



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 04:09 AM UTC

PDB ID : 3J9P / pdb_00003j9p
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

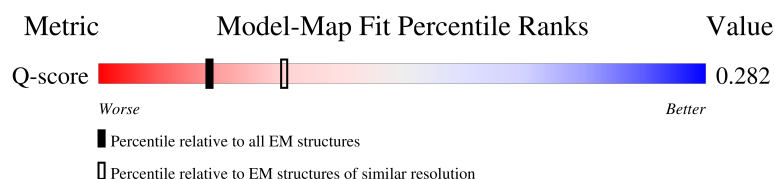
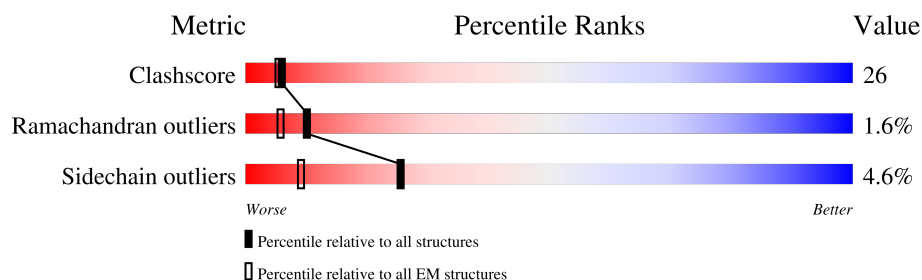
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.24 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4688 (3.74 - 4.74)

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	1528	
1	B	1528	
1	C	1528	
1	D	1528	

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

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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

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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

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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

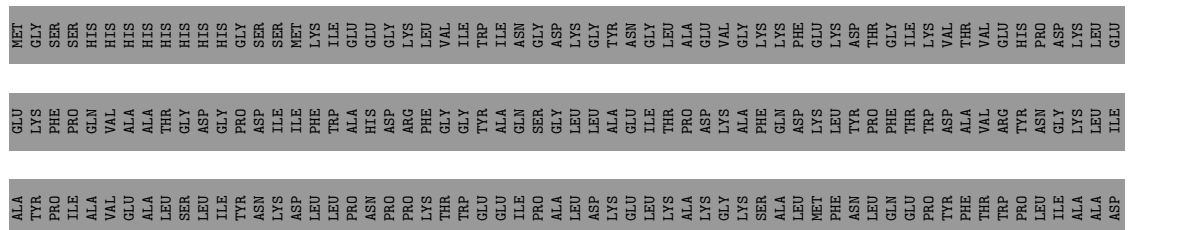
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-396	GLY	-	expression tag	UNP P0AEX9
C	-395	SER	-	expression tag	UNP P0AEX9
C	-394	SER	-	expression tag	UNP P0AEX9
C	-393	MET	-	expression tag	UNP P0AEX9
C	-26	ASN	-	linker	UNP O75762
C	-25	SER	-	linker	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











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	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	0.55	1/4326 (0.0%)	1.28	43/5872 (0.7%)
1	B	0.55	1/4326 (0.0%)	1.28	44/5872 (0.7%)
1	C	0.55	1/4326 (0.0%)	1.28	44/5872 (0.7%)
1	D	0.55	1/4326 (0.0%)	1.27	43/5872 (0.7%)
All	All	0.55	4/17304 (0.0%)	1.28	174/23488 (0.7%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	824	VAL	CA-CB	5.31	1.61	1.54
1	B	824	VAL	CA-CB	5.30	1.61	1.54
1	D	824	VAL	CA-CB	5.29	1.61	1.54
1	A	824	VAL	CA-CB	5.25	1.61	1.54

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	681	GLU	CA-C-N	9.43	129.49	119.78
1	C	681	GLU	C-N-CA	9.43	129.49	119.78
1	D	681	GLU	CA-C-N	9.40	129.47	119.78
1	D	681	GLU	C-N-CA	9.40	129.47	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	681	GLU	CA-C-N	9.40	129.46	119.78
1	A	681	GLU	C-N-CA	9.40	129.46	119.78
1	B	681	GLU	CA-C-N	9.38	129.44	119.78
1	B	681	GLU	C-N-CA	9.38	129.44	119.78
1	A	766	ASN	N-CA-CB	9.34	126.89	112.41
1	D	766	ASN	N-CA-CB	9.31	126.84	112.41
1	C	766	ASN	N-CA-CB	9.31	126.84	112.41
1	B	766	ASN	N-CA-CB	9.29	126.80	112.41
1	A	716	PHE	N-CA-C	-8.78	101.40	110.97
1	B	716	PHE	N-CA-C	-8.76	101.42	110.97
1	C	716	PHE	N-CA-C	-8.76	101.42	110.97
1	D	716	PHE	N-CA-C	-8.70	101.49	110.97
1	C	475	LEU	N-CA-C	8.40	120.52	111.36
1	D	475	LEU	N-CA-C	8.37	120.48	111.36
1	A	475	LEU	N-CA-C	8.37	120.48	111.36
1	B	475	LEU	N-CA-C	8.35	120.46	111.36
1	D	876	VAL	N-CA-C	7.74	118.53	110.72
1	C	876	VAL	N-CA-C	7.71	118.51	110.72
1	B	876	VAL	N-CA-C	7.68	118.48	110.72
1	A	876	VAL	N-CA-C	7.67	118.47	110.72
1	B	819	VAL	N-CA-C	7.54	119.34	112.17
1	C	819	VAL	N-CA-C	7.49	119.29	112.17
1	D	819	VAL	N-CA-C	7.48	119.27	112.17
1	A	819	VAL	N-CA-C	7.45	119.25	112.17
1	C	871	LEU	N-CA-C	7.42	120.43	111.82
1	D	871	LEU	N-CA-C	7.40	120.40	111.82
1	A	871	LEU	N-CA-C	7.38	120.38	111.82
1	B	871	LEU	N-CA-C	7.36	120.35	111.82
1	A	990	LEU	CA-C-N	7.12	127.55	119.93
1	A	990	LEU	C-N-CA	7.12	127.55	119.93
1	B	990	LEU	CA-C-N	7.12	127.54	119.93
1	B	990	LEU	C-N-CA	7.12	127.54	119.93
1	C	990	LEU	CA-C-N	7.10	127.53	119.93
1	C	990	LEU	C-N-CA	7.10	127.53	119.93
1	D	990	LEU	CA-C-N	7.09	127.51	119.93
1	D	990	LEU	C-N-CA	7.09	127.51	119.93
1	C	475	LEU	CA-C-N	6.81	133.95	121.70
1	C	475	LEU	C-N-CA	6.81	133.95	121.70
1	A	475	LEU	CA-C-N	6.80	133.94	121.70
1	A	475	LEU	C-N-CA	6.80	133.94	121.70
1	B	475	LEU	CA-C-N	6.79	133.93	121.70
1	B	475	LEU	C-N-CA	6.79	133.93	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	475	LEU	CA-C-N	6.77	133.89	121.70
1	D	475	LEU	C-N-CA	6.77	133.89	121.70
1	C	512	HIS	N-CA-C	6.47	119.65	111.69
1	D	781	SER	N-CA-C	6.47	118.12	111.14
1	D	916	ILE	N-CA-C	6.45	121.47	112.50
1	C	916	ILE	N-CA-C	6.44	121.45	112.50
1	B	916	ILE	N-CA-C	6.44	121.45	112.50
1	B	781	SER	N-CA-C	6.43	118.08	111.14
1	A	512	HIS	N-CA-C	6.43	119.60	111.69
1	D	512	HIS	N-CA-C	6.42	119.59	111.69
1	A	916	ILE	N-CA-C	6.42	121.43	112.50
1	B	512	HIS	N-CA-C	6.42	119.59	111.69
1	B	947	PHE	N-CA-C	6.42	121.90	113.30
1	C	781	SER	N-CA-C	6.41	118.06	111.14
1	A	947	PHE	N-CA-C	6.37	121.83	113.30
1	D	947	PHE	N-CA-C	6.36	121.82	113.30
1	A	781	SER	N-CA-C	6.35	118.00	111.14
1	C	947	PHE	N-CA-C	6.31	121.76	113.30
1	D	660	PHE	CA-C-N	6.28	133.01	121.70
1	D	660	PHE	C-N-CA	6.28	133.01	121.70
1	A	660	PHE	CA-C-N	6.26	132.97	121.70
1	A	660	PHE	C-N-CA	6.26	132.97	121.70
1	C	660	PHE	CA-C-N	6.25	132.95	121.70
1	C	660	PHE	C-N-CA	6.25	132.95	121.70
1	A	694	ARG	N-CA-C	6.23	118.15	111.36
1	C	694	ARG	N-CA-C	6.23	118.15	111.36
1	B	694	ARG	N-CA-C	6.21	118.13	111.36
1	B	660	PHE	CA-C-N	6.21	132.87	121.70
1	B	660	PHE	C-N-CA	6.21	132.87	121.70
1	D	694	ARG	N-CA-C	6.16	118.07	111.36
1	B	1033	ILE	CA-C-N	6.15	126.47	119.83
1	B	1033	ILE	C-N-CA	6.15	126.47	119.83
1	A	1033	ILE	CA-C-N	6.12	126.44	119.83
1	A	1033	ILE	C-N-CA	6.12	126.44	119.83
1	D	1033	ILE	CA-C-N	6.08	126.40	119.83
1	D	1033	ILE	C-N-CA	6.08	126.40	119.83
1	C	1033	ILE	CA-C-N	6.08	126.39	119.83
1	C	1033	ILE	C-N-CA	6.08	126.39	119.83
1	C	766	ASN	N-CA-C	-6.06	105.47	112.86
1	A	766	ASN	N-CA-C	-6.05	105.48	112.86
1	D	766	ASN	N-CA-C	-6.04	105.49	112.86
1	B	766	ASN	N-CA-C	-5.99	105.55	112.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	700	HIS	CA-C-N	5.98	125.19	118.97
1	D	700	HIS	C-N-CA	5.98	125.19	118.97
1	C	700	HIS	CA-C-N	5.97	125.18	118.97
1	C	700	HIS	C-N-CA	5.97	125.18	118.97
1	B	700	HIS	CA-C-N	5.94	125.15	118.97
1	B	700	HIS	C-N-CA	5.94	125.15	118.97
1	A	700	HIS	CA-C-N	5.92	125.13	118.97
1	A	700	HIS	C-N-CA	5.92	125.13	118.97
1	A	715	GLY	N-CA-C	-5.79	105.66	113.24
1	A	645	SER	CB-CA-C	-5.75	109.93	116.54
1	D	645	SER	CB-CA-C	-5.74	109.94	116.54
1	D	715	GLY	N-CA-C	-5.74	105.72	113.24
1	A	574	ILE	CB-CA-C	-5.72	104.97	111.55
1	B	715	GLY	N-CA-C	-5.72	105.75	113.24
1	C	645	SER	CB-CA-C	-5.72	109.96	116.54
1	B	645	SER	CB-CA-C	-5.72	109.97	116.54
1	C	715	GLY	N-CA-C	-5.70	105.77	113.24
1	B	574	ILE	CB-CA-C	-5.69	105.00	111.55
1	D	574	ILE	CB-CA-C	-5.69	105.01	111.55
1	C	817	ILE	N-CA-C	-5.69	104.82	110.62
1	D	714	TYR	N-CA-C	-5.67	105.10	111.28
1	B	714	TYR	N-CA-C	-5.67	105.09	111.28
1	C	574	ILE	CB-CA-C	-5.66	105.04	111.55
1	B	817	ILE	N-CA-C	-5.66	104.84	110.62
1	A	714	TYR	N-CA-C	-5.66	105.11	111.28
1	C	714	TYR	N-CA-C	-5.65	105.12	111.28
1	A	817	ILE	N-CA-C	-5.64	104.86	110.62
1	D	817	ILE	N-CA-C	-5.61	104.90	110.62
1	C	891	LEU	N-CA-C	5.61	117.47	111.36
1	B	891	LEU	N-CA-C	5.58	117.44	111.36
1	D	891	LEU	N-CA-C	5.58	117.44	111.36
1	A	891	LEU	N-CA-C	5.54	117.39	111.36
1	B	723	LEU	CA-C-N	5.44	125.87	119.94
1	B	723	LEU	C-N-CA	5.44	125.87	119.94
1	D	723	LEU	CA-C-N	5.43	125.86	119.94
1	D	723	LEU	C-N-CA	5.43	125.86	119.94
1	C	723	LEU	CA-C-N	5.42	125.84	119.94
1	C	723	LEU	C-N-CA	5.42	125.84	119.94
1	A	723	LEU	CA-C-N	5.42	125.84	119.94
1	A	723	LEU	C-N-CA	5.42	125.84	119.94
1	C	919	ARG	N-CA-C	-5.39	106.07	113.30
1	B	919	ARG	N-CA-C	-5.37	106.10	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	919	ARG	N-CA-C	-5.37	106.11	113.30
1	C	986	LEU	N-CA-C	-5.36	106.79	113.55
1	D	919	ARG	N-CA-C	-5.35	106.13	113.30
1	D	986	LEU	N-CA-C	-5.32	106.84	113.55
1	B	986	LEU	N-CA-C	-5.30	106.87	113.55
1	D	894	LEU	N-CA-C	-5.29	105.51	111.28
1	B	894	LEU	N-CA-C	-5.29	105.52	111.28
1	D	823	PHE	N-CA-C	5.29	119.42	112.92
1	C	823	PHE	N-CA-C	5.29	119.42	112.92
1	A	986	LEU	N-CA-C	-5.28	106.90	113.55
1	A	894	LEU	N-CA-C	-5.28	105.53	111.28
1	A	823	PHE	N-CA-C	5.27	119.40	112.92
1	C	894	LEU	N-CA-C	-5.26	105.55	111.28
1	B	823	PHE	N-CA-C	5.23	119.35	112.92
1	B	768	TYR	N-CA-C	5.20	117.03	111.36
1	D	768	TYR	N-CA-C	5.17	116.99	111.36
1	A	768	TYR	N-CA-C	5.17	116.99	111.36
1	C	768	TYR	N-CA-C	5.17	116.99	111.36
1	A	917	ASN	CA-C-N	5.15	130.97	121.70
1	A	917	ASN	C-N-CA	5.15	130.97	121.70
1	B	609	LEU	N-CA-C	5.14	117.78	111.82
1	A	609	LEU	N-CA-C	5.14	117.78	111.82
1	D	917	ASN	CA-C-N	5.13	130.94	121.70
1	D	917	ASN	C-N-CA	5.13	130.94	121.70
1	B	917	ASN	CA-C-N	5.13	130.94	121.70
1	B	917	ASN	C-N-CA	5.13	130.94	121.70
1	B	459	ILE	N-CA-C	5.13	115.35	110.42
1	D	609	LEU	N-CA-C	5.13	117.77	111.82
1	C	609	LEU	N-CA-C	5.12	117.76	111.82
1	C	917	ASN	CA-C-N	5.11	130.90	121.70
1	C	917	ASN	C-N-CA	5.11	130.90	121.70
1	D	900	SER	CA-C-N	5.10	124.27	118.97
1	D	900	SER	C-N-CA	5.10	124.27	118.97
1	C	459	ILE	N-CA-C	5.10	115.32	110.42
1	A	900	SER	CA-C-N	5.09	124.26	118.97
1	A	900	SER	C-N-CA	5.09	124.26	118.97
1	A	459	ILE	N-CA-C	5.07	115.29	110.42
1	B	900	SER	CA-C-N	5.07	124.24	118.97
1	B	900	SER	C-N-CA	5.07	124.24	118.97
1	C	900	SER	CA-C-N	5.06	124.23	118.97
1	C	900	SER	C-N-CA	5.06	124.23	118.97
1	D	459	ILE	N-CA-C	5.04	115.26	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	951	VAL	N-CA-C	5.03	115.26	110.53
1	B	951	VAL	N-CA-C	5.01	115.24	110.53

There are no chirality outliers.

All (93) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1032	GLU	Peptide
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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	239	0
1	B	4238	0	4110	238	0
1	C	4238	0	4110	243	0
1	D	4238	0	4110	248	0
All	All	16952	0	16440	885	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 26.

All (885) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:496:LYS:HZ2	1:D:496:LYS:HA	1.60	0.66
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1048:LYS:HZ3	1:C:1050:ARG:NH2	1.95	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
1:B:804:SER:HA	1:B:807:LEU:HD12	1.78	0.65
1:C:660:PHE:HB3	1:C:661:LYS:C	2.22	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:660:PHE:HB3	1:D:661:LYS:C	2.23	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:660:PHE:HB3	1:B:661:LYS:C	2.22	0.64
1:A:660:PHE:HB3	1:A:661:LYS:C	2.22	0.63
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:D:1048:LYS:HZ3	1:A:1050:ARG:NH2	1.96	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:A:496:LYS:HA	1:A:496:LYS:HZ2	1.64	0.62
1:A:496:LYS:HA	1:A:496:LYS:NZ	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:HA	1:D:496:LYS:NZ	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:480:LEU:HA	1:A:481:HIS:C	2.27	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:C:480:LEU:HA	1:C:481:HIS:C	2.27	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:A:916:ILE:N	1:A:917:ASN:HA	2.18	0.59
1:D:480:LEU:HA	1:D:481:HIS:C	2.27	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:C:496:LYS:HA	1:C:496:LYS:HZ2	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:480:LEU:HA	1:B:481:HIS:C	2.27	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:870:LEU:CD2	1:D:956:LEU:HD11	2.37	0.54
1:C:455:SER:HB2	1:C:488:LEU:HD23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:580:GLN:HG2	1:D:581:ALA:N	2.23	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:1042:MET:SD	1:C:1042:MET:C	2.93	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
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:1042:MET:SD	1:B:1042:MET:C	2.93	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:C:659:ASN:C	1:C:660:PHE:HD1	2.19	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:A:1042:MET:SD	1:A:1042:MET:C	2.93	0.51
1:B:659:ASN:C	1:B:660:PHE:HD1	2.19	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:D:1042:MET:SD	1:D:1042:MET:C	2.93	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:659:ASN:C	1:A:660:PHE:HD1	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:491:LYS:HG3	1:D:492:ASN:OD1	2.11	0.50
1:B:496:LYS:HA	1:B:496:LYS:HZ2	1.75	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:659:ASN:C	1:D:660:PHE:HD1	2.19	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: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
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:B:631:PRO:O	1:B:632:GLU:C	2.56	0.49
1:C:631:PRO:O	1:C:632:GLU:C	2.56	0.49
1:C:631:PRO:HA	1:C:634:MET:HE3	1.95	0.49
1:D:981:GLU:O	1:D:984:THR:HG22	2.12	0.49
1:A:631:PRO:HA	1:A:634:MET:HE3	1.95	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:D:631:PRO:HA	1:D:634:MET:HE3	1.95	0.49
1:C:918:TYR:CD1	1:C:921:SER:HB3	2.47	0.49
1:B:631:PRO:HA	1:B:634:MET:HE3	1.95	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:D:631:PRO:O	1:D:632:GLU:C	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:631:PRO:O	1:A:632:GLU:C	2.56	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:B:1042:MET:O	1:B:1043:GLU:C	2.57	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:1042:MET:O	1:A:1043:GLU:C	2.57	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
1:D:867:LEU:O	1:D:870:LEU:HB3	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:516:THR:HG22	1:C:517:ALA:N	2.28	0.47
1:C:547:ASP:OD1	1:C:547:ASP:N	2.48	0.47
1:A:547:ASP:OD1	1:A:547:ASP:N	2.48	0.47
1:B:829:HIS:ND1	1:B:829:HIS:C	2.73	0.47
1:C:690:VAL:HG21	1:C:977:ALA:HB2	1.97	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:C:1042:MET:O	1:C:1043:GLU:C	2.57	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
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:829:HIS:ND1	1:A:829:HIS:C	2.72	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:C:512:HIS:CD2	1:C:512:HIS:C	2.93	0.47
1:D:589:HIS:O	1:D:591:LYS:NZ	2.39	0.47
1:D:1042:MET:O	1:D:1043:GLU:C	2.57	0.47
1:B:742:PRO:HA	1:B:832:TRP:HE1	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:512:HIS:CD2	1:D:512:HIS:C	2.93	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:829:HIS:ND1	1:D:829:HIS:C	2.73	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:C:829:HIS:ND1	1:C:829:HIS:C	2.73	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:D:468:ASP:N	1:D:469:ILE:HA	2.23	0.46
1:D:839:VAL:O	1:D:842:TYR:HB3	2.15	0.46
1:A:512:HIS:CD2	1:A:512:HIS: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:1048:LYS:HZ1	1:A:1050:ARG:HH12	1.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:512:HIS:C	1:B:512:HIS:CD2	2.93	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:922:PHE:N	1:B:922:PHE:CD1	2.83	0.46
1:C:862:MET:HB2	1:C:862:MET:HE3	1.76	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1048:LYS:HZ3	1:A:1050:ARG:HH22	1.63	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: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:B:1048:LYS:HZ3	1:C:1050:ARG:HH22	1.62	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
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:852:ARG:HD3	1:B:982:LEU:HG	1.98	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:634:MET:HE3	1:C:634:MET:HB3	1.90	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:766:ASN:CG	1:C:769:LEU:CB	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:766:ASN:CG	1:D:769:LEU:CB	2.91	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:D:634:MET:HE3	1:D:634:MET:HB3	1.90	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:886:LEU:O	1:D:889:TYR:HB3	2.18	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:D:518:LEU:HD11	1:D:530:MET:HG3	2.00	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
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:D:862:MET:HE3	1:D:862:MET:HB2	1.76	0.43
1:A:766:ASN:CG	1:A:769:LEU:CB	2.91	0.43
1:A:852:ARG:HD3	1:A:982:LEU:HG	1.98	0.43
1:B:852:ARG:O	1:B:853:PHE:HB2	2.16	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:B:862:MET:HE3	1:B:862:MET:HB2	1.76	0.43
1:C:518:LEU:HD11	1:C:530:MET:HG3	2.00	0.43
1:C:569:SER:C	1:C:570:HIS:HD2	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:569:SER:C	1:D:570:HIS:HD2	2.26	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:B:569:SER:C	1:B:570:HIS:HD2	2.26	0.43
1:A:621:CYS:SG	1:A:622:PRO:HD3	2.58	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:569:SER:C	1:A:570:HIS:HD2	2.26	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:768:TYR:O	1:D:769:LEU:C	2.62	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
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:B:1048:LYS:HZ1	1:C:1050:ARG:HH12	1.66	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:766:ASN:CG	1:B:769:LEU:CB	2.91	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:A:768:TYR:O	1:A:769:LEU:C	2.62	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
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: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: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:D:946:ILE:C	1:D:947:PHE:HD1	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:639:ASP:C	1:B:640:PHE:HD1	2.28	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:743:GLY:H	1:C:832:TRP:NE1	2.13	0.42
1:C:768:TYR:O	1:C:769:LEU:C	2.62	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:D:948:VAL:HB	1:D:949:PRO:HD3	2.02	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: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:A:639:ASP:C	1:A:640:PHE:HD1	2.28	0.42
1:A:931:LEU:HD12	1:A:931:LEU:O	2.19	0.42
1:A:946:ILE:C	1:A:947:PHE:HD1	2.28	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:874:THR:HA	1:D:877:PHE:CE2	2.55	0.42
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:1048:LYS:HZ1	1:A:1050:ARG:NH1	2.17	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:C:639:ASP:C	1:C:640:PHE:HD1	2.28	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:639:ASP:C	1:D:640:PHE:HD1	2.28	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:C:946:ILE:C	1:C:947:PHE:HD1	2.27	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
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:970:HIS:HE1	1:B:974:LYS:NZ	2.18	0.41
1:B:994:PHE:C	1:B:995:LEU:HD22	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:835:GLY:O	1:A:839:VAL:HG23	2.21	0.41
1:C:994:PHE:C	1:C:995:LEU:HD22	2.46	0.41
1:A:468:ASP:N	1:A:469:ILE:HA	2.23	0.41
1:A:743:GLY:H	1:A:832:TRP:NE1	2.13	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:B:946:ILE:C	1:B:947:PHE:HD1	2.27	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:B:506:ALA:HA	1:B:507:LEU:C	2.46	0.41
1:B:628:GLU:C	1:B:630:LEU:H	2.29	0.41
1:C:602:SER:HA	1:C:603:LYS:HA	1.48	0.41
1:C:628:GLU:C	1:C:630:LEU:H	2.29	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:970:HIS:HE1	1:D:974:LYS:NZ	2.18	0.40
1:D:994:PHE:C	1:D:995:LEU:HD22	2.46	0.40
1:A:990:LEU:HD21	1:A:994:PHE:HD2	1.86	0.40
1:A:994:PHE:C	1:A:995:LEU:HD22	2.46	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:D:743:GLY:H	1:D:832:TRP:NE1	2.13	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 [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	550/1528 (36%)	485 (88%)	56 (10%)	9 (2%)	7	36
1	B	550/1528 (36%)	485 (88%)	56 (10%)	9 (2%)	7	36
1	C	550/1528 (36%)	485 (88%)	56 (10%)	9 (2%)	7	36
1	D	550/1528 (36%)	485 (88%)	56 (10%)	9 (2%)	7	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2200/6112 (36%)	1940 (88%)	224 (10%)	36 (2%)	10	36

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 ⓘ

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%)	396 (95%)	19 (5%)	24	46
1	B	415/1325 (31%)	396 (95%)	19 (5%)	24	46
1	C	415/1325 (31%)	395 (95%)	20 (5%)	23	45
1	D	415/1325 (31%)	396 (95%)	19 (5%)	24	46
All	All	1660/5300 (31%)	1583 (95%)	77 (5%)	25	46

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	480	LEU
1	D	496	LYS
1	D	503	LYS
1	D	527	THR
1	D	536	THR
1	D	550	THR
1	D	620	LYS
1	D	690	VAL
1	D	695	ILE
1	D	819	VAL
1	D	829	HIS
1	D	832	TRP
1	D	844	MET
1	D	922	PHE
1	D	945	THR
1	D	974	LYS
1	D	1050	ARG
1	D	1052	LYS
1	D	1067	LEU
1	A	480	LEU
1	A	496	LYS
1	A	503	LYS
1	A	527	THR
1	A	536	THR

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Mol	Chain	Res	Type
1	A	550	THR
1	A	620	LYS
1	A	690	VAL
1	A	695	ILE
1	A	819	VAL
1	A	829	HIS
1	A	832	TRP
1	A	844	MET
1	A	922	PHE
1	A	945	THR
1	A	974	LYS
1	A	1050	ARG
1	A	1052	LYS
1	A	1067	LEU
1	B	480	LEU
1	B	496	LYS
1	B	503	LYS
1	B	527	THR
1	B	536	THR
1	B	550	THR
1	B	620	LYS
1	B	690	VAL
1	B	695	ILE
1	B	819	VAL
1	B	829	HIS
1	B	832	TRP
1	B	844	MET
1	B	922	PHE
1	B	945	THR
1	B	974	LYS
1	B	1050	ARG
1	B	1052	LYS
1	B	1067	LEU
1	C	480	LEU
1	C	496	LYS
1	C	503	LYS
1	C	527	THR
1	C	536	THR
1	C	550	THR
1	C	620	LYS
1	C	690	VAL
1	C	695	ILE

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Mol	Chain	Res	Type
1	C	819	VAL
1	C	829	HIS
1	C	832	TRP
1	C	844	MET
1	C	920	GLU
1	C	922	PHE
1	C	945	THR
1	C	974	LYS
1	C	1050	ARG
1	C	1052	LYS
1	C	1067	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	460	ASN
1	D	553	HIS
1	D	739	ASN
1	D	954	ASN
1	D	1047	GLN
1	D	1061	GLN
1	A	460	ASN
1	A	549	ASN
1	A	553	HIS
1	A	739	ASN
1	A	954	ASN
1	A	1047	GLN
1	B	460	ASN
1	B	549	ASN
1	B	553	HIS
1	B	739	ASN
1	B	954	ASN
1	B	1047	GLN
1	B	1061	GLN
1	C	460	ASN
1	C	549	ASN
1	C	553	HIS
1	C	739	ASN
1	C	954	ASN
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

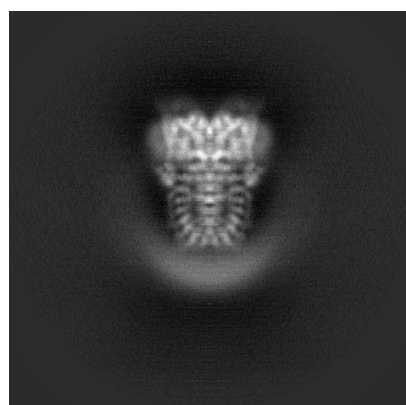
6 Map visualisation [i](#)

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

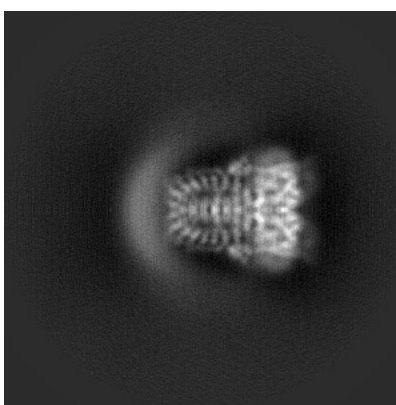
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

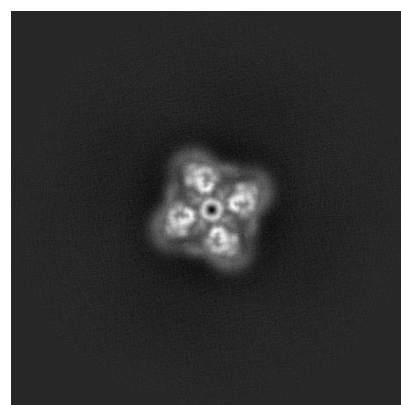
6.1.1 Primary map



X



Y

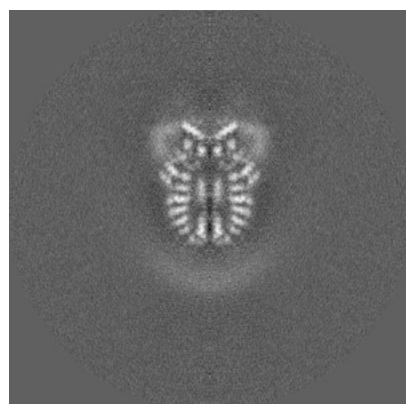


Z

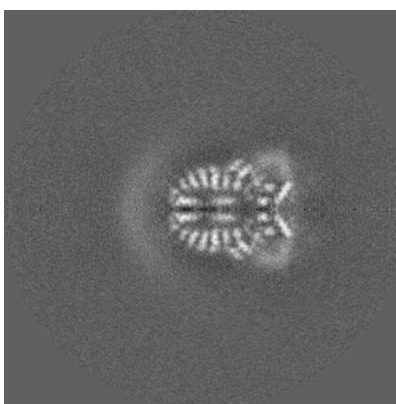
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

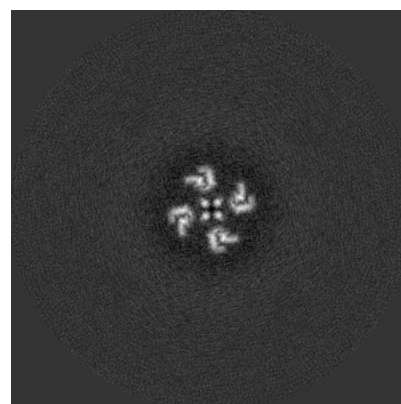
6.2.1 Primary map



X Index: 150



Y Index: 150

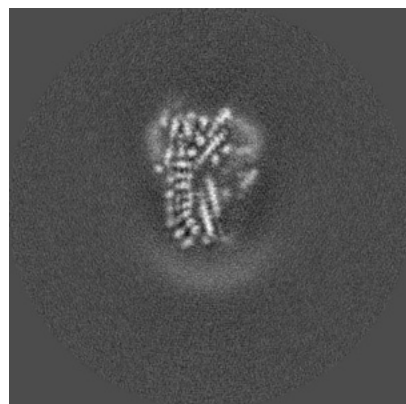


Z Index: 150

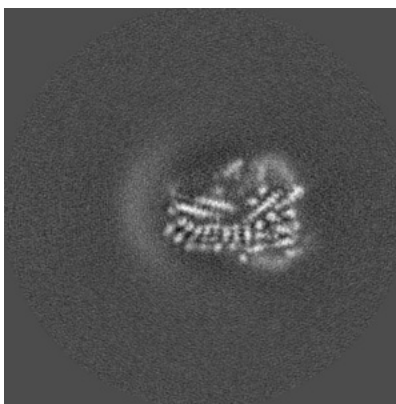
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

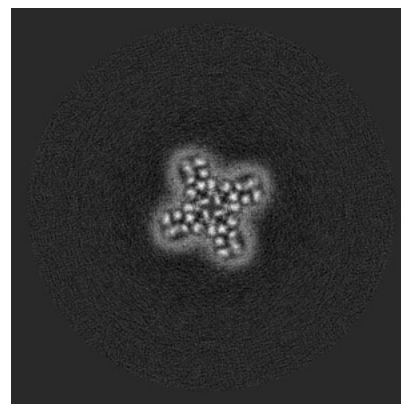
6.3.1 Primary map



X Index: 156



Y Index: 144

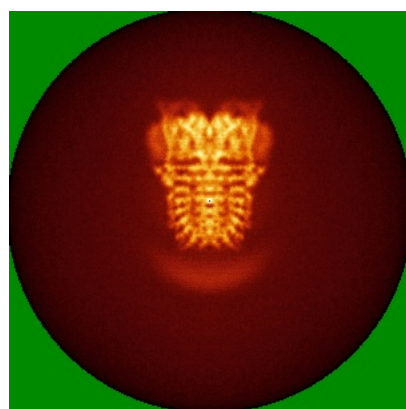


Z Index: 212

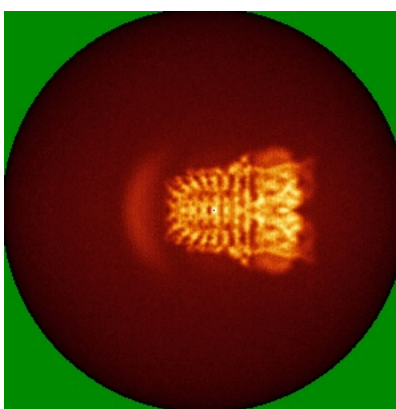
The images above show the largest variance slices of the map in three orthogonal directions.

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

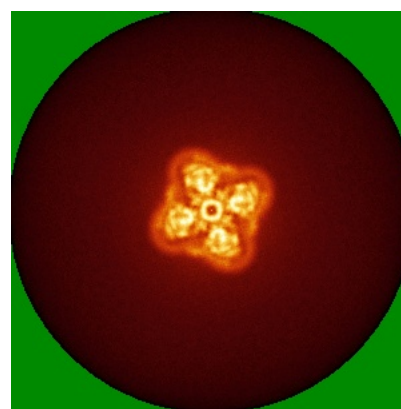
6.4.1 Primary map



X



Y

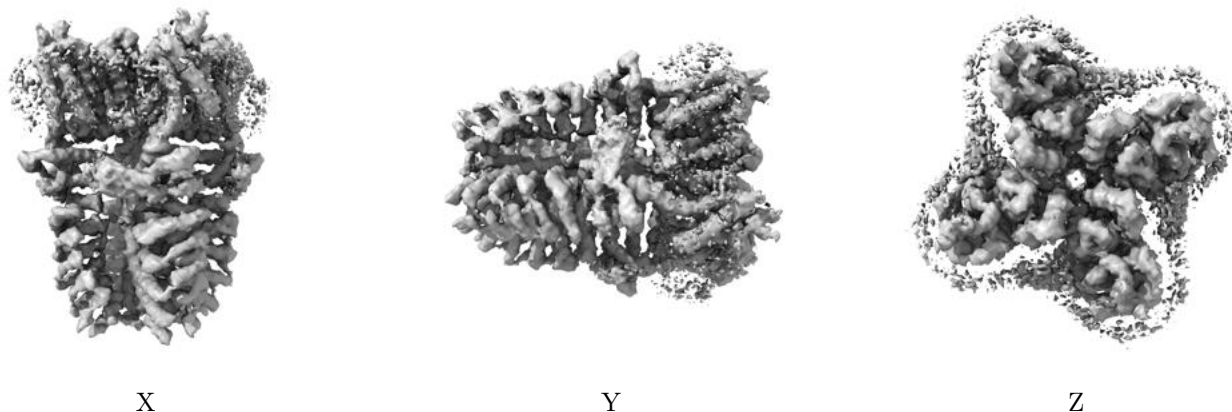


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

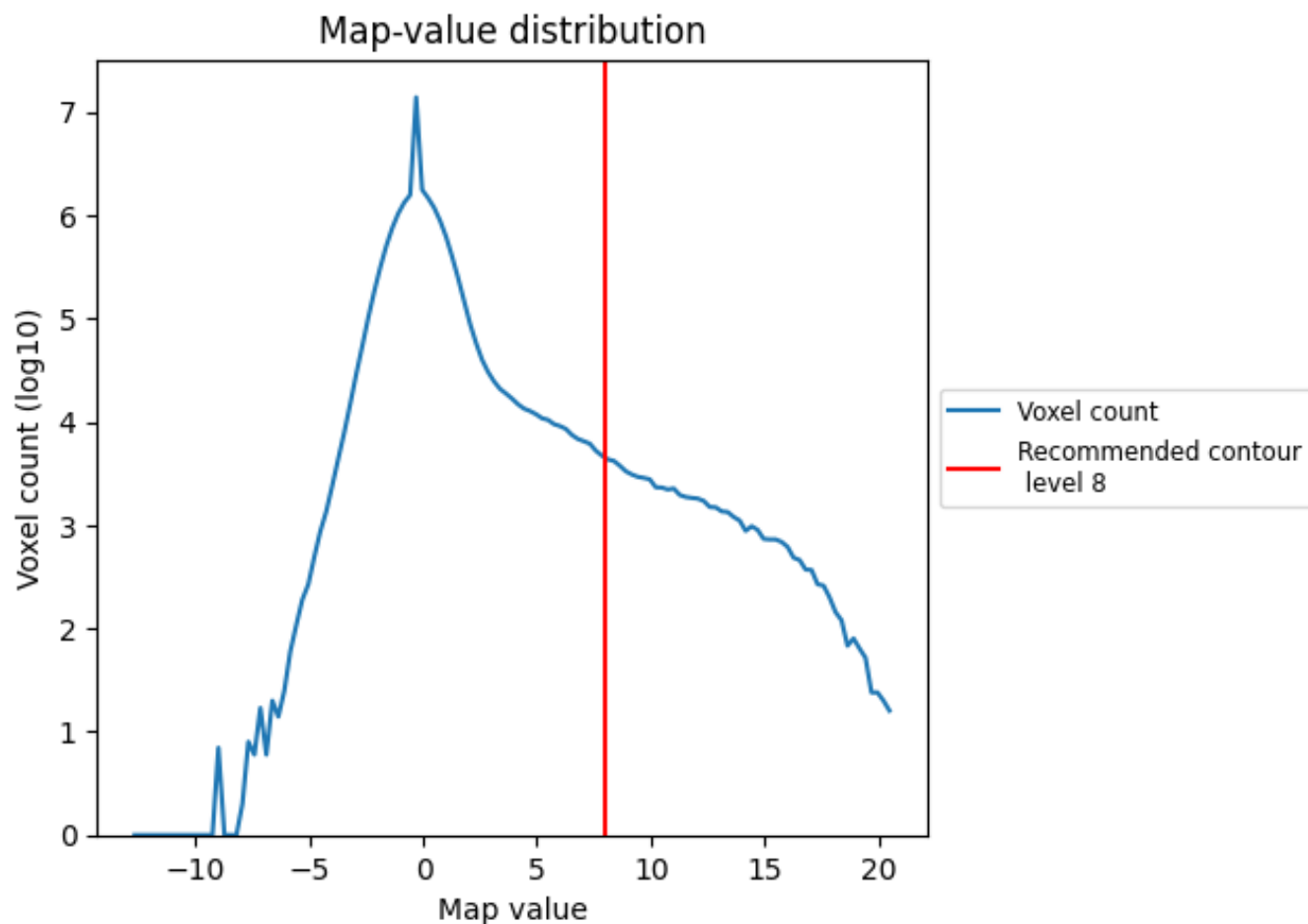
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

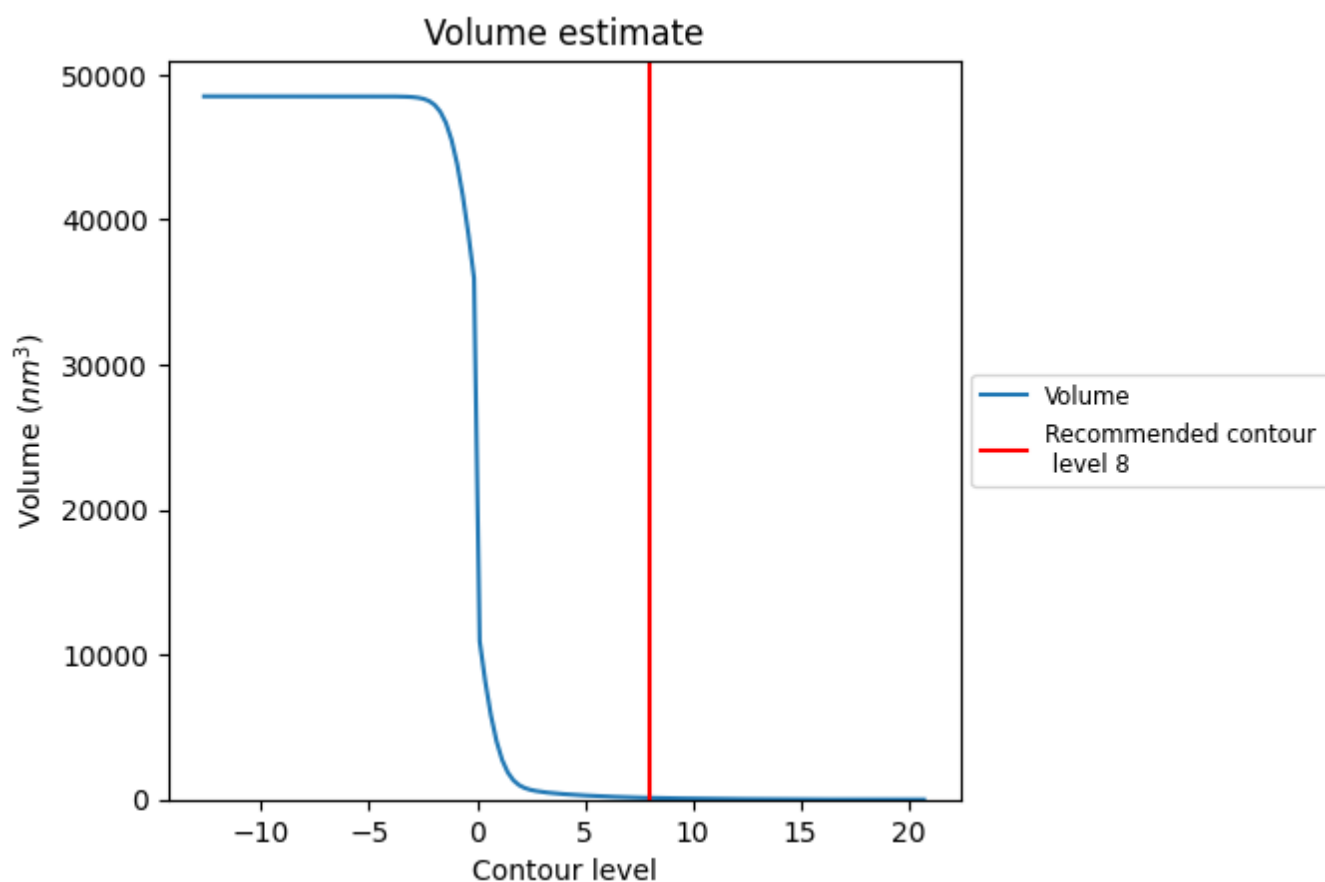
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

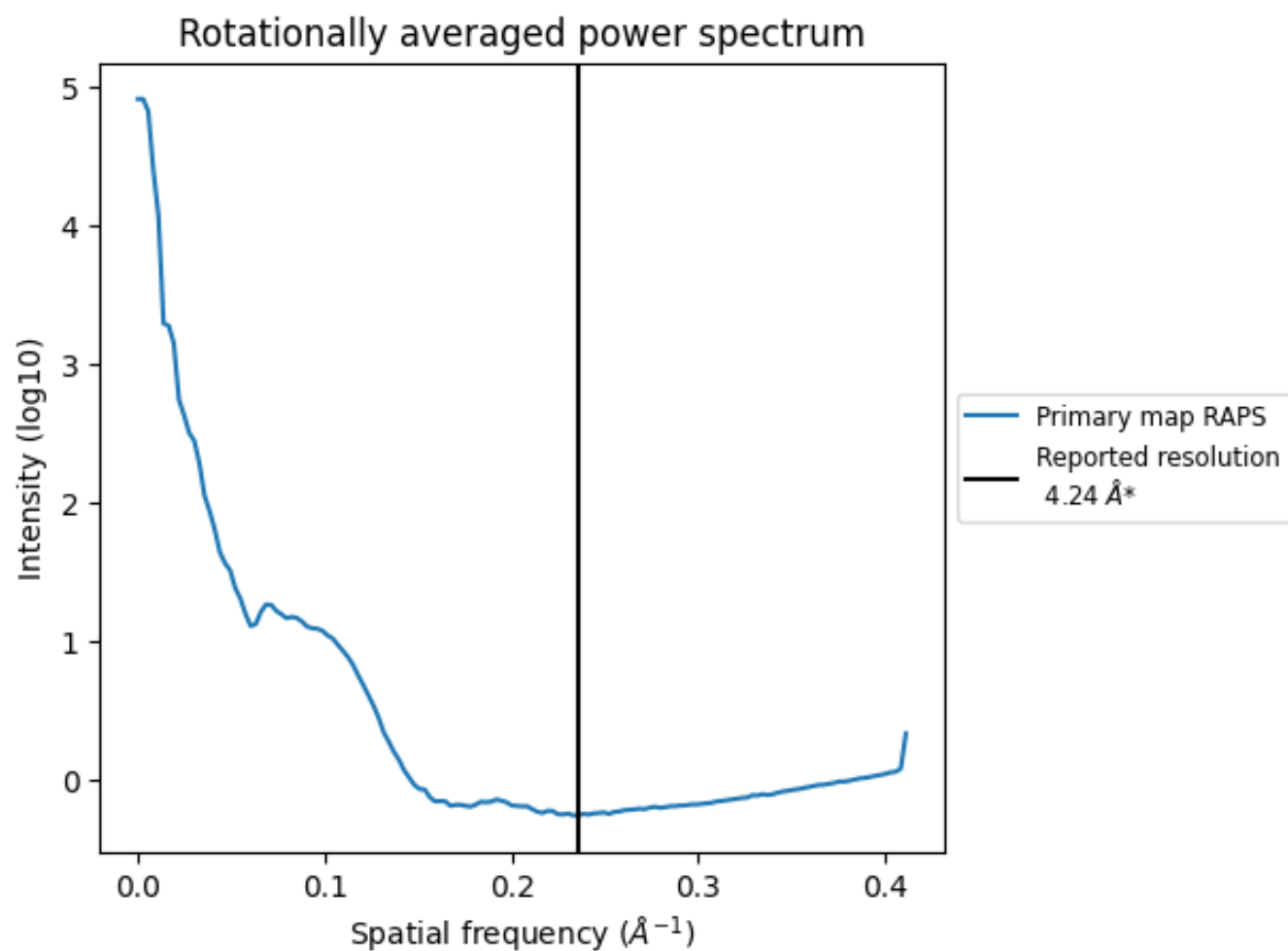
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 117 nm³; 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 Å⁻¹

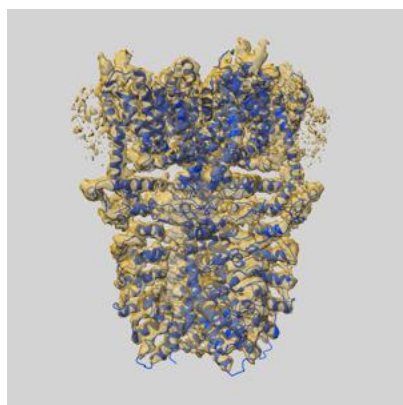
8 Fourier-Shell correlation

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

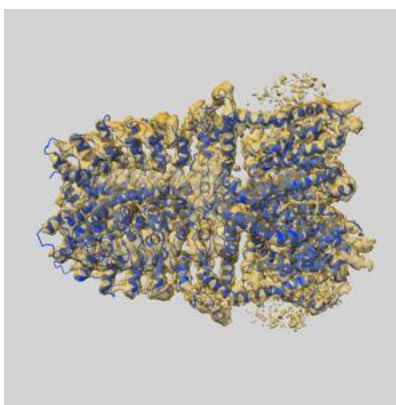
9 Map-model fit [i](#)

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

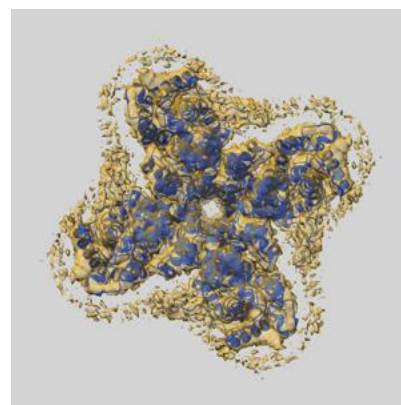
9.1 Map-model overlay [i](#)



X



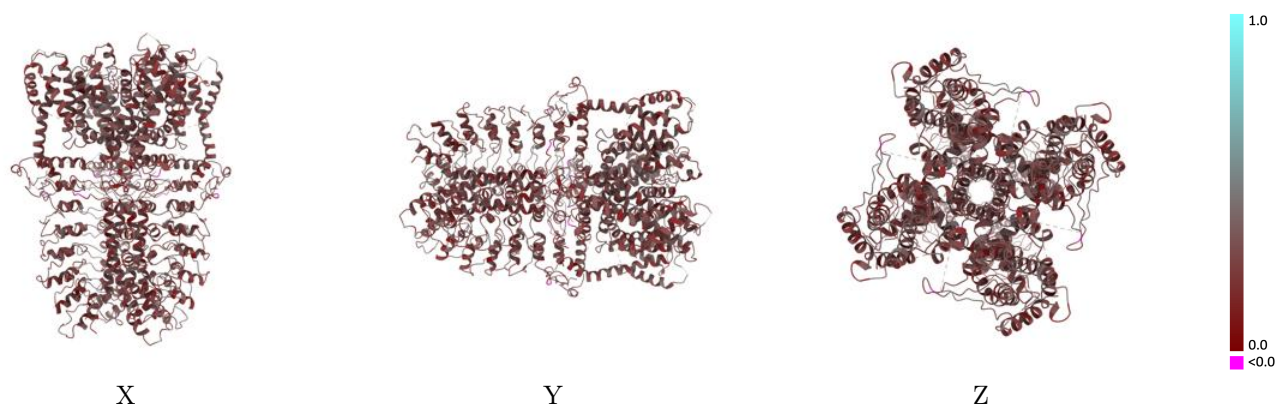
Y



Z

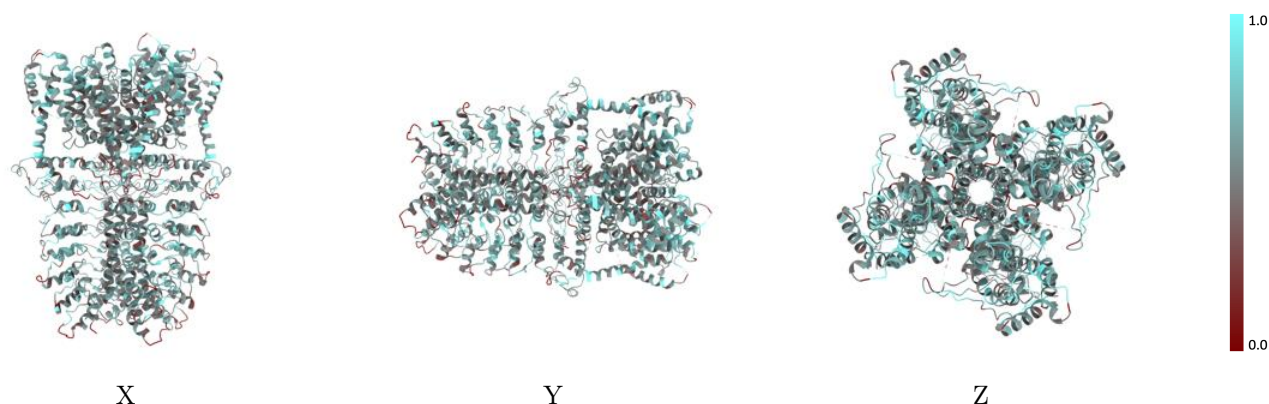
The images above show the 3D surface view of the map at the recommended contour level 8.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



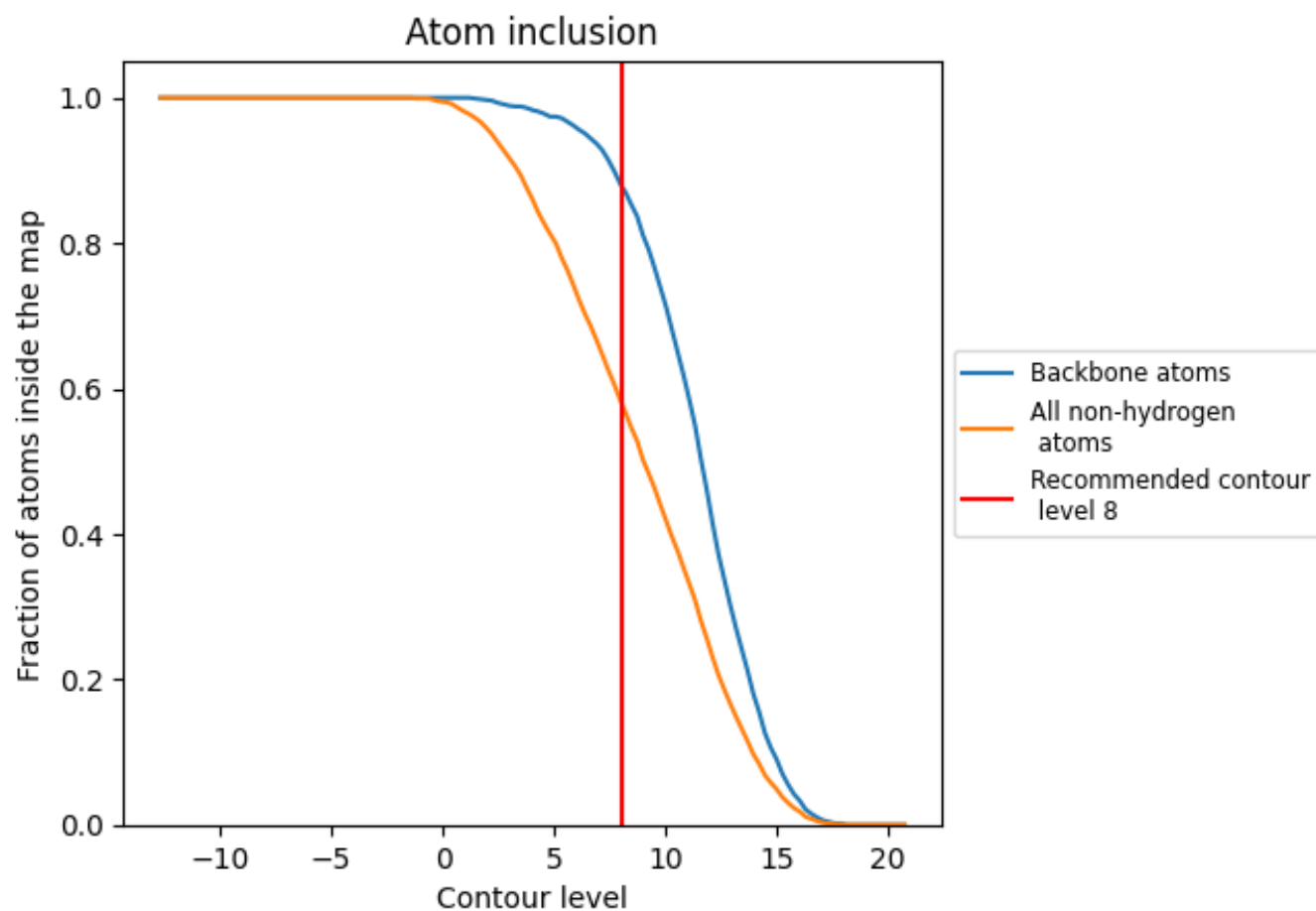
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5820	0.2820
A	0.5820	0.2810
B	0.5820	0.2810
C	0.5810	0.2810
D	0.5820	0.2820

