



## Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 11:32 PM EST

PDB ID : 3J9P  
EMDB ID : EMD-6267  
Title : Structure of the TRPA1 ion channel determined by electron cryo-microscopy  
Authors : Paulsen, C.E.; Armache, J.-P.; Gao, Y.; Cheng, Y.; Julius, D.  
Deposited on : 2015-02-14  
Resolution : 4.24 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](mailto: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.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

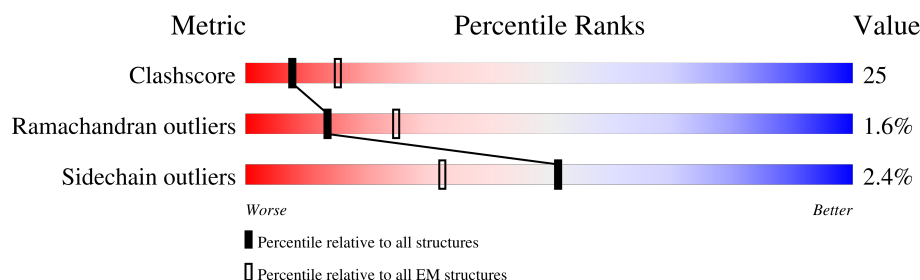
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.24 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	1528	<div> <div>5%</div> <div>20%</div> <div>15%</div> <div>•</div> <div>63%</div> </div>
1	B	1528	<div> <div>5%</div> <div>20%</div> <div>15%</div> <div>•</div> <div>63%</div> </div>
1	C	1528	<div> <div>5%</div> <div>20%</div> <div>15%</div> <div>•</div> <div>63%</div> </div>
1	D	1528	<div> <div>5%</div> <div>19%</div> <div>16%</div> <div>•</div> <div>63%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16952 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 Maltose-binding periplasmic protein, Transient receptor potential cation channel subfamily A member 1 chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	560	Total	C	N	O	S	0	0
			4238	2775	711	722	30		
1	A	560	Total	C	N	O	S	0	0
			4238	2775	711	722	30		
1	B	560	Total	C	N	O	S	0	0
			4238	2775	711	722	30		
1	C	560	Total	C	N	O	S	0	0
			4238	2775	711	722	30		

There are 180 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-408	MET	-	EXPRESSION TAG	UNP P0AEX9
D	-407	GLY	-	EXPRESSION TAG	UNP P0AEX9
D	-406	SER	-	EXPRESSION TAG	UNP P0AEX9
D	-405	SER	-	EXPRESSION TAG	UNP P0AEX9
D	-404	HIS	-	EXPRESSION TAG	UNP P0AEX9
D	-403	HIS	-	EXPRESSION TAG	UNP P0AEX9
D	-402	HIS	-	EXPRESSION TAG	UNP P0AEX9
D	-401	HIS	-	EXPRESSION TAG	UNP P0AEX9
D	-400	HIS	-	EXPRESSION TAG	UNP P0AEX9
D	-399	HIS	-	EXPRESSION TAG	UNP P0AEX9
D	-398	HIS	-	EXPRESSION TAG	UNP P0AEX9
D	-397	HIS	-	EXPRESSION TAG	UNP P0AEX9
D	-396	GLY	-	EXPRESSION TAG	UNP P0AEX9
D	-395	SER	-	EXPRESSION TAG	UNP P0AEX9
D	-394	SER	-	EXPRESSION TAG	UNP P0AEX9
D	-393	MET	-	EXPRESSION TAG	UNP P0AEX9
D	-26	ASN	-	LINKER	UNP O75762
D	-25	SER	-	LINKER	UNP O75762
D	-24	SER	-	LINKER	UNP O75762
D	-23	SER	-	LINKER	UNP O75762
D	-22	ASN	-	LINKER	UNP O75762

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	-21	ASN	-	LINKER	UNP O75762
D	-20	ASN	-	LINKER	UNP O75762
D	-19	ASN	-	LINKER	UNP O75762
D	-18	ASN	-	LINKER	UNP O75762
D	-17	ASN	-	LINKER	UNP O75762
D	-16	ASN	-	LINKER	UNP O75762
D	-15	ASN	-	LINKER	UNP O75762
D	-14	ASN	-	LINKER	UNP O75762
D	-13	ASN	-	LINKER	UNP O75762
D	-12	LEU	-	LINKER	UNP O75762
D	-11	GLY	-	LINKER	UNP O75762
D	-10	ILE	-	LINKER	UNP O75762
D	-9	GLU	-	LINKER	UNP O75762
D	-8	GLU	-	LINKER	UNP O75762
D	-7	ASN	-	LINKER	UNP O75762
D	-6	LEU	-	LINKER	UNP O75762
D	-5	TYR	-	LINKER	UNP O75762
D	-4	PHE	-	LINKER	UNP O75762
D	-3	GLN	-	LINKER	UNP O75762
D	-2	GLY	-	LINKER	UNP O75762
D	-1	ALA	-	LINKER	UNP O75762
D	0	GLY	-	LINKER	UNP O75762
D	1	SER	-	LINKER	UNP O75762
D	966	ASP	GLU	CONFLICT	UNP O75762
A	-408	MET	-	EXPRESSION TAG	UNP P0AEX9
A	-407	GLY	-	EXPRESSION TAG	UNP P0AEX9
A	-406	SER	-	EXPRESSION TAG	UNP P0AEX9
A	-405	SER	-	EXPRESSION TAG	UNP P0AEX9
A	-404	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	-403	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	-402	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	-401	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	-400	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	-399	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	-398	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	-397	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	-396	GLY	-	EXPRESSION TAG	UNP P0AEX9
A	-395	SER	-	EXPRESSION TAG	UNP P0AEX9
A	-394	SER	-	EXPRESSION TAG	UNP P0AEX9
A	-393	MET	-	EXPRESSION TAG	UNP P0AEX9
A	-26	ASN	-	LINKER	UNP O75762
A	-25	SER	-	LINKER	UNP O75762

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	SER	-	LINKER	UNP O75762
A	-23	SER	-	LINKER	UNP O75762
A	-22	ASN	-	LINKER	UNP O75762
A	-21	ASN	-	LINKER	UNP O75762
A	-20	ASN	-	LINKER	UNP O75762
A	-19	ASN	-	LINKER	UNP O75762
A	-18	ASN	-	LINKER	UNP O75762
A	-17	ASN	-	LINKER	UNP O75762
A	-16	ASN	-	LINKER	UNP O75762
A	-15	ASN	-	LINKER	UNP O75762
A	-14	ASN	-	LINKER	UNP O75762
A	-13	ASN	-	LINKER	UNP O75762
A	-12	LEU	-	LINKER	UNP O75762
A	-11	GLY	-	LINKER	UNP O75762
A	-10	ILE	-	LINKER	UNP O75762
A	-9	GLU	-	LINKER	UNP O75762
A	-8	GLU	-	LINKER	UNP O75762
A	-7	ASN	-	LINKER	UNP O75762
A	-6	LEU	-	LINKER	UNP O75762
A	-5	TYR	-	LINKER	UNP O75762
A	-4	PHE	-	LINKER	UNP O75762
A	-3	GLN	-	LINKER	UNP O75762
A	-2	GLY	-	LINKER	UNP O75762
A	-1	ALA	-	LINKER	UNP O75762
A	0	GLY	-	LINKER	UNP O75762
A	1	SER	-	LINKER	UNP O75762
A	966	ASP	GLU	CONFLICT	UNP O75762
B	-408	MET	-	EXPRESSION TAG	UNP P0AEX9
B	-407	GLY	-	EXPRESSION TAG	UNP P0AEX9
B	-406	SER	-	EXPRESSION TAG	UNP P0AEX9
B	-405	SER	-	EXPRESSION TAG	UNP P0AEX9
B	-404	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	-403	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	-402	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	-401	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	-400	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	-399	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	-398	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	-397	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	-396	GLY	-	EXPRESSION TAG	UNP P0AEX9
B	-395	SER	-	EXPRESSION TAG	UNP P0AEX9
B	-394	SER	-	EXPRESSION TAG	UNP P0AEX9

*Continued on next page...*

*Continued from previous page...*

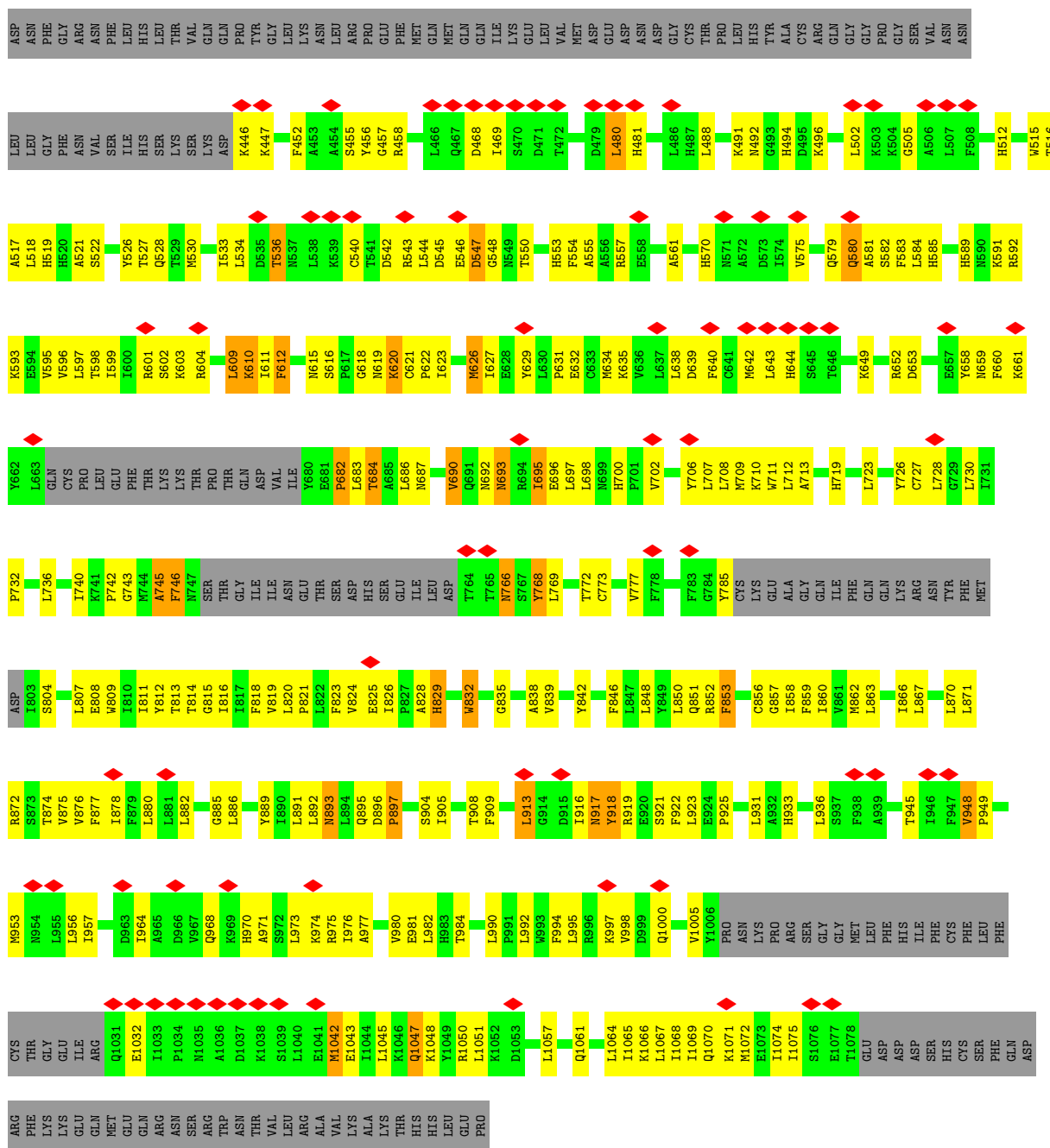
Chain	Residue	Modelled	Actual	Comment	Reference
B	-393	MET	-	EXPRESSION TAG	UNP P0AEX9
B	-26	ASN	-	LINKER	UNP O75762
B	-25	SER	-	LINKER	UNP O75762
B	-24	SER	-	LINKER	UNP O75762
B	-23	SER	-	LINKER	UNP O75762
B	-22	ASN	-	LINKER	UNP O75762
B	-21	ASN	-	LINKER	UNP O75762
B	-20	ASN	-	LINKER	UNP O75762
B	-19	ASN	-	LINKER	UNP O75762
B	-18	ASN	-	LINKER	UNP O75762
B	-17	ASN	-	LINKER	UNP O75762
B	-16	ASN	-	LINKER	UNP O75762
B	-15	ASN	-	LINKER	UNP O75762
B	-14	ASN	-	LINKER	UNP O75762
B	-13	ASN	-	LINKER	UNP O75762
B	-12	LEU	-	LINKER	UNP O75762
B	-11	GLY	-	LINKER	UNP O75762
B	-10	ILE	-	LINKER	UNP O75762
B	-9	GLU	-	LINKER	UNP O75762
B	-8	GLU	-	LINKER	UNP O75762
B	-7	ASN	-	LINKER	UNP O75762
B	-6	LEU	-	LINKER	UNP O75762
B	-5	TYR	-	LINKER	UNP O75762
B	-4	PHE	-	LINKER	UNP O75762
B	-3	GLN	-	LINKER	UNP O75762
B	-2	GLY	-	LINKER	UNP O75762
B	-1	ALA	-	LINKER	UNP O75762
B	0	GLY	-	LINKER	UNP O75762
B	1	SER	-	LINKER	UNP O75762
B	966	ASP	GLU	CONFLICT	UNP O75762
C	-408	MET	-	EXPRESSION TAG	UNP P0AEX9
C	-407	GLY	-	EXPRESSION TAG	UNP P0AEX9
C	-406	SER	-	EXPRESSION TAG	UNP P0AEX9
C	-405	SER	-	EXPRESSION TAG	UNP P0AEX9
C	-404	HIS	-	EXPRESSION TAG	UNP P0AEX9
C	-403	HIS	-	EXPRESSION TAG	UNP P0AEX9
C	-402	HIS	-	EXPRESSION TAG	UNP P0AEX9
C	-401	HIS	-	EXPRESSION TAG	UNP P0AEX9
C	-400	HIS	-	EXPRESSION TAG	UNP P0AEX9
C	-399	HIS	-	EXPRESSION TAG	UNP P0AEX9
C	-398	HIS	-	EXPRESSION TAG	UNP P0AEX9
C	-397	HIS	-	EXPRESSION TAG	UNP P0AEX9

*Continued on next page...*

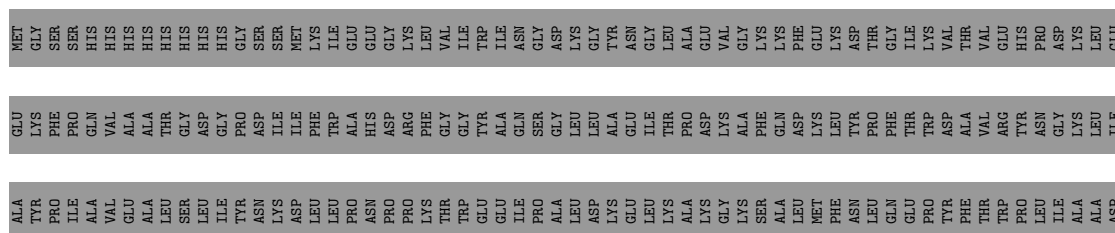
*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	-396	GLY	-	EXPRESSION TAG	UNP P0AEX9
C	-395	SER	-	EXPRESSION TAG	UNP P0AEX9
C	-394	SER	-	EXPRESSION TAG	UNP P0AEX9
C	-393	MET	-	EXPRESSION TAG	UNP P0AEX9
C	-26	ASN	-	LINKER	UNP O75762
C	-25	SER	-	LINKER	UNP O75762
C	-24	SER	-	LINKER	UNP O75762
C	-23	SER	-	LINKER	UNP O75762
C	-22	ASN	-	LINKER	UNP O75762
C	-21	ASN	-	LINKER	UNP O75762
C	-20	ASN	-	LINKER	UNP O75762
C	-19	ASN	-	LINKER	UNP O75762
C	-18	ASN	-	LINKER	UNP O75762
C	-17	ASN	-	LINKER	UNP O75762
C	-16	ASN	-	LINKER	UNP O75762
C	-15	ASN	-	LINKER	UNP O75762
C	-14	ASN	-	LINKER	UNP O75762
C	-13	ASN	-	LINKER	UNP O75762
C	-12	LEU	-	LINKER	UNP O75762
C	-11	GLY	-	LINKER	UNP O75762
C	-10	ILE	-	LINKER	UNP O75762
C	-9	GLU	-	LINKER	UNP O75762
C	-8	GLU	-	LINKER	UNP O75762
C	-7	ASN	-	LINKER	UNP O75762
C	-6	LEU	-	LINKER	UNP O75762
C	-5	TYR	-	LINKER	UNP O75762
C	-4	PHE	-	LINKER	UNP O75762
C	-3	GLN	-	LINKER	UNP O75762
C	-2	GLY	-	LINKER	UNP O75762
C	-1	ALA	-	LINKER	UNP O75762
C	0	GLY	-	LINKER	UNP O75762
C	1	SER	-	LINKER	UNP O75762
C	966	ASP	GLU	CONFLICT	UNP O75762



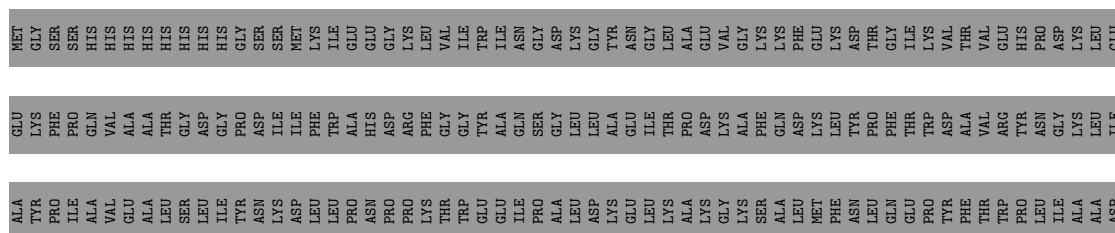


- Molecule 1: Maltose-binding periplasmic protein, Transient receptor potential cation channel subfamily A member 1 chimera

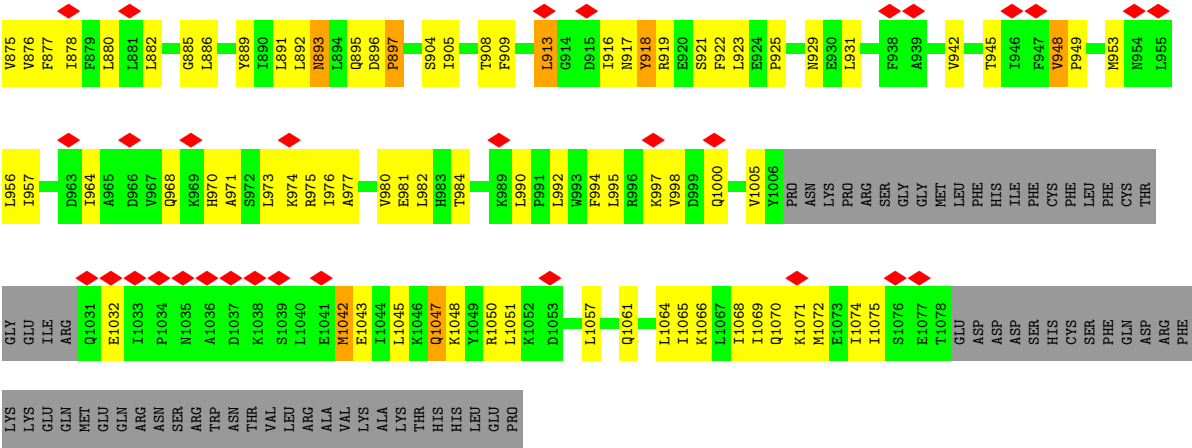












## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	43585	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	21	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	31000	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	20.724	Depositor
Minimum map value	-12.650	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	8.0	Depositor
Map size ( $\text{\AA}$ )	364.68, 364.68, 364.68	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.2156, 1.2156, 1.2156	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	0.41	0/4326	0.82	1/5872 (0.0%)
1	B	0.41	0/4326	0.82	1/5872 (0.0%)
1	C	0.42	0/4326	0.82	1/5872 (0.0%)
1	D	0.41	0/4326	0.82	1/5872 (0.0%)
All	All	0.41	0/17304	0.82	4/23488 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	23
1	B	0	23
1	C	0	23
1	D	0	24
All	All	0	93

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	766	ASN	N-CA-CB	9.05	126.89	110.60
1	D	766	ASN	N-CA-CB	9.02	126.84	110.60
1	C	766	ASN	N-CA-CB	9.02	126.84	110.60
1	B	766	ASN	N-CA-CB	9.00	126.80	110.60

There are no chirality outliers.

All (93) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1032	GLU	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	A	1047	GLN	Sidechain
1	A	547	ASP	Peptide
1	A	593	LYS	Peptide
1	A	604	ARG	Peptide
1	A	609	LEU	Peptide
1	A	610	LYS	Peptide
1	A	612	PHE	Peptide
1	A	626	MET	Peptide
1	A	643	LEU	Peptide
1	A	644	HIS	Peptide
1	A	682	PRO	Peptide
1	A	692	ASN	Peptide
1	A	693	ASN	Peptide
1	A	695	ILE	Peptide
1	A	696	GLU	Peptide
1	A	740	ILE	Peptide
1	A	745	ALA	Peptide
1	A	826	ILE	Peptide
1	A	893	ASN	Peptide
1	A	897	PRO	Peptide
1	A	913	LEU	Peptide
1	A	918	TYR	Peptide
1	B	1032	GLU	Peptide
1	B	1047	GLN	Sidechain
1	B	547	ASP	Peptide
1	B	593	LYS	Peptide
1	B	604	ARG	Peptide
1	B	609	LEU	Peptide
1	B	610	LYS	Peptide
1	B	612	PHE	Peptide
1	B	626	MET	Peptide
1	B	643	LEU	Peptide
1	B	644	HIS	Peptide
1	B	682	PRO	Peptide
1	B	692	ASN	Peptide
1	B	693	ASN	Peptide
1	B	695	ILE	Peptide
1	B	696	GLU	Peptide
1	B	740	ILE	Peptide
1	B	745	ALA	Peptide
1	B	826	ILE	Peptide
1	B	893	ASN	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	B	897	PRO	Peptide
1	B	913	LEU	Peptide
1	B	918	TYR	Peptide
1	C	1032	GLU	Peptide
1	C	1047	GLN	Sidechain
1	C	547	ASP	Peptide
1	C	593	LYS	Peptide
1	C	604	ARG	Peptide
1	C	609	LEU	Peptide
1	C	610	LYS	Peptide
1	C	612	PHE	Peptide
1	C	626	MET	Peptide
1	C	643	LEU	Peptide
1	C	644	HIS	Peptide
1	C	682	PRO	Peptide
1	C	692	ASN	Peptide
1	C	693	ASN	Peptide
1	C	695	ILE	Peptide
1	C	696	GLU	Peptide
1	C	740	ILE	Peptide
1	C	745	ALA	Peptide
1	C	826	ILE	Peptide
1	C	893	ASN	Peptide
1	C	897	PRO	Peptide
1	C	913	LEU	Peptide
1	C	918	TYR	Peptide
1	D	1032	GLU	Peptide
1	D	1047	GLN	Sidechain
1	D	547	ASP	Peptide
1	D	593	LYS	Peptide
1	D	604	ARG	Peptide
1	D	609	LEU	Peptide
1	D	610	LYS	Peptide
1	D	612	PHE	Peptide
1	D	626	MET	Peptide
1	D	643	LEU	Peptide
1	D	644	HIS	Peptide
1	D	682	PRO	Peptide
1	D	692	ASN	Peptide
1	D	693	ASN	Peptide
1	D	695	ILE	Peptide
1	D	696	GLU	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	D	740	ILE	Peptide
1	D	745	ALA	Peptide
1	D	826	ILE	Peptide
1	D	893	ASN	Peptide
1	D	897	PRO	Peptide
1	D	913	LEU	Peptide
1	D	917	ASN	Peptide
1	D	918	TYR	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4238	0	4110	232	0
1	B	4238	0	4110	230	0
1	C	4238	0	4110	233	0
1	D	4238	0	4110	239	0
All	All	16952	0	16440	851	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 25.

All (851) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1051:LEU:HD13	1:A:1047:GLN:NE2	1.39	1.37
1:A:1051:LEU:HD13	1:B:1047:GLN:NE2	1.40	1.32
1:B:1051:LEU:HD13	1:C:1047:GLN:NE2	1.41	1.32
1:D:1047:GLN:NE2	1:C:1051:LEU:HD13	1.40	1.30
1:D:1051:LEU:CD1	1:A:1047:GLN:NE2	2.26	0.97
1:A:1051:LEU:CD1	1:B:1047:GLN:NE2	2.27	0.96
1:D:1047:GLN:NE2	1:C:1051:LEU:CD1	2.27	0.96
1:D:1051:LEU:HD13	1:A:1047:GLN:HE22	1.14	0.95
1:B:1051:LEU:CD1	1:C:1047:GLN:NE2	2.29	0.95
1:B:1051:LEU:HD13	1:C:1047:GLN:HE22	1.17	0.94
1:D:1047:GLN:HE22	1:C:1051:LEU:HD13	1.14	0.93

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1051:LEU:HD13	1:B:1047:GLN:HE22	1.16	0.93
1:B:629:TYR:H	1:B:697:LEU:HD11	1.41	0.86
1:A:629:TYR:H	1:A:697:LEU:HD11	1.41	0.85
1:D:629:TYR:H	1:D:697:LEU:HD11	1.41	0.84
1:A:1072:MET:O	1:B:458:ARG:NH2	2.11	0.83
1:C:629:TYR:H	1:C:697:LEU:HD11	1.41	0.83
1:A:970:HIS:O	1:A:970:HIS:ND1	2.12	0.82
1:D:540:CYS:HA	1:D:543:ARG:HH21	1.44	0.82
1:D:970:HIS:O	1:D:970:HIS:ND1	2.12	0.82
1:A:540:CYS:HA	1:A:543:ARG:HH21	1.44	0.82
1:B:540:CYS:HA	1:B:543:ARG:HH21	1.44	0.82
1:D:1072:MET:O	1:A:458:ARG:NH2	2.13	0.81
1:B:1072:MET:O	1:C:458:ARG:NH2	2.12	0.81
1:C:970:HIS:ND1	1:C:970:HIS:O	2.12	0.81
1:C:540:CYS:HA	1:C:543:ARG:HH21	1.44	0.81
1:D:458:ARG:NH2	1:C:1072:MET:O	2.14	0.81
1:B:970:HIS:O	1:B:970:HIS:ND1	2.12	0.80
1:D:1051:LEU:HD13	1:A:1047:GLN:HE21	1.46	0.80
1:A:1051:LEU:HD13	1:B:1047:GLN:HE21	1.47	0.79
1:B:1051:LEU:HD13	1:C:1047:GLN:HE21	1.48	0.78
1:D:1047:GLN:HE21	1:C:1051:LEU:HD13	1.49	0.78
1:B:925:PRO:HB2	1:B:931:LEU:HD23	1.66	0.78
1:B:811:ILE:HD11	1:B:842:TYR:CD1	2.19	0.77
1:D:925:PRO:HB2	1:D:931:LEU:HD23	1.66	0.77
1:A:811:ILE:HD11	1:A:842:TYR:CD1	2.19	0.77
1:B:1051:LEU:CD1	1:C:1047:GLN:HE22	1.96	0.77
1:C:811:ILE:HD11	1:C:842:TYR:CD1	2.19	0.77
1:D:811:ILE:HD11	1:D:842:TYR:CD1	2.19	0.77
1:C:925:PRO:HB2	1:C:931:LEU:HD23	1.65	0.77
1:D:695:ILE:HD13	1:D:698:LEU:HB3	1.67	0.76
1:A:925:PRO:HB2	1:A:931:LEU:HD23	1.66	0.76
1:D:579:GLN:O	1:D:581:ALA:N	2.18	0.76
1:B:695:ILE:HD13	1:B:698:LEU:HB3	1.67	0.76
1:A:695:ILE:HD13	1:A:698:LEU:HB3	1.67	0.76
1:A:1051:LEU:CD1	1:B:1047:GLN:HE22	1.95	0.75
1:C:579:GLN:O	1:C:581:ALA:N	2.18	0.75
1:D:631:PRO:O	1:D:634:MET:N	2.20	0.75
1:A:631:PRO:O	1:A:634:MET:N	2.20	0.75
1:B:579:GLN:O	1:B:581:ALA:N	2.18	0.75
1:D:540:CYS:HA	1:D:543:ARG:NH2	2.01	0.75
1:B:882:LEU:HA	1:B:905:ILE:HD13	1.68	0.75

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:631:PRO:O	1:C:634:MET:N	2.20	0.75
1:B:631:PRO:O	1:B:634:MET:N	2.20	0.75
1:C:540:CYS:HA	1:C:543:ARG:NH2	2.01	0.75
1:C:882:LEU:HA	1:C:905:ILE:HD13	1.68	0.75
1:C:695:ILE:HD13	1:C:698:LEU:HB3	1.67	0.74
1:A:540:CYS:HA	1:A:543:ARG:NH2	2.01	0.74
1:B:540:CYS:HA	1:B:543:ARG:NH2	2.01	0.74
1:A:579:GLN:O	1:A:581:ALA:N	2.18	0.74
1:A:882:LEU:HA	1:A:905:ILE:HD13	1.68	0.73
1:D:1000:GLN:N	1:D:1000:GLN:OE1	2.21	0.73
1:D:1065:ILE:HA	1:D:1068:ILE:HG12	1.71	0.73
1:C:1000:GLN:N	1:C:1000:GLN:OE1	2.21	0.73
1:D:591:LYS:HA	1:D:627:ILE:HD11	1.70	0.73
1:D:882:LEU:HA	1:D:905:ILE:HD13	1.68	0.73
1:B:591:LYS:HA	1:B:627:ILE:HD11	1.70	0.73
1:A:832:TRP:HA	1:A:832:TRP:CE3	2.24	0.73
1:A:1065:ILE:HA	1:A:1068:ILE:HG12	1.71	0.73
1:C:832:TRP:HA	1:C:832:TRP:CE3	2.24	0.72
1:A:1000:GLN:N	1:A:1000:GLN:OE1	2.21	0.72
1:B:1000:GLN:OE1	1:B:1000:GLN:N	2.21	0.72
1:B:522:SER:HB3	1:B:555:ALA:HB2	1.71	0.72
1:B:832:TRP:HA	1:B:832:TRP:CE3	2.24	0.72
1:C:1065:ILE:HA	1:C:1068:ILE:HG12	1.71	0.72
1:D:832:TRP:HA	1:D:832:TRP:CE3	2.24	0.71
1:D:1051:LEU:CD1	1:A:1047:GLN:HE22	1.94	0.71
1:A:591:LYS:HA	1:A:627:ILE:HD11	1.70	0.71
1:B:832:TRP:HA	1:B:832:TRP:HE3	1.56	0.71
1:C:522:SER:HB3	1:C:555:ALA:HB2	1.71	0.71
1:C:832:TRP:HA	1:C:832:TRP:HE3	1.55	0.71
1:B:1065:ILE:HA	1:B:1068:ILE:HG12	1.71	0.71
1:C:591:LYS:HA	1:C:627:ILE:HD11	1.70	0.71
1:A:885:GLY:HA2	1:A:908:THR:HG21	1.73	0.71
1:B:885:GLY:HA2	1:B:908:THR:HG21	1.73	0.71
1:D:885:GLY:HA2	1:D:908:THR:HG21	1.73	0.71
1:D:1047:GLN:HE22	1:C:1051:LEU:CD1	1.94	0.71
1:A:522:SER:HB3	1:A:555:ALA:HB2	1.71	0.70
1:D:832:TRP:HA	1:D:832:TRP:HE3	1.55	0.70
1:A:832:TRP:HA	1:A:832:TRP:HE3	1.55	0.70
1:D:468:ASP:H	1:D:469:ILE:HA	1.56	0.70
1:B:468:ASP:H	1:B:469:ILE:HA	1.56	0.70
1:A:468:ASP:H	1:A:469:ILE:HA	1.56	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:468:ASP:H	1:C:469:ILE:HA	1.56	0.70
1:D:522:SER:HB3	1:D:555:ALA:HB2	1.71	0.69
1:B:638:LEU:HD11	1:B:653:ASP:HB2	1.75	0.69
1:C:638:LEU:HD11	1:C:653:ASP:HB2	1.75	0.69
1:C:885:GLY:HA2	1:C:908:THR:HG21	1.73	0.69
1:B:545:ASP:HB3	1:B:546:GLU:HA	1.75	0.69
1:D:638:LEU:HD11	1:D:653:ASP:HB2	1.75	0.68
1:B:631:PRO:HB2	1:B:697:LEU:HD22	1.76	0.68
1:D:544:LEU:O	1:D:548:GLY:HA2	1.94	0.68
1:C:545:ASP:HB3	1:C:546:GLU:HA	1.75	0.68
1:D:545:ASP:HB3	1:D:546:GLU:HA	1.75	0.68
1:A:544:LEU:O	1:A:548:GLY:HA2	1.93	0.68
1:A:638:LEU:HD11	1:A:653:ASP:HB2	1.75	0.68
1:B:516:THR:HG22	1:B:517:ALA:H	1.58	0.68
1:B:542:ASP:O	1:B:543:ARG:HD3	1.94	0.68
1:C:542:ASP:O	1:C:543:ARG:HD3	1.94	0.68
1:C:516:THR:HG22	1:C:517:ALA:H	1.58	0.68
1:A:743:GLY:H	1:A:832:TRP:HE1	1.42	0.67
1:B:544:LEU:O	1:B:548:GLY:HA2	1.93	0.67
1:C:631:PRO:HB2	1:C:697:LEU:HD22	1.75	0.67
1:D:516:THR:HG22	1:D:517:ALA:H	1.58	0.67
1:D:542:ASP:O	1:D:543:ARG:HD3	1.94	0.67
1:A:516:THR:HG22	1:A:517:ALA:H	1.58	0.67
1:A:631:PRO:HB2	1:A:697:LEU:HD22	1.76	0.67
1:C:544:LEU:O	1:C:548:GLY:HA2	1.93	0.67
1:C:743:GLY:H	1:C:832:TRP:HE1	1.43	0.67
1:D:631:PRO:HB2	1:D:697:LEU:HD22	1.75	0.67
1:B:743:GLY:H	1:B:832:TRP:HE1	1.43	0.66
1:A:542:ASP:O	1:A:543:ARG:HD3	1.94	0.66
1:A:545:ASP:HB3	1:A:546:GLU:HA	1.75	0.66
1:D:743:GLY:H	1:D:832:TRP:HE1	1.42	0.66
1:D:804:SER:HA	1:D:807:LEU:HD12	1.78	0.66
1:B:515:TRP:O	1:B:519:HIS:ND1	2.29	0.66
1:C:515:TRP:O	1:C:519:HIS:ND1	2.29	0.66
1:C:804:SER:HA	1:C:807:LEU:HD12	1.78	0.66
1:A:992:LEU:HA	1:A:995:LEU:HD23	1.78	0.65
1:A:1069:ILE:HD11	1:B:1064:LEU:HD21	1.78	0.65
1:B:992:LEU:HA	1:B:995:LEU:HD23	1.78	0.65
1:A:804:SER:HA	1:A:807:LEU:HD12	1.78	0.65
1:A:515:TRP:O	1:A:519:HIS:ND1	2.29	0.65
1:D:1064:LEU:HD21	1:C:1069:ILE:HD11	1.79	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:804:SER:HA	1:B:807:LEU:HD12	1.78	0.65
1:D:561:ALA:HB1	1:D:598:THR:HG21	1.80	0.64
1:D:1069:ILE:HD11	1:A:1064:LEU:HD21	1.79	0.64
1:B:1069:ILE:HD11	1:C:1064:LEU:HD21	1.78	0.64
1:D:515:TRP:O	1:D:519:HIS:ND1	2.29	0.64
1:D:992:LEU:HA	1:D:995:LEU:HD23	1.78	0.64
1:C:561:ALA:HB1	1:C:598:THR:HG21	1.79	0.64
1:A:561:ALA:HB1	1:A:598:THR:HG21	1.79	0.64
1:B:640:PHE:HD2	1:B:642:MET:HB3	1.63	0.63
1:A:640:PHE:HD2	1:A:642:MET:HB3	1.63	0.63
1:B:561:ALA:HB1	1:B:598:THR:HG21	1.80	0.63
1:C:992:LEU:HA	1:C:995:LEU:HD23	1.78	0.63
1:B:496:LYS:HA	1:B:496:LYS:NZ	2.15	0.62
1:D:640:PHE:HD2	1:D:642:MET:HB3	1.63	0.62
1:C:871:LEU:O	1:C:874:THR:HG22	2.00	0.62
1:D:889:TYR:O	1:D:893:ASN:ND2	2.33	0.62
1:D:1048:LYS:HZ3	1:A:1050:ARG:NH2	1.97	0.62
1:A:496:LYS:NZ	1:A:496:LYS:HA	2.15	0.62
1:C:640:PHE:HD2	1:C:642:MET:HB3	1.62	0.62
1:C:496:LYS:NZ	1:C:496:LYS:HA	2.14	0.62
1:A:889:TYR:O	1:A:893:ASN:ND2	2.33	0.62
1:B:811:ILE:HD11	1:B:842:TYR:HD1	1.64	0.62
1:D:496:LYS:NZ	1:D:496:LYS:HA	2.15	0.62
1:B:582:SER:O	1:B:585:HIS:HB2	2.00	0.61
1:B:889:TYR:O	1:B:893:ASN:ND2	2.33	0.61
1:C:889:TYR:O	1:C:893:ASN:ND2	2.33	0.61
1:D:871:LEU:O	1:D:874:THR:HG22	2.00	0.61
1:A:582:SER:O	1:A:585:HIS:HB2	2.00	0.61
1:A:923:LEU:HD22	1:B:897:PRO:HG3	1.82	0.61
1:D:917:ASN:H	1:D:918:TYR:CB	2.13	0.61
1:B:871:LEU:O	1:B:874:THR:HG22	2.00	0.61
1:D:875:VAL:O	1:D:878:ILE:HG22	2.01	0.61
1:B:997:LYS:HB2	1:B:998:VAL:HA	1.83	0.61
1:C:917:ASN:H	1:C:918:TYR:CB	2.13	0.61
1:B:875:VAL:O	1:B:878:ILE:HG22	2.01	0.61
1:A:871:LEU:O	1:A:874:THR:HG22	2.00	0.61
1:A:875:VAL:O	1:A:878:ILE:HG22	2.01	0.61
1:A:917:ASN:H	1:A:918:TYR:CB	2.13	0.61
1:A:811:ILE:HD11	1:A:842:TYR:HD1	1.64	0.60
1:C:997:LYS:HB2	1:C:998:VAL:HA	1.83	0.60
1:D:877:PHE:HA	1:D:880:LEU:HB3	1.82	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:HIS:CE1	1:A:583:PHE:HB3	2.37	0.60
1:A:997:LYS:HB2	1:A:998:VAL:HA	1.83	0.60
1:C:582:SER:O	1:C:585:HIS:HB2	2.00	0.60
1:C:875:VAL:O	1:C:878:ILE:HG22	2.01	0.60
1:D:811:ILE:HD11	1:D:842:TYR:HD1	1.64	0.60
1:B:923:LEU:HD22	1:C:897:PRO:HG3	1.83	0.60
1:B:917:ASN:H	1:B:918:TYR:CB	2.13	0.60
1:C:877:PHE:HA	1:C:880:LEU:HB3	1.82	0.60
1:D:582:SER:O	1:D:585:HIS:HB2	2.00	0.60
1:C:660:PHE:HB3	1:C:661:LYS:C	2.22	0.60
1:A:877:PHE:HA	1:A:880:LEU:HB3	1.82	0.60
1:A:1048:LYS:HZ3	1:B:1050:ARG:NH2	2.00	0.60
1:B:877:PHE:HA	1:B:880:LEU:HB3	1.82	0.60
1:C:553:HIS:CE1	1:C:583:PHE:HB3	2.37	0.60
1:D:660:PHE:HB3	1:D:661:LYS:C	2.23	0.60
1:B:553:HIS:CE1	1:B:583:PHE:HB3	2.36	0.59
1:C:809:TRP:O	1:C:813:THR:HG23	2.02	0.59
1:D:997:LYS:HB2	1:D:998:VAL:HA	1.83	0.59
1:D:1050:ARG:NH2	1:C:1048:LYS:HZ3	2.00	0.59
1:B:660:PHE:HB3	1:B:661:LYS:C	2.22	0.59
1:A:916:ILE:N	1:A:917:ASN:HA	2.18	0.59
1:D:891:LEU:HB3	1:D:892:LEU:HD22	1.85	0.59
1:A:891:LEU:HB3	1:A:892:LEU:HD22	1.85	0.59
1:A:990:LEU:HD11	1:A:994:PHE:HD2	1.68	0.59
1:B:809:TRP:O	1:B:813:THR:HG23	2.02	0.59
1:D:766:ASN:OD1	1:D:769:LEU:CB	2.51	0.59
1:A:766:ASN:OD1	1:A:769:LEU:CB	2.51	0.59
1:D:553:HIS:CE1	1:D:583:PHE:HB3	2.37	0.59
1:D:809:TRP:O	1:D:813:THR:HG23	2.02	0.59
1:D:818:PHE:HD2	1:D:835:GLY:HA2	1.67	0.59
1:D:916:ILE:N	1:D:917:ASN:HA	2.18	0.59
1:A:660:PHE:HB3	1:A:661:LYS:C	2.22	0.59
1:B:766:ASN:OD1	1:B:769:LEU:CB	2.51	0.59
1:A:824:VAL:HG12	1:A:825:GLU:N	2.18	0.58
1:B:818:PHE:HD2	1:B:835:GLY:HA2	1.67	0.58
1:C:891:LEU:HB3	1:C:892:LEU:HD22	1.85	0.58
1:B:891:LEU:HB3	1:B:892:LEU:HD22	1.85	0.58
1:D:990:LEU:HD11	1:D:994:PHE:HD2	1.68	0.58
1:B:824:VAL:HG12	1:B:825:GLU:N	2.18	0.58
1:D:824:VAL:HG12	1:D:825:GLU:N	2.18	0.58
1:A:990:LEU:HD11	1:A:994:PHE:CD2	2.39	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:990:LEU:HD11	1:B:994:PHE:CD2	2.39	0.58
1:B:990:LEU:HD11	1:B:994:PHE:HD2	1.68	0.58
1:A:809:TRP:O	1:A:813:THR:HG23	2.02	0.58
1:C:455:SER:HA	1:C:488:LEU:HB3	1.86	0.58
1:D:455:SER:HA	1:D:488:LEU:HB3	1.86	0.58
1:D:923:LEU:HD22	1:A:897:PRO:HG3	1.85	0.58
1:D:990:LEU:HD11	1:D:994:PHE:CD2	2.39	0.58
1:C:766:ASN:OD1	1:C:769:LEU:CB	2.51	0.58
1:C:990:LEU:HD11	1:C:994:PHE:CD2	2.39	0.58
1:B:452:PHE:CE1	1:B:1071:LYS:HE3	2.39	0.58
1:C:990:LEU:HD11	1:C:994:PHE:HD2	1.68	0.58
1:A:686:LEU:HD22	1:A:708:LEU:HD11	1.86	0.58
1:C:824:VAL:HG12	1:C:825:GLU:N	2.18	0.58
1:C:968:GLN:HA	1:C:971:ALA:HB2	1.85	0.58
1:B:1048:LYS:HZ3	1:C:1050:ARG:NH2	2.02	0.57
1:C:818:PHE:HD2	1:C:835:GLY:HA2	1.67	0.57
1:D:686:LEU:HD22	1:D:708:LEU:HD11	1.86	0.57
1:A:818:PHE:HD2	1:A:835:GLY:HA2	1.68	0.57
1:C:916:ILE:N	1:C:917:ASN:HA	2.18	0.57
1:B:851:GLN:O	1:B:857:GLY:HA2	2.05	0.57
1:B:916:ILE:N	1:B:917:ASN:HA	2.18	0.57
1:B:968:GLN:HA	1:B:971:ALA:HB2	1.85	0.57
1:A:851:GLN:O	1:A:857:GLY:HA2	2.05	0.57
1:D:452:PHE:CE1	1:D:1071:LYS:HE3	2.39	0.57
1:C:452:PHE:CE1	1:C:1071:LYS:HE3	2.39	0.57
1:B:455:SER:HA	1:B:488:LEU:HB3	1.86	0.57
1:C:480:LEU:HD12	1:C:481:HIS:HA	1.87	0.57
1:A:968:GLN:HA	1:A:971:ALA:HB2	1.85	0.57
1:B:686:LEU:HD22	1:B:708:LEU:HD11	1.86	0.57
1:B:480:LEU:HD12	1:B:481:HIS:HA	1.87	0.57
1:D:851:GLN:O	1:D:857:GLY:HA2	2.05	0.56
1:A:452:PHE:CE1	1:A:1071:LYS:HE3	2.39	0.56
1:A:480:LEU:HD12	1:A:481:HIS:HA	1.87	0.56
1:C:686:LEU:HD22	1:C:708:LEU:HD11	1.86	0.56
1:C:811:ILE:HD11	1:C:842:TYR:HD1	1.65	0.56
1:D:480:LEU:HD12	1:D:481:HIS:HA	1.87	0.56
1:D:968:GLN:HA	1:D:971:ALA:HB2	1.85	0.56
1:C:851:GLN:O	1:C:857:GLY:HA2	2.05	0.56
1:A:455:SER:HA	1:A:488:LEU:HB3	1.86	0.56
1:D:456:TYR:O	1:D:494:HIS:NE2	2.40	0.55
1:D:897:PRO:HG3	1:C:923:LEU:HD22	1.87	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:TYR:O	1:B:494:HIS:NE2	2.40	0.55
1:B:698:LEU:HD21	1:B:976:ILE:HG21	1.88	0.55
1:C:456:TYR:O	1:C:494:HIS:NE2	2.40	0.55
1:C:945:THR:HA	1:C:949:PRO:HD2	1.88	0.55
1:A:455:SER:HB2	1:A:488:LEU:HD23	1.89	0.55
1:C:698:LEU:HD21	1:C:976:ILE:HG21	1.87	0.55
1:C:480:LEU:HA	1:C:481:HIS:C	2.27	0.55
1:A:575:VAL:HA	1:A:610:LYS:HE3	1.88	0.55
1:A:698:LEU:HD21	1:A:976:ILE:HG21	1.87	0.55
1:D:698:LEU:HD21	1:D:976:ILE:HG21	1.88	0.55
1:D:945:THR:HA	1:D:949:PRO:HD2	1.88	0.55
1:A:687:ASN:O	1:A:690:VAL:HG12	2.07	0.55
1:A:480:LEU:HA	1:A:481:HIS:C	2.27	0.55
1:A:945:THR:HA	1:A:949:PRO:HD2	1.88	0.55
1:A:870:LEU:CD2	1:A:956:LEU:HD11	2.38	0.55
1:B:945:THR:HA	1:B:949:PRO:HD2	1.88	0.55
1:C:575:VAL:HA	1:C:610:LYS:HE3	1.88	0.55
1:D:687:ASN:O	1:D:690:VAL:HG12	2.07	0.54
1:D:1047:GLN:HE21	1:C:1051:LEU:CD1	2.13	0.54
1:A:456:TYR:O	1:A:494:HIS:NE2	2.39	0.54
1:A:876:VAL:HG11	1:B:859:PHE:CD2	2.42	0.54
1:B:455:SER:HB2	1:B:488:LEU:HD23	1.89	0.54
1:B:575:VAL:HA	1:B:610:LYS:HE3	1.88	0.54
1:B:870:LEU:CD2	1:B:956:LEU:HD11	2.37	0.54
1:B:876:VAL:HG11	1:C:859:PHE:CD2	2.42	0.54
1:B:687:ASN:O	1:B:690:VAL:HG12	2.07	0.54
1:D:480:LEU:HA	1:D:481:HIS:C	2.27	0.54
1:D:580:GLN:HG2	1:D:581:ALA:N	2.23	0.54
1:D:870:LEU:CD2	1:D:956:LEU:HD11	2.37	0.54
1:B:480:LEU:HA	1:B:481:HIS:C	2.27	0.54
1:C:455:SER:HB2	1:C:488:LEU:HD23	1.89	0.54
1:D:848:LEU:O	1:D:851:GLN:HB3	2.08	0.54
1:C:687:ASN:O	1:C:690:VAL:HG12	2.07	0.54
1:D:575:VAL:HA	1:D:610:LYS:HE3	1.88	0.54
1:B:848:LEU:O	1:B:851:GLN:HB3	2.08	0.54
1:B:1051:LEU:CD1	1:C:1047:GLN:HE21	2.13	0.54
1:D:455:SER:HB2	1:D:488:LEU:HD23	1.89	0.53
1:A:580:GLN:HG2	1:A:581:ALA:N	2.23	0.53
1:B:918:TYR:HD1	1:B:921:SER:HB3	1.74	0.53
1:A:848:LEU:O	1:A:851:GLN:HB3	2.08	0.53
1:B:977:ALA:HA	1:B:980:VAL:HG12	1.91	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:580:GLN:HG2	1:B:581:ALA:N	2.23	0.53
1:A:597:LEU:CD1	1:A:601:ARG:HH12	2.22	0.53
1:A:977:ALA:HA	1:A:980:VAL:HG12	1.91	0.53
1:C:870:LEU:CD2	1:C:956:LEU:HD11	2.37	0.53
1:C:977:ALA:HA	1:C:980:VAL:HG12	1.91	0.53
1:D:597:LEU:CD1	1:D:601:ARG:HH12	2.22	0.53
1:D:518:LEU:HD12	1:D:521:ALA:HB3	1.91	0.53
1:D:876:VAL:HG11	1:A:859:PHE:CD2	2.44	0.53
1:A:1047:GLN:HA	1:A:1050:ARG:HH21	1.74	0.53
1:C:710:LYS:O	1:C:713:ALA:N	2.41	0.53
1:B:619:ASN:O	1:B:622:PRO:HD2	2.09	0.53
1:C:580:GLN:HG2	1:C:581:ALA:N	2.23	0.53
1:D:710:LYS:O	1:D:713:ALA:N	2.40	0.52
1:A:918:TYR:HD1	1:A:921:SER:HB3	1.74	0.52
1:D:977:ALA:HA	1:D:980:VAL:HG12	1.91	0.52
1:A:917:ASN:H	1:A:918:TYR:HB2	1.74	0.52
1:B:874:THR:HA	1:B:877:PHE:CZ	2.44	0.52
1:C:918:TYR:HD1	1:C:921:SER:HB3	1.74	0.52
1:D:619:ASN:O	1:D:622:PRO:HD2	2.09	0.52
1:A:619:ASN:O	1:A:622:PRO:HD2	2.09	0.52
1:A:923:LEU:HD11	1:B:897:PRO:HB3	1.91	0.52
1:B:597:LEU:CD1	1:B:601:ARG:HH12	2.22	0.52
1:B:609:LEU:HB2	1:B:610:LYS:HG3	1.92	0.52
1:C:874:THR:HA	1:C:877:PHE:CZ	2.44	0.52
1:C:1047:GLN:HA	1:C:1050:ARG:HH21	1.74	0.52
1:D:859:PHE:O	1:D:862:MET:HB3	2.10	0.52
1:B:824:VAL:HG12	1:B:825:GLU:H	1.75	0.52
1:C:917:ASN:H	1:C:918:TYR:HB2	1.73	0.52
1:D:874:THR:HA	1:D:877:PHE:CZ	2.44	0.52
1:D:918:TYR:HD1	1:D:921:SER:HB3	1.74	0.52
1:C:859:PHE:O	1:C:862:MET:HB3	2.10	0.52
1:B:518:LEU:HD12	1:B:521:ALA:HB3	1.91	0.52
1:C:848:LEU:O	1:C:851:GLN:HB3	2.08	0.52
1:D:859:PHE:CD2	1:C:876:VAL:HG11	2.44	0.52
1:D:917:ASN:H	1:D:918:TYR:HB2	1.74	0.52
1:D:1047:GLN:HA	1:D:1050:ARG:HH21	1.74	0.52
1:B:917:ASN:H	1:B:918:TYR:HB2	1.74	0.52
1:A:859:PHE:O	1:A:862:MET:HB3	2.10	0.52
1:A:874:THR:HA	1:A:877:PHE:CZ	2.44	0.52
1:D:824:VAL:HG12	1:D:825:GLU:H	1.75	0.52
1:A:491:LYS:HG3	1:A:492:ASN:OD1	2.11	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1061:GLN:NE2	1:B:1061:GLN:HE22	2.08	0.52
1:A:518:LEU:HD12	1:A:521:ALA:HB3	1.91	0.51
1:B:491:LYS:HG3	1:B:492:ASN:OD1	2.11	0.51
1:B:1047:GLN:HA	1:B:1050:ARG:HH21	1.74	0.51
1:D:1061:GLN:NE2	1:A:1061:GLN:HE22	2.08	0.51
1:A:885:GLY:O	1:A:904:SER:OG	2.28	0.51
1:C:597:LEU:CD1	1:C:601:ARG:HH12	2.22	0.51
1:C:619:ASN:O	1:C:622:PRO:HD2	2.09	0.51
1:D:609:LEU:HB2	1:D:610:LYS:HG3	1.92	0.51
1:D:726:TYR:HE2	1:D:846:PHE:HB2	1.76	0.51
1:C:518:LEU:HD12	1:C:521:ALA:HB3	1.91	0.51
1:D:885:GLY:O	1:D:904:SER:OG	2.28	0.51
1:A:824:VAL:HG12	1:A:825:GLU:H	1.75	0.51
1:C:609:LEU:HB2	1:C:610:LYS:HG3	1.92	0.51
1:C:726:TYR:HE2	1:C:846:PHE:HB2	1.76	0.51
1:C:824:VAL:HG12	1:C:825:GLU:H	1.75	0.51
1:B:859:PHE:O	1:B:862:MET:HB3	2.10	0.51
1:B:1061:GLN:NE2	1:C:1061:GLN:HE22	2.09	0.51
1:C:885:GLY:O	1:C:904:SER:OG	2.29	0.51
1:A:620:LYS:O	1:A:623:ILE:HB	2.11	0.51
1:A:609:LEU:HB2	1:A:610:LYS:HG3	1.92	0.50
1:B:885:GLY:O	1:B:904:SER:OG	2.29	0.50
1:C:491:LYS:HG3	1:C:492:ASN:OD1	2.10	0.50
1:D:491:LYS:HG3	1:D:492:ASN:OD1	2.11	0.50
1:B:710:LYS:O	1:B:713:ALA:N	2.41	0.50
1:B:923:LEU:HD11	1:C:897:PRO:HB3	1.92	0.50
1:D:773:CYS:O	1:D:777:VAL:HG23	2.12	0.50
1:D:897:PRO:HB3	1:C:923:LEU:HD11	1.94	0.50
1:C:773:CYS:O	1:C:777:VAL:HG23	2.12	0.50
1:D:620:LYS:O	1:D:623:ILE:HB	2.11	0.50
1:D:723:LEU:HD23	1:D:727:CYS:HB2	1.94	0.50
1:A:710:LYS:O	1:A:713:ALA:N	2.40	0.50
1:B:620:LYS:O	1:B:623:ILE:HB	2.11	0.50
1:A:1048:LYS:HZ1	1:B:1050:ARG:HH12	1.60	0.50
1:A:723:LEU:HD23	1:A:727:CYS:HB2	1.94	0.50
1:A:726:TYR:HE2	1:A:846:PHE:HB2	1.76	0.50
1:B:773:CYS:O	1:B:777:VAL:HG23	2.12	0.50
1:B:723:LEU:HD23	1:B:727:CYS:HB2	1.94	0.49
1:B:1048:LYS:HZ1	1:C:1050:ARG:HH12	1.58	0.49
1:C:620:LYS:O	1:C:623:ILE:HB	2.11	0.49
1:C:723:LEU:HD23	1:C:727:CYS:HB2	1.94	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:981:GLU:O	1:A:984:THR:HG22	2.13	0.49
1:B:1047:GLN:HA	1:B:1050:ARG:NH2	2.28	0.49
1:B:726:TYR:HE2	1:B:846:PHE:HB2	1.76	0.49
1:C:872:ARG:O	1:C:875:VAL:HG12	2.13	0.49
1:D:918:TYR:CD1	1:D:921:SER:HB3	2.47	0.49
1:A:773:CYS:O	1:A:777:VAL:HG23	2.12	0.49
1:D:496:LYS:HA	1:D:496:LYS:HZ2	1.75	0.49
1:D:981:GLU:O	1:D:984:THR:HG22	2.12	0.49
1:C:1047:GLN:HA	1:C:1050:ARG:NH2	2.28	0.49
1:D:618:GLY:HA2	1:D:619:ASN:HA	1.61	0.49
1:C:918:TYR:CD1	1:C:921:SER:HB3	2.47	0.49
1:B:872:ARG:O	1:B:875:VAL:HG12	2.12	0.49
1:B:918:TYR:CD1	1:B:921:SER:HB3	2.47	0.49
1:D:516:THR:HG22	1:D:517:ALA:N	2.28	0.48
1:A:863:LEU:HA	1:A:866:ILE:HG22	1.95	0.48
1:C:468:ASP:N	1:C:469:ILE:HA	2.23	0.48
1:A:1047:GLN:HA	1:A:1050:ARG:NH2	2.28	0.48
1:B:446:LYS:HA	1:B:447:LYS:HA	1.54	0.48
1:D:863:LEU:HA	1:D:866:ILE:HG22	1.96	0.48
1:D:872:ARG:O	1:D:875:VAL:HG12	2.12	0.48
1:A:730:LEU:HA	1:A:842:TYR:CE2	2.48	0.48
1:A:872:ARG:O	1:A:875:VAL:HG12	2.12	0.48
1:A:918:TYR:CD1	1:A:921:SER:HB3	2.48	0.48
1:B:818:PHE:HD1	1:B:819:VAL:HG22	1.78	0.48
1:D:730:LEU:HA	1:D:842:TYR:CE2	2.49	0.48
1:D:745:ALA:O	1:D:746:PHE:HB2	2.14	0.48
1:C:863:LEU:HA	1:C:866:ILE:HG22	1.95	0.48
1:D:1047:GLN:HA	1:D:1050:ARG:NH2	2.28	0.48
1:B:981:GLU:O	1:B:984:THR:HG22	2.12	0.48
1:A:629:TYR:HA	1:A:697:LEU:HD21	1.96	0.48
1:A:745:ALA:O	1:A:746:PHE:HB2	2.14	0.48
1:A:818:PHE:HD1	1:A:819:VAL:HG22	1.78	0.48
1:B:863:LEU:HA	1:B:866:ILE:HG22	1.95	0.48
1:A:591:LYS:HD2	1:A:591:LYS:N	2.29	0.48
1:C:629:TYR:HA	1:C:697:LEU:HD21	1.96	0.48
1:C:818:PHE:HD1	1:C:819:VAL:HG22	1.78	0.48
1:D:818:PHE:HD1	1:D:819:VAL:HG22	1.78	0.47
1:B:591:LYS:N	1:B:591:LYS:HD2	2.29	0.47
1:B:730:LEU:HA	1:B:842:TYR:CE2	2.49	0.47
1:C:981:GLU:O	1:C:984:THR:HG22	2.13	0.47
1:D:629:TYR:HA	1:D:697:LEU:HD21	1.96	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:867:LEU:O	1:D:870:LEU:HB3	2.15	0.47
1:B:1048:LYS:HZ1	1:C:1050:ARG:NH1	2.13	0.47
1:C:730:LEU:HA	1:C:842:TYR:CE2	2.49	0.47
1:D:1061:GLN:HE22	1:C:1061:GLN:NE2	2.11	0.47
1:A:819:VAL:HG12	1:A:819:VAL:O	2.14	0.47
1:B:856:CYS:O	1:B:859:PHE:N	2.46	0.47
1:C:591:LYS:HD2	1:C:591:LYS:N	2.29	0.47
1:C:867:LEU:O	1:C:870:LEU:HB3	2.15	0.47
1:D:820:LEU:HD23	1:D:820:LEU:HA	1.74	0.47
1:A:649:LYS:HA	1:A:1005:VAL:O	2.15	0.47
1:A:1066:LYS:HA	1:A:1069:ILE:HD12	1.97	0.47
1:B:629:TYR:HA	1:B:697:LEU:HD21	1.96	0.47
1:C:745:ALA:O	1:C:746:PHE:HB2	2.14	0.47
1:B:922:PHE:HD1	1:B:922:PHE:N	2.13	0.47
1:C:516:THR:HG22	1:C:517:ALA:N	2.28	0.47
1:C:547:ASP:N	1:C:547:ASP:OD1	2.48	0.47
1:C:1042:MET:SD	1:C:1042:MET:C	2.93	0.47
1:A:547:ASP:OD1	1:A:547:ASP:N	2.48	0.47
1:B:1042:MET:SD	1:B:1042:MET:C	2.93	0.47
1:C:690:VAL:HG21	1:C:977:ALA:HB2	1.97	0.47
1:D:1048:LYS:HZ1	1:A:1050:ARG:HH12	1.63	0.47
1:D:1051:LEU:CD1	1:A:1047:GLN:HE21	2.11	0.47
1:A:446:LYS:HA	1:A:447:LYS:HA	1.54	0.47
1:A:516:THR:HG22	1:A:517:ALA:N	2.27	0.47
1:A:690:VAL:HG21	1:A:977:ALA:HB2	1.97	0.47
1:A:812:TYR:O	1:A:816:ILE:HG12	2.15	0.47
1:A:867:LEU:O	1:A:870:LEU:HB3	2.15	0.47
1:A:922:PHE:N	1:A:922:PHE:CD1	2.83	0.47
1:A:1051:LEU:CD1	1:B:1047:GLN:HE21	2.11	0.47
1:B:812:TYR:O	1:B:816:ILE:HG12	2.15	0.47
1:B:819:VAL:HG12	1:B:819:VAL:O	2.14	0.47
1:B:867:LEU:O	1:B:870:LEU:HB3	2.15	0.47
1:B:878:ILE:HD12	1:B:878:ILE:HA	1.80	0.47
1:C:640:PHE:CD2	1:C:642:MET:HB3	2.47	0.47
1:C:693:ASN:O	1:C:695:ILE:HG22	2.14	0.47
1:C:922:PHE:HD1	1:C:922:PHE:N	2.13	0.47
1:D:652:ARG:NH1	1:D:702:VAL:O	2.42	0.47
1:D:819:VAL:HG12	1:D:819:VAL:O	2.14	0.47
1:D:923:LEU:HD11	1:A:897:PRO:HB3	1.97	0.47
1:B:649:LYS:HA	1:B:1005:VAL:O	2.15	0.47
1:B:690:VAL:HG21	1:B:977:ALA:HB2	1.97	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:819:VAL:HG12	1:C:819:VAL:O	2.14	0.47
1:D:534:LEU:HD22	1:D:570:HIS:ND1	2.30	0.47
1:D:591:LYS:N	1:D:591:LYS:HD2	2.29	0.47
1:D:615:ASN:HA	1:D:616:SER:HA	1.50	0.47
1:D:690:VAL:HG21	1:D:977:ALA:HB2	1.97	0.47
1:A:693:ASN:O	1:A:695:ILE:HG22	2.14	0.47
1:A:808:GLU:O	1:A:812:TYR:HD2	1.97	0.47
1:A:839:VAL:O	1:A:842:TYR:HB3	2.15	0.47
1:A:922:PHE:N	1:A:922:PHE:HD1	2.13	0.47
1:B:693:ASN:O	1:B:695:ILE:HG22	2.14	0.47
1:D:589:HIS:O	1:D:591:LYS:NZ	2.39	0.47
1:A:1042:MET:SD	1:A:1042:MET:C	2.93	0.47
1:B:659:ASN:C	1:B:660:PHE:HD1	2.19	0.47
1:B:742:PRO:HA	1:B:832:TRP:HE1	1.80	0.47
1:B:808:GLU:O	1:B:812:TYR:HD2	1.97	0.47
1:B:1042:MET:O	1:B:1045:LEU:N	2.48	0.47
1:B:1066:LYS:HA	1:B:1069:ILE:HD12	1.97	0.47
1:C:922:PHE:N	1:C:922:PHE:CD1	2.83	0.47
1:C:1042:MET:O	1:C:1045:LEU:N	2.48	0.47
1:D:526:TYR:O	1:D:530:MET:HE3	2.15	0.46
1:D:693:ASN:O	1:D:695:ILE:HG22	2.14	0.46
1:D:742:PRO:HA	1:D:832:TRP:HE1	1.81	0.46
1:D:922:PHE:N	1:D:922:PHE:HD1	2.13	0.46
1:D:1057:LEU:O	1:D:1057:LEU:HD23	2.15	0.46
1:A:682:PRO:O	1:A:683:LEU:HB2	2.15	0.46
1:B:652:ARG:NH1	1:B:702:VAL:O	2.41	0.46
1:C:534:LEU:HD22	1:C:570:HIS:ND1	2.30	0.46
1:C:1066:LYS:HA	1:C:1069:ILE:HD12	1.97	0.46
1:D:649:LYS:HA	1:D:1005:VAL:O	2.15	0.46
1:D:1042:MET:O	1:D:1045:LEU:N	2.48	0.46
1:A:534:LEU:HD22	1:A:570:HIS:ND1	2.30	0.46
1:B:534:LEU:HD22	1:B:570:HIS:ND1	2.30	0.46
1:B:658:TYR:N	1:B:659:ASN:HA	2.30	0.46
1:B:707:LEU:O	1:B:711:TRP:HB2	2.16	0.46
1:B:745:ALA:O	1:B:746:PHE:HB2	2.14	0.46
1:C:649:LYS:HA	1:C:1005:VAL:O	2.15	0.46
1:D:658:TYR:N	1:D:659:ASN:HA	2.30	0.46
1:D:1074:ILE:H	1:A:458:ARG:NH2	2.13	0.46
1:B:547:ASP:OD1	1:B:547:ASP:N	2.48	0.46
1:C:659:ASN:C	1:C:660:PHE:HD1	2.19	0.46
1:D:468:ASP:N	1:D:469:ILE:HA	2.23	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:839:VAL:O	1:D:842:TYR:HB3	2.15	0.46
1:D:1042:MET:SD	1:D:1042:MET:C	2.93	0.46
1:A:557:ARG:O	1:A:592:ARG:NE	2.48	0.46
1:A:658:TYR:N	1:A:659:ASN:HA	2.30	0.46
1:A:1042:MET:O	1:A:1045:LEU:N	2.48	0.46
1:A:1057:LEU:HD23	1:A:1057:LEU:O	2.15	0.46
1:B:839:VAL:O	1:B:842:TYR:HB3	2.15	0.46
1:C:557:ARG:O	1:C:592:ARG:NE	2.48	0.46
1:D:659:ASN:C	1:D:660:PHE:HD1	2.19	0.46
1:A:496:LYS:HA	1:A:496:LYS:HZ3	1.80	0.46
1:A:742:PRO:HA	1:A:832:TRP:HE1	1.80	0.46
1:B:602:SER:HA	1:B:603:LYS:HA	1.48	0.46
1:C:808:GLU:O	1:C:812:TYR:HD2	1.97	0.46
1:C:839:VAL:O	1:C:842:TYR:HB3	2.15	0.46
1:D:808:GLU:O	1:D:812:TYR:HD2	1.97	0.46
1:D:812:TYR:O	1:D:816:ILE:HG12	2.15	0.46
1:D:922:PHE:N	1:D:922:PHE:CD1	2.83	0.46
1:A:550:THR:O	1:A:553:HIS:N	2.48	0.46
1:B:550:THR:O	1:B:553:HIS:N	2.48	0.46
1:C:682:PRO:O	1:C:683:LEU:HB2	2.15	0.46
1:C:742:PRO:HA	1:C:832:TRP:HE1	1.80	0.46
1:D:707:LEU:O	1:D:711:TRP:HB2	2.16	0.46
1:A:659:ASN:C	1:A:660:PHE:HD1	2.19	0.46
1:B:682:PRO:O	1:B:683:LEU:HB2	2.15	0.46
1:D:547:ASP:OD1	1:D:547:ASP:N	2.48	0.46
1:D:632:GLU:OE1	1:D:700:HIS:ND1	2.49	0.46
1:D:820:LEU:O	1:D:823:PHE:N	2.46	0.46
1:A:1074:ILE:H	1:B:458:ARG:NH2	2.14	0.46
1:C:707:LEU:O	1:C:711:TRP:HB2	2.16	0.46
1:D:1066:LYS:HA	1:D:1069:ILE:HD12	1.97	0.46
1:A:632:GLU:OE1	1:A:700:HIS:ND1	2.49	0.46
1:A:707:LEU:O	1:A:711:TRP:HB2	2.16	0.46
1:B:557:ARG:O	1:B:592:ARG:NE	2.48	0.46
1:A:856:CYS:O	1:A:858:ILE:N	2.49	0.46
1:B:526:TYR:O	1:B:530:MET:HE3	2.16	0.46
1:B:922:PHE:N	1:B:922:PHE:CD1	2.83	0.46
1:C:1057:LEU:HD23	1:C:1057:LEU:O	2.15	0.46
1:B:1051:LEU:HD22	1:C:1047:GLN:HE22	1.82	0.45
1:B:913:LEU:O	1:B:913:LEU:HD12	2.17	0.45
1:D:446:LYS:HA	1:D:447:LYS:HA	1.54	0.45
1:D:640:PHE:CD2	1:D:642:MET:HB3	2.47	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:682:PRO:O	1:D:683:LEU:HB2	2.15	0.45
1:D:852:ARG:HD3	1:D:982:LEU:HG	1.98	0.45
1:A:640:PHE:CD2	1:A:642:MET:HB3	2.47	0.45
1:A:815:GLY:O	1:A:818:PHE:HB3	2.16	0.45
1:B:808:GLU:O	1:B:812:TYR:CD2	2.70	0.45
1:C:652:ARG:NH1	1:C:702:VAL:O	2.42	0.45
1:C:812:TYR:O	1:C:816:ILE:HG12	2.15	0.45
1:C:856:CYS:O	1:C:858:ILE:N	2.49	0.45
1:C:913:LEU:HD12	1:C:913:LEU:O	2.17	0.45
1:D:815:GLY:O	1:D:818:PHE:HB3	2.16	0.45
1:A:526:TYR:O	1:A:530:MET:HE3	2.17	0.45
1:A:913:LEU:HD12	1:A:913:LEU:O	2.17	0.45
1:B:533:ILE:O	1:B:536:THR:OG1	2.34	0.45
1:B:632:GLU:OE1	1:B:700:HIS:ND1	2.49	0.45
1:C:658:TYR:N	1:C:659:ASN:HA	2.30	0.45
1:C:925:PRO:O	1:C:929:ASN:N	2.48	0.45
1:D:557:ARG:O	1:D:592:ARG:NE	2.48	0.45
1:A:602:SER:HA	1:A:603:LYS:HA	1.48	0.45
1:C:527:THR:OG1	1:C:528:GLN:N	2.50	0.45
1:C:815:GLY:O	1:C:818:PHE:HB3	2.16	0.45
1:D:1050:ARG:HH12	1:C:1048:LYS:HZ1	1.64	0.45
1:A:808:GLU:O	1:A:812:TYR:CD2	2.70	0.45
1:A:1048:LYS:HZ1	1:B:1050:ARG:NH1	2.14	0.45
1:C:856:CYS:O	1:C:859:PHE:N	2.46	0.45
1:D:856:CYS:O	1:D:858:ILE:N	2.49	0.45
1:B:815:GLY:O	1:B:818:PHE:HB3	2.16	0.45
1:B:852:ARG:O	1:B:853:PHE:HB2	2.16	0.45
1:D:533:ILE:O	1:D:536:THR:OG1	2.34	0.45
1:A:615:ASN:HA	1:A:616:SER:HA	1.50	0.45
1:C:533:ILE:O	1:C:536:THR:OG1	2.34	0.45
1:C:820:LEU:O	1:C:823:PHE:N	2.46	0.45
1:A:852:ARG:O	1:A:853:PHE:HB2	2.16	0.45
1:A:876:VAL:HG11	1:B:859:PHE:CE2	2.52	0.45
1:B:1057:LEU:O	1:B:1057:LEU:HD23	2.15	0.45
1:C:808:GLU:O	1:C:812:TYR:CD2	2.70	0.45
1:C:852:ARG:O	1:C:853:PHE:HB2	2.16	0.45
1:D:527:THR:OG1	1:D:528:GLN:N	2.50	0.45
1:A:553:HIS:ND1	1:A:583:PHE:HB3	2.32	0.45
1:A:618:GLY:HA2	1:A:619:ASN:HA	1.61	0.45
1:A:871:LEU:HA	1:A:874:THR:HG22	1.99	0.45
1:A:1051:LEU:HD22	1:B:1047:GLN:HE22	1.82	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:THR:HG22	1:B:517:ALA:N	2.27	0.45
1:A:533:ILE:O	1:A:536:THR:OG1	2.34	0.44
1:B:631:PRO:O	1:B:632:GLU:C	2.56	0.44
1:B:852:ARG:HD3	1:B:982:LEU:HG	1.98	0.44
1:C:526:TYR:O	1:C:530:MET:HE3	2.16	0.44
1:C:631:PRO:O	1:C:632:GLU:C	2.56	0.44
1:C:632:GLU:OE1	1:C:700:HIS:ND1	2.49	0.44
1:C:878:ILE:HD12	1:C:878:ILE:HA	1.80	0.44
1:D:553:HIS:ND1	1:D:583:PHE:HB3	2.32	0.44
1:D:596:VAL:HA	1:D:599:ILE:HG22	1.99	0.44
1:B:856:CYS:O	1:B:858:ILE:N	2.49	0.44
1:C:728:LEU:O	1:C:732:PRO:HG2	2.17	0.44
1:D:852:ARG:O	1:D:853:PHE:HB2	2.16	0.44
1:B:640:PHE:CD2	1:B:642:MET:HB3	2.47	0.44
1:C:695:ILE:HB	1:C:973:LEU:HD21	1.99	0.44
1:C:820:LEU:HD23	1:C:820:LEU:HA	1.74	0.44
1:D:808:GLU:O	1:D:812:TYR:CD2	2.70	0.44
1:A:695:ILE:HB	1:A:973:LEU:HD21	1.99	0.44
1:D:913:LEU:HD12	1:D:913:LEU:O	2.17	0.44
1:B:695:ILE:HB	1:B:973:LEU:HD21	1.99	0.44
1:C:852:ARG:HD3	1:C:982:LEU:HG	1.98	0.44
1:D:550:THR:O	1:D:553:HIS:N	2.48	0.44
1:A:558:GLU:H	1:A:558:GLU:HG2	1.64	0.44
1:A:596:VAL:HA	1:A:599:ILE:HG22	1.99	0.44
1:A:652:ARG:NH1	1:A:702:VAL:O	2.42	0.44
1:B:728:LEU:O	1:B:732:PRO:HG2	2.17	0.44
1:C:553:HIS:ND1	1:C:583:PHE:HB3	2.32	0.44
1:C:871:LEU:HA	1:C:874:THR:HG22	1.99	0.44
1:D:458:ARG:NH2	1:C:1074:ILE:H	2.15	0.44
1:D:631:PRO:O	1:D:632:GLU:C	2.56	0.44
1:D:886:LEU:O	1:D:889:TYR:HB3	2.18	0.44
1:D:1048:LYS:HZ3	1:A:1050:ARG:HH22	1.64	0.44
1:A:527:THR:OG1	1:A:528:GLN:N	2.50	0.44
1:B:553:HIS:ND1	1:B:583:PHE:HB3	2.32	0.44
1:B:876:VAL:HG11	1:C:859:PHE:CE2	2.53	0.44
1:C:446:LYS:HA	1:C:447:LYS:HA	1.54	0.44
1:C:496:LYS:HA	1:C:496:LYS:HZ2	1.81	0.44
1:D:518:LEU:HD11	1:D:530:MET:HG3	2.00	0.44
1:A:631:PRO:O	1:A:632:GLU:C	2.56	0.44
1:B:527:THR:OG1	1:B:528:GLN:N	2.50	0.44
1:B:615:ASN:HA	1:B:616:SER:HA	1.50	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:886:LEU:O	1:B:889:TYR:HB3	2.18	0.44
1:C:886:LEU:O	1:C:889:TYR:HB3	2.18	0.44
1:B:871:LEU:HA	1:B:874:THR:HG22	1.99	0.44
1:D:695:ILE:HB	1:D:973:LEU:HD21	1.99	0.43
1:A:852:ARG:HD3	1:A:982:LEU:HG	1.98	0.43
1:B:1042:MET:O	1:B:1043:GLU:C	2.57	0.43
1:C:596:VAL:HA	1:C:599:ILE:HG22	1.99	0.43
1:D:728:LEU:O	1:D:732:PRO:HG2	2.17	0.43
1:D:768:TYR:O	1:D:772:THR:HG23	2.18	0.43
1:D:933:HIS:NE2	1:A:833:GLN:CB	2.81	0.43
1:A:710:LYS:HG3	1:A:711:TRP:H	1.83	0.43
1:A:728:LEU:O	1:A:732:PRO:HG2	2.17	0.43
1:C:518:LEU:HD11	1:C:530:MET:HG3	2.00	0.43
1:D:709:MET:O	1:D:712:LEU:HB3	2.18	0.43
1:D:856:CYS:O	1:D:859:PHE:N	2.46	0.43
1:D:871:LEU:HA	1:D:874:THR:HG22	1.99	0.43
1:D:1047:GLN:HE22	1:C:1051:LEU:HD22	1.83	0.43
1:A:709:MET:O	1:A:712:LEU:HB3	2.18	0.43
1:A:768:TYR:O	1:A:772:THR:HG23	2.19	0.43
1:A:621:CYS:SG	1:A:622:PRO:HD3	2.58	0.43
1:A:1042:MET:O	1:A:1043:GLU:C	2.57	0.43
1:B:496:LYS:HA	1:B:496:LYS:HZ2	1.80	0.43
1:B:621:CYS:SG	1:B:622:PRO:HD3	2.58	0.43
1:B:710:LYS:HG3	1:B:711:TRP:H	1.84	0.43
1:A:818:PHE:HD2	1:A:835:GLY:CA	2.32	0.43
1:C:502:LEU:HA	1:C:505:GLY:HA2	2.01	0.43
1:C:743:GLY:N	1:C:832:TRP:HE1	2.14	0.43
1:C:768:TYR:O	1:C:772:THR:HG23	2.18	0.43
1:C:1070:GLN:O	1:C:1070:GLN:NE2	2.52	0.43
1:A:997:LYS:CB	1:A:998:VAL:HA	2.46	0.43
1:B:618:GLY:HA2	1:B:619:ASN:HA	1.61	0.43
1:C:656:ILE:H	1:C:656:ILE:HG13	1.64	0.43
1:C:709:MET:O	1:C:712:LEU:HB3	2.19	0.43
1:D:874:THR:O	1:D:878:ILE:HB	2.19	0.43
1:B:596:VAL:HA	1:B:599:ILE:HG22	1.99	0.43
1:B:1074:ILE:H	1:C:458:ARG:NH2	2.17	0.43
1:C:710:LYS:HG3	1:C:711:TRP:H	1.84	0.43
1:D:502:LEU:HA	1:D:505:GLY:HA2	2.01	0.43
1:D:621:CYS:SG	1:D:622:PRO:HD3	2.58	0.43
1:D:632:GLU:OE1	1:D:632:GLU:HA	2.19	0.43
1:B:611:ILE:O	1:B:612:PHE:HB2	2.19	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:709:MET:O	1:B:712:LEU:HB3	2.18	0.43
1:B:818:PHE:HD2	1:B:835:GLY:CA	2.32	0.43
1:B:997:LYS:CB	1:B:998:VAL:HA	2.46	0.43
1:C:457:GLY:HA3	1:C:494:HIS:CD2	2.54	0.43
1:C:611:ILE:O	1:C:612:PHE:HB2	2.19	0.43
1:D:1070:GLN:O	1:D:1070:GLN:NE2	2.52	0.43
1:A:632:GLU:OE1	1:A:632:GLU:HA	2.19	0.43
1:A:874:THR:O	1:A:878:ILE:HB	2.19	0.43
1:C:1042:MET:O	1:C:1043:GLU:C	2.57	0.43
1:D:457:GLY:HA3	1:D:494:HIS:CD2	2.54	0.43
1:D:936:LEU:HD13	1:A:837:ILE:HD11	2.01	0.43
1:A:603:LYS:HE2	1:A:603:LYS:HB2	1.77	0.43
1:A:730:LEU:N	1:A:842:TYR:OH	2.52	0.43
1:B:502:LEU:HA	1:B:505:GLY:HA2	2.01	0.43
1:B:518:LEU:HD11	1:B:530:MET:HG3	2.00	0.43
1:B:632:GLU:OE1	1:B:632:GLU:HA	2.19	0.43
1:B:730:LEU:N	1:B:842:TYR:OH	2.52	0.43
1:B:925:PRO:O	1:B:929:ASN:N	2.48	0.43
1:C:621:CYS:SG	1:C:622:PRO:HD3	2.58	0.43
1:C:931:LEU:HD12	1:C:931:LEU:O	2.19	0.43
1:D:730:LEU:N	1:D:842:TYR:OH	2.52	0.42
1:D:909:PHE:CE2	1:C:942:VAL:HG23	2.54	0.42
1:A:502:LEU:HA	1:A:505:GLY:HA2	2.01	0.42
1:C:895:GLN:NE2	1:C:896:ASP:O	2.52	0.42
1:D:611:ILE:O	1:D:612:PHE:HB2	2.19	0.42
1:D:916:ILE:CG2	1:D:919:ARG:HB2	2.50	0.42
1:D:1051:LEU:HD22	1:A:1047:GLN:HE22	1.84	0.42
1:A:518:LEU:HD11	1:A:530:MET:HG3	2.00	0.42
1:A:811:ILE:HD12	1:A:842:TYR:HA	2.01	0.42
1:A:886:LEU:O	1:A:889:TYR:HB3	2.18	0.42
1:A:1070:GLN:O	1:A:1070:GLN:NE2	2.52	0.42
1:B:457:GLY:HA3	1:B:494:HIS:CD2	2.54	0.42
1:B:695:ILE:HG21	1:B:973:LEU:HD11	2.02	0.42
1:C:695:ILE:HG21	1:C:973:LEU:HD11	2.02	0.42
1:D:584:LEU:HD22	1:D:619:ASN:OD1	2.20	0.42
1:D:629:TYR:N	1:D:697:LEU:HD11	2.23	0.42
1:D:695:ILE:HG21	1:D:973:LEU:HD11	2.02	0.42
1:D:743:GLY:N	1:D:832:TRP:HE1	2.14	0.42
1:B:973:LEU:HA	1:B:973:LEU:HD23	1.86	0.42
1:C:584:LEU:HD22	1:C:619:ASN:OD1	2.20	0.42
1:C:874:THR:O	1:C:878:ILE:HB	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:850:LEU:HD23	1:D:850:LEU:HA	1.79	0.42
1:D:895:GLN:NE2	1:D:896:ASP:O	2.52	0.42
1:D:1048:LYS:HZ1	1:A:1050:ARG:NH1	2.17	0.42
1:B:468:ASP:N	1:B:469:ILE:HA	2.23	0.42
1:B:811:ILE:HD12	1:B:842:TYR:HA	2.01	0.42
1:B:829:HIS:ND1	1:B:829:HIS:C	2.73	0.42
1:C:719:HIS:NE2	1:C:852:ARG:HD2	2.35	0.42
1:C:730:LEU:N	1:C:842:TYR:OH	2.52	0.42
1:D:597:LEU:HD13	1:D:601:ARG:HH12	1.84	0.42
1:D:736:LEU:HD13	1:D:773:CYS:SG	2.60	0.42
1:A:611:ILE:O	1:A:612:PHE:HB2	2.19	0.42
1:A:990:LEU:HA	1:A:991:PRO:HD3	1.88	0.42
1:B:768:TYR:O	1:B:772:THR:HG23	2.18	0.42
1:D:818:PHE:HD2	1:D:835:GLY:CA	2.32	0.42
1:A:695:ILE:HG21	1:A:973:LEU:HD11	2.02	0.42
1:A:916:ILE:CG2	1:A:919:ARG:HB2	2.50	0.42
1:B:719:HIS:NE2	1:B:852:ARG:HD2	2.35	0.42
1:B:874:THR:O	1:B:878:ILE:HB	2.19	0.42
1:C:948:VAL:HB	1:C:949:PRO:HD3	2.02	0.42
1:D:931:LEU:HD12	1:D:931:LEU:O	2.19	0.42
1:A:584:LEU:HD22	1:A:619:ASN:OD1	2.20	0.42
1:A:719:HIS:NE2	1:A:852:ARG:HD2	2.35	0.42
1:B:948:VAL:HB	1:B:949:PRO:HD3	2.02	0.42
1:B:1070:GLN:O	1:B:1070:GLN:NE2	2.52	0.42
1:C:512:HIS:CD2	1:C:512:HIS:C	2.93	0.42
1:D:948:VAL:HB	1:D:949:PRO:HD3	2.02	0.42
1:D:1042:MET:O	1:D:1043:GLU:C	2.57	0.42
1:A:457:GLY:HA3	1:A:494:HIS:CD2	2.54	0.42
1:A:597:LEU:HD13	1:A:601:ARG:HH12	1.84	0.42
1:A:829:HIS:ND1	1:A:829:HIS:C	2.72	0.42
1:B:931:LEU:HD12	1:B:931:LEU:O	2.20	0.42
1:C:632:GLU:OE1	1:C:632:GLU:HA	2.19	0.42
1:D:602:SER:HA	1:D:603:LYS:HA	1.48	0.42
1:D:710:LYS:HG3	1:D:711:TRP:H	1.84	0.42
1:D:829:HIS:ND1	1:D:829:HIS:C	2.73	0.42
1:A:931:LEU:HD12	1:A:931:LEU:O	2.19	0.42
1:B:916:ILE:CG2	1:B:919:ARG:HB2	2.49	0.42
1:C:736:LEU:HD13	1:C:773:CYS:SG	2.60	0.42
1:C:916:ILE:CG2	1:C:919:ARG:HB2	2.49	0.42
1:D:512:HIS:CD2	1:D:512:HIS:C	2.93	0.42
1:D:874:THR:HA	1:D:877:PHE:CE2	2.55	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:895:GLN:NE2	1:A:896:ASP:O	2.52	0.42
1:A:923:LEU:CD1	1:B:897:PRO:HB3	2.50	0.42
1:C:550:THR:O	1:C:553:HIS:N	2.47	0.42
1:C:829:HIS:ND1	1:C:829:HIS:C	2.73	0.42
1:D:684:THR:O	1:D:687:ASN:HB3	2.20	0.41
1:A:719:HIS:CD2	1:A:852:ARG:HD2	2.55	0.41
1:A:731:ILE:H	1:A:731:ILE:HG13	1.69	0.41
1:A:949:PRO:HB3	1:B:913:LEU:CD1	2.50	0.41
1:A:970:HIS:HE1	1:A:974:LYS:NZ	2.18	0.41
1:B:862:MET:SD	1:B:964:ILE:HG23	2.60	0.41
1:B:975:ARG:HG2	1:B:976:ILE:HD13	2.02	0.41
1:C:580:GLN:HG3	1:C:615:ASN:O	2.20	0.41
1:C:629:TYR:N	1:C:697:LEU:HD11	2.23	0.41
1:C:684:THR:O	1:C:687:ASN:HB3	2.20	0.41
1:A:512:HIS:CD2	1:A:512:HIS:C	2.93	0.41
1:A:736:LEU:HD13	1:A:773:CYS:SG	2.60	0.41
1:A:874:THR:HA	1:A:877:PHE:CE2	2.55	0.41
1:A:948:VAL:HB	1:A:949:PRO:HD3	2.02	0.41
1:B:736:LEU:HD13	1:B:773:CYS:SG	2.60	0.41
1:B:949:PRO:HB3	1:C:913:LEU:CD1	2.50	0.41
1:D:719:HIS:CD2	1:D:852:ARG:HD2	2.55	0.41
1:A:891:LEU:O	1:A:892:LEU:HD13	2.20	0.41
1:A:919:ARG:O	1:A:919:ARG:HG3	2.20	0.41
1:C:597:LEU:HD13	1:C:601:ARG:HH12	1.84	0.41
1:D:862:MET:SD	1:D:964:ILE:HG23	2.60	0.41
1:A:635:LYS:HB2	1:A:635:LYS:HE2	1.81	0.41
1:A:923:LEU:CD2	1:B:897:PRO:HG3	2.49	0.41
1:B:895:GLN:NE2	1:B:896:ASP:O	2.52	0.41
1:B:919:ARG:O	1:B:919:ARG:HG3	2.20	0.41
1:C:891:LEU:O	1:C:892:LEU:HD13	2.20	0.41
1:D:997:LYS:CB	1:D:998:VAL:HA	2.46	0.41
1:A:580:GLN:HG3	1:A:615:ASN:O	2.20	0.41
1:B:554:PHE:O	1:B:557:ARG:N	2.54	0.41
1:B:580:GLN:HG3	1:B:615:ASN:O	2.20	0.41
1:B:584:LEU:HD22	1:B:619:ASN:OD1	2.20	0.41
1:B:595:VAL:O	1:B:598:THR:HG22	2.21	0.41
1:B:638:LEU:HD21	1:B:653:ASP:O	2.21	0.41
1:C:919:ARG:O	1:C:919:ARG:HG3	2.20	0.41
1:C:975:ARG:HG2	1:C:976:ILE:HD13	2.02	0.41
1:D:635:LYS:HE2	1:D:635:LYS:HB2	1.81	0.41
1:D:835:GLY:O	1:D:839:VAL:HG23	2.21	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1050:ARG:NH1	1:C:1048:LYS:HZ1	2.18	0.41
1:A:862:MET:SD	1:A:964:ILE:HG23	2.60	0.41
1:B:512:HIS:CD2	1:B:512:HIS:C	2.93	0.41
1:B:970:HIS:HE1	1:B:974:LYS:NZ	2.18	0.41
1:B:1075:ILE:HA	1:B:1076:SER:HA	1.94	0.41
1:C:874:THR:HA	1:C:877:PHE:CE2	2.55	0.41
1:D:719:HIS:NE2	1:D:852:ARG:HD2	2.35	0.41
1:D:859:PHE:CE2	1:C:876:VAL:HG11	2.55	0.41
1:A:835:GLY:O	1:A:839:VAL:HG23	2.21	0.41
1:A:468:ASP:N	1:A:469:ILE:HA	2.23	0.41
1:B:719:HIS:CD2	1:B:852:ARG:HD2	2.55	0.41
1:B:835:GLY:O	1:B:839:VAL:HG23	2.21	0.41
1:B:874:THR:HA	1:B:877:PHE:CE2	2.55	0.41
1:C:719:HIS:CD2	1:C:852:ARG:HD2	2.55	0.41
1:D:811:ILE:HD12	1:D:842:TYR:HA	2.02	0.41
1:D:919:ARG:O	1:D:919:ARG:HG3	2.20	0.41
1:A:554:PHE:O	1:A:557:ARG:N	2.54	0.41
1:A:638:LEU:HD21	1:A:653:ASP:O	2.21	0.41
1:A:684:THR:O	1:A:687:ASN:HB3	2.20	0.41
1:A:856:CYS:O	1:A:859:PHE:N	2.46	0.41
1:C:602:SER:HA	1:C:603:LYS:HA	1.48	0.41
1:C:635:LYS:HB2	1:C:635:LYS:HE2	1.81	0.41
1:C:638:LEU:HD21	1:C:653:ASP:O	2.21	0.41
1:C:811:ILE:HD12	1:C:842:TYR:HA	2.02	0.41
1:C:835:GLY:O	1:C:839:VAL:HG23	2.21	0.41
1:C:970:HIS:HE1	1:C:974:LYS:NZ	2.18	0.41
1:D:580:GLN:HG3	1:D:615:ASN:O	2.20	0.41
1:A:975:ARG:HG2	1:A:976:ILE:HD13	2.02	0.41
1:B:684:THR:O	1:B:687:ASN:HB3	2.20	0.41
1:B:891:LEU:O	1:B:892:LEU:HD13	2.20	0.41
1:C:616:SER:HA	1:C:617:PRO:HD3	1.90	0.41
1:C:862:MET:SD	1:C:964:ILE:HG23	2.60	0.41
1:C:953:MET:O	1:C:957:ILE:HG13	2.21	0.41
1:D:595:VAL:O	1:D:598:THR:HG22	2.21	0.40
1:D:626:MET:O	1:D:627:ILE:HG13	2.21	0.40
1:D:876:VAL:HG11	1:A:859:PHE:CE2	2.56	0.40
1:D:990:LEU:HD21	1:D:994:PHE:HD2	1.86	0.40
1:C:595:VAL:O	1:C:598:THR:HG22	2.21	0.40
1:C:818:PHE:HD2	1:C:835:GLY:CA	2.32	0.40
1:C:850:LEU:HD23	1:C:850:LEU:HA	1.79	0.40
1:D:554:PHE:O	1:D:557:ARG:N	2.54	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:891:LEU:O	1:D:892:LEU:HD13	2.20	0.40
1:D:913:LEU:CD1	1:C:949:PRO:HB3	2.51	0.40
1:D:970:HIS:HE1	1:D:974:LYS:NZ	2.18	0.40
1:A:990:LEU:HD21	1:A:994:PHE:HD2	1.86	0.40
1:C:851:GLN:HA	1:C:860:ILE:HD13	2.04	0.40
1:D:603:LYS:HB2	1:D:603:LYS:HE2	1.77	0.40
1:A:595:VAL:O	1:A:598:THR:HG22	2.21	0.40
1:A:626:MET:O	1:A:627:ILE:HG13	2.21	0.40
1:B:603:LYS:HE2	1:B:603:LYS:HB2	1.77	0.40
1:D:814:THR:HG21	1:D:838:ALA:HA	2.03	0.40
1:D:975:ARG:HG2	1:D:976:ILE:HD13	2.02	0.40
1:B:942:VAL:HG23	1:C:909:PHE:CE2	2.57	0.40
1:D:638:LEU:HD21	1:D:653:ASP:O	2.21	0.40
1:D:851:GLN:HA	1:D:860:ILE:HD13	2.04	0.40
1:D:953:MET:O	1:D:957:ILE:HG13	2.21	0.40
1:D:1050:ARG:HH22	1:C:1048:LYS:HZ3	1.69	0.40
1:D:1067:LEU:HD13	1:D:1067:LEU:O	2.22	0.40
1:B:953:MET:O	1:B:957:ILE:HG13	2.21	0.40
1:B:990:LEU:HD21	1:B:994:PHE:HD2	1.86	0.40
1:C:990:LEU:HD21	1:C:994:PHE:HD2	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	550/1528 (36%)	485 (88%)	56 (10%)	9 (2%)	9	45
1	B	550/1528 (36%)	485 (88%)	56 (10%)	9 (2%)	9	45
1	C	550/1528 (36%)	485 (88%)	56 (10%)	9 (2%)	9	45
1	D	550/1528 (36%)	485 (88%)	56 (10%)	9 (2%)	9	45
All	All	2200/6112 (36%)	1940 (88%)	224 (10%)	36 (2%)	13	45

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	580	GLN
1	D	639	ASP
1	A	580	GLN
1	A	639	ASP
1	B	580	GLN
1	B	639	ASP
1	C	580	GLN
1	C	639	ASP
1	D	746	PHE
1	D	853	PHE
1	D	1075	ILE
1	A	746	PHE
1	A	853	PHE
1	A	1075	ILE
1	B	746	PHE
1	B	853	PHE
1	B	1075	ILE
1	C	746	PHE
1	C	853	PHE
1	C	1075	ILE
1	D	828	ALA
1	D	948	VAL
1	A	828	ALA
1	A	948	VAL
1	B	828	ALA
1	B	948	VAL
1	C	828	ALA
1	C	948	VAL
1	D	684	THR
1	A	684	THR
1	B	684	THR
1	C	684	THR
1	D	821	PRO
1	A	821	PRO
1	B	821	PRO
1	C	821	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	415/1325 (31%)	405 (98%)	10 (2%)	49	69
1	B	415/1325 (31%)	405 (98%)	10 (2%)	49	69
1	C	415/1325 (31%)	405 (98%)	10 (2%)	49	69
1	D	415/1325 (31%)	405 (98%)	10 (2%)	49	69
All	All	1660/5300 (31%)	1620 (98%)	40 (2%)	51	69

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	480	LEU
1	D	536	THR
1	D	620	LYS
1	D	690	VAL
1	D	706	TYR
1	D	768	TYR
1	D	785	TYR
1	D	829	HIS
1	D	832	TRP
1	D	1042	MET
1	A	480	LEU
1	A	536	THR
1	A	620	LYS
1	A	690	VAL
1	A	706	TYR
1	A	768	TYR
1	A	785	TYR
1	A	829	HIS
1	A	832	TRP
1	A	1042	MET
1	B	480	LEU
1	B	536	THR
1	B	620	LYS
1	B	690	VAL
1	B	706	TYR
1	B	768	TYR
1	B	785	TYR
1	B	829	HIS
1	B	832	TRP
1	B	1042	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	480	LEU
1	C	536	THR
1	C	620	LYS
1	C	690	VAL
1	C	706	TYR
1	C	768	TYR
1	C	785	TYR
1	C	829	HIS
1	C	832	TRP
1	C	1042	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	954	ASN
1	D	1047	GLN
1	D	1061	GLN
1	A	1047	GLN
1	B	1047	GLN
1	B	1061	GLN
1	C	1047	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

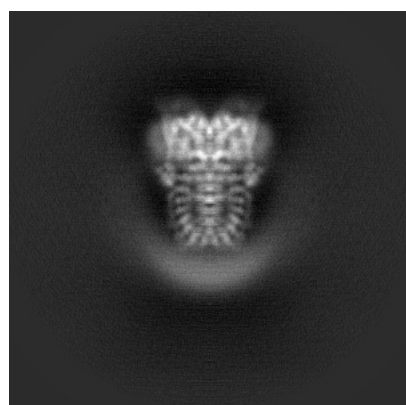
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6267. These allow visual inspection of the internal detail of the map and identification of artifacts.

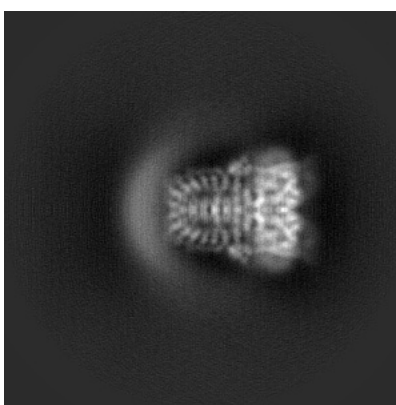
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

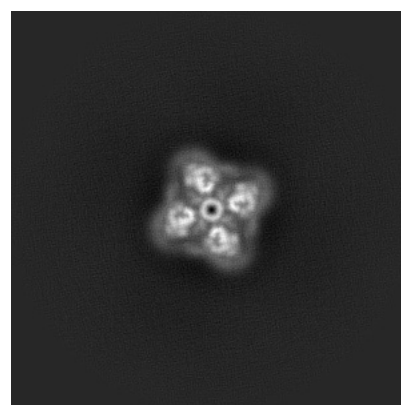
#### 6.1.1 Primary map



X



Y

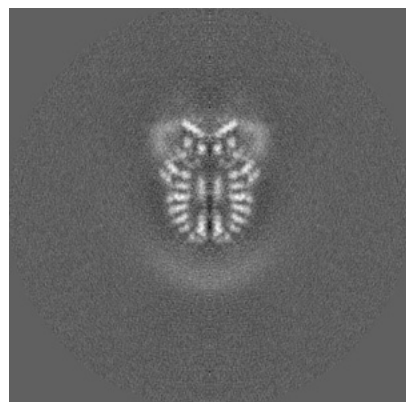


Z

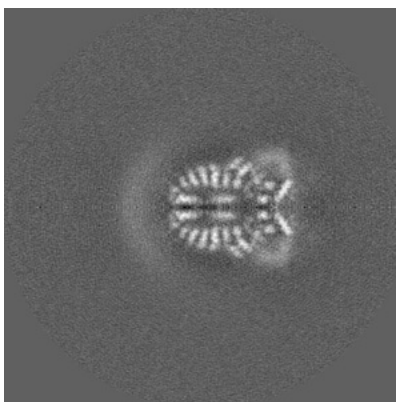
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

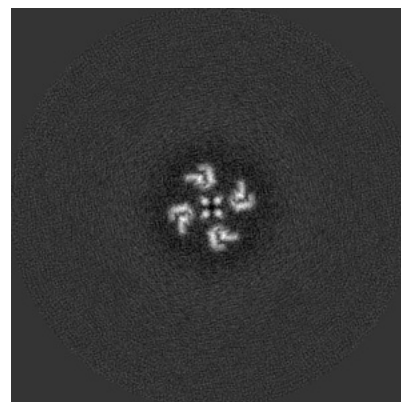
#### 6.2.1 Primary map



X Index: 150



Y Index: 150

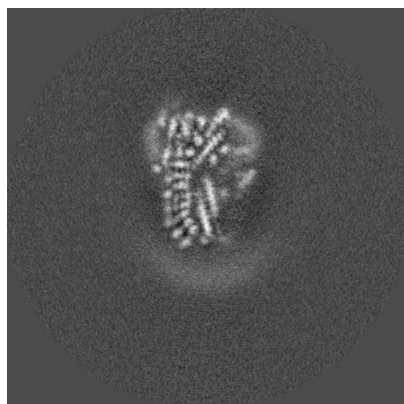


Z Index: 150

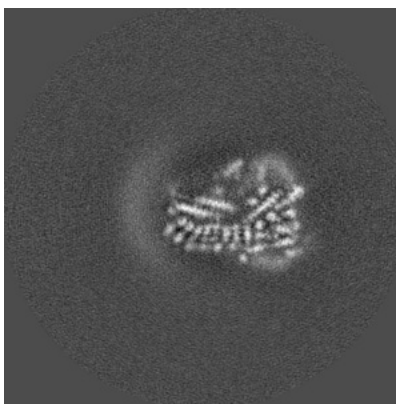
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

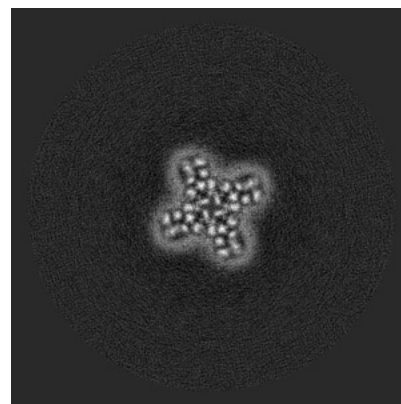
### 6.3.1 Primary map



X Index: 156



Y Index: 144



Z Index: 212

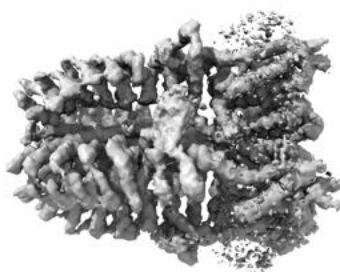
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

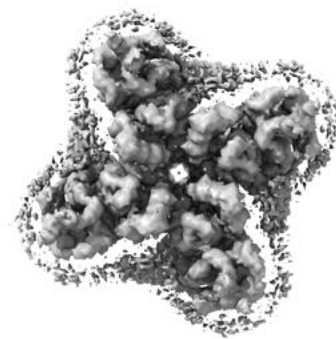
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 8.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

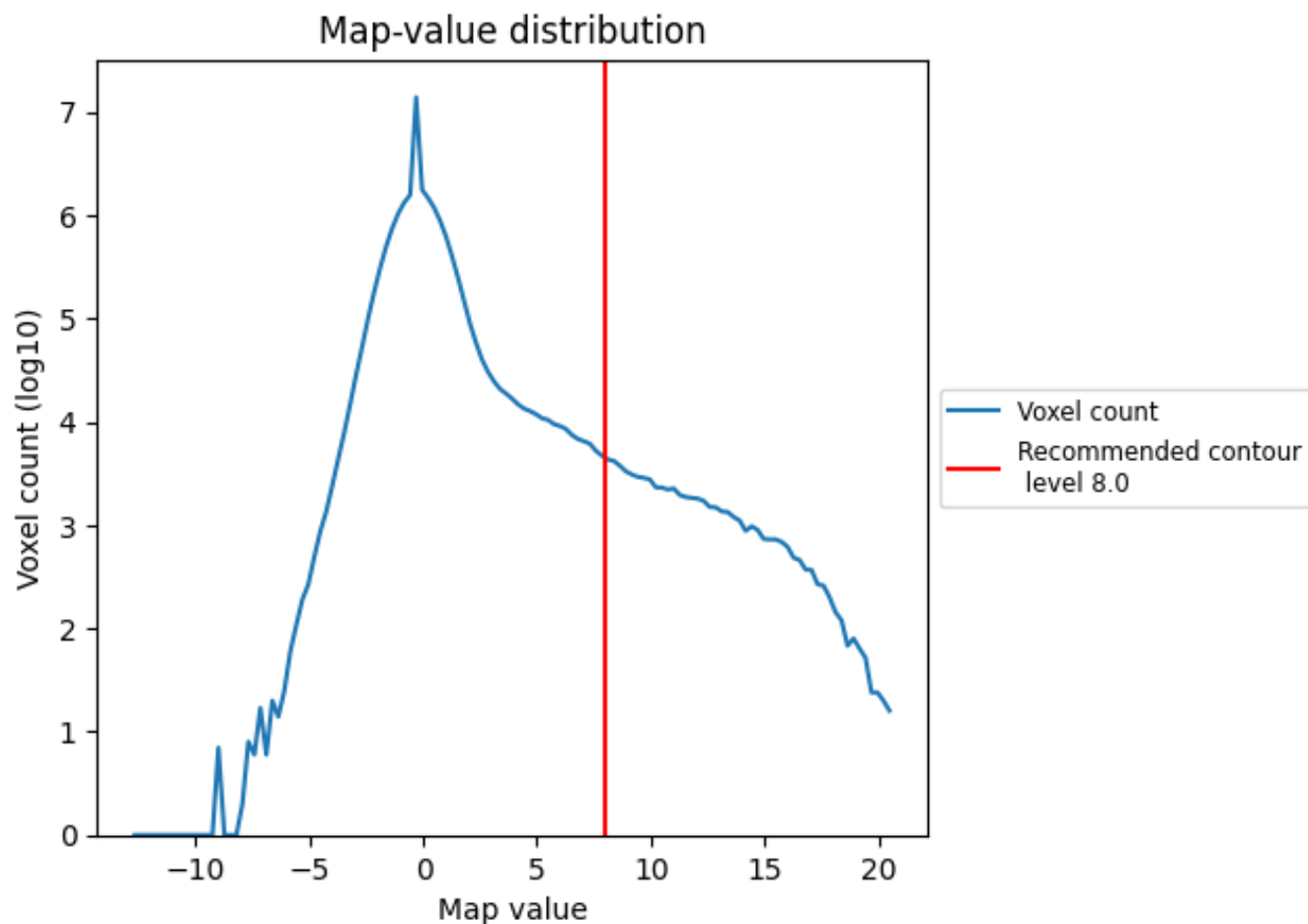
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

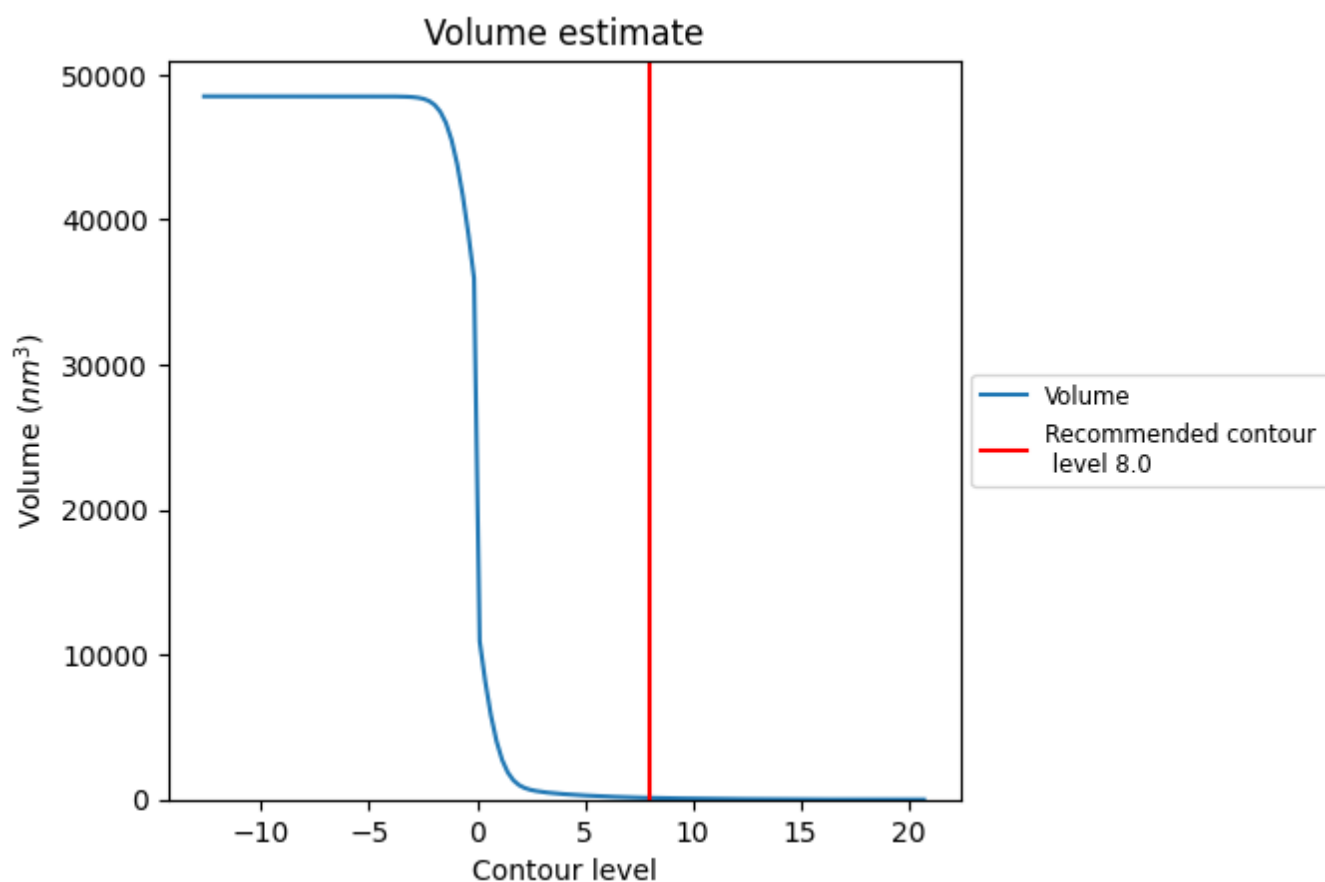
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

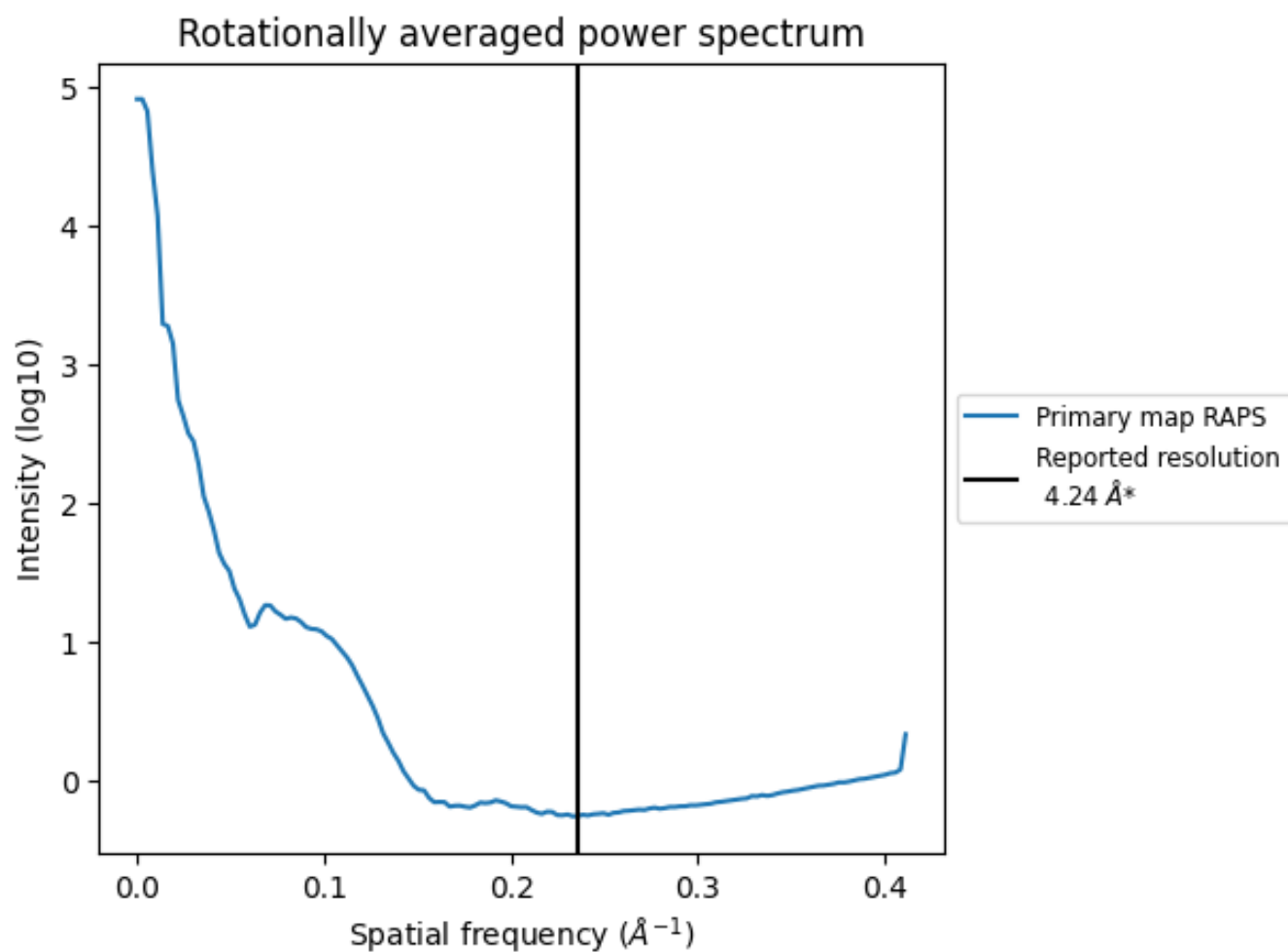
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 117 nm<sup>3</sup>; this corresponds to an approximate mass of 105 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 0.236  $\text{\AA}^{-1}$

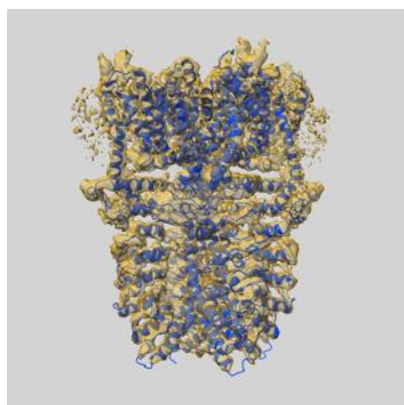
## 8 Fourier-Shell correlation

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

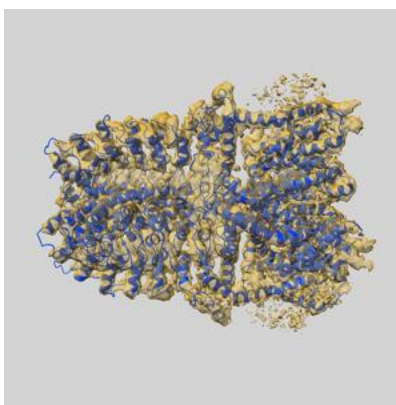
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6267 and PDB model 3J9P. Per-residue inclusion information can be found in section [3](#) on page [8](#).

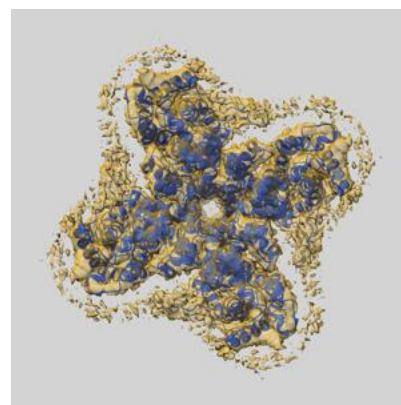
### 9.1 Map-model overlay [i](#)



X



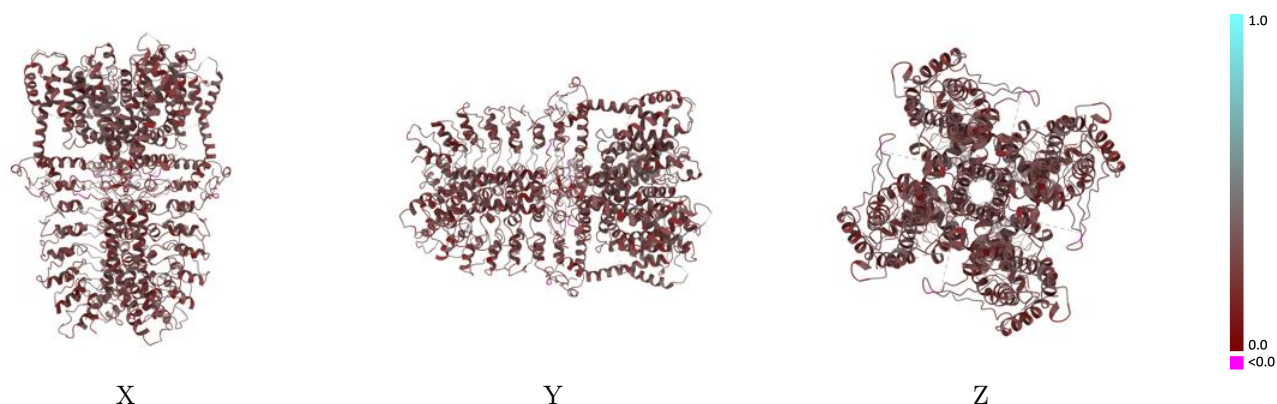
Y



Z

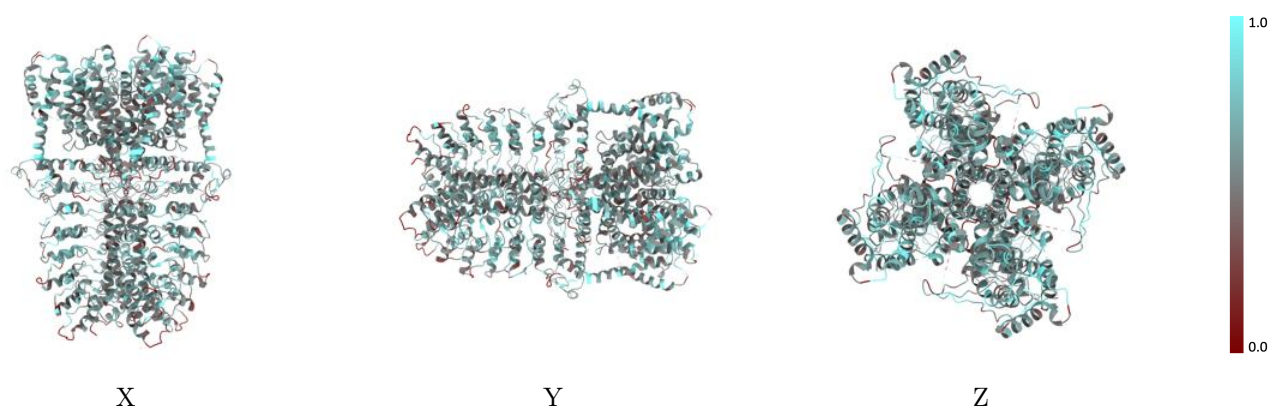
The images above show the 3D surface view of the map at the recommended contour level 8.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



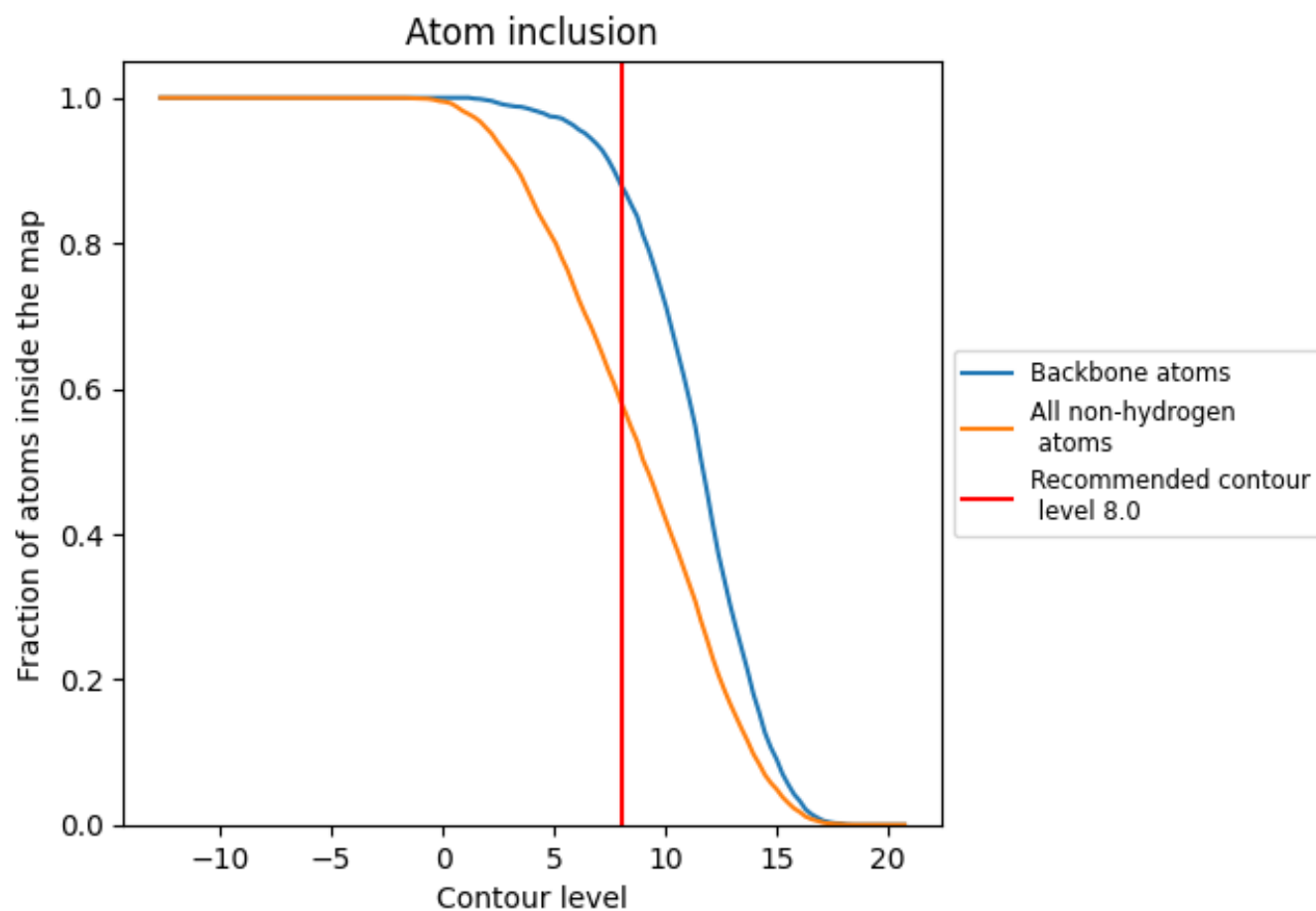
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (8.0).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 58% 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 (8.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5817	<div></div> 0.2820
A	<div></div> 0.5819	<div></div> 0.2810
B	<div></div> 0.5816	<div></div> 0.2810
C	<div></div> 0.5814	<div></div> 0.2810
D	<div></div> 0.5819	<div></div> 0.2820

