.56	0.44
1:L:424:GLU:HA	1:L:438:GLU:HA	1.98	0.44
1:M:424:GLU:HA	1:M:438:GLU:HA	1.98	0.44
1:M:463:GLY:O	1:M:474:TRP:HD1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:463:GLY:O	1:N:474:TRP:HD1	2.00	0.44
1:O:447:ARG:HE	1:O:472:THR:HG23	1.82	0.44
1:O:463:GLY:O	1:O:474:TRP:HD1	2.00	0.44
1:Q:424:GLU:HA	1:Q:438:GLU:HA	1.98	0.44
1:R:463:GLY:O	1:R:474:TRP:HD1	2.00	0.44
1:A:389:ALA:C	1:A:391:ASN:H	2.24	0.44
1:A:448:GLU:OE1	1:A:488:LEU:HB3	2.17	0.44
1:C:443:TYR:CG	1:C:444:LEU:N	2.85	0.44
1:C:447:ARG:HE	1:C:472:THR:HG23	1.82	0.44
1:D:463:GLY:O	1:D:474:TRP:HD1	2.00	0.44
1:F:443:TYR:CG	1:F:444:LEU:N	2.85	0.44
1:J:665:MET:HE3	1:J:665:MET:HB3	1.90	0.44
1:M:448:GLU:OE1	1:M:488:LEU:HB3	2.17	0.44
1:O:443:TYR:CG	1:O:444:LEU:N	2.85	0.44
1:P:463:GLY:O	1:P:474:TRP:HD1	2.00	0.44
1:R:443:TYR:CG	1:R:444:LEU:N	2.85	0.44
1:R:522:LEU:HD11	1:R:545:MET:SD	2.56	0.44
1:C:448:GLU:OE1	1:C:488:LEU:HB3	2.17	0.44
1:D:443:TYR:CG	1:D:444:LEU:N	2.85	0.44
1:F:522:LEU:HD11	1:F:545:MET:SD	2.56	0.44
1:G:448:GLU:OE1	1:G:488:LEU:HB3	2.17	0.44
1:G:519:ARG:HG2	1:H:531:GLU:CG	2.43	0.44
1:L:408:PRO:HG3	1:L:521:LEU:HD21	2.00	0.44
1:N:408:PRO:HG3	1:N:521:LEU:HD21	2.00	0.44
1:O:448:GLU:OE1	1:O:488:LEU:HB3	2.17	0.44
1:A:373:LEU:HD22	1:A:412:ILE:HG23	1.99	0.44
1:A:408:PRO:HG3	1:A:521:LEU:HD21	2.00	0.44
1:J:443:TYR:CG	1:J:444:LEU:N	2.85	0.44
1:J:448:GLU:OE1	1:J:488:LEU:HB3	2.17	0.44
1:M:373:LEU:HD22	1:M:412:ILE:HG23	1.99	0.44
1:M:389:ALA:C	1:M:391:ASN:H	2.24	0.44
1:M:408:PRO:HG3	1:M:521:LEU:HD21	2.00	0.44
1:P:443:TYR:CG	1:P:444:LEU:N	2.85	0.44
1:P:466:LEU:O	1:P:466:LEU:HD23	2.17	0.44
1:R:448:GLU:OE1	1:R:488:LEU:HB3	2.17	0.44
1:R:656:GLN:O	1:R:657:SER:OG	2.31	0.44
1:F:448:GLU:OE1	1:F:488:LEU:HB3	2.17	0.44
1:G:443:TYR:CG	1:G:444:LEU:N	2.85	0.44
1:M:656:GLN:O	1:M:657:SER:OG	2.31	0.44
1:Q:466:LEU:HD23	1:Q:466:LEU:O	2.17	0.44
1:K:450:VAL:HB	1:K:488:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:448:GLU:OE1	1:Q:488:LEU:HB3	2.17	0.44
1:B:379:SER:O	1:B:380:SER:OG	2.26	0.44
1:B:447:ARG:HE	1:B:472:THR:HG23	1.82	0.44
1:E:448:GLU:OE1	1:E:488:LEU:HB3	2.17	0.44
1:F:450:VAL:HB	1:F:488:LEU:HD22	2.00	0.44
1:H:450:VAL:HB	1:H:488:LEU:HD22	2.00	0.44
1:J:450:VAL:HB	1:J:488:LEU:HD22	2.00	0.44
1:L:450:VAL:HB	1:L:488:LEU:HD22	2.00	0.44
1:L:466:LEU:HD23	1:L:466:LEU:O	2.17	0.44
1:D:373:LEU:HD22	1:D:412:ILE:HG23	1.99	0.44
1:E:466:LEU:HD23	1:E:466:LEU:O	2.17	0.44
1:G:450:VAL:HB	1:G:488:LEU:HD22	2.00	0.44
1:I:450:VAL:HB	1:I:488:LEU:HD22	2.00	0.44
1:K:665:MET:HE3	1:K:665:MET:HB3	1.90	0.44
1:R:450:VAL:HB	1:R:488:LEU:HD22	2.00	0.44
1:C:408:PRO:HG3	1:C:521:LEU:HD21	1.99	0.44
1:C:483:LEU:HD12	1:C:486:SER:HB2	2.00	0.44
1:F:373:LEU:HD22	1:F:412:ILE:HG23	1.99	0.44
1:G:408:PRO:HG3	1:G:521:LEU:HD21	2.00	0.44
1:H:408:PRO:HG3	1:H:521:LEU:HD21	2.00	0.44
1:I:466:LEU:HD23	1:I:466:LEU:O	2.17	0.44
1:J:408:PRO:HG3	1:J:521:LEU:HD21	2.00	0.44
1:K:408:PRO:HG3	1:K:521:LEU:HD21	2.00	0.44
1:N:447:ARG:HE	1:N:472:THR:HG23	1.82	0.44
1:O:408:PRO:HG3	1:O:521:LEU:HD21	2.00	0.44
1:O:483:LEU:HD12	1:O:486:SER:HB2	2.00	0.44
1:P:373:LEU:HD22	1:P:412:ILE:HG23	1.99	0.44
1:R:373:LEU:HD22	1:R:412:ILE:HG23	1.99	0.44
1:A:450:VAL:HB	1:A:488:LEU:HD22	2.00	0.43
1:D:448:GLU:OE1	1:D:488:LEU:HB3	2.17	0.43
1:E:450:VAL:HB	1:E:488:LEU:HD22	2.00	0.43
1:G:373:LEU:HD22	1:G:412:ILE:HG23	1.99	0.43
1:J:373:LEU:HD22	1:J:412:ILE:HG23	1.99	0.43
1:J:398:ARG:NH2	1:R:363:GLU:O	2.51	0.43
1:M:450:VAL:HB	1:M:488:LEU:HD22	2.00	0.43
1:Q:450:VAL:HB	1:Q:488:LEU:HD22	2.00	0.43
1:D:690:LEU:HD13	1:D:696:ILE:HD11	2.00	0.43
1:H:447:ARG:HE	1:H:472:THR:HG23	1.82	0.43
1:O:690:LEU:HD13	1:O:696:ILE:HD11	2.00	0.43
1:P:690:LEU:HD13	1:P:696:ILE:HD11	2.00	0.43
1:B:483:LEU:HD12	1:B:486:SER:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:690:LEU:HD13	1:C:696:ILE:HD11	2.00	0.43
1:D:450:VAL:HB	1:D:488:LEU:HD22	2.00	0.43
1:H:373:LEU:HD22	1:H:412:ILE:HG23	1.99	0.43
1:H:665:MET:HE3	1:H:665:MET:HB3	1.90	0.43
1:K:373:LEU:HD22	1:K:412:ILE:HG23	1.99	0.43
1:K:447:ARG:HE	1:K:472:THR:HG23	1.82	0.43
1:N:379:SER:O	1:N:380:SER:OG	2.26	0.43
1:N:448:GLU:OE1	1:N:488:LEU:HB3	2.17	0.43
1:N:483:LEU:HD12	1:N:486:SER:HB2	2.00	0.43
1:P:448:GLU:OE1	1:P:488:LEU:HB3	2.17	0.43
1:P:450:VAL:HB	1:P:488:LEU:HD22	2.00	0.43
1:B:448:GLU:OE1	1:B:488:LEU:HB3	2.17	0.43
1:B:466:LEU:HD23	1:B:466:LEU:O	2.17	0.43
1:C:440:LYS:HZ3	1:C:474:TRP:NE1	2.16	0.43
1:D:408:PRO:HG3	1:D:521:LEU:HD21	1.99	0.43
1:D:483:LEU:HD12	1:D:486:SER:HB2	2.00	0.43
1:E:587:ARG:NH2	1:E:689:GLU:OE1	2.47	0.43
1:B:450:VAL:HB	1:B:488:LEU:HD22	2.00	0.43
1:E:483:LEU:HD12	1:E:486:SER:HB2	2.00	0.43
1:H:488:LEU:HA	1:H:488:LEU:HD23	1.80	0.43
1:H:598:TYR:CD2	1:H:685:LEU:HD21	2.54	0.43
1:K:488:LEU:HA	1:K:488:LEU:HD23	1.80	0.43
1:K:598:TYR:CD2	1:K:685:LEU:HD21	2.54	0.43
1:L:373:LEU:HD22	1:L:412:ILE:HG23	1.99	0.43
1:M:549:LEU:HD23	1:M:549:LEU:HA	1.83	0.43
1:P:483:LEU:HD12	1:P:486:SER:HB2	2.00	0.43
1:B:447:ARG:HG2	1:B:491:PHE:HB2	2.01	0.43
1:E:690:LEU:HD13	1:E:696:ILE:HD11	2.00	0.43
1:G:483:LEU:HD12	1:G:486:SER:HB2	2.00	0.43
1:L:443:TYR:CG	1:L:444:LEU:N	2.85	0.43
1:N:450:VAL:HB	1:N:488:LEU:HD22	2.00	0.43
1:Q:483:LEU:HD12	1:Q:486:SER:HB2	2.00	0.43
1:B:598:TYR:CD2	1:B:685:LEU:HD21	2.54	0.43
1:B:690:LEU:HD13	1:B:696:ILE:HD11	2.00	0.43
1:E:373:LEU:HD22	1:E:412:ILE:HG23	1.99	0.43
1:H:483:LEU:HD12	1:H:486:SER:HB2	2.00	0.43
1:I:373:LEU:HD22	1:I:412:ILE:HG23	1.99	0.43
1:I:443:TYR:CG	1:I:444:LEU:N	2.85	0.43
1:J:483:LEU:HD12	1:J:486:SER:HB2	2.00	0.43
1:N:447:ARG:HG2	1:N:491:PHE:HB2	2.01	0.43
1:N:466:LEU:HD23	1:N:466:LEU:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:690:LEU:HD13	1:N:696:ILE:HD11	2.00	0.43
1:O:656:GLN:O	1:O:657:SER:OG	2.31	0.43
1:Q:690:LEU:HD13	1:Q:696:ILE:HD11	2.00	0.43
1:A:447:ARG:HG2	1:A:491:PHE:HB2	2.01	0.43
1:A:690:LEU:HD13	1:A:696:ILE:HD11	2.00	0.43
1:C:450:VAL:HB	1:C:488:LEU:HD22	2.00	0.43
1:E:440:LYS:HG2	1:E:474:TRP:CE2	2.54	0.43
1:K:483:LEU:HD12	1:K:486:SER:HB2	2.00	0.43
1:M:447:ARG:HG2	1:M:491:PHE:HB2	2.01	0.43
1:M:598:TYR:CD2	1:M:685:LEU:HD21	2.54	0.43
1:N:598:TYR:CD2	1:N:685:LEU:HD21	2.54	0.43
1:O:440:LYS:HG2	1:O:474:TRP:CE2	2.54	0.43
1:P:408:PRO:HG3	1:P:521:LEU:HD21	2.00	0.43
1:P:440:LYS:HG2	1:P:474:TRP:CE2	2.54	0.43
1:P:665:MET:HE3	1:P:665:MET:HB3	1.90	0.43
1:Q:373:LEU:HD22	1:Q:412:ILE:HG23	1.99	0.43
1:Q:408:PRO:HG3	1:Q:521:LEU:HD21	2.00	0.43
1:Q:440:LYS:HG2	1:Q:474:TRP:CE2	2.54	0.43
1:Q:587:ARG:NH2	1:Q:689:GLU:OE1	2.47	0.43
1:R:690:LEU:HD13	1:R:696:ILE:HD11	2.00	0.43
1:A:483:LEU:HD12	1:A:486:SER:HB2	2.00	0.43
1:A:598:TYR:CD2	1:A:685:LEU:HD21	2.54	0.43
1:C:440:LYS:HG2	1:C:474:TRP:CE2	2.54	0.43
1:C:447:ARG:HG2	1:C:491:PHE:HB2	2.01	0.43
1:C:598:TYR:CD2	1:C:685:LEU:HD21	2.54	0.43
1:D:440:LYS:HG2	1:D:474:TRP:CE2	2.54	0.43
1:F:408:PRO:HG3	1:F:521:LEU:HD21	2.00	0.43
1:F:452:GLN:CD	1:F:453:LEU:HG	2.44	0.43
1:I:598:TYR:CD2	1:I:685:LEU:HD21	2.54	0.43
1:J:598:TYR:CD2	1:J:685:LEU:HD21	2.54	0.43
1:M:483:LEU:HD12	1:M:486:SER:HB2	2.00	0.43
1:M:690:LEU:HD13	1:M:696:ILE:HD11	2.00	0.43
1:O:447:ARG:HG2	1:O:491:PHE:HB2	2.01	0.43
1:O:450:VAL:HB	1:O:488:LEU:HD22	2.00	0.43
1:R:452:GLN:CD	1:R:453:LEU:HG	2.44	0.43
1:B:488:LEU:HA	1:B:488:LEU:HD23	1.80	0.43
1:B:610:PHE:CE2	1:B:661:LEU:HD21	2.54	0.43
1:D:375:ILE:HD11	1:D:501:LEU:HD12	2.01	0.43
1:D:665:MET:HE3	1:D:665:MET:HB3	1.90	0.43
1:E:408:PRO:HG3	1:E:521:LEU:HD21	2.00	0.43
1:F:440:LYS:HG2	1:F:474:TRP:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:690:LEU:HD13	1:F:696:ILE:HD11	2.00	0.43
1:G:598:TYR:CD2	1:G:685:LEU:HD21	2.54	0.43
1:I:483:LEU:HD12	1:I:486:SER:HB2	2.00	0.43
1:L:483:LEU:HD12	1:L:486:SER:HB2	2.00	0.43
1:L:665:MET:HE3	1:L:665:MET:HB3	1.90	0.43
1:R:408:PRO:HG3	1:R:521:LEU:HD21	2.00	0.43
1:A:610:PHE:CE2	1:A:661:LEU:HD21	2.54	0.42
1:F:375:ILE:HD11	1:F:501:LEU:HD12	2.01	0.42
1:G:460:TYR:HB3	1:G:479:TYR:CD1	2.54	0.42
1:I:447:ARG:HG2	1:I:491:PHE:HB2	2.01	0.42
1:J:531:GLU:CG	1:R:519:ARG:HG2	2.47	0.42
1:L:598:TYR:CD2	1:L:685:LEU:HD21	2.54	0.42
1:N:610:PHE:CE2	1:N:661:LEU:HD21	2.54	0.42
1:O:598:TYR:CD2	1:O:685:LEU:HD21	2.54	0.42
1:R:375:ILE:HD11	1:R:501:LEU:HD12	2.01	0.42
1:R:440:LYS:HG2	1:R:474:TRP:CE2	2.54	0.42
1:A:549:LEU:HD23	1:A:549:LEU:HA	1.83	0.42
1:E:452:GLN:CD	1:E:453:LEU:HG	2.44	0.42
1:F:610:PHE:CE2	1:F:661:LEU:HD21	2.54	0.42
1:J:460:TYR:HB3	1:J:479:TYR:CD1	2.54	0.42
1:O:440:LYS:HZ3	1:O:474:TRP:NE1	2.17	0.42
1:P:375:ILE:HD11	1:P:501:LEU:HD12	2.01	0.42
1:P:598:TYR:CD2	1:P:685:LEU:HD21	2.54	0.42
1:Q:375:ILE:HD11	1:Q:501:LEU:HD12	2.01	0.42
1:R:610:PHE:CE2	1:R:661:LEU:HD21	2.54	0.42
1:B:440:LYS:HG2	1:B:474:TRP:CE2	2.54	0.42
1:C:375:ILE:HD11	1:C:501:LEU:HD12	2.01	0.42
1:D:598:TYR:CD2	1:D:685:LEU:HD21	2.54	0.42
1:E:375:ILE:HD11	1:E:501:LEU:HD12	2.01	0.42
1:H:393:GLU:HG3	1:H:498:THR:HG21	2.02	0.42
1:K:393:GLU:HG3	1:K:498:THR:HG21	2.02	0.42
1:L:447:ARG:HG2	1:L:491:PHE:HB2	2.01	0.42
1:M:610:PHE:CE2	1:M:661:LEU:HD21	2.54	0.42
1:N:440:LYS:HG2	1:N:474:TRP:CE2	2.54	0.42
1:O:375:ILE:HD11	1:O:501:LEU:HD12	2.01	0.42
1:P:447:ARG:HG2	1:P:491:PHE:HB2	2.01	0.42
1:Q:452:GLN:CD	1:Q:453:LEU:HG	2.44	0.42
1:Q:598:TYR:CD2	1:Q:685:LEU:HD21	2.54	0.42
1:C:452:GLN:CD	1:C:453:LEU:HG	2.44	0.42
1:C:610:PHE:CE2	1:C:661:LEU:HD21	2.54	0.42
1:E:460:TYR:HB3	1:E:479:TYR:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:598:TYR:CD2	1:E:685:LEU:HD21	2.54	0.42
1:G:610:PHE:CE2	1:G:661:LEU:HD21	2.54	0.42
1:H:447:ARG:HH21	1:H:472:THR:HG1	1.57	0.42
1:H:452:GLN:CD	1:H:453:LEU:HG	2.44	0.42
1:H:634:ASP:CG	1:H:636:ALA:H	2.28	0.42
1:J:610:PHE:CE2	1:J:661:LEU:HD21	2.54	0.42
1:K:452:GLN:CD	1:K:453:LEU:HG	2.44	0.42
1:K:634:ASP:CG	1:K:636:ALA:H	2.28	0.42
1:N:389:ALA:HB1	1:N:392:ASP:H	1.85	0.42
1:O:610:PHE:CE2	1:O:661:LEU:HD21	2.54	0.42
1:Q:460:TYR:HB3	1:Q:479:TYR:CD1	2.55	0.42
1:R:598:TYR:CD2	1:R:685:LEU:HD21	2.54	0.42
1:A:443:TYR:CG	1:A:444:LEU:N	2.85	0.42
1:B:389:ALA:HB1	1:B:392:ASP:H	1.85	0.42
1:B:452:GLN:CD	1:B:453:LEU:HG	2.44	0.42
1:D:447:ARG:HG2	1:D:491:PHE:HB2	2.01	0.42
1:E:634:ASP:CG	1:E:636:ALA:H	2.28	0.42
1:G:452:GLN:CD	1:G:453:LEU:HG	2.44	0.42
1:I:665:MET:HE3	1:I:665:MET:HB3	1.90	0.42
1:J:375:ILE:HD11	1:J:501:LEU:HD12	2.01	0.42
1:J:452:GLN:CD	1:J:453:LEU:HG	2.44	0.42
1:N:488:LEU:HA	1:N:488:LEU:HD23	1.80	0.42
1:O:452:GLN:CD	1:O:453:LEU:HG	2.44	0.42
1:P:566:LEU:HA	1:P:566:LEU:HD23	1.78	0.42
1:Q:610:PHE:CE2	1:Q:661:LEU:HD21	2.54	0.42
1:A:460:TYR:HB3	1:A:479:TYR:CD1	2.54	0.42
1:B:460:TYR:HB3	1:B:479:TYR:CD1	2.54	0.42
1:F:393:GLU:HG3	1:F:498:THR:HG21	2.02	0.42
1:F:483:LEU:HD12	1:F:486:SER:HB2	2.00	0.42
1:F:598:TYR:CD2	1:F:685:LEU:HD21	2.54	0.42
1:I:440:LYS:HG2	1:I:474:TRP:CE2	2.54	0.42
1:M:443:TYR:CG	1:M:444:LEU:N	2.85	0.42
1:N:452:GLN:CD	1:N:453:LEU:HG	2.44	0.42
1:O:460:TYR:HB3	1:O:479:TYR:CD1	2.54	0.42
1:Q:634:ASP:CG	1:Q:636:ALA:H	2.28	0.42
1:R:483:LEU:HD12	1:R:486:SER:HB2	2.00	0.42
1:A:393:GLU:HG3	1:A:498:THR:HG21	2.02	0.42
1:B:375:ILE:HD11	1:B:501:LEU:HD12	2.01	0.42
1:B:634:ASP:CG	1:B:636:ALA:H	2.28	0.42
1:D:566:LEU:HA	1:D:566:LEU:HD23	1.78	0.42
1:E:610:PHE:CE2	1:E:661:LEU:HD21	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:375:ILE:HD11	1:G:501:LEU:HD12	2.01	0.42
1:H:690:LEU:HD13	1:H:696:ILE:HD11	2.00	0.42
1:I:690:LEU:HD13	1:I:696:ILE:HD11	2.00	0.42
1:J:447:ARG:HG2	1:J:491:PHE:HB2	2.01	0.42
1:K:690:LEU:HD13	1:K:696:ILE:HD11	2.00	0.42
1:L:440:LYS:HG2	1:L:474:TRP:CE2	2.54	0.42
1:M:460:TYR:HB3	1:M:479:TYR:CD1	2.55	0.42
1:N:375:ILE:HD11	1:N:501:LEU:HD12	2.01	0.42
1:N:460:TYR:HB3	1:N:479:TYR:CD1	2.55	0.42
1:N:634:ASP:CG	1:N:636:ALA:H	2.28	0.42
1:Q:447:ARG:HG2	1:Q:491:PHE:HB2	2.01	0.42
1:R:393:GLU:HG3	1:R:498:THR:HG21	2.02	0.42
1:A:440:LYS:HG2	1:A:474:TRP:CE2	2.54	0.42
1:C:389:ALA:HB1	1:C:392:ASP:H	1.85	0.42
1:C:460:TYR:HB3	1:C:479:TYR:CD1	2.55	0.42
1:D:542:LEU:HD23	1:D:542:LEU:HA	1.91	0.42
1:F:460:TYR:HB3	1:F:479:TYR:CD1	2.55	0.42
1:G:690:LEU:HD13	1:G:696:ILE:HD11	2.00	0.42
1:I:610:PHE:CE2	1:I:661:LEU:HD21	2.54	0.42
1:J:690:LEU:HD13	1:J:696:ILE:HD11	2.00	0.42
1:M:440:LYS:HG2	1:M:474:TRP:CE2	2.54	0.42
1:O:634:ASP:CG	1:O:636:ALA:H	2.28	0.42
1:P:542:LEU:HD23	1:P:542:LEU:HA	1.91	0.42
1:R:447:ARG:HG2	1:R:491:PHE:HB2	2.01	0.42
1:C:634:ASP:CG	1:C:636:ALA:H	2.28	0.42
1:F:447:ARG:HG2	1:F:491:PHE:HB2	2.01	0.42
1:G:447:ARG:HG2	1:G:491:PHE:HB2	2.01	0.42
1:H:447:ARG:HG2	1:H:491:PHE:HB2	2.01	0.42
1:I:389:ALA:HB1	1:I:392:ASP:H	1.85	0.42
1:J:634:ASP:CG	1:J:636:ALA:H	2.28	0.42
1:L:389:ALA:HB1	1:L:392:ASP:H	1.85	0.42
1:L:690:LEU:HD13	1:L:696:ILE:HD11	2.00	0.42
1:M:393:GLU:HG3	1:M:498:THR:HG21	2.02	0.42
1:N:393:GLU:HG3	1:N:498:THR:HG21	2.02	0.42
1:O:389:ALA:HB1	1:O:392:ASP:H	1.85	0.42
1:Q:389:ALA:HB1	1:Q:392:ASP:H	1.85	0.42
1:R:460:TYR:HB3	1:R:479:TYR:CD1	2.54	0.42
1:R:634:ASP:CG	1:R:636:ALA:H	2.28	0.42
1:B:393:GLU:HG3	1:B:498:THR:HG21	2.02	0.42
1:B:542:LEU:HD23	1:B:542:LEU:HA	1.91	0.42
1:D:452:GLN:CD	1:D:453:LEU:HG	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:389:ALA:HB1	1:E:392:ASP:H	1.85	0.42
1:E:447:ARG:HG2	1:E:491:PHE:HB2	2.01	0.42
1:F:417:ASN:HB2	1:F:420:MET:HE2	2.02	0.42
1:G:634:ASP:CG	1:G:636:ALA:H	2.28	0.42
1:H:440:LYS:HG2	1:H:474:TRP:CE2	2.54	0.42
1:K:440:LYS:HG2	1:K:474:TRP:CE2	2.54	0.42
1:L:610:PHE:CE2	1:L:661:LEU:HD21	2.54	0.42
1:P:610:PHE:CE2	1:P:661:LEU:HD21	2.54	0.42
1:A:452:GLN:CD	1:A:453:LEU:HG	2.44	0.41
1:E:393:GLU:HG3	1:E:498:THR:HG21	2.02	0.41
1:E:665:MET:HE3	1:E:665:MET:HB3	1.90	0.41
1:F:634:ASP:CG	1:F:636:ALA:H	2.28	0.41
1:H:389:ALA:HB1	1:H:392:ASP:H	1.85	0.41
1:I:375:ILE:HD11	1:I:501:LEU:HD12	2.01	0.41
1:K:385:LEU:C	1:K:387:ALA:N	2.79	0.41
1:K:389:ALA:HB1	1:K:392:ASP:H	1.85	0.41
1:K:447:ARG:HG2	1:K:491:PHE:HB2	2.01	0.41
1:L:375:ILE:HD11	1:L:501:LEU:HD12	2.01	0.41
1:P:452:GLN:CD	1:P:453:LEU:HG	2.44	0.41
1:R:417:ASN:HB2	1:R:420:MET:HE2	2.02	0.41
1:A:656:GLN:O	1:A:657:SER:OG	2.31	0.41
1:D:610:PHE:CE2	1:D:661:LEU:HD21	2.54	0.41
1:G:385:LEU:C	1:G:387:ALA:N	2.79	0.41
1:H:417:ASN:HB2	1:H:420:MET:HE2	2.02	0.41
1:I:460:TYR:HB3	1:I:479:TYR:CD1	2.55	0.41
1:K:417:ASN:HB2	1:K:420:MET:HE2	2.02	0.41
1:L:452:GLN:CD	1:L:453:LEU:HG	2.44	0.41
1:M:452:GLN:CD	1:M:453:LEU:HG	2.44	0.41
1:R:566:LEU:HD23	1:R:566:LEU:HA	1.78	0.41
1:A:634:ASP:CG	1:A:636:ALA:H	2.28	0.41
1:A:690:LEU:HD23	1:A:690:LEU:HA	1.80	0.41
1:D:460:TYR:HB3	1:D:479:TYR:CD1	2.55	0.41
1:D:488:LEU:HD23	1:D:488:LEU:HA	1.80	0.41
1:G:440:LYS:HG2	1:G:474:TRP:CE2	2.54	0.41
1:H:443:TYR:CG	1:H:444:LEU:N	2.85	0.41
1:H:497:LEU:HA	1:H:497:LEU:HD12	1.79	0.41
1:J:385:LEU:C	1:J:387:ALA:N	2.79	0.41
1:J:389:ALA:HB1	1:J:392:ASP:H	1.85	0.41
1:J:440:LYS:HG2	1:J:474:TRP:CE2	2.54	0.41
1:K:367:PHE:CD2	1:L:524:GLN:HG2	2.55	0.41
1:K:379:SER:O	1:K:380:SER:OG	2.26	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:443:TYR:CG	1:K:444:LEU:N	2.85	0.41
1:K:610:PHE:CE2	1:K:661:LEU:HD21	2.54	0.41
1:L:367:PHE:CD2	1:M:524:GLN:HG2	2.56	0.41
1:L:393:GLU:HG3	1:L:498:THR:HG21	2.02	0.41
1:L:460:TYR:HB3	1:L:479:TYR:CD1	2.55	0.41
1:L:634:ASP:CG	1:L:636:ALA:H	2.28	0.41
1:O:488:LEU:HD23	1:O:488:LEU:HA	1.80	0.41
1:P:460:TYR:HB3	1:P:479:TYR:CD1	2.55	0.41
1:P:488:LEU:HD23	1:P:488:LEU:HA	1.80	0.41
1:P:663:VAL:O	1:P:686:SER:HA	2.21	0.41
1:Q:393:GLU:HG3	1:Q:498:THR:HG21	2.02	0.41
1:Q:417:ASN:HB2	1:Q:420:MET:HE2	2.02	0.41
1:A:460:TYR:OH	1:A:482:ARG:HD2	2.21	0.41
1:A:524:GLN:HG2	1:I:367:PHE:CD2	2.56	0.41
1:B:460:TYR:OH	1:B:482:ARG:HD2	2.21	0.41
1:B:634:ASP:O	1:B:638:THR:OG1	2.39	0.41
1:C:656:GLN:O	1:C:657:SER:OG	2.31	0.41
1:C:663:VAL:O	1:C:686:SER:HA	2.21	0.41
1:D:663:VAL:O	1:D:686:SER:HA	2.21	0.41
1:G:389:ALA:HB1	1:G:392:ASP:H	1.85	0.41
1:G:656:GLN:O	1:G:657:SER:OG	2.31	0.41
1:I:452:GLN:CD	1:I:453:LEU:HG	2.44	0.41
1:I:523:GLU:HA	1:I:526:GLU:HG2	2.02	0.41
1:I:542:LEU:HD23	1:I:542:LEU:HA	1.91	0.41
1:J:417:ASN:HB2	1:J:420:MET:HE2	2.02	0.41
1:K:460:TYR:HB3	1:K:479:TYR:CD1	2.55	0.41
1:L:566:LEU:HD23	1:L:566:LEU:HA	1.78	0.41
1:M:460:TYR:OH	1:M:482:ARG:HD2	2.21	0.41
1:M:634:ASP:CG	1:M:636:ALA:H	2.28	0.41
1:N:460:TYR:OH	1:N:482:ARG:HD2	2.21	0.41
1:N:542:LEU:HD23	1:N:542:LEU:HA	1.91	0.41
1:Q:665:MET:HE3	1:Q:665:MET:HB3	1.90	0.41
1:A:389:ALA:HB1	1:A:392:ASP:H	1.85	0.41
1:D:389:ALA:HB1	1:D:392:ASP:H	1.85	0.41
1:D:417:ASN:HB2	1:D:420:MET:HE2	2.02	0.41
1:D:497:LEU:HD12	1:D:497:LEU:HA	1.79	0.41
1:E:417:ASN:HB2	1:E:420:MET:HE2	2.02	0.41
1:E:488:LEU:HD23	1:E:488:LEU:HA	1.80	0.41
1:G:417:ASN:HB2	1:G:420:MET:HE2	2.03	0.41
1:H:375:ILE:HD11	1:H:501:LEU:HD12	2.01	0.41
1:H:610:PHE:CE2	1:H:661:LEU:HD21	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:393:GLU:HG3	1:I:498:THR:HG21	2.02	0.41
1:I:417:ASN:HB2	1:I:420:MET:HE2	2.02	0.41
1:I:634:ASP:CG	1:I:636:ALA:H	2.28	0.41
1:J:656:GLN:O	1:J:657:SER:OG	2.31	0.41
1:K:447:ARG:HH21	1:K:472:THR:HG1	1.57	0.41
1:K:497:LEU:HD12	1:K:497:LEU:HA	1.79	0.41
1:L:523:GLU:HA	1:L:526:GLU:HG2	2.03	0.41
1:M:690:LEU:HD23	1:M:690:LEU:HA	1.80	0.41
1:N:367:PHE:CD2	1:O:524:GLN:HG2	2.56	0.41
1:N:634:ASP:O	1:N:638:THR:OG1	2.39	0.41
1:O:663:VAL:O	1:O:686:SER:HA	2.21	0.41
1:P:389:ALA:HB1	1:P:392:ASP:H	1.85	0.41
1:P:417:ASN:HB2	1:P:420:MET:HE2	2.02	0.41
1:Q:488:LEU:HD23	1:Q:488:LEU:HA	1.80	0.41
1:C:488:LEU:HD23	1:C:488:LEU:HA	1.80	0.41
1:F:500:HIS:O	1:F:504:VAL:N	2.53	0.41
1:F:566:LEU:HD23	1:F:566:LEU:HA	1.78	0.41
1:H:367:PHE:CD2	1:I:524:GLN:HG2	2.56	0.41
1:H:390:LEU:HD13	1:H:390:LEU:HA	1.95	0.41
1:H:443:TYR:CD2	1:H:444:LEU:N	2.88	0.41
1:H:460:TYR:HB3	1:H:479:TYR:CD1	2.55	0.41
1:I:566:LEU:HD23	1:I:566:LEU:HA	1.78	0.41
1:I:690:LEU:HD23	1:I:690:LEU:HA	1.80	0.41
1:K:375:ILE:HD11	1:K:501:LEU:HD12	2.01	0.41
1:M:389:ALA:HB1	1:M:392:ASP:H	1.85	0.41
1:M:523:GLU:HA	1:M:526:GLU:HG2	2.02	0.41
1:P:367:PHE:CD2	1:Q:524:GLN:HG2	2.56	0.41
1:R:385:LEU:C	1:R:387:ALA:N	2.79	0.41
1:D:634:ASP:CG	1:D:636:ALA:H	2.28	0.41
1:E:367:PHE:CD2	1:F:524:GLN:HG2	2.56	0.41
1:G:663:VAL:O	1:G:686:SER:HA	2.21	0.41
1:I:634:ASP:O	1:I:638:THR:OG1	2.38	0.41
1:J:663:VAL:O	1:J:686:SER:HA	2.21	0.41
1:K:443:TYR:CD2	1:K:444:LEU:N	2.88	0.41
1:M:367:PHE:CD2	1:N:524:GLN:HG2	2.56	0.41
1:M:390:LEU:HD13	1:M:390:LEU:HA	1.95	0.41
1:O:542:LEU:HD23	1:O:542:LEU:HA	1.91	0.41
1:R:500:HIS:O	1:R:504:VAL:N	2.53	0.41
1:A:523:GLU:HA	1:A:526:GLU:HG2	2.03	0.41
1:C:417:ASN:HB2	1:C:420:MET:HE2	2.02	0.41
1:G:393:GLU:HG3	1:G:498:THR:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:367:PHE:CD2	1:K:524:GLN:HG2	2.56	0.41
1:K:390:LEU:HD13	1:K:390:LEU:HA	1.95	0.41
1:L:417:ASN:HB2	1:L:420:MET:HE2	2.03	0.41
1:L:634:ASP:O	1:L:638:THR:OG1	2.38	0.41
1:L:690:LEU:HD23	1:L:690:LEU:HA	1.80	0.41
1:O:417:ASN:HB2	1:O:420:MET:HE2	2.02	0.41
1:P:634:ASP:CG	1:P:636:ALA:H	2.28	0.41
1:Q:500:HIS:O	1:Q:504:VAL:N	2.53	0.41
1:A:367:PHE:CD2	1:B:524:GLN:HG2	2.56	0.41
1:A:375:ILE:HD11	1:A:501:LEU:HD12	2.01	0.41
1:A:390:LEU:HD13	1:A:390:LEU:HA	1.95	0.41
1:B:523:GLU:HA	1:B:526:GLU:HG2	2.03	0.41
1:C:456:LEU:HD23	1:C:462:LYS:HE3	2.03	0.41
1:C:542:LEU:HD23	1:C:542:LEU:HA	1.91	0.41
1:D:634:ASP:O	1:D:638:THR:OG1	2.38	0.41
1:E:460:TYR:OH	1:E:482:ARG:HD2	2.21	0.41
1:E:500:HIS:O	1:E:504:VAL:N	2.53	0.41
1:F:389:ALA:HB1	1:F:392:ASP:H	1.85	0.41
1:G:500:HIS:O	1:G:504:VAL:N	2.53	0.41
1:I:460:TYR:OH	1:I:482:ARG:HD2	2.21	0.41
1:J:393:GLU:HG3	1:J:498:THR:HG21	2.02	0.41
1:J:497:LEU:HA	1:J:497:LEU:HD12	1.79	0.41
1:L:460:TYR:OH	1:L:482:ARG:HD2	2.21	0.41
1:M:375:ILE:HD11	1:M:501:LEU:HD12	2.01	0.41
1:M:663:VAL:O	1:M:686:SER:HA	2.21	0.41
1:N:523:GLU:HA	1:N:526:GLU:HG2	2.03	0.41
1:O:456:LEU:HD23	1:O:462:LYS:HE3	2.03	0.41
1:P:497:LEU:HD12	1:P:497:LEU:HA	1.79	0.41
1:Q:460:TYR:OH	1:Q:482:ARG:HD2	2.21	0.41
1:Q:663:VAL:O	1:Q:686:SER:HA	2.21	0.41
1:R:389:ALA:HB1	1:R:392:ASP:H	1.85	0.41
1:A:417:ASN:HB2	1:A:420:MET:HE2	2.02	0.41
1:A:559:ILE:O	1:A:560:ARG:C	2.64	0.41
1:A:663:VAL:O	1:A:686:SER:HA	2.21	0.41
1:B:367:PHE:CD2	1:C:524:GLN:HG2	2.56	0.41
1:B:456:LEU:HD23	1:B:462:LYS:HE3	2.03	0.41
1:E:523:GLU:HA	1:E:526:GLU:HG2	2.03	0.41
1:E:663:VAL:O	1:E:686:SER:HA	2.21	0.41
1:F:460:TYR:OH	1:F:482:ARG:HD2	2.21	0.41
1:G:423:GLY:O	1:G:439:LEU:HG	2.21	0.41
1:G:497:LEU:HA	1:G:497:LEU:HD12	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:423:GLY:O	1:I:439:LEU:HG	2.21	0.41
1:J:423:GLY:O	1:J:439:LEU:HG	2.21	0.41
1:J:500:HIS:O	1:J:504:VAL:N	2.53	0.41
1:J:559:ILE:O	1:J:560:ARG:C	2.64	0.41
1:L:423:GLY:O	1:L:439:LEU:HG	2.21	0.41
1:L:542:LEU:HD23	1:L:542:LEU:HA	1.91	0.41
1:M:417:ASN:HB2	1:M:420:MET:HE2	2.02	0.41
1:M:559:ILE:O	1:M:560:ARG:C	2.64	0.41
1:N:417:ASN:HB2	1:N:420:MET:HE2	2.02	0.41
1:O:367:PHE:CD2	1:P:524:GLN:HG2	2.56	0.41
1:O:460:TYR:OH	1:O:482:ARG:HD2	2.21	0.41
1:P:634:ASP:O	1:P:638:THR:OG1	2.39	0.41
1:Q:523:GLU:HA	1:Q:526:GLU:HG2	2.03	0.41
1:Q:559:ILE:O	1:Q:560:ARG:C	2.64	0.41
1:B:417:ASN:HB2	1:B:420:MET:HE2	2.02	0.40
1:C:460:TYR:OH	1:C:482:ARG:HD2	2.21	0.40
1:E:559:ILE:O	1:E:560:ARG:C	2.64	0.40
1:G:443:TYR:CD2	1:G:444:LEU:N	2.88	0.40
1:G:559:ILE:O	1:G:560:ARG:C	2.64	0.40
1:J:443:TYR:CD2	1:J:444:LEU:N	2.88	0.40
1:K:523:GLU:HA	1:K:526:GLU:HG2	2.03	0.40
1:N:456:LEU:HD23	1:N:462:LYS:HE3	2.03	0.40
1:O:393:GLU:HG3	1:O:498:THR:HG21	2.02	0.40
1:P:432:VAL:HA	1:P:433:PRO:HD2	1.98	0.40
1:A:456:LEU:HD23	1:A:462:LYS:HE3	2.03	0.40
1:B:379:SER:C	1:B:381:GLN:H	2.30	0.40
1:B:623:ARG:O	1:B:625:THR:HG23	2.21	0.40
1:C:379:SER:C	1:C:381:GLN:H	2.30	0.40
1:C:393:GLU:HG3	1:C:498:THR:HG21	2.02	0.40
1:H:523:GLU:HA	1:H:526:GLU:HG2	2.03	0.40
1:I:544:ARG:HH22	1:I:577:LYS:HA	1.86	0.40
1:K:379:SER:C	1:K:381:GLN:H	2.30	0.40
1:M:456:LEU:HD23	1:M:462:LYS:HE3	2.03	0.40
1:M:544:ARG:HH22	1:M:577:LYS:HA	1.87	0.40
1:N:379:SER:C	1:N:381:GLN:H	2.30	0.40
1:N:423:GLY:O	1:N:439:LEU:HG	2.21	0.40
1:N:623:ARG:O	1:N:625:THR:HG23	2.21	0.40
1:O:623:ARG:O	1:O:625:THR:HG23	2.21	0.40
1:P:523:GLU:HA	1:P:526:GLU:HG2	2.03	0.40
1:Q:379:SER:C	1:Q:381:GLN:H	2.30	0.40
1:R:460:TYR:OH	1:R:482:ARG:HD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:GLY:O	1:B:439:LEU:HG	2.21	0.40
1:C:623:ARG:O	1:C:625:THR:HG23	2.21	0.40
1:D:379:SER:C	1:D:381:GLN:H	2.30	0.40
1:D:432:VAL:HA	1:D:433:PRO:HD2	1.98	0.40
1:E:445:LEU:HD12	1:E:445:LEU:HA	1.93	0.40
1:E:542:LEU:HD23	1:E:542:LEU:HA	1.91	0.40
1:G:390:LEU:HD13	1:G:390:LEU:HA	1.95	0.40
1:G:460:TYR:OH	1:G:482:ARG:HD2	2.21	0.40
1:G:488:LEU:HA	1:G:488:LEU:HD23	1.80	0.40
1:G:523:GLU:HA	1:G:526:GLU:HG2	2.02	0.40
1:H:379:SER:C	1:H:381:GLN:H	2.30	0.40
1:H:559:ILE:O	1:H:560:ARG:C	2.64	0.40
1:H:663:VAL:O	1:H:686:SER:HA	2.21	0.40
1:J:460:TYR:OH	1:J:482:ARG:HD2	2.21	0.40
1:J:488:LEU:HA	1:J:488:LEU:HD23	1.80	0.40
1:J:523:GLU:HA	1:J:526:GLU:HG2	2.02	0.40
1:K:623:ARG:O	1:K:625:THR:HG23	2.21	0.40
1:K:634:ASP:O	1:K:638:THR:OG1	2.38	0.40
1:K:663:VAL:O	1:K:686:SER:HA	2.21	0.40
1:L:544:ARG:HH22	1:L:577:LYS:HA	1.87	0.40
1:M:646:ARG:NH1	1:M:678:GLU:OE1	2.54	0.40
1:O:646:ARG:NH1	1:O:678:GLU:OE1	2.53	0.40
1:P:379:SER:C	1:P:381:GLN:H	2.30	0.40
1:Q:367:PHE:CD2	1:R:524:GLN:HG2	2.56	0.40
1:A:544:ARG:HH22	1:A:577:LYS:HA	1.87	0.40
1:A:646:ARG:NH1	1:A:678:GLU:OE1	2.54	0.40
1:C:559:ILE:O	1:C:560:ARG:C	2.64	0.40
1:C:646:ARG:NH1	1:C:678:GLU:OE1	2.53	0.40
1:D:523:GLU:HA	1:D:526:GLU:HG2	2.03	0.40
1:D:623:ARG:O	1:D:625:THR:HG23	2.21	0.40
1:E:379:SER:C	1:E:381:GLN:H	2.30	0.40
1:F:663:VAL:O	1:F:686:SER:HA	2.21	0.40
1:H:623:ARG:O	1:H:625:THR:HG23	2.21	0.40
1:J:390:LEU:HD13	1:J:390:LEU:HA	1.95	0.40
1:J:456:LEU:CD2	1:J:462:LYS:HE3	2.52	0.40
1:K:559:ILE:O	1:K:560:ARG:C	2.64	0.40
1:L:456:LEU:HD23	1:L:462:LYS:HE3	2.03	0.40
1:M:665:MET:HE3	1:M:665:MET:HB3	1.90	0.40
1:O:379:SER:C	1:O:381:GLN:H	2.30	0.40
1:O:559:ILE:O	1:O:560:ARG:C	2.64	0.40
1:Q:423:GLY:O	1:Q:439:LEU:HG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:462:LYS:HB3	1:Q:473:PHE:HD1	1.87	0.40
1:Q:544:ARG:HH22	1:Q:577:LYS:HA	1.87	0.40
1:A:623:ARG:O	1:A:625:THR:HG23	2.21	0.40
1:B:544:ARG:HH22	1:B:577:LYS:HA	1.87	0.40
1:B:663:VAL:O	1:B:686:SER:HA	2.21	0.40
1:C:467:LEU:HB3	1:C:472:THR:OG1	2.22	0.40
1:D:393:GLU:HG3	1:D:498:THR:HG21	2.02	0.40
1:D:456:LEU:HD23	1:D:462:LYS:HE3	2.03	0.40
1:E:462:LYS:HB3	1:E:473:PHE:HD1	1.87	0.40
1:E:544:ARG:HH22	1:E:577:LYS:HA	1.87	0.40
1:G:456:LEU:CD2	1:G:462:LYS:HE3	2.52	0.40
1:I:456:LEU:HD23	1:I:462:LYS:HE3	2.03	0.40
1:M:462:LYS:HB3	1:M:473:PHE:HD1	1.87	0.40
1:M:623:ARG:O	1:M:625:THR:HG23	2.21	0.40
1:N:544:ARG:HH22	1:N:577:LYS:HA	1.86	0.40
1:O:467:LEU:HB3	1:O:472:THR:OG1	2.22	0.40
1:O:523:GLU:HA	1:O:526:GLU:HG2	2.02	0.40
1:P:623:ARG:O	1:P:625:THR:HG23	2.21	0.40
1:Q:542:LEU:HD23	1:Q:542:LEU:HA	1.91	0.40
1:R:544:ARG:HH22	1:R:577:LYS:HA	1.86	0.40
1:R:634:ASP:O	1:R:638:THR:OG1	2.38	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	342/710 (48%)	282 (82%)	59 (17%)	1 (0%)	36	65
1	B	342/710 (48%)	282 (82%)	59 (17%)	1 (0%)	36	65
1	C	342/710 (48%)	282 (82%)	59 (17%)	1 (0%)	36	65
1	D	342/710 (48%)	282 (82%)	59 (17%)	1 (0%)	36	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	342/710 (48%)	282 (82%)	59 (17%)	1 (0%)	36	65
1	F	342/710 (48%)	282 (82%)	59 (17%)	1 (0%)	36	65
1	G	342/710 (48%)	281 (82%)	60 (18%)	1 (0%)	36	65
1	H	342/710 (48%)	281 (82%)	60 (18%)	1 (0%)	36	65
1	I	342/710 (48%)	281 (82%)	60 (18%)	1 (0%)	36	65
1	J	342/710 (48%)	282 (82%)	59 (17%)	1 (0%)	36	65
1	K	342/710 (48%)	281 (82%)	60 (18%)	1 (0%)	36	65
1	L	342/710 (48%)	281 (82%)	60 (18%)	1 (0%)	36	65
1	M	342/710 (48%)	282 (82%)	59 (17%)	1 (0%)	36	65
1	N	342/710 (48%)	282 (82%)	59 (17%)	1 (0%)	36	65
1	O	342/710 (48%)	282 (82%)	59 (17%)	1 (0%)	36	65
1	P	342/710 (48%)	282 (82%)	59 (17%)	1 (0%)	36	65
1	Q	342/710 (48%)	282 (82%)	59 (17%)	1 (0%)	36	65
1	R	342/710 (48%)	282 (82%)	59 (17%)	1 (0%)	36	65
All	All	6156/12780 (48%)	5071 (82%)	1067 (17%)	18 (0%)	37	65

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	386	GLU
1	B	386	GLU
1	C	386	GLU
1	D	386	GLU
1	E	386	GLU
1	F	386	GLU
1	G	386	GLU
1	H	386	GLU
1	I	386	GLU
1	J	386	GLU
1	K	386	GLU
1	L	386	GLU
1	M	386	GLU
1	N	386	GLU
1	O	386	GLU
1	P	386	GLU
1	Q	386	GLU
1	R	386	GLU

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	306/605 (51%)	303 (99%)	3 (1%)	68	74
1	B	306/605 (51%)	303 (99%)	3 (1%)	68	74
1	C	306/605 (51%)	303 (99%)	3 (1%)	68	74
1	D	306/605 (51%)	303 (99%)	3 (1%)	68	74
1	E	306/605 (51%)	303 (99%)	3 (1%)	68	74
1	F	306/605 (51%)	303 (99%)	3 (1%)	68	74
1	G	306/605 (51%)	303 (99%)	3 (1%)	68	74
1	H	306/605 (51%)	303 (99%)	3 (1%)	68	74
1	I	306/605 (51%)	303 (99%)	3 (1%)	68	74
1	J	306/605 (51%)	303 (99%)	3 (1%)	68	74
1	K	306/605 (51%)	303 (99%)	3 (1%)	68	74
1	L	306/605 (51%)	303 (99%)	3 (1%)	68	74
1	M	306/605 (51%)	303 (99%)	3 (1%)	68	74
1	N	306/605 (51%)	303 (99%)	3 (1%)	68	74
1	O	306/605 (51%)	303 (99%)	3 (1%)	68	74
1	P	306/605 (51%)	303 (99%)	3 (1%)	68	74
1	Q	306/605 (51%)	303 (99%)	3 (1%)	68	74
1	R	306/605 (51%)	303 (99%)	3 (1%)	68	74
All	All	5508/10890 (51%)	5454 (99%)	54 (1%)	65	74

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	480	GLU
1	A	503	HIS
1	A	638	THR
1	B	480	GLU
1	B	503	HIS
1	B	638	THR

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Continued from previous page...

Mol	Chain	Res	Type
1	C	480	GLU
1	C	503	HIS
1	C	638	THR
1	D	480	GLU
1	D	503	HIS
1	D	638	THR
1	E	480	GLU
1	E	503	HIS
1	E	638	THR
1	F	480	GLU
1	F	503	HIS
1	F	638	THR
1	G	480	GLU
1	G	503	HIS
1	G	638	THR
1	H	480	GLU
1	H	503	HIS
1	H	638	THR
1	I	480	GLU
1	I	503	HIS
1	I	638	THR
1	J	480	GLU
1	J	503	HIS
1	J	638	THR
1	K	480	GLU
1	K	503	HIS
1	K	638	THR
1	L	480	GLU
1	L	503	HIS
1	L	638	THR
1	M	480	GLU
1	M	503	HIS
1	M	638	THR
1	N	480	GLU
1	N	503	HIS
1	N	638	THR
1	O	480	GLU
1	O	503	HIS
1	O	638	THR
1	P	480	GLU
1	P	503	HIS
1	P	638	THR

Continued on next page...

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Mol	Chain	Res	Type
1	Q	480	GLU
1	Q	503	HIS
1	Q	638	THR
1	R	480	GLU
1	R	503	HIS
1	R	638	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	381	GLN
1	A	543	GLN
1	A	561	ASN
1	B	543	GLN
1	B	561	ASN
1	C	543	GLN
1	C	561	ASN
1	D	430	GLN
1	D	543	GLN
1	D	561	ASN
1	E	381	GLN
1	E	543	GLN
1	E	561	ASN
1	F	543	GLN
1	F	561	ASN
1	G	543	GLN
1	G	561	ASN
1	H	543	GLN
1	H	561	ASN
1	I	543	GLN
1	I	561	ASN
1	J	543	GLN
1	J	561	ASN
1	K	543	GLN
1	K	561	ASN
1	L	543	GLN
1	L	561	ASN
1	M	381	GLN
1	M	543	GLN
1	M	561	ASN
1	N	543	GLN
1	N	561	ASN

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Mol	Chain	Res	Type
1	O	561	ASN
1	P	561	ASN
1	Q	381	GLN
1	Q	543	GLN
1	Q	561	ASN
1	R	543	GLN
1	R	561	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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.

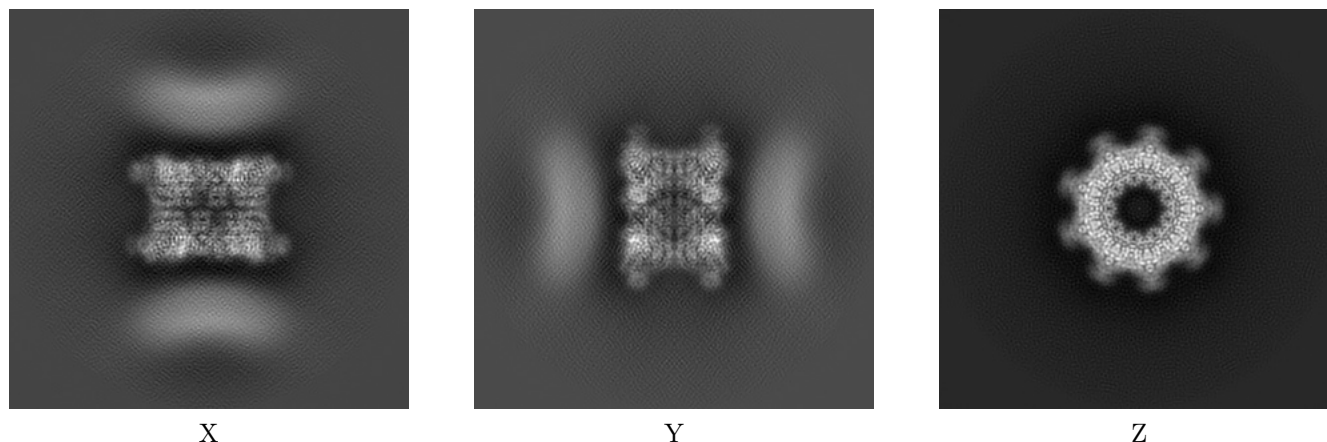
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11820. These allow visual inspection of the internal detail of the map and identification of artifacts.

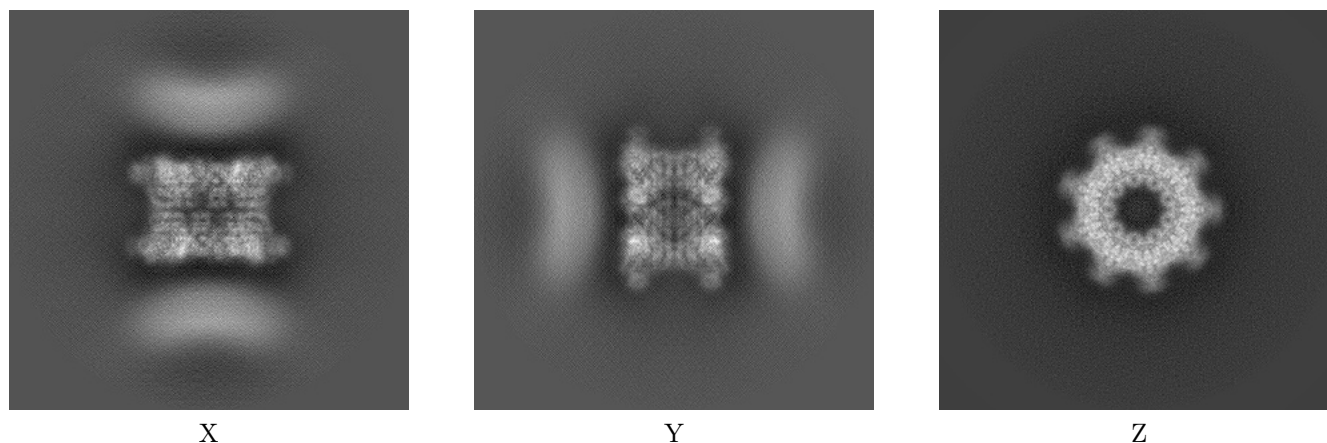
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



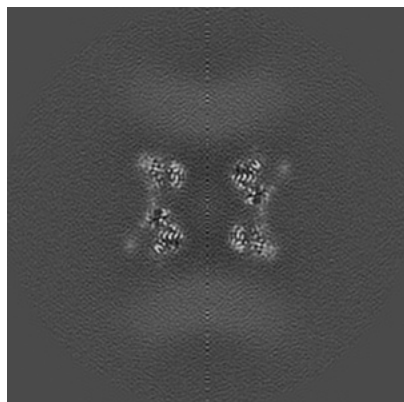
6.1.2 Raw map



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

6.2 Central slices [i](#)

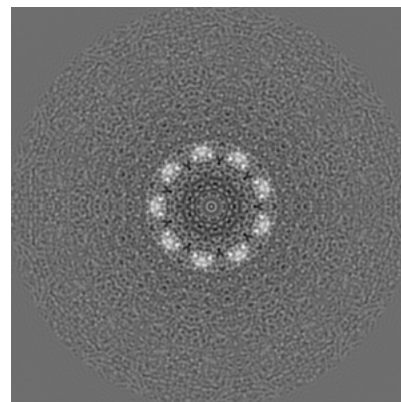
6.2.1 Primary map



X Index: 256

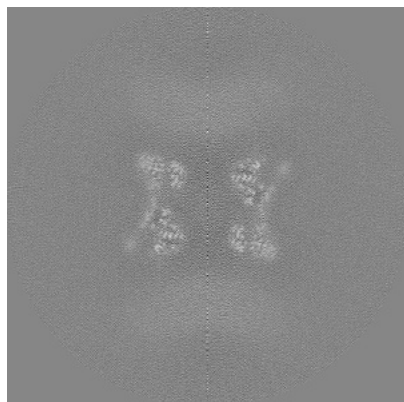


Y Index: 256

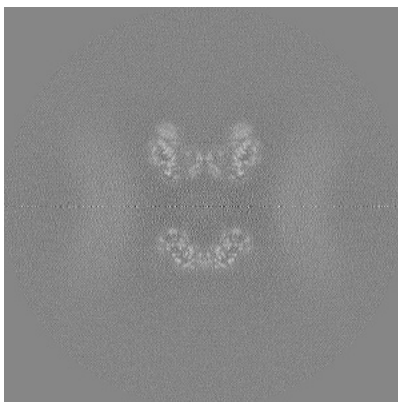


Z Index: 256

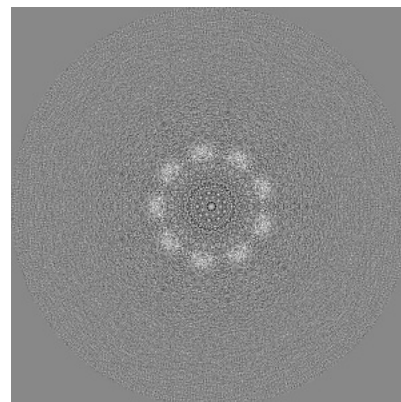
6.2.2 Raw map



X Index: 256



Y Index: 256

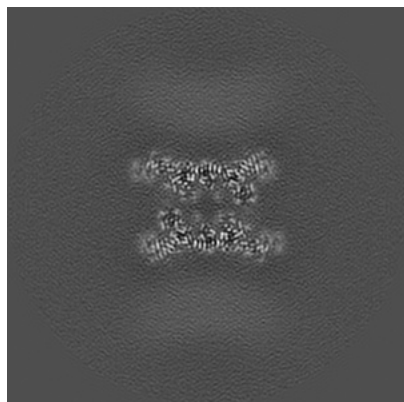


Z Index: 256

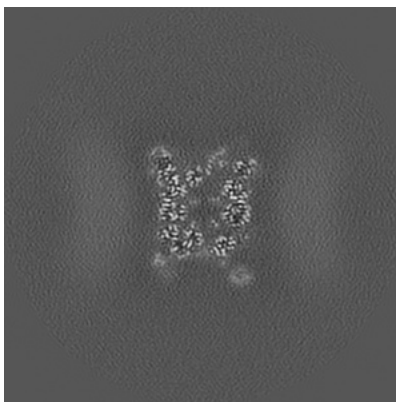
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

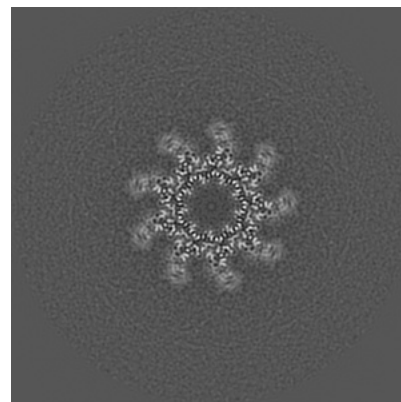
6.3.1 Primary map



X Index: 216

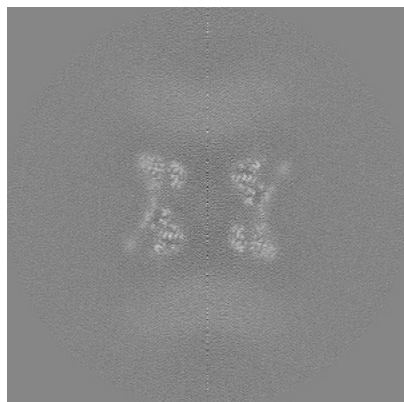


Y Index: 214

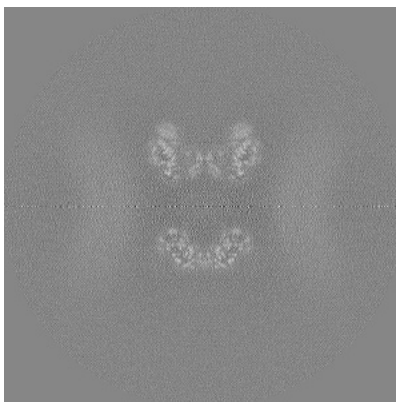


Z Index: 303

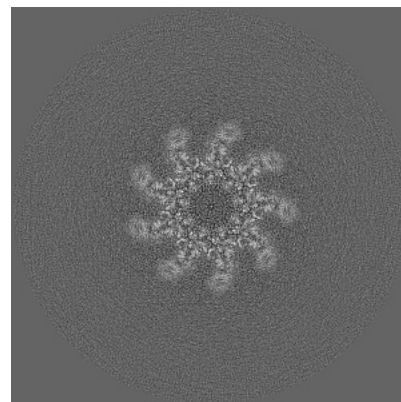
6.3.2 Raw map



X Index: 256



Y Index: 256

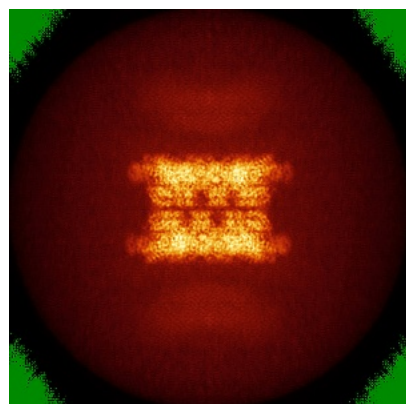


Z Index: 209

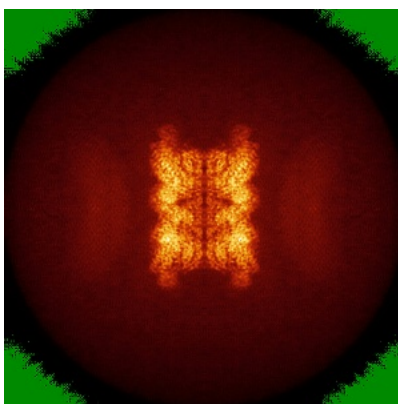
The images above show the largest variance slices of the map in three orthogonal directions.

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

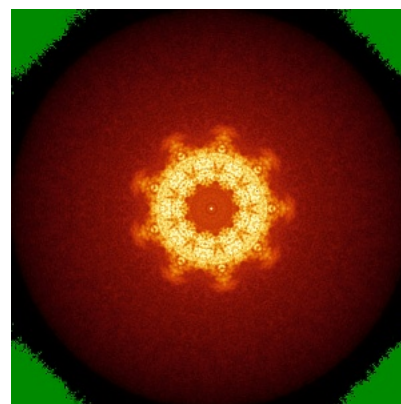
6.4.1 Primary map



X

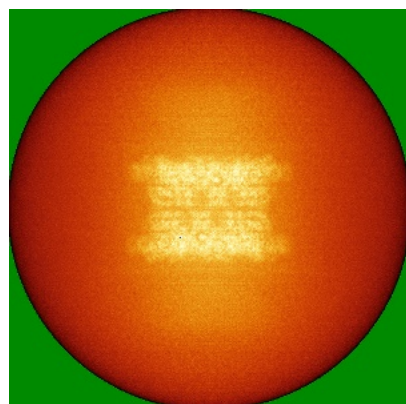


Y

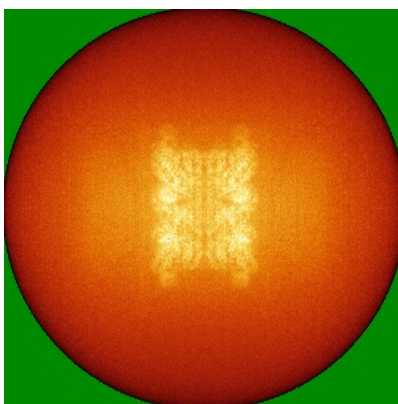


Z

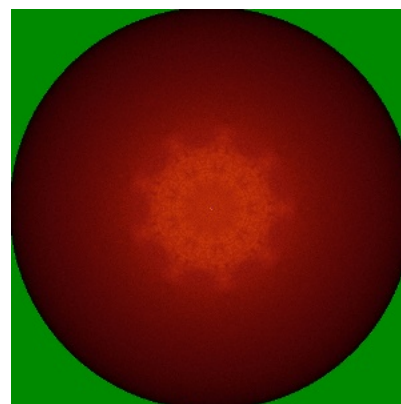
6.4.2 Raw map



X



Y

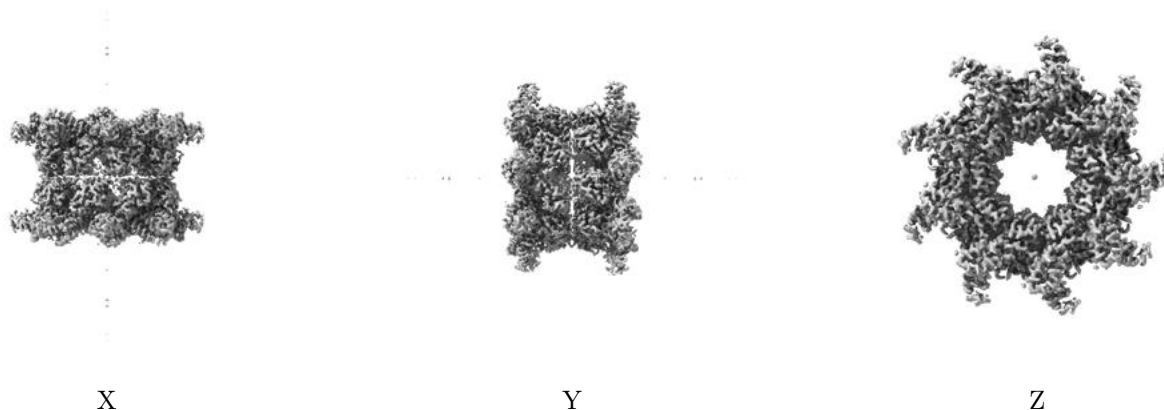


Z

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

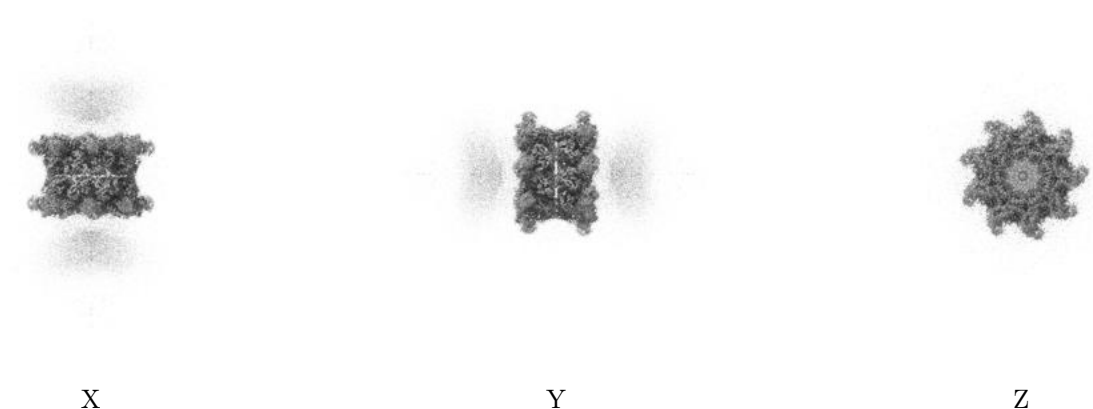
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0112. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

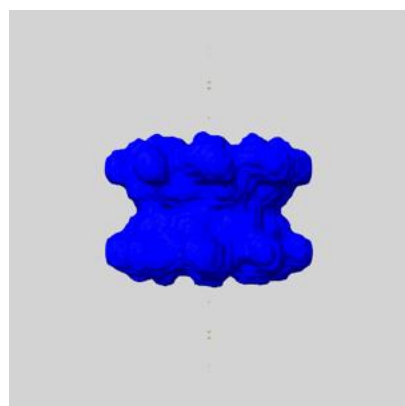
6.6 Mask visualisation [i](#)

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

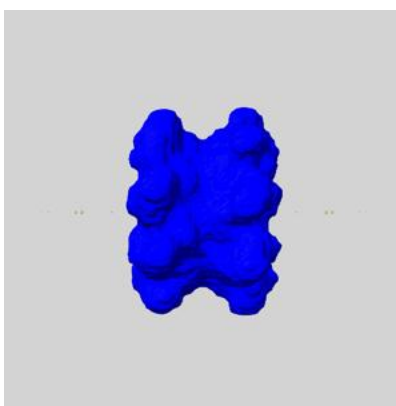
A mask typically either:

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

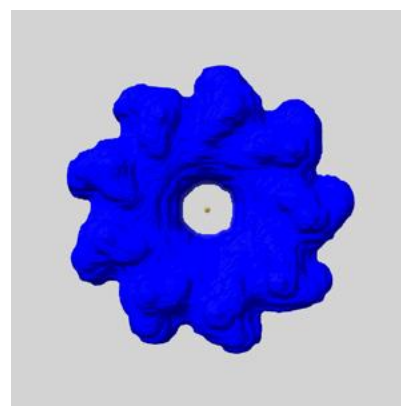
6.6.1 emd_11820_msk_1.map [i](#)



X



Y

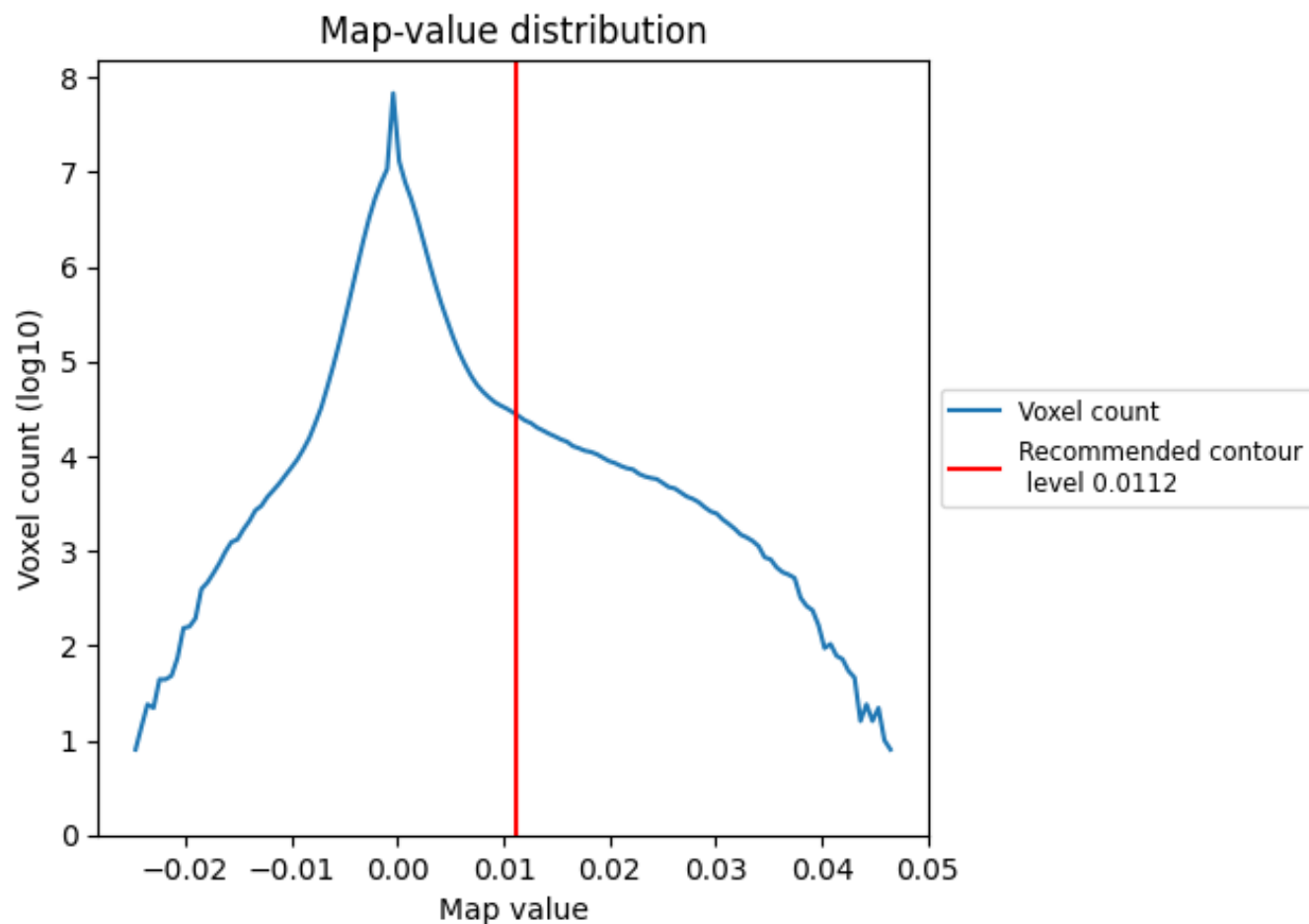


Z

7 Map analysis [i](#)

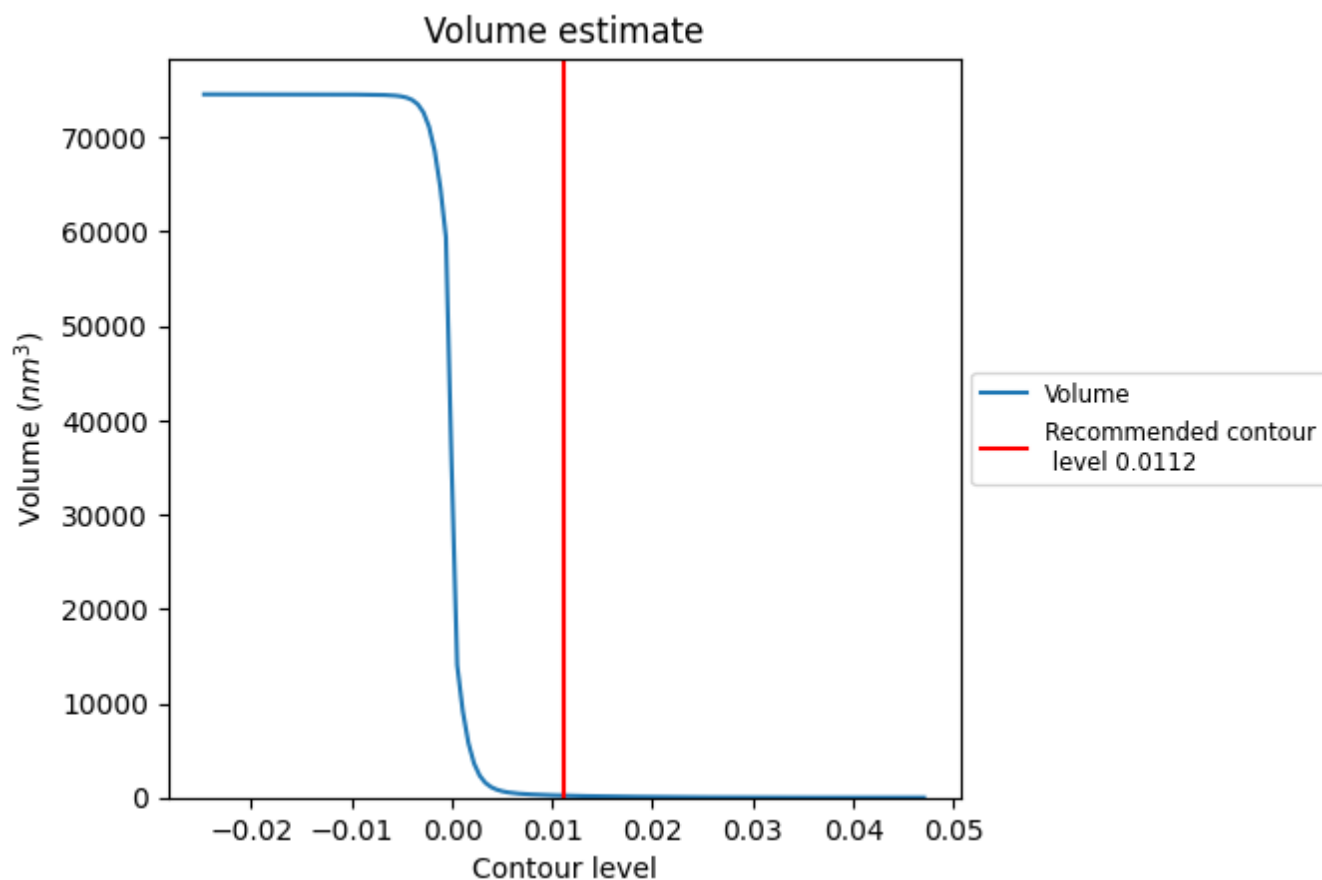
This section contains the results of statistical analysis of the map.

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.

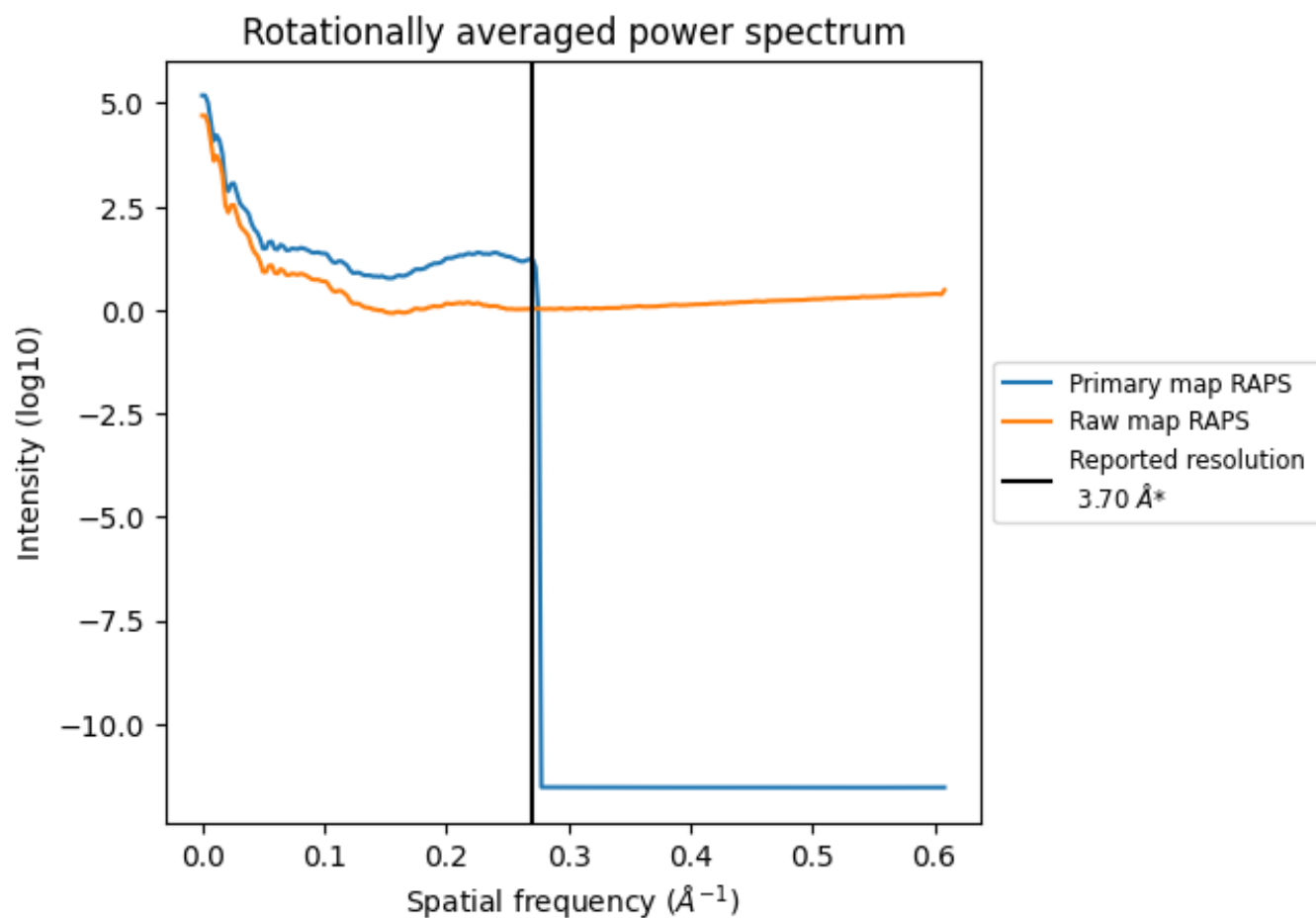
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 207 nm³; this corresponds to an approximate mass of 187 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 ⓘ

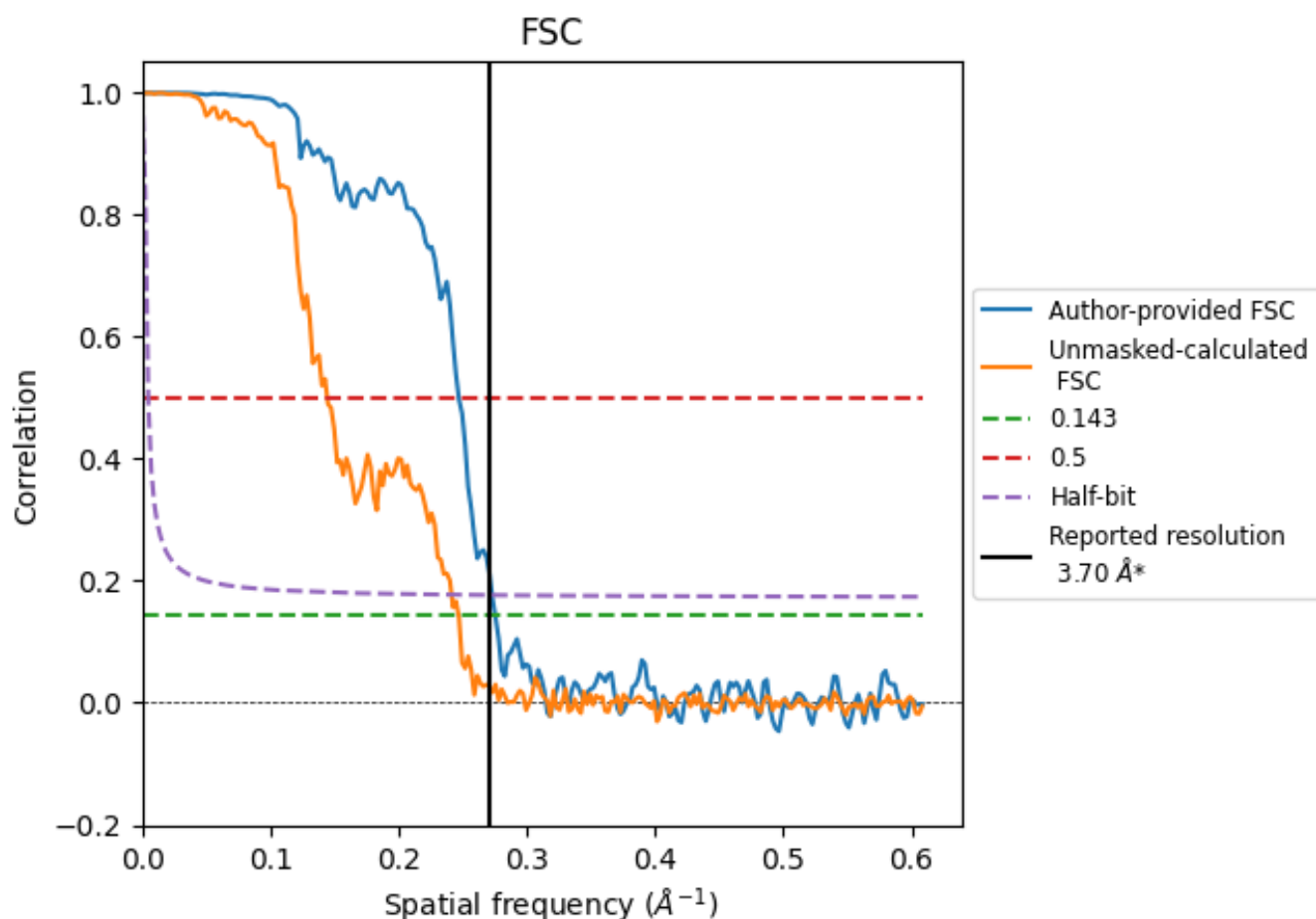


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.63	4.05	3.66
Unmasked-calculated*	4.05	6.93	4.15

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

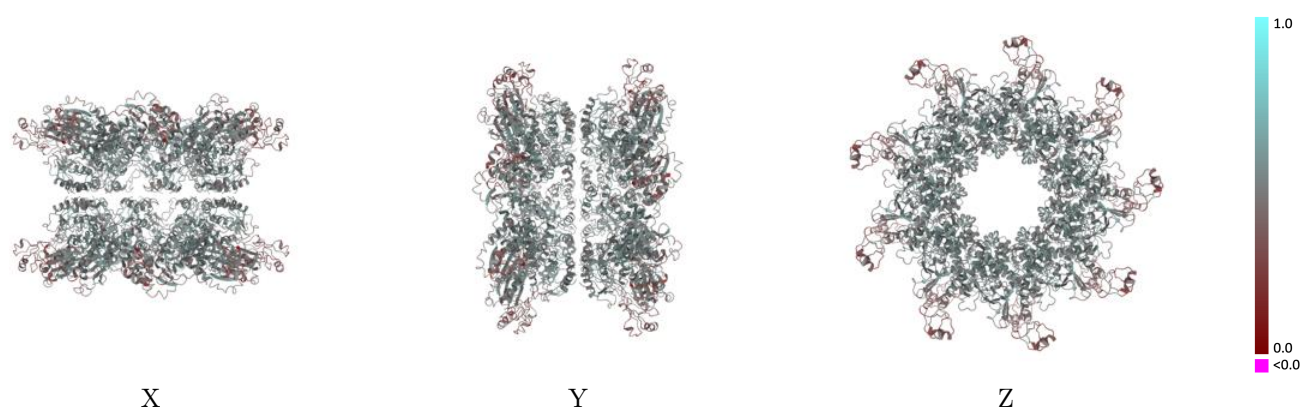
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11820 and PDB model 7ALW. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)

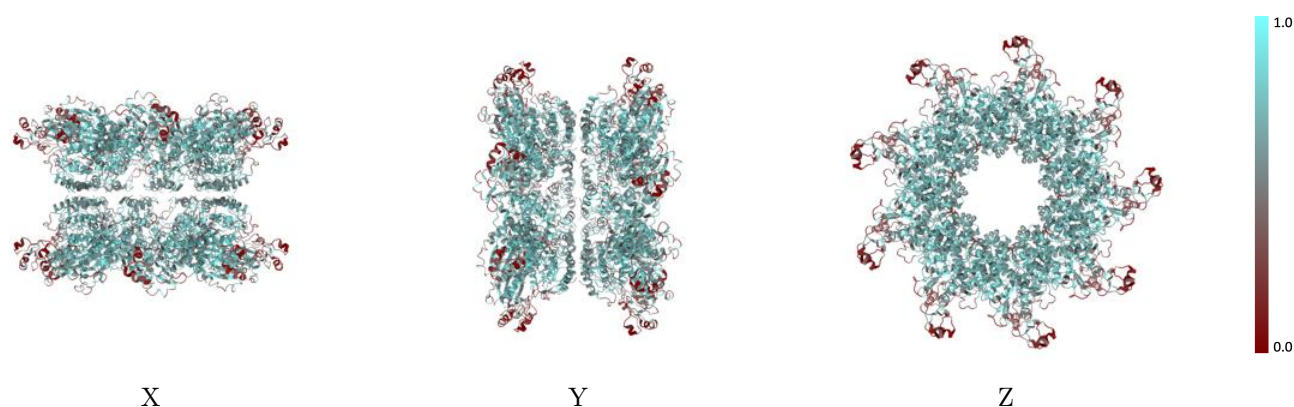
This section was not generated.

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



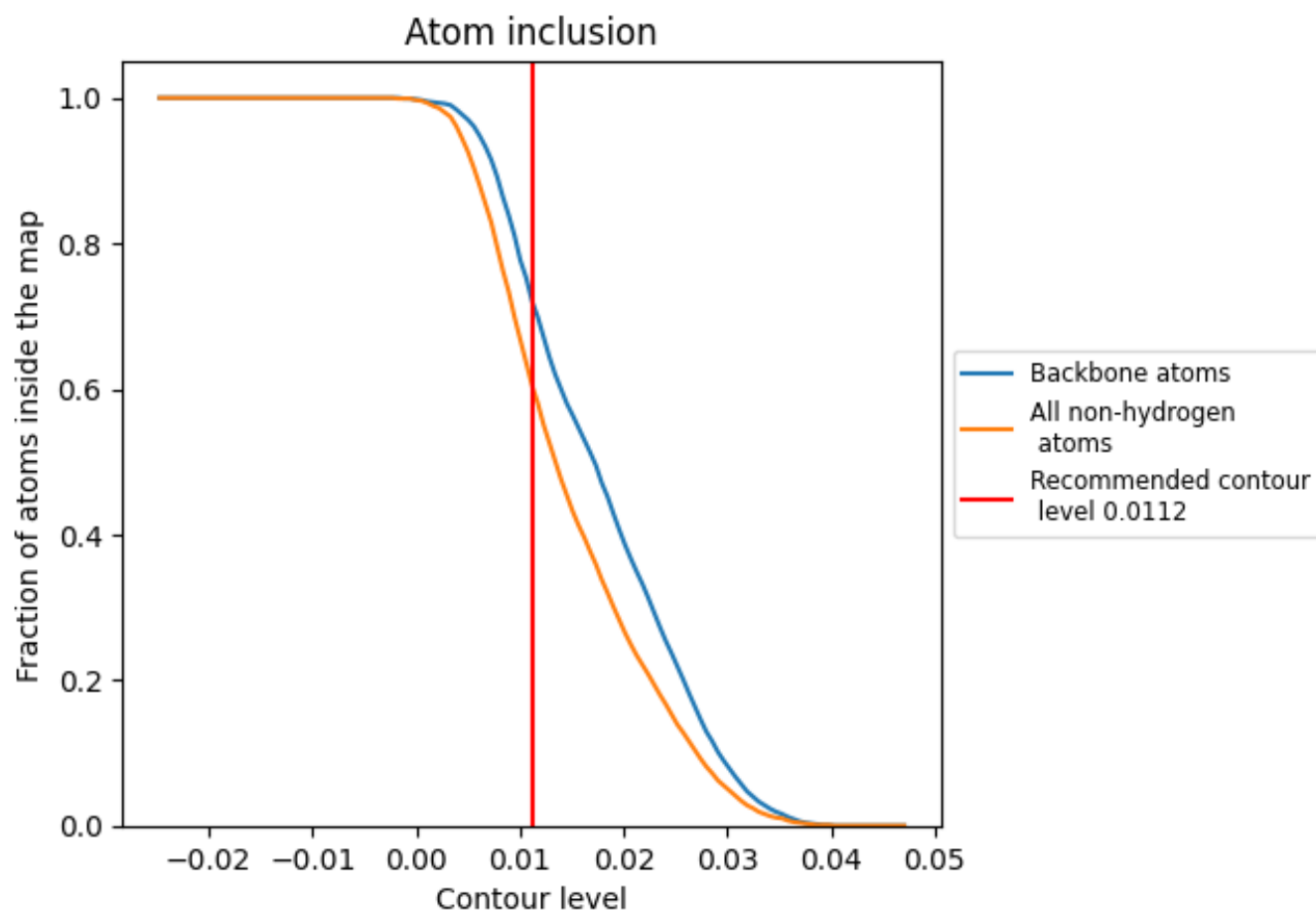
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0112).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0112) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6040	0.4790
A	0.6070	0.4790
B	0.6020	0.4780
C	0.6050	0.4780
D	0.6080	0.4780
E	0.6010	0.4800
F	0.6060	0.4800
G	0.6080	0.4800
H	0.6040	0.4800
I	0.6020	0.4790
J	0.6050	0.4790
K	0.6040	0.4810
L	0.6020	0.4800
M	0.6080	0.4800
N	0.6020	0.4790
O	0.6050	0.4780
P	0.6040	0.4780
Q	0.6010	0.4790
R	0.6050	0.4790

1.0

0.0

<0.0