



Full wwPDB EM Validation Report ⓘ

Jul 14, 2024 – 08:47 AM JST

PDB ID : 8Y7O
EMDB ID : EMD-39022
Title : FluPol-NS2 complex (hexamer)
Authors : Peng, Q.; Sun, J.Q.
Deposited on : 2024-02-04
Resolution : 3.00 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:

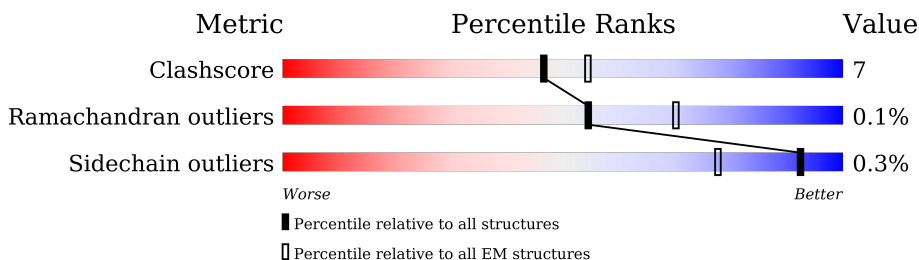
EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

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 3.00 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 ≥ 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	729	
1	E	729	
1	I	729	
1	L	729	
1	M	729	
1	Q	729	
2	B	757	
2	F	757	

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Mol	Chain	Length	Quality of chain
2	H	757	71% 17% 12%
2	J	757	77% 13% 9%
2	N	757	81% 10% 9%
2	R	757	70% 18% 12%
3	C	792	34% 5% 61%
3	D	792	24% 7% 70%
3	G	792	36% 8% 57%
3	K	792	6% 32% 6% 61%
3	O	792	6% 31% 7% 61%
3	P	792	24% 6% 70%
4	S	121	68% 29% .
4	T	121	8% 74% 22% ..
4	U	121	7% 65% 31% ..
4	V	121	12% 69% 26% ..
4	W	121	11% 74% 22% ..
4	X	121	12% 70% 25% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 86104 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 Polymerase acidic protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	E	687	Total	C	N	O	S	0	0
			5552	3515	944	1053	40		
1	A	712	Total	C	N	O	S	0	0
			5779	3665	977	1095	42		
1	I	687	Total	C	N	O	S	0	0
			5558	3521	944	1053	40		
1	L	712	Total	C	N	O	S	0	0
			5779	3665	977	1095	42		
1	Q	687	Total	C	N	O	S	0	0
			5558	3521	944	1053	40		
1	M	712	Total	C	N	O	S	0	0
			5779	3665	977	1095	42		

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-12	MET	-	initiating methionine	UNP P03434
E	-11	HIS	-	expression tag	UNP P03434
E	-10	HIS	-	expression tag	UNP P03434
E	-9	HIS	-	expression tag	UNP P03434
E	-8	HIS	-	expression tag	UNP P03434
E	-7	HIS	-	expression tag	UNP P03434
E	-6	HIS	-	expression tag	UNP P03434
E	-5	HIS	-	expression tag	UNP P03434
E	-4	HIS	-	expression tag	UNP P03434
E	-3	GLY	-	expression tag	UNP P03434
E	-2	SER	-	expression tag	UNP P03434
E	-1	GLY	-	expression tag	UNP P03434
E	0	SER	-	expression tag	UNP P03434
A	-12	MET	-	initiating methionine	UNP P03434
A	-11	HIS	-	expression tag	UNP P03434
A	-10	HIS	-	expression tag	UNP P03434
A	-9	HIS	-	expression tag	UNP P03434
A	-8	HIS	-	expression tag	UNP P03434

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	HIS	-	expression tag	UNP P03434
A	-6	HIS	-	expression tag	UNP P03434
A	-5	HIS	-	expression tag	UNP P03434
A	-4	HIS	-	expression tag	UNP P03434
A	-3	GLY	-	expression tag	UNP P03434
A	-2	SER	-	expression tag	UNP P03434
A	-1	GLY	-	expression tag	UNP P03434
A	0	SER	-	expression tag	UNP P03434
I	-12	MET	-	initiating methionine	UNP P03434
I	-11	HIS	-	expression tag	UNP P03434
I	-10	HIS	-	expression tag	UNP P03434
I	-9	HIS	-	expression tag	UNP P03434
I	-8	HIS	-	expression tag	UNP P03434
I	-7	HIS	-	expression tag	UNP P03434
I	-6	HIS	-	expression tag	UNP P03434
I	-5	HIS	-	expression tag	UNP P03434
I	-4	HIS	-	expression tag	UNP P03434
I	-3	GLY	-	expression tag	UNP P03434
I	-2	SER	-	expression tag	UNP P03434
I	-1	GLY	-	expression tag	UNP P03434
I	0	SER	-	expression tag	UNP P03434
L	-12	MET	-	initiating methionine	UNP P03434
L	-11	HIS	-	expression tag	UNP P03434
L	-10	HIS	-	expression tag	UNP P03434
L	-9	HIS	-	expression tag	UNP P03434
L	-8	HIS	-	expression tag	UNP P03434
L	-7	HIS	-	expression tag	UNP P03434
L	-6	HIS	-	expression tag	UNP P03434
L	-5	HIS	-	expression tag	UNP P03434
L	-4	HIS	-	expression tag	UNP P03434
L	-3	GLY	-	expression tag	UNP P03434
L	-2	SER	-	expression tag	UNP P03434
L	-1	GLY	-	expression tag	UNP P03434
L	0	SER	-	expression tag	UNP P03434
Q	-12	MET	-	initiating methionine	UNP P03434
Q	-11	HIS	-	expression tag	UNP P03434
Q	-10	HIS	-	expression tag	UNP P03434
Q	-9	HIS	-	expression tag	UNP P03434
Q	-8	HIS	-	expression tag	UNP P03434
Q	-7	HIS	-	expression tag	UNP P03434
Q	-6	HIS	-	expression tag	UNP P03434
Q	-5	HIS	-	expression tag	UNP P03434

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	-4	HIS	-	expression tag	UNP P03434
Q	-3	GLY	-	expression tag	UNP P03434
Q	-2	SER	-	expression tag	UNP P03434
Q	-1	GLY	-	expression tag	UNP P03434
Q	0	SER	-	expression tag	UNP P03434
M	-12	MET	-	initiating methionine	UNP P03434
M	-11	HIS	-	expression tag	UNP P03434
M	-10	HIS	-	expression tag	UNP P03434
M	-9	HIS	-	expression tag	UNP P03434
M	-8	HIS	-	expression tag	UNP P03434
M	-7	HIS	-	expression tag	UNP P03434
M	-6	HIS	-	expression tag	UNP P03434
M	-5	HIS	-	expression tag	UNP P03434
M	-4	HIS	-	expression tag	UNP P03434
M	-3	GLY	-	expression tag	UNP P03434
M	-2	SER	-	expression tag	UNP P03434
M	-1	GLY	-	expression tag	UNP P03434
M	0	SER	-	expression tag	UNP P03434

- Molecule 2 is a protein called RNA-directed RNA polymerase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	F	668	5297	3341	909	1006	41	0	0
2	B	686	5457	3439	941	1035	42	0	0
2	H	668	5297	3341	909	1006	41	0	0
2	J	686	5457	3439	941	1035	42	0	0
2	R	668	5297	3341	909	1006	41	0	0
2	N	686	5457	3439	941	1035	42	0	0

- Molecule 3 is a protein called Polymerase basic protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	308	2463	1553	443	448	19	0	0
3	K	308	2463	1553	443	448	19	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	O	308	2463	1553	443	448	19	0	0
3	D	241	1943	1239	336	351	17	0	0
3	G	344	2724	1719	487	496	22	0	0
3	P	241	1943	1239	336	351	17	0	0

There are 204 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	691	ARG	LEU	engineered mutation	UNP P03429
C	760	GLY	-	expression tag	UNP P03429
C	761	TRP	-	expression tag	UNP P03429
C	762	SER	-	expression tag	UNP P03429
C	763	HIS	-	expression tag	UNP P03429
C	764	PRO	-	expression tag	UNP P03429
C	765	GLN	-	expression tag	UNP P03429
C	766	PHE	-	expression tag	UNP P03429
C	767	GLU	-	expression tag	UNP P03429
C	768	LYS	-	expression tag	UNP P03429
C	769	GLY	-	expression tag	UNP P03429
C	770	GLY	-	expression tag	UNP P03429
C	771	GLY	-	expression tag	UNP P03429
C	772	SER	-	expression tag	UNP P03429
C	773	GLY	-	expression tag	UNP P03429
C	774	GLY	-	expression tag	UNP P03429
C	775	GLY	-	expression tag	UNP P03429
C	776	SER	-	expression tag	UNP P03429
C	777	GLY	-	expression tag	UNP P03429
C	778	GLY	-	expression tag	UNP P03429
C	779	SER	-	expression tag	UNP P03429
C	780	ALA	-	expression tag	UNP P03429
C	781	TRP	-	expression tag	UNP P03429
C	782	SER	-	expression tag	UNP P03429
C	783	HIS	-	expression tag	UNP P03429
C	784	PRO	-	expression tag	UNP P03429
C	785	GLN	-	expression tag	UNP P03429
C	786	PHE	-	expression tag	UNP P03429
C	787	GLU	-	expression tag	UNP P03429
C	788	LYS	-	expression tag	UNP P03429
C	789	GLY	-	expression tag	UNP P03429

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Chain	Residue	Modelled	Actual	Comment	Reference
C	790	ARG	-	expression tag	UNP P03429
C	791	SER	-	expression tag	UNP P03429
C	792	GLY	-	expression tag	UNP P03429
K	691	ARG	LEU	engineered mutation	UNP P03429
K	760	GLY	-	expression tag	UNP P03429
K	761	TRP	-	expression tag	UNP P03429
K	762	SER	-	expression tag	UNP P03429
K	763	HIS	-	expression tag	UNP P03429
K	764	PRO	-	expression tag	UNP P03429
K	765	GLN	-	expression tag	UNP P03429
K	766	PHE	-	expression tag	UNP P03429
K	767	GLU	-	expression tag	UNP P03429
K	768	LYS	-	expression tag	UNP P03429
K	769	GLY	-	expression tag	UNP P03429
K	770	GLY	-	expression tag	UNP P03429
K	771	GLY	-	expression tag	UNP P03429
K	772	SER	-	expression tag	UNP P03429
K	773	GLY	-	expression tag	UNP P03429
K	774	GLY	-	expression tag	UNP P03429
K	775	GLY	-	expression tag	UNP P03429
K	776	SER	-	expression tag	UNP P03429
K	777	GLY	-	expression tag	UNP P03429
K	778	GLY	-	expression tag	UNP P03429
K	779	SER	-	expression tag	UNP P03429
K	780	ALA	-	expression tag	UNP P03429
K	781	TRP	-	expression tag	UNP P03429
K	782	SER	-	expression tag	UNP P03429
K	783	HIS	-	expression tag	UNP P03429
K	784	PRO	-	expression tag	UNP P03429
K	785	GLN	-	expression tag	UNP P03429
K	786	PHE	-	expression tag	UNP P03429
K	787	GLU	-	expression tag	UNP P03429
K	788	LYS	-	expression tag	UNP P03429
K	789	GLY	-	expression tag	UNP P03429
K	790	ARG	-	expression tag	UNP P03429
K	791	SER	-	expression tag	UNP P03429
K	792	GLY	-	expression tag	UNP P03429
O	691	ARG	LEU	engineered mutation	UNP P03429
O	760	GLY	-	expression tag	UNP P03429
O	761	TRP	-	expression tag	UNP P03429
O	762	SER	-	expression tag	UNP P03429
O	763	HIS	-	expression tag	UNP P03429

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Chain	Residue	Modelled	Actual	Comment	Reference
O	764	PRO	-	expression tag	UNP P03429
O	765	GLN	-	expression tag	UNP P03429
O	766	PHE	-	expression tag	UNP P03429
O	767	GLU	-	expression tag	UNP P03429
O	768	LYS	-	expression tag	UNP P03429
O	769	GLY	-	expression tag	UNP P03429
O	770	GLY	-	expression tag	UNP P03429
O	771	GLY	-	expression tag	UNP P03429
O	772	SER	-	expression tag	UNP P03429
O	773	GLY	-	expression tag	UNP P03429
O	774	GLY	-	expression tag	UNP P03429
O	775	GLY	-	expression tag	UNP P03429
O	776	SER	-	expression tag	UNP P03429
O	777	GLY	-	expression tag	UNP P03429
O	778	GLY	-	expression tag	UNP P03429
O	779	SER	-	expression tag	UNP P03429
O	780	ALA	-	expression tag	UNP P03429
O	781	TRP	-	expression tag	UNP P03429
O	782	SER	-	expression tag	UNP P03429
O	783	HIS	-	expression tag	UNP P03429
O	784	PRO	-	expression tag	UNP P03429
O	785	GLN	-	expression tag	UNP P03429
O	786	PHE	-	expression tag	UNP P03429
O	787	GLU	-	expression tag	UNP P03429
O	788	LYS	-	expression tag	UNP P03429
O	789	GLY	-	expression tag	UNP P03429
O	790	ARG	-	expression tag	UNP P03429
O	791	SER	-	expression tag	UNP P03429
O	792	GLY	-	expression tag	UNP P03429
D	691	ARG	LEU	engineered mutation	UNP P03429
D	760	GLY	-	expression tag	UNP P03429
D	761	TRP	-	expression tag	UNP P03429
D	762	SER	-	expression tag	UNP P03429
D	763	HIS	-	expression tag	UNP P03429
D	764	PRO	-	expression tag	UNP P03429
D	765	GLN	-	expression tag	UNP P03429
D	766	PHE	-	expression tag	UNP P03429
D	767	GLU	-	expression tag	UNP P03429
D	768	LYS	-	expression tag	UNP P03429
D	769	GLY	-	expression tag	UNP P03429
D	770	GLY	-	expression tag	UNP P03429
D	771	GLY	-	expression tag	UNP P03429

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Chain	Residue	Modelled	Actual	Comment	Reference
D	772	SER	-	expression tag	UNP P03429
D	773	GLY	-	expression tag	UNP P03429
D	774	GLY	-	expression tag	UNP P03429
D	775	GLY	-	expression tag	UNP P03429
D	776	SER	-	expression tag	UNP P03429
D	777	GLY	-	expression tag	UNP P03429
D	778	GLY	-	expression tag	UNP P03429
D	779	SER	-	expression tag	UNP P03429
D	780	ALA	-	expression tag	UNP P03429
D	781	TRP	-	expression tag	UNP P03429
D	782	SER	-	expression tag	UNP P03429
D	783	HIS	-	expression tag	UNP P03429
D	784	PRO	-	expression tag	UNP P03429
D	785	GLN	-	expression tag	UNP P03429
D	786	PHE	-	expression tag	UNP P03429
D	787	GLU	-	expression tag	UNP P03429
D	788	LYS	-	expression tag	UNP P03429
D	789	GLY	-	expression tag	UNP P03429
D	790	ARG	-	expression tag	UNP P03429
D	791	SER	-	expression tag	UNP P03429
D	792	GLY	-	expression tag	UNP P03429
G	691	ARG	LEU	engineered mutation	UNP P03429
G	760	GLY	-	expression tag	UNP P03429
G	761	TRP	-	expression tag	UNP P03429
G	762	SER	-	expression tag	UNP P03429
G	763	HIS	-	expression tag	UNP P03429
G	764	PRO	-	expression tag	UNP P03429
G	765	GLN	-	expression tag	UNP P03429
G	766	PHE	-	expression tag	UNP P03429
G	767	GLU	-	expression tag	UNP P03429
G	768	LYS	-	expression tag	UNP P03429
G	769	GLY	-	expression tag	UNP P03429
G	770	GLY	-	expression tag	UNP P03429
G	771	GLY	-	expression tag	UNP P03429
G	772	SER	-	expression tag	UNP P03429
G	773	GLY	-	expression tag	UNP P03429
G	774	GLY	-	expression tag	UNP P03429
G	775	GLY	-	expression tag	UNP P03429
G	776	SER	-	expression tag	UNP P03429
G	777	GLY	-	expression tag	UNP P03429
G	778	GLY	-	expression tag	UNP P03429
G	779	SER	-	expression tag	UNP P03429

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Chain	Residue	Modelled	Actual	Comment	Reference
G	780	ALA	-	expression tag	UNP P03429
G	781	TRP	-	expression tag	UNP P03429
G	782	SER	-	expression tag	UNP P03429
G	783	HIS	-	expression tag	UNP P03429
G	784	PRO	-	expression tag	UNP P03429
G	785	GLN	-	expression tag	UNP P03429
G	786	PHE	-	expression tag	UNP P03429
G	787	GLU	-	expression tag	UNP P03429
G	788	LYS	-	expression tag	UNP P03429
G	789	GLY	-	expression tag	UNP P03429
G	790	ARG	-	expression tag	UNP P03429
G	791	SER	-	expression tag	UNP P03429
G	792	GLY	-	expression tag	UNP P03429
P	691	ARG	LEU	engineered mutation	UNP P03429
P	760	GLY	-	expression tag	UNP P03429
P	761	TRP	-	expression tag	UNP P03429
P	762	SER	-	expression tag	UNP P03429
P	763	HIS	-	expression tag	UNP P03429
P	764	PRO	-	expression tag	UNP P03429
P	765	GLN	-	expression tag	UNP P03429
P	766	PHE	-	expression tag	UNP P03429
P	767	GLU	-	expression tag	UNP P03429
P	768	LYS	-	expression tag	UNP P03429
P	769	GLY	-	expression tag	UNP P03429
P	770	GLY	-	expression tag	UNP P03429
P	771	GLY	-	expression tag	UNP P03429
P	772	SER	-	expression tag	UNP P03429
P	773	GLY	-	expression tag	UNP P03429
P	774	GLY	-	expression tag	UNP P03429
P	775	GLY	-	expression tag	UNP P03429
P	776	SER	-	expression tag	UNP P03429
P	777	GLY	-	expression tag	UNP P03429
P	778	GLY	-	expression tag	UNP P03429
P	779	SER	-	expression tag	UNP P03429
P	780	ALA	-	expression tag	UNP P03429
P	781	TRP	-	expression tag	UNP P03429
P	782	SER	-	expression tag	UNP P03429
P	783	HIS	-	expression tag	UNP P03429
P	784	PRO	-	expression tag	UNP P03429
P	785	GLN	-	expression tag	UNP P03429
P	786	PHE	-	expression tag	UNP P03429
P	787	GLU	-	expression tag	UNP P03429

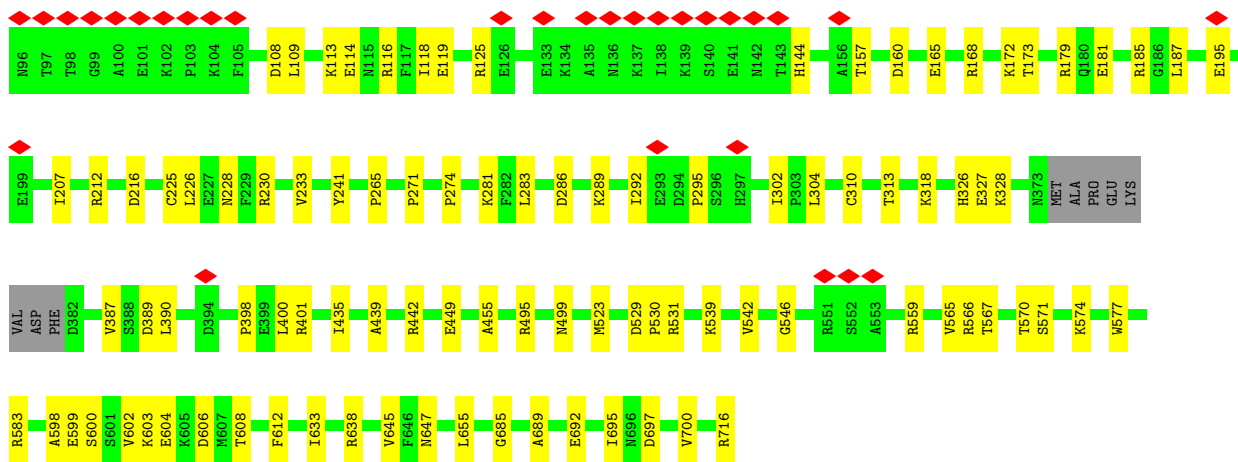
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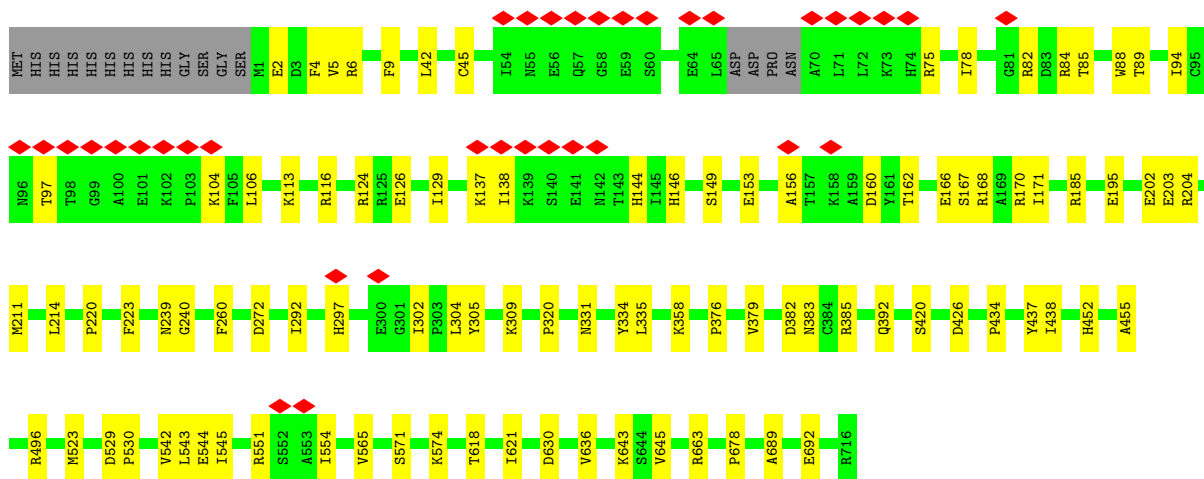
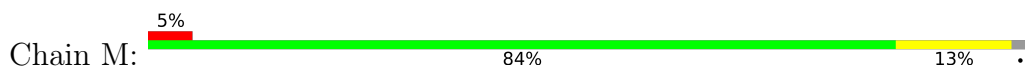
Chain	Residue	Modelled	Actual	Comment	Reference
P	788	LYS	-	expression tag	UNP P03429
P	789	GLY	-	expression tag	UNP P03429
P	790	ARG	-	expression tag	UNP P03429
P	791	SER	-	expression tag	UNP P03429
P	792	GLY	-	expression tag	UNP P03429

- Molecule 4 is a protein called Nuclear export protein.

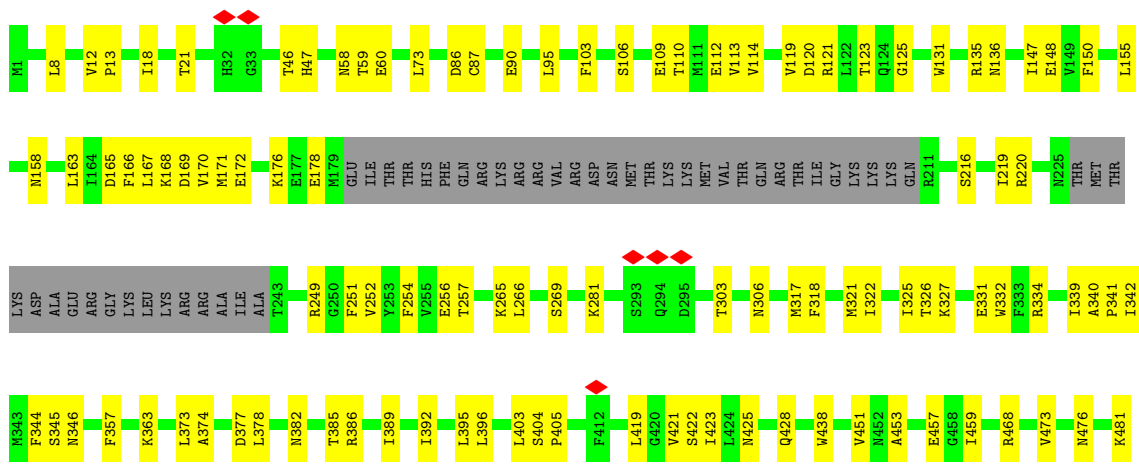
Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			S
4	S	117	975	614	170	185	6	0	0
4	T	117	971	612	169	184	6	0	0
4	U	117	975	614	170	185	6	0	0
4	V	117	971	612	169	184	6	0	0
4	W	117	975	614	170	185	6	0	0
4	X	117	971	612	169	184	6	0	0

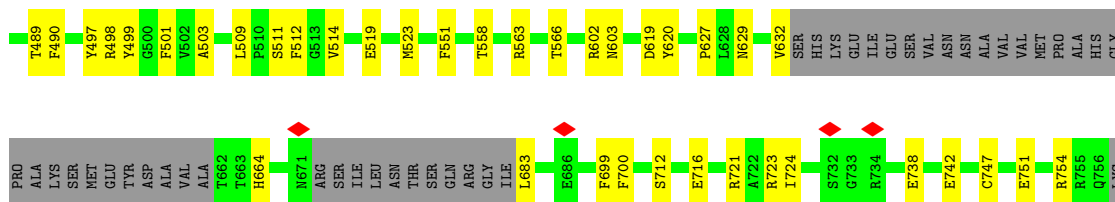


• Molecule 1: Polymerase acidic protein

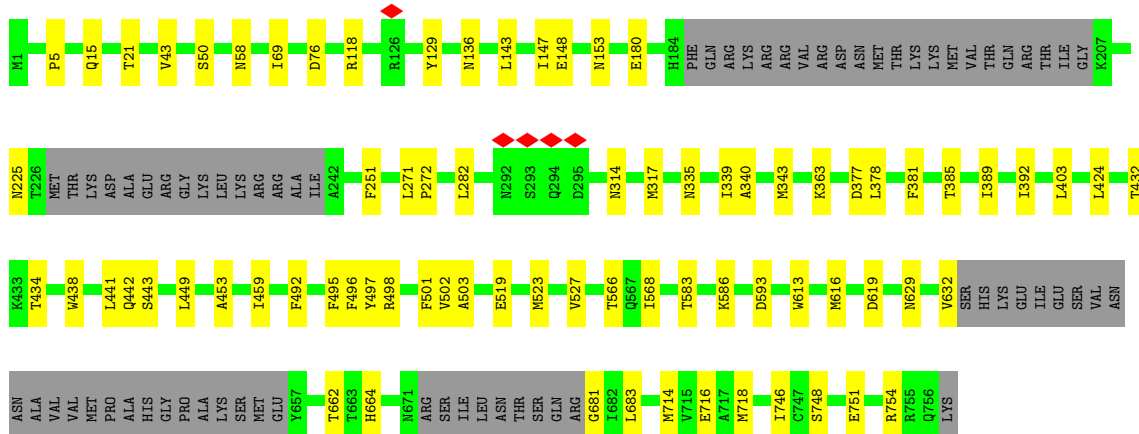
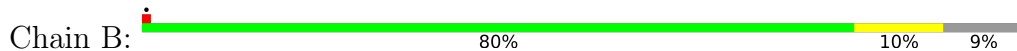


• Molecule 2: RNA-directed RNA polymerase catalytic subunit

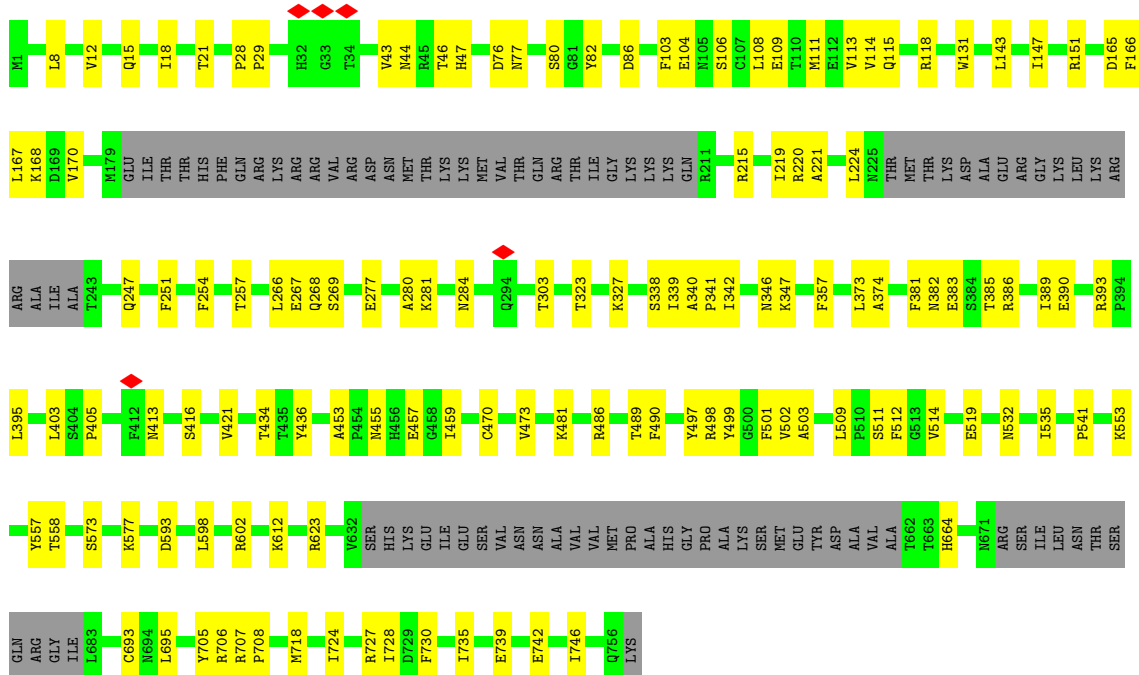




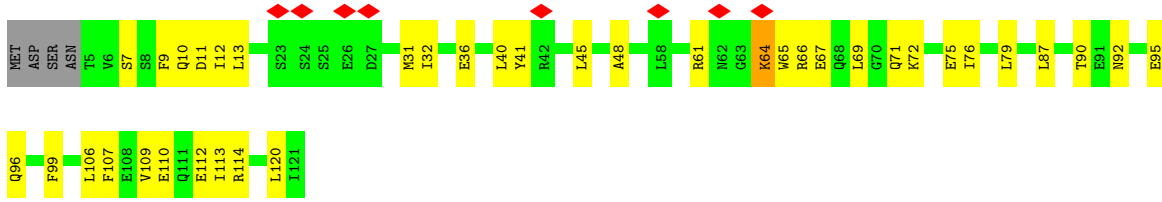
• Molecule 2: RNA-directed RNA polymerase catalytic subunit



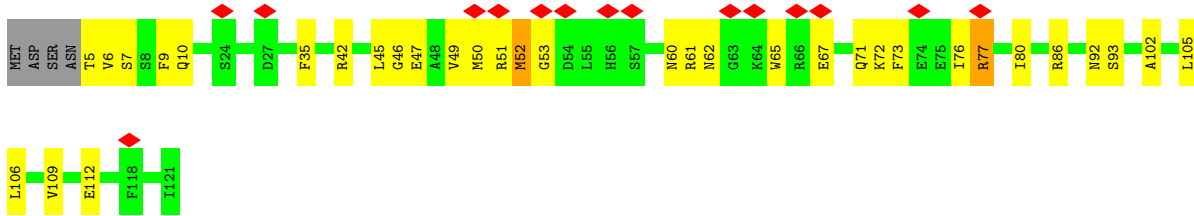
• Molecule 2: RNA-directed RNA polymerase catalytic subunit



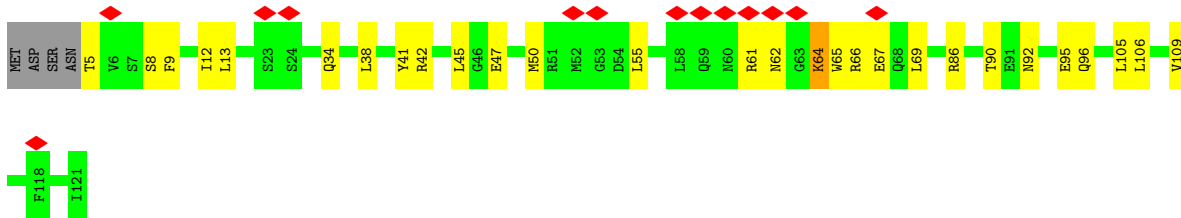
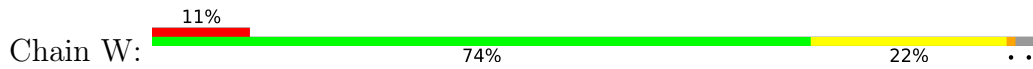
• Molecule 2: RNA-directed RNA polymerase catalytic subunit



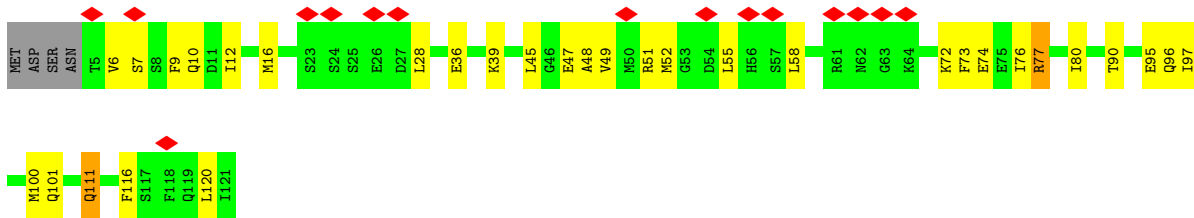
• Molecule 4: Nuclear export protein



• Molecule 4: Nuclear export protein



• Molecule 4: Nuclear export protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	351243	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.793	Depositor
Minimum map value	-0.005	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	498.4, 498.4, 498.4	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.89, 0.89, 0.89	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.25	0/5902	0.49	0/7957
1	E	0.24	0/5669	0.49	0/7645
1	I	0.24	0/5676	0.49	0/7654
1	L	0.24	0/5902	0.49	0/7957
1	M	0.24	0/5902	0.48	0/7957
1	Q	0.24	0/5676	0.49	0/7654
2	B	0.24	0/5563	0.48	0/7508
2	F	0.25	0/5402	0.50	0/7295
2	H	0.24	0/5402	0.49	0/7295
2	J	0.25	0/5563	0.49	0/7508
2	N	0.24	0/5563	0.49	0/7508
2	R	0.25	0/5402	0.49	0/7295
3	C	0.23	0/2504	0.53	0/3368
3	D	0.23	0/1975	0.50	0/2653
3	G	0.24	0/2766	0.52	0/3722
3	K	0.24	0/2504	0.52	0/3368
3	O	0.23	0/2504	0.53	0/3368
3	P	0.24	0/1975	0.50	0/2653
4	S	0.26	0/989	0.55	0/1321
4	T	0.27	0/985	0.57	0/1316
4	U	0.28	0/989	0.56	0/1321
4	V	0.24	0/985	0.53	0/1316
4	W	0.28	0/989	0.56	0/1321
4	X	0.27	0/985	0.54	0/1316
All	All	0.24	0/87772	0.50	0/118276

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5779	0	5689	64	0
1	E	5552	0	5441	76	0
1	I	5558	0	5448	58	0
1	L	5779	0	5689	83	0
1	M	5779	0	5689	64	0
1	Q	5558	0	5448	69	0
2	B	5457	0	5403	50	0
2	F	5297	0	5214	104	0
2	H	5297	0	5214	96	0
2	J	5457	0	5403	67	0
2	N	5457	0	5403	48	0
2	R	5297	0	5214	95	0
3	C	2463	0	2537	27	0
3	D	1943	0	1992	38	0
3	G	2724	0	2800	43	0
3	K	2463	0	2537	38	0
3	O	2463	0	2537	37	0
3	P	1943	0	1992	38	0
4	S	975	0	970	26	0
4	T	971	0	964	26	0
4	U	975	0	970	26	0
4	V	971	0	964	25	0
4	W	975	0	970	19	0
4	X	971	0	964	25	0
All	All	86104	0	85452	1121	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 7.

All (1121) 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)
3:K:59:ALA:O	3:K:88:ARG:HA	1.68	0.93
3:D:59:ALA:O	3:D:88:ARG:HA	1.75	0.86
1:E:204:ARG:HB3	2:F:332:TRP:HB2	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:28:MET:SD	3:O:32:LYS:NZ	2.51	0.83
1:L:207:ILE:O	1:L:208:THR:HG22	1.82	0.79
1:M:124:ARG:HH21	1:M:195:GLU:HB3	1.47	0.78
4:X:36:GLU:HA	4:X:39:LYS:HZ3	1.49	0.77
4:T:6:VAL:HA	4:T:9:PHE:HD2	1.48	0.77
1:L:320:PRO:HA	1:L:544:GLU:O	1.84	0.77
4:S:101:GLN:HB2	4:T:12:ILE:HD11	1.67	0.76
1:A:114:GLU:HG2	1:A:116:ARG:HE	1.52	0.75
2:F:425:ASN:HD22	2:F:428:GLN:HE22	1.34	0.75
1:Q:530:PRO:HG2	1:Q:542:VAL:HG11	1.67	0.75
3:O:744:LEU:HD12	3:O:746:ASP:H	1.52	0.75
2:H:280:ALA:O	2:H:284:ASN:ND2	2.20	0.74
2:H:708:PRO:HB3	3:G:728:GLN:HG3	1.70	0.74
1:E:571:SER:HB3	1:E:574:LYS:HG2	1.69	0.74
2:J:434:THR:HG22	2:J:435:THR:H	1.54	0.72
3:P:59:ALA:O	3:P:88:ARG:HA	1.90	0.72
2:N:210:GLN:NE2	2:N:211:ARG:O	2.23	0.71
4:T:35:PHE:O	4:T:39:LYS:HG2	1.91	0.71
2:H:498:ARG:HG3	2:H:499:TYR:H	1.55	0.71
3:O:1:MET:SD	3:O:5:LYS:NZ	2.64	0.71
3:O:59:ALA:O	3:O:88:ARG:HA	1.90	0.71
1:A:530:PRO:HG2	1:A:542:VAL:HG11	1.73	0.71
1:A:320:PRO:HA	1:A:544:GLU:O	1.90	0.71
3:K:708:LEU:HB3	3:K:724:VAL:HG12	1.73	0.70
3:K:2:GLU:HA	3:K:5:LYS:HE2	1.74	0.70
3:C:744:LEU:HD12	3:C:746:ASP:H	1.57	0.70
4:U:112:GLU:OE1	4:V:42:ARG:NH1	2.25	0.70
2:F:723:ARG:HH12	2:F:747:CYS:HB3	1.57	0.70
1:E:209:GLY:H	1:E:212:ARG:HG3	1.56	0.70
1:Q:173:THR:HG22	3:P:696:ILE:HG12	1.74	0.70
2:H:489:THR:HA	2:H:497:TYR:O	1.91	0.69
1:Q:583:ARG:NH2	2:R:509:LEU:O	2.25	0.69
1:Q:76:PHE:HB3	1:Q:109:LEU:HD11	1.75	0.69
2:F:378:LEU:O	2:F:386:ARG:NH1	2.26	0.69
2:J:131:TRP:O	2:J:220:ARG:NH2	2.25	0.69
1:L:208:THR:HG23	1:L:208:THR:O	1.93	0.68
4:X:36:GLU:HA	4:X:39:LYS:NZ	2.08	0.68
3:K:737:ARG:HE	3:K:738:LYS:H	1.41	0.68
2:H:76:ASP:OD1	2:H:77:ASN:N	2.22	0.68
1:I:571:SER:HB3	1:I:574:LYS:HG2	1.76	0.68
1:L:643:LYS:HD2	2:J:5:PRO:HG2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:744:LEU:HD12	3:K:746:ASP:H	1.56	0.68
2:J:453:ALA:HB3	2:J:459:ILE:HG13	1.75	0.68
2:R:403:LEU:HG	2:R:405:PRO:HD3	1.76	0.68
1:E:530:PRO:HG2	1:E:542:VAL:HG11	1.75	0.67
1:Q:165:GLU:HA	1:Q:168:ARG:HH21	1.59	0.67
2:N:662:THR:HG22	2:N:664:HIS:H	1.60	0.67
1:A:621:ILE:HD13	1:A:636:VAL:HG12	1.77	0.67
4:U:31:MET:SD	4:V:86:ARG:NH1	2.67	0.67
1:L:618:THR:HB	1:L:630:ASP:HB3	1.77	0.67
3:P:696:ILE:HG22	3:P:734:VAL:HG22	1.77	0.67
2:B:453:ALA:HB3	2:B:459:ILE:HG13	1.77	0.67
1:L:629:GLU:OE1	2:J:1:MET:HB2	1.95	0.67
1:E:539:LYS:HD3	1:E:566:ARG:HH21	1.60	0.66
3:D:114:VAL:HG11	3:D:203:VAL:HG23	1.77	0.66
1:Q:75:ARG:HH21	1:Q:113:LYS:HD3	1.60	0.66
1:L:239:ASN:OD1	1:L:240:GLY:N	2.28	0.66
1:Q:442:ARG:HE	1:Q:608:THR:HG21	1.61	0.66
1:Q:574:LYS:HA	1:Q:577:TRP:HB3	1.77	0.66
3:O:715:ASN:OD1	3:O:716:LEU:N	2.26	0.66
2:R:614:GLU:HG2	2:R:615:LEU:HD12	1.77	0.66
1:L:352:GLU:HG2	1:L:353:LYS:HG3	1.78	0.65
3:C:716:LEU:HG	3:C:717:ALA:H	1.59	0.65
2:J:43:VAL:HG22	2:J:403:LEU:HD12	1.77	0.65
1:L:449:GLU:OE2	1:L:638:ARG:NH1	2.29	0.65
3:C:143:ARG:NH1	3:C:220:VAL:O	2.30	0.65
2:J:662:THR:HG23	2:J:664:HIS:H	1.60	0.65
1:I:214:LEU:HD22	2:H:346:ASN:HD21	1.61	0.65
1:L:583:ARG:HE	2:J:25:THR:HG21	1.60	0.65
1:E:583:ARG:NH2	2:F:509:LEU:O	2.28	0.64
2:R:273:VAL:HB	2:R:277:GLU:HG3	1.78	0.64
1:M:320:PRO:HA	1:M:544:GLU:O	1.97	0.64
2:R:511:SER:OG	2:R:512:PHE:N	2.31	0.64
2:F:699:PHE:HZ	3:D:7:LEU:HD11	1.62	0.64
3:O:701:ASP:OD2	3:O:703:ARG:NH1	2.31	0.64
1:I:478:ASP:OD1	1:I:510:HIS:NE2	2.30	0.64
2:H:511:SER:OG	2:H:512:PHE:N	2.31	0.64
4:V:51:ARG:O	4:V:53:GLY:N	2.30	0.64
2:F:176:LYS:NZ	2:F:178:GLU:O	2.31	0.64
2:R:489:THR:HG22	2:R:498:ARG:HA	1.80	0.63
3:P:700:GLU:HB2	3:P:731:VAL:HG13	1.81	0.63
2:J:279:LYS:NZ	2:J:502:VAL:O	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:693:GLY:HA3	3:O:737:ARG:HD3	1.80	0.63
2:B:662:THR:HG22	2:B:664:HIS:H	1.64	0.63
2:R:716:GLU:HA	2:R:719:VAL:HG22	1.80	0.63
1:E:455:ALA:HB1	1:E:645:VAL:HG21	1.79	0.63
4:V:6:VAL:HA	4:V:9:PHE:HD2	1.63	0.63
2:H:381:PHE:O	2:H:386:ARG:NH1	2.32	0.63
2:R:519:GLU:OE2	2:R:664:HIS:ND1	2.31	0.63
2:F:511:SER:OG	2:F:512:PHE:N	2.32	0.63
2:H:373:LEU:HD21	2:H:389:ILE:HD12	1.81	0.63
1:L:635:LYS:HE3	2:J:1:MET:HE1	1.79	0.63
2:H:742:GLU:O	2:H:746:ILE:HG13	1.99	0.62
2:R:383:GLU:OE1	2:R:387:LYS:NZ	2.32	0.62
2:H:598:LEU:HD13	2:H:612:LYS:HE2	1.80	0.62
1:Q:539:LYS:HD3	1:Q:566:ARG:HH21	1.64	0.62
3:O:737:ARG:NH2	3:O:740:ASP:O	2.32	0.62
4:W:47:GLU:HA	4:W:50:MET:HG3	1.80	0.62
3:G:59:ALA:O	3:G:88:ARG:HA	1.99	0.62
1:A:318:LYS:HG2	1:A:546:GLY:HA2	1.81	0.62
3:P:235:THR:HA	3:P:242:GLN:HB3	1.82	0.62
2:R:125:GLY:HA3	2:R:249:ARG:HH12	1.65	0.62
1:M:621:ILE:HG21	1:M:636:VAL:HG12	1.81	0.62
3:D:116:LYS:O	3:D:119:PHE:N	2.32	0.62
2:N:453:ALA:HB3	2:N:459:ILE:HG13	1.81	0.62
2:F:147:ILE:HD11	2:F:158:ASN:HD22	1.65	0.62
2:J:183:THR:O	2:J:207:LYS:HA	2.00	0.62
1:Q:599:GLU:O	1:Q:602:VAL:HG22	1.98	0.62
2:H:413:ASN:ND2	2:H:416:SER:OG	2.32	0.62
4:U:79:LEU:HG	4:U:106:LEU:HD21	1.82	0.62
1:E:76:PHE:HB3	1:E:109:LEU:HD11	1.80	0.61
4:T:20:GLN:NE2	4:T:29:ASN:OD1	2.34	0.61
1:Q:114:GLU:HB3	1:Q:116:ARG:HG2	1.80	0.61
2:F:629:ASN:HB2	2:F:632:VAL:HG12	1.82	0.61
1:I:1:MET:HB2	1:I:187:LEU:HD22	1.83	0.61
2:H:453:ALA:HB3	2:H:459:ILE:HG13	1.82	0.61
1:L:75:ARG:HH22	1:L:113:LYS:HD2	1.64	0.61
3:O:78:TRP:HB3	3:O:91:VAL:HG12	1.82	0.61
4:X:73:PHE:O	4:X:77:ARG:NH1	2.34	0.61
1:E:214:LEU:HD23	1:E:217:GLN:HE21	1.65	0.61
2:J:455:ASN:ND2	2:J:457:GLU:OE2	2.34	0.61
4:V:73:PHE:O	4:V:77:ARG:NH1	2.32	0.61
1:M:204:ARG:O	2:N:168:LYS:NZ	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:710:ILE:HD11	3:C:726:ILE:HG22	1.83	0.61
2:H:113:VAL:HG11	2:H:257:THR:HG21	1.82	0.61
3:O:143:ARG:NH1	3:O:220:VAL:O	2.34	0.61
2:H:165:ASP:HA	2:H:168:LYS:HG2	1.83	0.60
2:H:489:THR:HG22	2:H:498:ARG:HA	1.83	0.60
2:J:614:GLU:HG2	2:J:615:LEU:HD12	1.81	0.60
3:C:161:ASP:OD2	3:C:175:ARG:NH1	2.32	0.60
4:V:72:LYS:O	4:V:76:ILE:HG12	2.02	0.60
1:M:618:THR:HB	1:M:630:ASP:HB3	1.83	0.60
2:J:335:ASN:O	2:J:339:ILE:HG12	2.02	0.60
3:P:184:THR:O	3:P:187:LYS:HG3	2.01	0.60
1:E:75:ARG:HH21	1:E:113:LYS:HD3	1.66	0.60
2:J:687:GLN:HB3	2:J:690:GLN:HE21	1.67	0.60
1:A:13:ILE:HG23	1:A:42:LEU:HD23	1.83	0.60
1:E:574:LYS:HA	1:E:577:TRP:HB3	1.84	0.59
2:H:131:TRP:O	2:H:220:ARG:NH2	2.35	0.59
1:M:211:MET:HA	1:M:214:LEU:HB2	1.84	0.59
3:O:12:SER:O	3:O:17:ARG:NH2	2.35	0.59
3:G:264:ARG:HB3	3:G:268:ARG:HH12	1.67	0.59
2:H:339:ILE:HA	2:H:342:ILE:HD12	1.84	0.59
4:U:64:LYS:O	4:U:67:GLU:HG3	2.02	0.59
2:H:303:THR:HG21	2:H:490:PHE:HB2	1.82	0.59
2:R:690:GLN:O	2:R:693:CYS:HB2	2.03	0.59
2:B:148:GLU:OE1	3:C:15:ARG:NH2	2.31	0.59
1:I:442:ARG:HE	1:I:608:THR:HG21	1.67	0.59
2:H:695:LEU:HD23	2:H:718:MET:HE1	1.84	0.59
3:D:130:PHE:HE1	3:D:234:LEU:HD21	1.67	0.59
2:F:135:ARG:HG2	2:F:136:ASN:H	1.68	0.59
4:S:74:GLU:OE1	4:S:77:ARG:NH2	2.33	0.59
2:H:170:VAL:HG11	2:H:247:GLN:HB2	1.85	0.59
1:A:289:LYS:HB3	1:A:499:ASN:HB3	1.85	0.59
3:G:264:ARG:HB3	3:G:268:ARG:NH1	2.17	0.59
2:B:118:ARG:HD2	3:C:30:ILE:HD11	1.85	0.58
1:A:618:THR:HB	1:A:630:ASP:HB3	1.83	0.58
3:K:165:GLU:HG2	3:K:691:ARG:HH22	1.68	0.58
1:L:510:HIS:O	1:L:512:ARG:NH1	2.36	0.58
4:X:72:LYS:O	4:X:76:ILE:HG12	2.03	0.58
1:A:134:LYS:HB3	1:A:145:ILE:HD13	1.85	0.58
1:L:114:GLU:HB3	1:L:116:ARG:HG2	1.85	0.58
1:L:514:ASP:HB3	1:L:573:ILE:HG13	1.85	0.58
3:D:118:TYR:O	3:D:121:LYS:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:374:ALA:HB2	2:F:396:LEU:HD23	1.85	0.58
4:U:106:LEU:HA	4:U:109:VAL:HG12	1.85	0.58
1:Q:600:SER:HB2	1:Q:606:ASP:OD1	2.04	0.58
2:R:455:ASN:ND2	2:R:457:GLU:OE1	2.37	0.58
1:Q:181:GLU:OE2	1:Q:185:ARG:NH2	2.37	0.58
1:I:289:LYS:HB3	1:I:499:ASN:HB3	1.86	0.58
2:H:43:VAL:HG12	2:H:47:HIS:HE1	1.69	0.58
2:R:378:LEU:O	2:R:386:ARG:NH1	2.37	0.58
1:E:387:VAL:HG12	1:E:389:ASP:H	1.68	0.58
1:L:173:THR:OG1	3:K:696:ILE:HG22	2.04	0.58
4:V:77:ARG:HA	4:V:80:ILE:HG22	1.85	0.58
1:Q:435:ILE:HD11	3:P:234:LEU:HD12	1.86	0.58
1:Q:571:SER:HB3	1:Q:574:LYS:HG2	1.86	0.58
2:R:453:ALA:HB3	2:R:459:ILE:HG13	1.86	0.58
1:A:11:PRO:O	1:A:14:VAL:N	2.37	0.57
3:C:161:ASP:HB3	3:C:176:ILE:HD12	1.85	0.57
1:I:530:PRO:HG2	1:I:542:VAL:HG11	1.84	0.57
1:M:149:SER:HB3	1:M:153:GLU:H	1.68	0.57
2:N:335:ASN:O	2:N:339:ILE:HG12	2.04	0.57
1:I:583:ARG:NH2	2:H:509:LEU:O	2.33	0.57
3:D:157:LYS:HA	3:D:160:GLN:HG2	1.86	0.57
1:Q:179:ARG:HD2	2:R:711:ILE:HD11	1.85	0.57
3:D:30:ILE:O	3:D:33:LYS:NZ	2.38	0.57
1:A:689:ALA:HA	1:A:692:GLU:HG2	1.87	0.57
2:H:46:THR:HG22	2:H:405:PRO:HG2	1.86	0.57
2:H:708:PRO:HA	3:G:728:GLN:HE21	1.69	0.57
4:U:66:ARG:HH22	4:U:120:LEU:HD23	1.69	0.57
1:M:292:ILE:HD11	1:M:309:LYS:HE2	1.86	0.57
2:F:700:PHE:HE1	2:F:721:ARG:HH21	1.53	0.57
1:I:196:ARG:HE	1:I:204:ARG:HH12	1.51	0.57
3:D:4:ILE:HD12	3:D:7:LEU:HD12	1.86	0.57
4:S:79:LEU:HD22	4:S:106:LEU:HD21	1.85	0.57
2:H:167:LEU:HD23	2:H:251:PHE:CE1	2.40	0.57
4:U:72:LYS:O	4:U:76:ILE:HG12	2.04	0.57
1:M:239:ASN:OD1	1:M:240:GLY:N	2.35	0.57
2:F:123:THR:HG21	3:D:33:LYS:HD2	1.85	0.57
2:H:266:LEU:HD13	2:H:421:VAL:HG11	1.85	0.57
1:L:161:TYR:HB3	1:L:168:ARG:HH12	1.70	0.57
1:M:523:MET:HG2	1:M:565:VAL:HG22	1.87	0.57
2:N:583:THR:O	2:N:586:LYS:NZ	2.38	0.57
3:G:118:TYR:OH	3:G:209:ARG:NH1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:716:GLU:OE2	2:B:754:ARG:NH1	2.38	0.57
1:M:689:ALA:HA	1:M:692:GLU:HG2	1.86	0.57
1:I:387:VAL:HG12	1:I:389:ASP:H	1.69	0.56
3:D:117:THR:OG1	3:D:209:ARG:NH1	2.38	0.56
1:E:241:TYR:OH	2:F:86:ASP:O	2.21	0.56
1:L:455:ALA:HB1	1:L:645:VAL:HG21	1.86	0.56
2:F:8:LEU:O	2:F:12:VAL:N	2.32	0.56
2:F:423:ILE:HD11	2:F:473:VAL:HG21	1.87	0.56
2:F:453:ALA:HB3	2:F:459:ILE:HG13	1.86	0.56
2:F:489:THR:HA	2:F:497:TYR:O	2.05	0.56
2:B:335:ASN:O	2:B:339:ILE:HG12	2.05	0.56
1:Q:289:LYS:HB3	1:Q:499:ASN:HB3	1.86	0.56
2:R:619:ASP:OD1	2:R:620:TYR:N	2.38	0.56
2:N:519:GLU:HG3	2:N:664:HIS:HB3	1.87	0.56
3:O:710:ILE:HA	3:O:713:LEU:HD12	1.86	0.56
3:D:113:LYS:HG3	3:D:114:VAL:HG13	1.86	0.56
3:G:136:ARG:O	3:G:138:GLN:NE2	2.38	0.56
1:A:455:ALA:HB1	1:A:645:VAL:HG21	1.87	0.56
1:L:318:LYS:HG2	1:L:546:GLY:HA2	1.87	0.56
1:L:420:SER:O	1:L:452:HIS:ND1	2.38	0.56
1:Q:78:ILE:O	1:Q:82:ARG:NE	2.39	0.56
2:R:724:ILE:HD12	2:R:727:ARG:HD2	1.87	0.56
2:N:378:LEU:HD23	2:N:386:ARG:HG3	1.87	0.56
2:B:339:ILE:HG22	2:B:343:MET:HE2	1.88	0.56
1:I:233:VAL:HG11	2:H:323:THR:HG23	1.86	0.56
3:K:130:PHE:O	4:U:71:GLN:NE2	2.39	0.56
1:Q:387:VAL:HG12	1:Q:389:ASP:H	1.71	0.56
3:O:175:ARG:O	3:O:176:ILE:HG22	2.06	0.56
1:A:605:LYS:HD2	4:T:29:ASN:HB3	1.86	0.56
1:M:137:LYS:HB3	1:M:138:ILE:HD12	1.87	0.56
3:G:701:ASP:O	3:G:723:ASN:ND2	2.37	0.56
2:F:120:ASP:OD1	2:F:121:ARG:N	2.39	0.56
1:A:173:THR:HG22	3:C:696:ILE:HG12	1.86	0.56
2:R:413:ASN:ND2	2:R:416:SER:OG	2.39	0.56
4:X:97:ILE:O	4:X:101:GLN:HG3	2.06	0.56
3:K:175:ARG:O	3:K:176:ILE:HG22	2.06	0.56
3:P:111:TYR:HB3	3:P:112:PRO:HD3	1.88	0.56
1:L:685:GLY:HA3	2:J:480:LYS:HE3	1.87	0.55
3:O:57:ILE:HG13	3:O:91:VAL:HG23	1.88	0.55
3:P:13:GLN:HB2	3:P:16:THR:HG22	1.88	0.55
2:H:553:LYS:NZ	2:H:557:TYR:OH	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:128:THR:OG1	2:R:249:ARG:NH2	2.38	0.55
1:A:326:HIS:O	1:A:327:GLU:HG3	2.06	0.55
1:L:676:LEU:HD22	2:J:486:ARG:HB3	1.88	0.55
2:H:382:ASN:OD1	2:H:383:GLU:N	2.38	0.55
2:J:147:ILE:HG23	2:J:158:ASN:HD21	1.71	0.55
1:Q:449:GLU:OE2	1:Q:638:ARG:NH2	2.40	0.55
2:N:507:MET:SD	2:N:537:ASN:ND2	2.79	0.55
4:X:96:GLN:O	4:X:100:MET:HG2	2.06	0.55
4:U:10:GLN:NE2	4:U:11:ASP:OD1	2.40	0.55
1:L:207:ILE:O	1:L:208:THR:CG2	2.52	0.55
1:Q:118:ILE:HG12	1:Q:144:HIS:HB3	1.89	0.55
1:M:643:LYS:HD2	2:N:5:PRO:HG2	1.88	0.55
2:B:377:ASP:OD2	2:B:378:LEU:N	2.39	0.55
4:T:73:PHE:O	4:T:77:ARG:NH1	2.36	0.55
1:I:455:ALA:HB1	1:I:645:VAL:HG21	1.88	0.55
3:K:143:ARG:NH1	3:K:220:VAL:O	2.40	0.55
3:D:113:LYS:O	3:D:116:LYS:NZ	2.36	0.55
3:O:188:GLU:O	3:O:192:GLU:HG3	2.06	0.55
1:L:152:GLY:HA2	1:L:172:LYS:HD3	1.88	0.55
1:A:292:ILE:HG23	1:A:295:PRO:HD3	1.88	0.54
1:A:75:ARG:HH21	1:A:113:LYS:HD2	1.72	0.54
1:I:420:SER:O	1:I:452:HIS:ND1	2.41	0.54
1:E:118:ILE:HG12	1:E:144:HIS:HB3	1.89	0.54
1:E:219:LEU:HD11	1:E:226:LEU:HD23	1.89	0.54
2:F:519:GLU:HG3	2:F:664:HIS:HB3	1.90	0.54
1:L:576:LYS:HE2	3:K:45:LEU:HD11	1.89	0.54
2:J:135:ARG:HG2	2:J:136:ASN:H	1.73	0.54
4:U:71:GLN:O	4:U:75:GLU:HG3	2.07	0.54
2:N:514:VAL:O	3:O:44:SER:OG	2.25	0.54
2:F:303:THR:HG21	2:F:490:PHE:HB2	1.88	0.54
2:B:282:LEU:HD23	2:B:441:LEU:HD21	1.89	0.54
3:C:746:ASP:O	3:C:749:THR:OG1	2.20	0.54
4:S:97:ILE:O	4:S:101:GLN:HG3	2.07	0.54
4:X:77:ARG:HA	4:X:80:ILE:HG22	1.89	0.54
2:F:377:ASP:OD1	2:F:378:LEU:N	2.38	0.54
3:C:59:ALA:O	3:C:88:ARG:HA	2.07	0.54
3:P:700:GLU:HG3	3:P:723:ASN:HD22	1.72	0.54
2:F:619:ASP:OD1	2:F:620:TYR:N	2.41	0.54
1:A:493:GLU:OE2	1:A:495:ARG:NH2	2.39	0.54
1:Q:326:HIS:O	1:Q:327:GLU:HG3	2.08	0.54
1:Q:529:ASP:OD1	1:Q:531:ARG:NH1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:420:SER:O	1:M:452:HIS:ND1	2.40	0.54
2:H:434:THR:HG23	2:H:436:TYR:H	1.73	0.54
2:J:143:LEU:O	2:J:147:ILE:HG12	2.08	0.54
1:M:124:ARG:NH2	1:M:195:GLU:HB3	2.19	0.54
2:J:583:THR:O	2:J:586:LYS:NZ	2.40	0.54
2:R:339:ILE:HA	2:R:342:ILE:HD12	1.88	0.54
1:M:202:GLU:HG2	1:M:203:GLU:H	1.73	0.54
3:O:132:PRO:HD2	3:O:243:MET:HE3	1.90	0.54
2:H:43:VAL:HG12	2:H:47:HIS:CE1	2.43	0.54
1:L:568:ASN:OD1	1:L:569:GLY:N	2.36	0.54
4:X:6:VAL:O	4:X:9:PHE:N	2.41	0.54
3:D:159:ALA:O	3:D:163:ILE:HG12	2.07	0.54
2:H:727:ARG:NH2	3:G:707:ALA:O	2.41	0.54
1:E:442:ARG:HH21	1:E:608:THR:HG21	1.72	0.53
2:F:325:ILE:HG23	2:F:326:THR:HG23	1.90	0.53
2:H:739:GLU:HA	2:H:742:GLU:HG3	1.90	0.53
1:Q:455:ALA:HB1	1:Q:645:VAL:HG21	1.88	0.53
2:R:489:THR:HA	2:R:497:TYR:O	2.07	0.53
1:M:146:HIS:ND1	1:M:156:ALA:HB2	2.23	0.53
2:J:180:GLU:OE1	2:J:209:LYS:NZ	2.41	0.53
2:F:119:VAL:HA	2:F:163:LEU:HD12	1.91	0.53
2:F:723:ARG:NH1	2:F:747:CYS:HB3	2.23	0.53
1:I:241:TYR:OH	2:H:86:ASP:O	2.20	0.53
3:G:61:LYS:HZ2	3:G:88:ARG:N	2.07	0.53
1:A:380:ASP:OD1	1:A:381:PHE:N	2.41	0.53
2:J:147:ILE:HD12	2:J:158:ASN:HD22	1.73	0.53
1:Q:12:MET:SD	1:Q:13:ILE:HG13	2.49	0.53
3:P:55:TYR:HB3	3:P:90:MET:HB3	1.91	0.53
2:F:18:ILE:O	2:F:21:THR:OG1	2.27	0.53
1:A:352:GLU:HG3	1:A:353:LYS:HG3	1.90	0.53
1:A:663:ARG:HB2	2:B:21:THR:HG21	1.90	0.53
3:K:141:ILE:HG13	3:K:143:ARG:HH11	1.74	0.53
1:E:147:ILE:HB	1:E:155:MET:HB2	1.89	0.53
2:F:46:THR:HG22	2:F:405:PRO:HG2	1.89	0.53
1:I:677:GLU:OE2	2:H:486:ARG:NH2	2.38	0.53
3:D:163:ILE:HD12	3:D:207:LEU:HB3	1.89	0.53
4:T:49:VAL:HG13	1:L:554:ILE:HD13	1.91	0.53
1:Q:108:ASP:HB2	1:Q:119:GLU:HA	1.91	0.53
3:O:141:ILE:HG13	3:O:143:ARG:HH11	1.73	0.53
1:E:196:ARG:HG3	1:E:201:ILE:HD13	1.90	0.53
1:E:623:GLU:OE1	1:E:709:SER:OG	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:292:ILE:HG23	1:Q:295:PRO:HD3	1.91	0.53
2:R:690:GLN:OE1	3:P:35:THR:OG1	2.21	0.53
1:A:302:ILE:HD13	1:A:305:TYR:HE2	1.74	0.52
2:J:177:GLU:OE1	2:J:178:GLU:HG2	2.09	0.52
3:P:78:TRP:HB3	3:P:91:VAL:HG12	1.90	0.52
1:E:212:ARG:NH2	1:E:227:GLU:OE1	2.42	0.52
1:E:331:ASN:HA	1:E:334:TYR:HD1	1.75	0.52
2:F:148:GLU:HG2	2:F:683:LEU:HD13	1.90	0.52
2:F:403:LEU:HG	2:F:405:PRO:HD3	1.92	0.52
2:R:165:ASP:HA	2:R:168:LYS:HG2	1.92	0.52
3:O:29:ALA:HA	3:O:32:LYS:NZ	2.24	0.52
3:O:159:ALA:O	3:O:163:ILE:HG12	2.09	0.52
3:G:110:HIS:HD1	3:G:196:CYS:HG	0.67	0.52
2:F:150:PHE:HE2	2:F:170:VAL:HG22	1.74	0.52
2:F:498:ARG:HG3	2:F:499:TYR:H	1.74	0.52
2:B:497:TYR:HD1	2:B:502:VAL:HG22	1.75	0.52
2:R:501:PHE:CE1	2:R:503:ALA:HB2	2.44	0.52
1:E:246:LEU:HD11	2:F:468:ARG:HE	1.74	0.52
3:C:735:MET:SD	3:C:738:LYS:NZ	2.82	0.52
2:H:251:PHE:HB3	2:H:340:ALA:HB2	1.90	0.52
1:Q:125:ARG:HD3	1:Q:195:GLU:HG3	1.91	0.52
2:R:371:GLU:HG2	2:R:399:GLY:HA3	1.91	0.52
4:W:64:LYS:O	4:W:67:GLU:HG3	2.08	0.52
1:E:530:PRO:O	1:E:531:ARG:HG2	2.09	0.52
1:I:664:LYS:HE3	2:H:481:LYS:HD2	1.90	0.52
1:E:604:GLU:OE2	3:D:136:ARG:NH2	2.43	0.52
2:F:86:ASP:OD1	2:F:87:CYS:N	2.43	0.52
2:F:165:ASP:OD1	2:F:166:PHE:N	2.42	0.52
2:R:317:MET:O	2:R:321:MET:HG3	2.09	0.52
1:Q:281:LYS:HE2	1:Q:570:THR:HG23	1.91	0.52
3:G:55:TYR:HB3	3:G:90:MET:HB3	1.91	0.52
3:G:135:PHE:HA	3:G:240:TRP:HA	1.92	0.52
1:E:249:MET:HB2	2:F:73:LEU:HD13	1.92	0.52
2:F:113:VAL:HG11	2:F:257:THR:HG21	1.91	0.52
1:A:657:GLY:O	1:A:661:GLU:HG2	2.09	0.52
1:I:274:PRO:HG2	1:I:401:ARG:HD3	1.90	0.52
3:K:11:MET:O	3:K:17:ARG:NH2	2.43	0.52
2:R:382:ASN:OD1	2:R:383:GLU:N	2.40	0.52
1:M:75:ARG:HH21	1:M:113:LYS:HD2	1.74	0.52
3:O:737:ARG:NH1	3:O:739:ARG:H	2.08	0.52
3:K:78:TRP:HB3	3:K:91:VAL:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:563:ARG:O	2:R:566:THR:OG1	2.26	0.52
4:S:5:THR:HG21	4:S:42:ARG:HH12	1.75	0.52
1:I:11:PRO:O	1:I:14:VAL:N	2.43	0.52
2:J:330:PRO:HB2	2:J:332:TRP:CD1	2.45	0.52
1:E:566:ARG:NH1	1:E:568:ASN:OD1	2.42	0.51
1:M:663:ARG:HB2	2:N:21:THR:HG21	1.91	0.51
4:W:62:ASN:C	4:W:66:ARG:HH22	2.14	0.51
3:P:184:THR:O	3:P:187:LYS:N	2.42	0.51
1:E:664:LYS:HE2	2:F:481:LYS:HB3	1.91	0.51
4:V:7:SER:HA	4:V:10:GLN:NE2	2.25	0.51
2:R:267:GLU:OE2	2:R:268:GLN:NE2	2.43	0.51
4:W:92:ASN:HB3	4:W:95:GLU:OE2	2.10	0.51
2:F:339:ILE:HA	2:F:342:ILE:HD12	1.91	0.51
1:Q:390:LEU:HB3	2:R:357:PHE:CZ	2.45	0.51
3:D:58:THR:HB	3:D:88:ARG:HD2	1.92	0.51
3:P:111:TYR:HA	3:P:198:ILE:HD11	1.92	0.51
2:F:501:PHE:CE2	2:F:503:ALA:HB2	2.45	0.51
2:H:224:LEU:HD12	2:H:347:LYS:HD3	1.92	0.51
2:R:251:PHE:HB3	2:R:340:ALA:HB2	1.93	0.51
1:E:694:LEU:HD22	1:E:701:LEU:HD23	1.93	0.51
2:F:266:LEU:HD13	2:F:421:VAL:HG11	1.91	0.51
4:W:12:ILE:HD11	4:X:101:GLN:HB2	1.92	0.51
1:E:555:GLY:HA3	4:T:116:PHE:HZ	1.76	0.51
2:F:373:LEU:HD21	2:F:389:ILE:HD12	1.93	0.51
2:F:514:VAL:HG11	2:F:558:THR:HG21	1.92	0.51
3:K:14:SER:O	3:K:17:ARG:N	2.44	0.51
2:F:327:LYS:HA	2:F:334:ARG:HH21	1.76	0.51
4:T:48:ALA:HA	4:T:51:ARG:HH11	1.75	0.51
1:I:326:HIS:O	1:I:327:GLU:HG3	2.11	0.51
2:H:114:VAL:HG23	2:H:254:PHE:CZ	2.46	0.51
3:K:737:ARG:HE	3:K:738:LYS:N	2.07	0.51
1:Q:530:PRO:O	1:Q:531:ARG:HG2	2.10	0.51
2:R:18:ILE:O	2:R:21:THR:OG1	2.26	0.51
3:G:264:ARG:NH1	3:G:268:ARG:HH22	2.09	0.51
2:H:501:PHE:CE2	2:H:503:ALA:HB2	2.46	0.51
2:H:502:VAL:HG12	2:H:502:VAL:O	2.11	0.51
1:L:621:ILE:HG21	1:L:636:VAL:HG12	1.93	0.51
1:M:302:ILE:HD13	1:M:305:TYR:HE2	1.75	0.51
2:N:167:LEU:HD12	2:N:251:PHE:CZ	2.46	0.51
2:B:15:GLN:OE1	2:B:498:ARG:NH1	2.44	0.51
2:J:148:GLU:HA	2:J:151:ARG:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:302:ILE:HG22	1:I:304:LEU:H	1.76	0.50
2:H:519:GLU:OE2	2:H:664:HIS:ND1	2.43	0.50
1:L:179:ARG:CZ	2:J:711:ILE:HD11	2.41	0.50
1:M:392:GLN:HA	2:N:357:PHE:CE2	2.47	0.50
4:X:45:LEU:O	4:X:49:VAL:HG23	2.11	0.50
2:F:317:MET:O	2:F:321:MET:HG3	2.10	0.50
2:J:112:GLU:O	2:J:116:GLN:HG3	2.11	0.50
2:R:177:GLU:HG2	2:R:214:LYS:HE2	1.94	0.50
3:D:78:TRP:HB3	3:D:91:VAL:HG12	1.94	0.50
1:E:225:CYS:HB3	1:E:228:ASN:ND2	2.27	0.50
1:Q:84:ARG:HE	1:Q:88:TRP:HE1	1.58	0.50
2:R:419:LEU:O	2:R:423:ILE:HG12	2.12	0.50
3:G:54:LYS:HE2	3:G:55:TYR:CZ	2.46	0.50
2:H:43:VAL:O	2:H:47:HIS:ND1	2.45	0.50
2:F:419:LEU:O	2:F:423:ILE:HG12	2.11	0.50
2:H:111:MET:O	2:H:115:GLN:HG2	2.12	0.50
2:H:730:PHE:HA	2:H:735:ILE:HG22	1.94	0.50
2:R:118:ARG:NH1	2:R:120:ASP:OD2	2.44	0.50
2:B:381:PHE:HB3	2:B:385:THR:HB	1.94	0.50
1:L:164:ASP:O	1:L:168:ARG:NE	2.45	0.50
2:R:327:LYS:HA	2:R:334:ARG:HH21	1.76	0.50
2:R:713:SER:N	2:R:716:GLU:OE2	2.45	0.50
1:M:455:ALA:HB1	1:M:645:VAL:HG21	1.92	0.50
3:G:113:LYS:HG3	3:G:114:VAL:HG13	1.93	0.50
3:P:189:LYS:HZ1	3:P:211:LEU:HD21	1.76	0.50
1:A:27:ASP:OD1	1:A:28:LEU:N	2.45	0.50
1:A:272:ASP:OD2	1:A:272:ASP:N	2.45	0.50
1:I:574:LYS:HA	1:I:577:TRP:HB3	1.92	0.50
2:B:443:SER:HB2	2:B:492:PHE:CZ	2.47	0.50
2:H:374:ALA:O	2:H:393:ARG:NH1	2.40	0.50
1:Q:697:ASP:HB3	1:Q:700:VAL:HG12	1.94	0.50
2:R:713:SER:OG	2:R:716:GLU:OE1	2.29	0.50
2:N:143:LEU:O	2:N:147:ILE:HG12	2.12	0.50
2:F:13:PRO:HB3	2:F:498:ARG:HH22	1.77	0.49
1:A:514:ASP:HB3	1:A:573:ILE:HG13	1.93	0.49
3:C:41:LYS:HB3	3:C:46:ARG:HH12	1.77	0.49
1:L:621:ILE:HD13	1:L:636:VAL:HG12	1.93	0.49
2:N:34:THR:HG22	2:N:35:GLY:H	1.77	0.49
3:D:700:GLU:HB2	3:D:731:VAL:HB	1.95	0.49
2:F:519:GLU:OE1	2:F:664:HIS:ND1	2.40	0.49
4:S:31:MET:HG2	4:S:35:PHE:HE2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:571:SER:HB3	1:L:574:LYS:HB2	1.93	0.49
2:R:384:SER:O	2:R:388:LYS:HG3	2.13	0.49
4:X:90:THR:OG1	4:X:95:GLU:OE1	2.30	0.49
3:D:697:LEU:HB2	3:D:733:LEU:HD22	1.94	0.49
2:F:340:ALA:HB3	2:F:341:PRO:HD3	1.95	0.49
3:C:14:SER:O	3:C:17:ARG:N	2.43	0.49
4:T:9:PHE:HD1	4:T:39:LYS:HZ3	1.58	0.49
4:U:92:ASN:HB3	4:U:95:GLU:OE1	2.11	0.49
2:F:47:HIS:NE2	2:F:395:LEU:HD21	2.27	0.49
2:H:111:MET:HA	2:H:114:VAL:HG12	1.95	0.49
1:E:697:ASP:HB3	1:E:700:VAL:HG12	1.94	0.49
1:A:643:LYS:HD2	2:B:5:PRO:HG2	1.94	0.49
2:H:735:ILE:HG13	2:H:739:GLU:OE2	2.12	0.49
1:Q:233:VAL:HG11	2:R:323:THR:HG23	1.93	0.49
4:S:109:VAL:O	4:S:113:ILE:HG12	2.13	0.49
1:Q:302:ILE:HG22	1:Q:304:LEU:H	1.77	0.49
2:R:113:VAL:HG11	2:R:257:THR:HG21	1.93	0.49
2:R:143:LEU:O	2:R:147:ILE:HG12	2.13	0.49
3:P:721:LYS:HD3	3:P:721:LYS:N	2.28	0.49
2:H:18:ILE:O	2:H:21:THR:OG1	2.29	0.49
2:H:166:PHE:HD2	2:H:167:LEU:HD12	1.78	0.49
1:L:108:ASP:HB2	1:L:119:GLU:HA	1.94	0.49
2:R:501:PHE:HE1	2:R:503:ALA:HB2	1.78	0.49
1:E:11:PRO:O	1:E:14:VAL:N	2.45	0.49
1:L:85:THR:O	1:L:89:THR:HG23	2.13	0.49
1:L:302:ILE:HD13	1:L:305:TYR:HE2	1.77	0.49
2:N:309:TRP:HZ2	2:N:416:SER:HB2	1.78	0.49
2:H:151:ARG:HH22	3:G:18:GLU:HG3	1.77	0.49
1:Q:600:SER:O	1:Q:603:LYS:O	2.31	0.49
1:L:133:GLU:O	1:L:137:LYS:HB2	2.13	0.49
1:L:326:HIS:O	1:L:327:GLU:HG3	2.13	0.49
1:I:6:ARG:HH11	1:I:6:ARG:HG2	1.78	0.48
1:L:207:ILE:C	1:L:208:THR:HG22	2.31	0.48
2:F:120:ASP:HA	3:D:33:LYS:HE3	1.94	0.48
2:J:497:TYR:HD1	2:J:502:VAL:HG22	1.78	0.48
2:N:131:TRP:HB2	2:N:220:ARG:HG2	1.94	0.48
3:P:57:ILE:HB	3:P:91:VAL:HG23	1.95	0.48
1:E:445:TYR:OH	1:E:613:GLU:OE2	2.28	0.48
4:V:92:ASN:OD1	4:V:93:SER:N	2.46	0.48
2:R:145:ASN:O	2:R:148:GLU:HG3	2.13	0.48
4:W:90:THR:HG23	4:W:96:GLN:NE2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:572:LYS:HA	1:E:575:MET:HE3	1.95	0.48
2:J:50:SER:HB3	2:J:68:PRO:HB3	1.96	0.48
2:N:362:MET:HB3	2:N:364:LEU:HD23	1.95	0.48
2:N:443:SER:HB2	2:N:492:PHE:CZ	2.48	0.48
3:D:106:THR:HG22	3:D:108:THR:HG23	1.95	0.48
2:F:58:ASN:OD1	2:F:59:THR:N	2.47	0.48
1:I:265:PRO:HG2	1:I:716:ARG:HG2	1.95	0.48
1:L:320:PRO:HB3	1:L:545:ILE:HG22	1.95	0.48
1:L:382:ASP:HA	1:L:385:ARG:HH11	1.78	0.48
1:L:657:GLY:O	1:L:661:GLU:HG2	2.13	0.48
4:V:60:ASN:CG	4:V:61:ARG:H	2.17	0.48
1:L:42:LEU:HG	1:L:46:PHE:HE2	1.79	0.48
2:J:260:ARG:O	2:J:264:GLU:HG2	2.14	0.48
2:J:681:GLY:O	2:J:683:LEU:N	2.46	0.48
3:K:11:MET:HB3	3:K:17:ARG:HH22	1.79	0.48
3:K:713:LEU:HD11	3:K:724:VAL:HG11	1.95	0.48
1:Q:318:LYS:HG2	1:Q:546:GLY:HA2	1.95	0.48
2:R:266:LEU:HD13	2:R:421:VAL:HG11	1.95	0.48
2:N:50:SER:HB2	2:N:68:PRO:HB3	1.96	0.48
3:O:737:ARG:NH1	3:O:739:ARG:O	2.47	0.48
2:R:118:ARG:HH11	3:P:30:ILE:HG22	1.77	0.48
3:O:136:ARG:NH2	3:O:241:GLU:OE1	2.46	0.48
3:D:111:TYR:HB3	3:D:112:PRO:HD3	1.95	0.48
3:G:54:LYS:HE2	3:G:55:TYR:CE2	2.48	0.48
1:E:50:ASP:O	1:E:52:HIS:ND1	2.46	0.48
2:B:424:LEU:HD11	2:B:442:GLN:HB2	1.96	0.48
1:L:161:TYR:CB	1:L:168:ARG:HH12	2.27	0.48
4:W:5:THR:HG21	4:W:42:ARG:HH12	1.78	0.48
1:A:383:ASN:OD1	1:A:384:CYS:N	2.47	0.48
4:S:8:SER:HB3	4:T:105:LEU:HD12	1.94	0.48
4:T:5:THR:HG22	4:T:9:PHE:CE2	2.49	0.48
1:E:575:MET:O	1:E:579:MET:HG3	2.14	0.48
4:V:61:ARG:HG2	4:V:65:TRP:HZ3	1.79	0.48
2:R:340:ALA:HB3	2:R:341:PRO:HD3	1.96	0.48
2:N:86:ASP:OD1	2:N:86:ASP:N	2.47	0.48
3:O:230:GLU:HG3	3:O:231:VAL:HG13	1.96	0.48
4:W:86:ARG:HH12	4:X:28:LEU:HD21	1.78	0.48
1:E:326:HIS:O	1:E:327:GLU:HG3	2.13	0.47
1:E:390:LEU:HB3	2:F:357:PHE:CZ	2.49	0.47
1:E:516:ASP:OD1	1:E:516:ASP:N	2.47	0.47
2:F:110:THR:HA	2:F:113:VAL:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:64:LYS:O	4:S:67:GLU:HG3	2.13	0.47
3:K:231:VAL:HG12	3:K:231:VAL:O	2.14	0.47
2:R:134:ASN:OD1	2:R:220:ARG:NH1	2.47	0.47
2:F:724:ILE:HD11	3:D:707:ALA:HB3	1.95	0.47
1:A:399:GLU:O	1:A:696:ASN:ND2	2.32	0.47
3:K:61:LYS:HZ2	3:K:88:ARG:N	2.12	0.47
2:J:566:THR:HG22	2:J:568:ILE:H	1.79	0.47
1:Q:326:HIS:ND1	1:Q:328:LYS:O	2.40	0.47
2:R:723:ARG:HH22	3:P:707:ALA:HB3	1.78	0.47
2:N:681:GLY:O	2:N:683:LEU:N	2.46	0.47
1:E:302:ILE:HD12	1:E:302:ILE:H	1.79	0.47
1:A:133:GLU:O	1:A:137:LYS:HB2	2.14	0.47
2:B:153:ASN:HD21	2:B:180:GLU:H	1.61	0.47
2:H:15:GLN:HB2	2:H:498:ARG:NH2	2.29	0.47
2:H:44:ASN:HA	2:H:47:HIS:HD1	1.78	0.47
2:F:131:TRP:O	2:F:220:ARG:NH2	2.48	0.47
2:F:318:PHE:O	2:F:322:ILE:HG12	2.15	0.47
2:F:523:MET:HA	2:F:551:PHE:HZ	1.79	0.47
2:B:583:THR:O	2:B:586:LYS:NZ	2.46	0.47
4:T:72:LYS:O	4:T:76:ILE:HG12	2.14	0.47
1:I:15:GLU:HA	1:I:18:GLU:HG2	1.97	0.47
1:M:2:GLU:O	1:M:6:ARG:HG2	2.14	0.47
1:M:166:GLU:HG2	1:M:170:ARG:NH1	2.29	0.47
3:D:55:TYR:HB3	3:D:90:MET:HB3	1.96	0.47
1:E:214:LEU:HD22	2:F:346:ASN:HD21	1.79	0.47
1:E:284:LEU:HB3	1:E:458:TYR:CZ	2.49	0.47
2:F:95:LEU:HD22	2:F:422:SER:HB3	1.96	0.47
1:A:126:GLU:OE2	1:A:129:ILE:HG12	2.15	0.47
2:B:442:GLN:NE2	2:B:443:SER:O	2.47	0.47
3:K:155:SER:OG	3:K:158:GLU:OE1	2.32	0.47
2:R:345:SER:O	2:R:404:SER:OG	2.31	0.47
2:R:535:ILE:HD11	3:P:232:LEU:HD23	1.96	0.47
2:F:251:PHE:HB3	2:F:340:ALA:HB2	1.96	0.47
4:S:78:TRP:O	4:S:81:GLU:HG3	2.14	0.47
1:I:118:ILE:HG22	1:I:144:HIS:HB3	1.96	0.47
1:I:164:ASP:OD1	1:I:165:GLU:N	2.39	0.47
2:H:8:LEU:O	2:H:12:VAL:N	2.36	0.47
1:L:326:HIS:ND1	1:L:328:LYS:O	2.35	0.47
4:V:45:LEU:O	4:V:49:VAL:HG23	2.14	0.47
4:V:49:VAL:HG12	1:M:554:ILE:HD13	1.97	0.47
1:Q:495:ARG:HG2	1:Q:495:ARG:HH11	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:133:LEU:HB3	2:R:135:ARG:HH11	1.79	0.47
1:M:5:VAL:HG13	1:M:9:PHE:HE2	1.80	0.47
2:N:403:LEU:HD12	2:N:403:LEU:O	2.13	0.47
3:O:195:ASP:N	3:O:195:ASP:OD1	2.46	0.47
3:G:189:LYS:HE2	3:G:207:LEU:HD11	1.97	0.47
1:E:217:GLN:NE2	2:F:58:ASN:OD1	2.47	0.47
4:T:20:GLN:HA	4:T:28:LEU:HD21	1.96	0.47
1:I:550:LEU:HB3	1:I:557:MET:HB2	1.96	0.47
2:H:277:GLU:O	2:H:281:LYS:HG3	2.15	0.47
1:L:203:GLU:OE2	2:J:332:TRP:NE1	2.47	0.47
4:U:110:GLU:HA	4:U:113:ILE:HG22	1.97	0.47
2:F:627:PRO:HB3	3:D:198:ILE:HG23	1.95	0.47
1:I:200:THR:HG23	1:I:201:ILE:HG13	1.97	0.47
2:H:455:ASN:ND2	2:H:457:GLU:OE1	2.48	0.47
2:J:147:ILE:HD12	2:J:158:ASN:ND2	2.30	0.47
4:U:41:TYR:HE2	4:U:45:LEU:HD22	1.79	0.47
2:N:389:ILE:HA	2:N:392:ILE:HG22	1.96	0.47
1:E:604:GLU:O	1:E:604:GLU:HG3	2.15	0.47
1:L:137:LYS:HB3	1:L:138:ILE:HD12	1.96	0.47
1:L:376:PRO:HA	2:J:363:LYS:HG3	1.97	0.47
2:J:385:THR:O	2:J:389:ILE:HG12	2.14	0.47
4:U:9:PHE:O	4:U:13:LEU:HD23	2.15	0.47
4:V:106:LEU:HA	4:V:109:VAL:HG12	1.97	0.47
1:E:288:LEU:HD13	1:E:527:LEU:HG	1.95	0.46
1:I:292:ILE:HG23	1:I:295:PRO:HD3	1.97	0.46
2:R:712:SER:HB3	3:P:730:ASP:HB3	1.96	0.46
1:M:335:LEU:HD23	1:M:543:LEU:HD13	1.96	0.46
4:W:65:TRP:O	4:W:69:LEU:HD23	2.14	0.46
2:F:389:ILE:HA	2:F:392:ILE:HG22	1.96	0.46
2:H:221:ALA:O	2:H:247:GLN:NE2	2.48	0.46
2:J:120:ASP:OD2	2:J:120:ASP:N	2.48	0.46
2:R:492:PHE:O	2:R:495:PHE:HB2	2.14	0.46
3:D:120:GLU:O	3:D:124:ARG:N	2.48	0.46
4:S:31:MET:HG2	4:S:35:PHE:CE2	2.50	0.46
2:H:340:ALA:HB3	2:H:341:PRO:HD3	1.98	0.46
1:L:382:ASP:HA	1:L:385:ARG:NH1	2.30	0.46
2:J:744:MET:HA	2:J:747:CYS:SG	2.55	0.46
1:M:379:VAL:HG22	2:N:364:LEU:HD12	1.98	0.46
4:X:74:GLU:HA	4:X:77:ARG:NH1	2.30	0.46
3:K:697:LEU:HD11	3:K:735:MET:HG3	1.97	0.46
4:U:7:SER:O	4:U:10:GLN:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:604:GLU:HB3	3:P:136:ARG:HH21	1.80	0.46
2:R:593:ASP:OD1	2:R:593:ASP:N	2.47	0.46
2:N:377:ASP:OD1	2:N:378:LEU:N	2.48	0.46
3:G:735:MET:SD	3:G:736:LYS:HG3	2.55	0.46
2:F:109:GLU:O	2:F:112:GLU:HG3	2.16	0.46
2:B:613:TRP:HA	2:B:616:MET:HE2	1.98	0.46
1:L:84:ARG:HG3	1:L:88:TRP:CD1	2.51	0.46
1:M:571:SER:HB3	1:M:574:LYS:HB2	1.97	0.46
4:W:41:TYR:O	4:W:45:LEU:HD23	2.14	0.46
2:B:129:TYR:HB2	2:B:225:ASN:HD22	1.80	0.46
3:C:195:ASP:OD1	3:C:195:ASP:N	2.49	0.46
4:S:64:LYS:HB3	4:S:64:LYS:HE3	1.67	0.46
2:H:497:TYR:HD1	2:H:502:VAL:HG22	1.79	0.46
2:J:724:ILE:HD11	3:K:707:ALA:HB3	1.96	0.46
3:K:5:LYS:HA	3:K:8:ARG:CD	2.45	0.46
3:G:146:ASP:HA	3:G:215:THR:HA	1.97	0.46
1:I:530:PRO:O	1:I:531:ARG:HG2	2.16	0.46
1:Q:1:MET:HB2	1:Q:187:LEU:HD22	1.97	0.46
1:M:78:ILE:O	1:M:82:ARG:NE	2.42	0.46
2:B:251:PHE:HB3	2:B:340:ALA:HB2	1.98	0.46
4:S:86:ARG:HH22	4:T:27:ASP:HB2	1.80	0.46
4:T:45:LEU:O	4:T:49:VAL:HG23	2.15	0.46
1:I:26:GLU:HG3	1:I:34:LYS:NZ	2.31	0.46
2:H:118:ARG:NH1	2:H:707:ARG:HH12	2.14	0.46
1:A:114:GLU:HB3	1:A:116:ARG:HG2	1.98	0.46
2:B:50:SER:O	2:B:50:SER:OG	2.34	0.46
2:H:403:LEU:HG	2:H:405:PRO:HD3	1.97	0.46
1:L:84:ARG:HG3	1:L:88:TRP:HD1	1.81	0.46
1:M:85:THR:O	1:M:89:THR:HG23	2.15	0.46
2:N:497:TYR:HD1	2:N:502:VAL:HG22	1.80	0.46
4:W:105:LEU:HD11	4:X:9:PHE:CE1	2.50	0.46
3:D:161:ASP:OD2	3:D:162:VAL:N	2.47	0.46
4:T:9:PHE:HD1	4:T:39:LYS:NZ	2.14	0.46
4:V:5:THR:HG22	4:V:9:PHE:HE2	1.81	0.46
2:N:59:THR:OG1	2:N:60:GLU:OE2	2.24	0.46
2:N:720:SER:O	2:N:724:ILE:HG12	2.16	0.46
2:F:602:ARG:NH1	2:F:603:ASN:OD1	2.49	0.45
1:A:137:LYS:HB3	1:A:138:ILE:HD12	1.98	0.45
2:B:271:LEU:HB3	2:B:272:PRO:HD3	1.97	0.45
1:I:34:LYS:O	1:I:38:ILE:HG12	2.16	0.45
1:L:583:ARG:NH2	2:J:510:PRO:O	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:663:ARG:HB2	2:J:21:THR:HG21	1.98	0.45
4:W:9:PHE:O	4:W:13:LEU:HD23	2.16	0.45
2:F:699:PHE:CZ	3:D:7:LEU:HD11	2.45	0.45
1:A:600:SER:OG	1:A:605:LYS:O	2.29	0.45
1:L:4:PHE:HE2	1:L:181:GLU:HG3	1.81	0.45
4:V:62:ASN:HA	4:V:65:TRP:CH2	2.51	0.45
2:R:114:VAL:HG23	2:R:254:PHE:CZ	2.50	0.45
1:I:686:LEU:O	1:I:690:ILE:HG12	2.15	0.45
1:I:697:ASP:HB3	1:I:700:VAL:HG12	1.98	0.45
4:U:90:THR:HG23	4:U:96:GLN:NE2	2.32	0.45
1:M:160:ASP:OD1	1:M:162:THR:OG1	2.30	0.45
4:X:12:ILE:O	4:X:16:MET:HG3	2.16	0.45
1:E:84:ARG:HE	1:E:88:TRP:HE1	1.64	0.45
1:E:151:THR:HG22	1:E:151:THR:O	2.16	0.45
1:E:230:ARG:NH1	2:F:331:GLU:OE2	2.49	0.45
2:F:168:LYS:O	2:F:171:MET:HB2	2.16	0.45
2:B:681:GLY:O	2:B:683:LEU:N	2.47	0.45
2:H:267:GLU:OE2	2:H:268:GLN:NE2	2.49	0.45
2:J:443:SER:HB2	2:J:492:PHE:CZ	2.51	0.45
1:Q:598:ALA:O	1:Q:602:VAL:HG13	2.16	0.45
2:N:178:GLU:OE2	2:N:211:ARG:HB3	2.17	0.45
3:G:237:GLY:HA3	3:G:240:TRP:CE2	2.51	0.45
1:E:555:GLY:HA3	4:T:116:PHE:CZ	2.51	0.45
2:F:125:GLY:CA	2:F:249:ARG:HH22	2.30	0.45
1:A:217:GLN:NE2	2:B:58:ASN:OD1	2.49	0.45
2:H:395:LEU:HD12	2:H:395:LEU:O	2.16	0.45
2:H:519:GLU:HG3	2:H:664:HIS:HB3	1.98	0.45
1:L:3:ASP:OD1	1:L:4:PHE:N	2.50	0.45
1:L:446:PHE:O	1:L:450:VAL:HG22	2.16	0.45
1:Q:612:PHE:HA	1:Q:633:ILE:HD13	1.99	0.45
4:S:82:GLU:OE2	4:S:83:VAL:HG23	2.16	0.45
1:L:302:ILE:HG22	1:L:304:LEU:H	1.82	0.45
2:R:174:MET:HA	2:R:217:TYR:HE2	1.81	0.45
1:M:331:ASN:HA	1:M:334:TYR:HD2	1.81	0.45
4:X:116:PHE:O	4:X:120:LEU:HB2	2.16	0.45
1:E:326:HIS:ND1	1:E:328:LYS:O	2.38	0.45
2:F:751:GLU:O	2:F:754:ARG:HG2	2.16	0.45
2:B:76:ASP:N	2:B:76:ASP:OD1	2.50	0.45
4:U:87:LEU:HD12	4:U:99:PHE:HB3	1.98	0.45
3:O:151:HIS:HB3	3:O:154:LEU:HD12	1.99	0.45
2:F:269:SER:O	2:F:281:LYS:NZ	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:78:TRP:HB3	3:C:91:VAL:HG12	1.99	0.45
1:Q:226:LEU:HD21	1:Q:230:ARG:HH21	1.82	0.45
1:M:382:ASP:HA	1:M:385:ARG:NH1	2.31	0.45
1:E:420:SER:O	1:E:452:HIS:ND1	2.50	0.45
2:F:712:SER:HB3	2:F:716:GLU:OE2	2.17	0.45
2:B:502:VAL:HG12	2:B:502:VAL:O	2.17	0.45
2:H:143:LEU:O	2:H:147:ILE:HG12	2.17	0.45
2:J:15:GLN:OE1	2:J:498:ARG:NH1	2.50	0.45
1:M:84:ARG:HG3	1:M:88:TRP:CD1	2.52	0.45
1:M:272:ASP:N	1:M:272:ASP:OD1	2.48	0.45
2:F:103:PHE:HZ	2:F:327:LYS:H	1.65	0.45
1:I:6:ARG:HG2	1:I:6:ARG:NH1	2.32	0.45
1:L:225:CYS:SG	1:L:226:LEU:N	2.90	0.45
1:L:238:PRO:HA	1:L:241:TYR:HE2	1.80	0.45
1:L:530:PRO:HG3	1:L:542:VAL:HG11	1.99	0.45
4:V:49:VAL:HA	4:V:52:MET:HE2	1.99	0.45
2:R:383:GLU:HA	2:R:386:ARG:HD2	1.98	0.45
1:E:207:ILE:H	1:E:207:ILE:HD12	1.82	0.44
2:H:269:SER:O	2:H:281:LYS:NZ	2.37	0.44
2:J:519:GLU:HG3	2:J:664:HIS:HB3	1.98	0.44
1:M:167:SER:HA	1:M:170:ARG:HH11	1.82	0.44
4:X:7:SER:HA	4:X:10:GLN:NE2	2.31	0.44
3:P:110:HIS:CG	3:P:196:CYS:HB2	2.51	0.44
2:H:80:SER:HB2	2:H:82:TYR:CD2	2.52	0.44
2:R:165:ASP:OD1	2:R:166:PHE:N	2.51	0.44
3:G:163:ILE:O	3:G:167:VAL:HG22	2.16	0.44
1:E:302:ILE:HG22	1:E:304:LEU:H	1.82	0.44
2:F:341:PRO:HA	2:F:344:PHE:HB2	2.00	0.44
2:B:136:ASN:OD1	2:B:225:ASN:ND2	2.50	0.44
2:B:746:ILE:HD11	3:C:8:ARG:HB2	1.98	0.44
2:R:269:SER:O	2:R:281:LYS:NZ	2.40	0.44
1:M:302:ILE:HG22	1:M:304:LEU:H	1.83	0.44
4:X:48:ALA:HA	4:X:51:ARG:HH11	1.83	0.44
3:P:237:GLY:HA3	3:P:240:TRP:CE2	2.53	0.44
2:F:125:GLY:HA2	2:F:249:ARG:HH22	1.81	0.44
1:A:322:ILE:HA	1:A:543:LEU:HD23	1.99	0.44
2:B:523:MET:O	2:B:527:VAL:HG22	2.18	0.44
2:H:385:THR:O	2:H:389:ILE:HG12	2.17	0.44
1:Q:144:HIS:HE1	1:Q:160:ASP:HB2	1.81	0.44
3:G:283:MET:O	3:G:287:THR:OG1	2.25	0.44
3:K:696:ILE:CD1	3:K:732:VAL:HB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:12:ILE:HD12	4:V:105:LEU:HD22	2.00	0.44
1:Q:685:GLY:HA3	2:R:480:LYS:HG2	1.99	0.44
2:R:292:ASN:ND2	2:R:295:ASP:OD1	2.51	0.44
2:B:519:GLU:OE2	2:B:664:HIS:ND1	2.33	0.44
1:I:12:MET:O	1:I:16:LEU:HD23	2.18	0.44
2:H:724:ILE:O	2:H:728:ILE:HG12	2.17	0.44
1:L:694:LEU:HD22	1:L:701:LEU:HD23	2.00	0.44
2:J:311:GLU:OE2	2:J:311:GLU:N	2.51	0.44
3:K:11:MET:HB3	3:K:17:ARG:NH2	2.32	0.44
4:U:90:THR:HG23	4:U:96:GLN:HE21	1.83	0.44
2:N:502:VAL:O	2:N:502:VAL:HG12	2.17	0.44
2:F:155:LEU:HD12	2:F:169:ASP:OD1	2.18	0.44
2:B:143:LEU:O	2:B:147:ILE:HG12	2.17	0.44
1:L:404:SER:HG	1:L:406:TRP:HD1	1.64	0.44
1:M:126:GLU:OE2	1:M:129:ILE:HG12	2.17	0.44
2:N:443:SER:HB2	2:N:492:PHE:HZ	1.81	0.44
3:O:746:ASP:O	3:O:749:THR:OG1	2.20	0.44
4:X:49:VAL:O	4:X:52:MET:HG2	2.18	0.44
1:E:265:PRO:HG2	1:E:716:ARG:HG2	1.99	0.44
1:E:281:LYS:HE2	1:E:570:THR:HG23	1.99	0.44
2:F:327:LYS:HA	2:F:334:ARG:NH2	2.33	0.44
2:F:489:THR:HG22	2:F:498:ARG:HD3	2.00	0.44
1:A:220:PRO:HG2	1:A:223:PHE:HD2	1.83	0.44
2:B:501:PHE:CE2	2:B:503:ALA:HB2	2.53	0.44
1:I:85:THR:O	1:I:89:THR:HG23	2.18	0.44
1:I:509:SER:HB3	1:I:518:VAL:HG21	2.00	0.44
4:U:45:LEU:HD12	4:U:48:ALA:HB3	2.00	0.44
2:R:215:ARG:O	2:R:219:ILE:HG12	2.17	0.44
3:O:28:MET:O	3:O:31:ILE:HG12	2.18	0.44
1:E:548:MET:O	1:E:558:SER:HA	2.18	0.44
2:B:492:PHE:O	2:B:495:PHE:HB2	2.18	0.44
1:I:439:ALA:HB2	2:H:541:PRO:HB2	2.00	0.44
2:H:593:ASP:OD1	2:H:593:ASP:N	2.49	0.44
3:K:57:ILE:HG13	3:K:91:VAL:HG23	2.00	0.44
1:Q:225:CYS:HB3	1:Q:228:ASN:ND2	2.33	0.44
1:Q:283:LEU:HD13	1:Q:286:ASP:HB2	2.00	0.44
2:N:151:ARG:HH22	3:O:15:ARG:NE	2.16	0.44
2:H:106:SER:HA	2:H:109:GLU:OE1	2.18	0.43
1:Q:271:PRO:HB3	1:Q:400:LEU:HD23	2.00	0.43
1:Q:606:ASP:OD2	3:P:135:PHE:HB3	2.18	0.43
2:R:692:CYS:SG	3:P:10:LEU:HD21	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:166:GLU:O	1:M:170:ARG:HG2	2.18	0.43
1:M:168:ARG:HA	1:M:171:ILE:HG22	1.99	0.43
3:D:110:HIS:CG	3:D:196:CYS:HB2	2.53	0.43
3:G:189:LYS:O	3:G:193:LEU:HG	2.18	0.43
3:G:721:LYS:HA	3:G:734:VAL:O	2.17	0.43
1:A:382:ASP:OD1	1:A:383:ASN:N	2.52	0.43
2:B:619:ASP:N	2:B:619:ASP:OD1	2.50	0.43
1:L:1:MET:HG2	1:L:3:ASP:OD1	2.18	0.43
3:P:113:LYS:HG3	3:P:114:VAL:HG13	1.99	0.43
2:F:457:GLU:OE2	2:F:457:GLU:N	2.50	0.43
2:B:43:VAL:HG13	2:B:403:LEU:HD13	2.01	0.43
2:B:385:THR:O	2:B:389:ILE:HG12	2.18	0.43
3:C:16:THR:HG22	3:C:20:LEU:HD23	1.99	0.43
4:S:7:SER:O	4:S:10:GLN:HG3	2.18	0.43
2:J:502:VAL:O	2:J:502:VAL:HG12	2.18	0.43
2:J:624:LEU:HD12	2:J:663:THR:HG22	1.99	0.43
2:J:720:SER:O	2:J:724:ILE:HG12	2.18	0.43
1:M:392:GLN:HA	2:N:357:PHE:HE2	1.83	0.43
1:M:426:ASP:OD2	2:N:553:LYS:HB2	2.18	0.43
1:M:434:PRO:HA	1:M:437:TYR:HD1	1.83	0.43
3:O:121:LYS:NZ	3:O:230:GLU:OE1	2.48	0.43
3:P:163:ILE:O	3:P:167:VAL:HG12	2.19	0.43
2:H:118:ARG:NH1	2:H:707:ARG:HH22	2.16	0.43
2:H:151:ARG:NH1	3:G:18:GLU:OE1	2.46	0.43
1:L:606:ASP:OD2	1:L:608:THR:HG22	2.19	0.43
2:J:184:HIS:ND1	2:J:682:ILE:O	2.45	0.43
2:R:109:GLU:HA	2:R:112:GLU:HG3	2.00	0.43
2:R:750:ILE:HA	2:R:753:LEU:HG	2.00	0.43
2:N:282:LEU:HD23	2:N:441:LEU:HD21	2.00	0.43
2:N:697:GLU:HG3	2:N:703:SER:HB2	2.01	0.43
3:D:19:ILE:O	3:D:23:THR:HG22	2.19	0.43
3:G:266:ILE:HG23	3:G:283:MET:SD	2.59	0.43
3:P:697:LEU:HB2	3:P:733:LEU:HD22	1.99	0.43
1:E:557:MET:SD	4:T:112:GLU:HG2	2.58	0.43
4:T:77:ARG:HA	4:T:80:ILE:HG22	2.01	0.43
2:H:532:ASN:HA	2:H:535:ILE:HG22	2.01	0.43
2:R:277:GLU:O	2:R:281:LYS:HG3	2.18	0.43
2:R:395:LEU:HD11	2:R:403:LEU:HD13	2.00	0.43
1:M:4:PHE:HD1	1:M:185:ARG:HH11	1.65	0.43
3:G:120:GLU:O	3:G:124:ARG:N	2.51	0.43
1:E:320:PRO:HG2	1:E:335:LEU:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:34:GLN:CD	4:T:79:LEU:HD12	2.39	0.43
1:Q:144:HIS:CE1	1:Q:157:THR:HB	2.54	0.43
1:Q:600:SER:HB2	1:Q:606:ASP:HA	1.99	0.43
2:F:385:THR:O	2:F:389:ILE:HG12	2.19	0.43
1:I:207:ILE:HB	1:I:212:ARG:HH11	1.84	0.43
1:L:382:ASP:OD1	1:L:383:ASN:N	2.51	0.43
3:D:162:VAL:HA	3:D:165:GLU:HG2	1.99	0.43
2:F:498:ARG:HD3	2:F:498:ARG:HA	1.87	0.43
4:T:87:LEU:HD13	4:T:99:PHE:HB2	2.00	0.43
2:H:111:MET:O	2:H:114:VAL:HG12	2.19	0.43
4:U:107:PHE:O	4:U:110:GLU:HG3	2.19	0.43
1:Q:265:PRO:HG2	1:Q:716:ARG:HG2	2.00	0.43
1:Q:523:MET:HG2	1:Q:565:VAL:HG22	2.01	0.43
1:M:220:PRO:HG2	1:M:223:PHE:CD2	2.54	0.43
3:G:18:GLU:OE2	3:G:22:LYS:HG3	2.19	0.43
2:F:167:LEU:O	2:F:171:MET:HG2	2.19	0.43
1:I:214:LEU:HD22	2:H:346:ASN:ND2	2.31	0.43
2:J:130:ASP:OD1	2:J:132:THR:OG1	2.33	0.43
4:V:46:GLY:HA2	4:V:49:VAL:HB	2.01	0.43
2:N:713:SER:N	2:N:716:GLU:OE2	2.39	0.43
2:F:425:ASN:ND2	2:F:428:GLN:HE22	2.11	0.43
1:A:34:LYS:O	1:A:38:ILE:HG12	2.19	0.43
2:B:566:THR:HG22	2:B:568:ILE:H	1.84	0.43
4:S:96:GLN:O	4:S:100:MET:HG2	2.19	0.43
1:L:699:TRP:O	1:L:703:ASN:ND2	2.37	0.43
2:R:47:HIS:NE2	2:R:395:LEU:HD13	2.34	0.43
3:O:56:PRO:HD2	3:O:92:SER:HA	2.01	0.43
4:W:106:LEU:HA	4:W:109:VAL:HG12	2.01	0.43
1:A:88:TRP:O	1:A:92:ASN:ND2	2.52	0.42
1:A:108:ASP:HB2	1:A:119:GLU:HA	2.00	0.42
2:H:434:THR:HG21	2:H:436:TYR:CZ	2.54	0.42
1:M:94:ILE:HA	1:M:97:THR:HG22	2.00	0.42
1:M:144:HIS:CE1	1:M:160:ASP:HB3	2.54	0.42
1:M:434:PRO:O	1:M:438:ILE:HG13	2.19	0.42
3:G:106:THR:HG22	3:G:108:THR:HG23	2.01	0.42
4:S:111:GLN:O	4:S:115:THR:HG23	2.19	0.42
1:L:169:ALA:O	1:L:173:THR:OG1	2.25	0.42
4:U:32:ILE:O	4:U:36:GLU:OE1	2.37	0.42
1:Q:439:ALA:HB2	2:R:541:PRO:HB2	2.00	0.42
1:M:144:HIS:HE2	1:M:156:ALA:HB1	1.84	0.42
1:M:382:ASP:OD1	1:M:383:ASN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:55:LEU:HD13	4:X:58:LEU:HD21	2.01	0.42
1:A:144:HIS:NE2	1:A:156:ALA:HB1	2.34	0.42
1:A:420:SER:O	1:A:452:HIS:ND1	2.51	0.42
2:B:69:ILE:HD12	2:B:317:MET:HE2	2.01	0.42
3:C:14:SER:HA	3:C:17:ARG:HB3	2.01	0.42
3:C:155:SER:OG	3:C:158:GLU:OE1	2.37	0.42
1:I:124:ARG:NH2	1:I:194:SER:HB2	2.34	0.42
2:H:338:SER:O	2:H:341:PRO:HD2	2.19	0.42
4:U:36:GLU:O	4:U:40:LEU:HD23	2.19	0.42
4:V:47:GLU:HA	4:V:50:MET:SD	2.59	0.42
2:R:307:THR:HG23	2:R:478:SER:HB2	2.00	0.42
1:M:260:PHE:HB3	1:M:678:PRO:HG2	2.00	0.42
3:O:717:ALA:HB3	3:O:720:GLU:HG2	2.01	0.42
2:B:629:ASN:HB2	2:B:632:VAL:HG12	2.01	0.42
4:S:19:MET:SD	4:T:95:GLU:HG2	2.59	0.42
1:I:84:ARG:HE	1:I:88:TRP:HE1	1.67	0.42
1:I:150:PHE:HE2	1:I:182:MET:HE1	1.84	0.42
1:I:390:LEU:HB3	2:H:357:PHE:CZ	2.54	0.42
2:R:86:ASP:OD1	2:R:87:CYS:N	2.53	0.42
2:N:424:LEU:HD11	2:N:442:GLN:HB2	2.01	0.42
3:O:162:VAL:O	3:O:166:VAL:HG23	2.19	0.42
3:D:725:LEU:HG	3:D:731:VAL:HG22	2.01	0.42
2:B:593:ASP:N	2:B:593:ASP:OD1	2.53	0.42
1:I:49:SER:HB3	1:I:109:LEU:HD21	2.01	0.42
1:I:84:ARG:NE	1:I:88:TRP:HE1	2.18	0.42
2:H:215:ARG:O	2:H:219:ILE:HG12	2.20	0.42
3:K:56:PRO:HD2	3:K:92:SER:HA	2.02	0.42
1:M:84:ARG:HG3	1:M:88:TRP:HD1	1.85	0.42
2:N:251:PHE:HB3	2:N:340:ALA:HB2	2.02	0.42
3:G:78:TRP:HB3	3:G:91:VAL:HG12	2.01	0.42
3:P:78:TRP:HZ3	3:P:80:LYS:HZ2	1.67	0.42
1:E:292:ILE:HG23	1:E:295:PRO:HD3	2.01	0.42
1:E:510:HIS:HB3	1:E:512:ARG:NH1	2.34	0.42
2:F:363:LYS:HD2	2:F:363:LYS:HA	1.92	0.42
4:S:67:GLU:OE2	4:S:68:GLN:NE2	2.53	0.42
2:H:470:CYS:HA	2:H:473:VAL:HG12	2.00	0.42
2:H:623:ARG:HE	3:G:103:GLY:H	1.66	0.42
1:L:84:ARG:HE	1:L:106:LEU:HD11	1.83	0.42
1:L:288:LEU:HD23	1:L:288:LEU:H	1.84	0.42
3:K:195:ASP:OD1	3:K:195:ASP:N	2.53	0.42
4:U:72:LYS:HA	4:U:72:LYS:HD3	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:530:PRO:CG	1:M:542:VAL:HG11	2.50	0.42
2:N:519:GLU:OE2	2:N:666:TRP:NE1	2.37	0.42
3:D:189:LYS:NZ	3:D:211:LEU:HD21	2.35	0.42
1:E:330:ILE:HG22	1:E:332:PRO:HD2	2.02	0.42
1:E:479:ASP:OD1	1:E:479:ASP:N	2.53	0.42
1:A:576:LYS:NZ	3:C:42:ASN:OD1	2.53	0.42
1:A:603:LYS:O	1:A:605:LYS:N	2.50	0.42
1:A:713:HIS:CE1	1:A:716:ARG:HH21	2.37	0.42
4:S:79:LEU:HD22	4:S:106:LEU:CD2	2.48	0.42
1:I:190:SER:HA	1:I:193:GLN:HG2	2.02	0.42
2:J:132:THR:HG21	2:J:149:VAL:HG21	2.02	0.42
3:K:696:ILE:HD12	3:K:733:LEU:O	2.20	0.42
2:R:629:ASN:HD21	2:R:632:VAL:HG13	1.85	0.42
1:M:358:LYS:HD2	1:M:358:LYS:HA	1.88	0.42
1:E:683:LEU:HD12	1:E:686:LEU:HD21	2.02	0.42
2:B:432:THR:HB	2:B:434:THR:HG22	2.02	0.42
1:I:479:ASP:N	1:I:479:ASP:OD1	2.52	0.42
2:H:390:GLU:HA	2:H:393:ARG:HG2	2.02	0.42
2:J:309:TRP:HZ2	2:J:416:SER:HB2	1.84	0.42
3:K:748:GLN:O	3:K:751:THR:OG1	2.31	0.42
1:Q:310:CYS:O	1:Q:313:THR:HG22	2.20	0.42
1:Q:559:ARG:NH2	4:X:111:GLN:HG3	2.35	0.42
1:M:42:LEU:HA	1:M:45:CYS:SG	2.59	0.42
1:M:376:PRO:HA	2:N:363:LYS:HG3	2.01	0.42
3:O:696:ILE:HG23	3:O:732:VAL:HB	2.01	0.42
3:G:114:VAL:HG11	3:G:203:VAL:HG13	2.01	0.42
2:F:216:SER:HA	2:F:219:ILE:HG12	2.02	0.42
2:F:738:GLU:O	2:F:742:GLU:OE1	2.38	0.42
1:A:220:PRO:HG2	1:A:223:PHE:CD2	2.55	0.42
1:A:370:LEU:HD13	1:A:507:GLY:HA2	2.02	0.42
2:B:69:ILE:HD11	2:B:314:ASN:HD22	1.83	0.42
2:H:705:TYR:CD2	2:H:706:ARG:HG3	2.55	0.42
1:L:119:GLU:HB3	1:L:145:ILE:HG22	2.02	0.42
1:Q:241:TYR:CE2	2:R:86:ASP:HB2	2.55	0.42
1:Q:606:ASP:HB2	3:P:135:PHE:HB3	2.01	0.42
2:R:43:VAL:HG12	2:R:47:HIS:CE1	2.54	0.42
3:D:189:LYS:O	3:D:193:LEU:HG	2.20	0.42
3:G:297:ILE:O	3:G:301:ASN:HB2	2.20	0.42
2:F:106:SER:OG	2:F:265:LYS:NZ	2.53	0.42
3:C:63:ILE:HD13	3:C:91:VAL:HG11	2.02	0.42
3:C:140:LYS:HA	3:C:221:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:144:HIS:CE1	1:L:156:ALA:HB1	2.54	0.42
1:L:322:ILE:HA	1:L:543:LEU:HD23	2.01	0.42
2:R:498:ARG:HG2	2:R:499:TYR:H	1.84	0.42
3:D:57:ILE:HB	3:D:91:VAL:HG23	2.02	0.42
3:G:225:SER:O	3:G:229:ILE:HG12	2.20	0.42
3:G:261:ILE:HG22	3:G:264:ARG:NH2	2.34	0.42
1:E:229:PHE:O	1:E:233:VAL:HG12	2.19	0.41
1:I:697:ASP:HA	1:I:698:PRO:HD3	1.93	0.41
1:Q:274:PRO:HG2	1:Q:401:ARG:HD3	2.03	0.41
1:M:529:ASP:HA	1:M:530:PRO:HD3	1.95	0.41
3:O:175:ARG:C	3:O:177:LEU:H	2.23	0.41
3:G:57:ILE:HB	3:G:91:VAL:HG23	2.02	0.41
1:E:16:LEU:HD23	1:E:16:LEU:HA	1.91	0.41
1:E:175:LEU:HA	1:E:178:ILE:HG22	2.02	0.41
2:F:345:SER:O	2:F:404:SER:OG	2.33	0.41
2:F:382:ASN:O	2:F:386:ARG:HG3	2.20	0.41
1:A:175:LEU:HA	1:A:178:ILE:HG22	2.01	0.41
1:A:697:ASP:HB3	1:A:700:VAL:HG23	2.02	0.41
3:C:696:ILE:HG22	3:C:734:VAL:HG12	2.02	0.41
1:I:602:VAL:HG23	1:I:603:LYS:HZ2	1.85	0.41
1:I:694:LEU:HD22	1:I:701:LEU:HD23	2.02	0.41
2:J:575:GLU:OE1	3:K:101:ARG:NH2	2.46	0.41
2:R:721:ARG:HA	2:R:724:ILE:HG22	2.02	0.41
4:X:55:LEU:HA	4:X:58:LEU:HD12	2.01	0.41
3:G:141:ILE:HG22	3:G:143:ARG:HG3	2.02	0.41
1:E:134:LYS:HB3	1:E:145:ILE:HD13	2.02	0.41
4:S:41:TYR:HE2	4:T:113:ILE:HD11	1.85	0.41
4:T:90:THR:OG1	4:T:95:GLU:OE1	2.30	0.41
2:H:118:ARG:HH12	2:H:707:ARG:HH12	1.67	0.41
2:H:498:ARG:HG3	2:H:499:TYR:N	2.28	0.41
4:W:8:SER:O	4:W:12:ILE:HG12	2.20	0.41
4:W:106:LEU:HA	4:W:106:LEU:HD23	1.95	0.41
2:F:114:VAL:HG23	2:F:254:PHE:CZ	2.54	0.41
1:A:667:LEU:HD11	2:B:496:PHE:HE1	1.84	0.41
2:H:514:VAL:HG11	2:H:558:THR:HG21	2.03	0.41
1:L:260:PHE:CD2	1:L:672:LEU:HD22	2.55	0.41
1:Q:647:ASN:OD1	1:Q:655:LEU:HD21	2.20	0.41
2:R:167:LEU:HD13	2:R:251:PHE:CE2	2.54	0.41
2:R:710:GLY:N	3:P:26:ASP:OD1	2.48	0.41
1:M:166:GLU:HG2	1:M:170:ARG:HH12	1.85	0.41
1:M:297:HIS:HA	1:M:496:ARG:HH21	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:182:GLN:HG3	3:O:187:LYS:NZ	2.35	0.41
1:E:242:ILE:HG13	2:F:90:GLU:OE1	2.20	0.41
1:E:461:LYS:HD2	1:E:501:TYR:CZ	2.56	0.41
2:H:28:PRO:HA	2:H:29:PRO:HD3	1.87	0.41
2:J:271:LEU:HB3	2:J:272:PRO:HD3	2.02	0.41
4:V:67:GLU:O	4:V:71:GLN:HG3	2.21	0.41
2:R:334:ARG:O	2:R:338:SER:OG	2.27	0.41
2:R:517:ILE:HG13	2:R:518:ASN:N	2.34	0.41
3:D:30:ILE:HG13	3:D:31:ILE:HG23	2.03	0.41
1:E:114:GLU:HB2	1:E:116:ARG:HG2	2.02	0.41
1:A:288:LEU:HD23	1:A:288:LEU:H	1.85	0.41
1:A:376:PRO:HA	2:B:363:LYS:HG3	2.02	0.41
1:A:459:ILE:HG23	1:A:581:MET:HB2	2.02	0.41
1:L:288:LEU:HD13	1:L:527:LEU:HD11	2.02	0.41
1:L:358:LYS:HD2	1:L:358:LYS:HA	1.83	0.41
2:J:685:ASP:OD1	2:J:688:MET:HB3	2.20	0.41
3:K:9:ASN:OD1	3:K:10:LEU:N	2.54	0.41
1:Q:225:CYS:SG	1:Q:226:LEU:N	2.94	0.41
1:Q:566:ARG:NH1	1:Q:567:THR:O	2.53	0.41
2:R:720:SER:HA	2:R:723:ARG:NE	2.35	0.41
2:N:131:TRP:O	2:N:220:ARG:HD3	2.21	0.41
3:G:174:ALA:HB2	3:G:726:ILE:HD12	2.02	0.41
3:P:694:PHE:HD1	3:P:736:LYS:HA	1.85	0.41
1:E:172:LYS:NZ	3:D:697:LEU:O	2.39	0.41
1:E:390:LEU:HB3	2:F:357:PHE:CE2	2.56	0.41
1:E:446:PHE:O	1:E:450:VAL:HG12	2.21	0.41
2:F:252:VAL:O	2:F:256:GLU:HG2	2.20	0.41
1:A:2:GLU:O	1:A:6:ARG:HG2	2.20	0.41
2:H:104:GLU:O	2:H:108:LEU:HG	2.19	0.41
2:H:573:SER:O	2:H:577:LYS:HG2	2.21	0.41
2:J:460:GLN:NE2	2:J:464:ASP:OD2	2.50	0.41
2:J:492:PHE:O	2:J:495:PHE:HB2	2.20	0.41
2:J:501:PHE:CE2	2:J:503:ALA:HB2	2.55	0.41
4:U:106:LEU:HD11	4:V:35:PHE:CZ	2.55	0.41
1:Q:390:LEU:HB3	2:R:357:PHE:HZ	1.84	0.41
1:Q:398:PRO:HG2	1:Q:695:ILE:HG21	2.03	0.41
1:Q:689:ALA:O	1:Q:692:GLU:HG2	2.21	0.41
2:R:39:THR:O	2:R:43:VAL:HG23	2.20	0.41
2:R:693:CYS:HA	3:P:32:LYS:NZ	2.36	0.41
1:M:116:ARG:HD2	1:M:144:HIS:HB2	2.01	0.41
3:G:28:MET:O	3:G:32:LYS:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:168:LYS:O	2:F:172:GLU:OE1	2.38	0.41
2:B:389:ILE:HA	2:B:392:ILE:HG22	2.03	0.41
2:J:706:ARG:HD2	2:J:707:ARG:N	2.35	0.41
3:K:154:LEU:HD11	3:K:185:ILE:HD13	2.02	0.41
1:Q:172:LYS:NZ	3:P:697:LEU:O	2.45	0.41
1:M:84:ARG:HE	1:M:106:LEU:HD11	1.84	0.41
3:G:148:ASN:HB2	3:G:214:LYS:HB3	2.02	0.41
2:F:438:TRP:HB3	2:F:451:VAL:HG12	2.02	0.41
2:F:563:ARG:HB2	2:F:566:THR:HG23	2.03	0.41
1:A:3:ASP:OD1	1:A:4:PHE:N	2.54	0.41
1:A:103:PRO:O	1:A:104:LYS:HB2	2.19	0.41
1:A:605:LYS:HG3	1:A:607:MET:CE	2.51	0.41
2:B:438:TRP:CD1	2:B:449:LEU:HD11	2.56	0.41
2:B:748:SER:O	2:B:751:GLU:HG3	2.20	0.41
3:C:735:MET:O	3:C:737:ARG:NH1	2.52	0.41
1:I:46:PHE:HE2	1:I:78:ILE:HG21	1.86	0.41
1:I:294:ASP:HA	1:I:496:ARG:O	2.20	0.41
2:H:103:PHE:HZ	2:H:327:LYS:H	1.67	0.41
1:L:94:ILE:HA	1:L:97:THR:HG22	2.02	0.41
1:L:171:ILE:O	1:L:175:LEU:HG	2.21	0.41
2:J:1:MET:HE3	2:J:1:MET:HB3	1.71	0.41
2:J:151:ARG:NH2	3:K:18:GLU:HG2	2.36	0.41
2:J:387:LYS:HA	2:J:390:GLU:HG3	2.02	0.41
3:K:175:ARG:C	3:K:177:LEU:H	2.24	0.41
4:U:65:TRP:O	4:U:69:LEU:HD23	2.21	0.41
4:V:102:ALA:O	4:V:106:LEU:HD23	2.20	0.41
4:V:109:VAL:O	4:V:112:GLU:HG3	2.21	0.41
2:R:159:GLU:OE2	2:R:159:GLU:N	2.52	0.41
2:R:347:LYS:HG2	2:R:404:SER:HB3	2.02	0.41
1:M:320:PRO:HB3	1:M:545:ILE:HG22	2.03	0.41
2:N:714:MET:O	2:N:718:MET:HG3	2.21	0.41
4:W:34:GLN:O	4:W:38:LEU:HD23	2.21	0.41
1:E:529:ASP:OD1	1:E:531:ARG:NH1	2.53	0.41
2:F:59:THR:HG23	2:F:60:GLU:OE1	2.20	0.41
2:F:395:LEU:O	2:F:395:LEU:HD12	2.21	0.41
2:F:498:ARG:CG	2:F:499:TYR:H	2.34	0.41
1:A:160:ASP:OD1	1:A:160:ASP:O	2.39	0.41
4:S:92:ASN:O	4:S:96:GLN:HG3	2.21	0.41
1:L:42:LEU:HG	1:L:46:PHE:CE2	2.55	0.41
1:L:529:ASP:HB3	1:L:532:LEU:HD13	2.03	0.41
1:M:214:LEU:HD22	2:N:346:ASN:HD21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:624:LEU:HD12	2:N:663:THR:HG22	2.03	0.41
4:X:6:VAL:O	4:X:9:PHE:HB2	2.20	0.41
3:P:185:ILE:HA	3:P:188:GLU:OE2	2.20	0.41
2:F:165:ASP:HA	2:F:168:LYS:HG2	2.03	0.40
1:A:131:TYR:OH	1:A:157:THR:HG22	2.21	0.40
1:I:271:PRO:HB3	1:I:400:LEU:HD23	2.02	0.40
2:H:693:CYS:HA	3:G:32:LYS:NZ	2.36	0.40
1:L:238:PRO:HA	1:L:241:TYR:CE2	2.56	0.40
1:L:571:SER:HB2	1:L:574:LYS:HE3	2.02	0.40
2:J:600:ASN:O	2:J:604:LEU:HG	2.21	0.40
2:R:338:SER:O	2:R:341:PRO:HD2	2.21	0.40
2:R:403:LEU:HD12	2:R:403:LEU:HA	1.99	0.40
2:R:532:ASN:HA	2:R:535:ILE:HG22	2.03	0.40
2:N:492:PHE:O	2:N:495:PHE:HB2	2.20	0.40
4:W:47:GLU:HA	4:W:50:MET:CG	2.50	0.40
4:W:105:LEU:HD11	4:X:9:PHE:HE1	1.86	0.40
3:P:230:GLU:HG3	3:P:231:VAL:HG13	2.03	0.40
1:E:330:ILE:HB	1:E:333:ASN:ND2	2.37	0.40
1:A:687:TYR:O	1:A:690:ILE:N	2.54	0.40
4:S:58:LEU:HA	4:S:61:ARG:HG2	2.03	0.40
1:L:428:ILE:HD11	1:L:443:ARG:HH21	1.87	0.40
2:J:714:MET:O	2:J:718:MET:HG3	2.22	0.40
2:R:168:LYS:HA	2:R:171:MET:HE3	2.03	0.40
1:E:539:LYS:HB2	1:E:566:ARG:HE	1.86	0.40
2:F:306:ASN:HB2	2:F:476:ASN:O	2.21	0.40
1:A:85:THR:O	1:A:89:THR:HG23	2.21	0.40
3:C:176:ILE:HG12	3:C:691:ARG:HH12	1.85	0.40
4:S:106:LEU:HD11	4:T:35:PHE:CE1	2.56	0.40
1:I:201:ILE:HG21	1:I:204:ARG:HH11	1.86	0.40
1:L:331:ASN:HA	1:L:334:TYR:HD2	1.86	0.40
3:K:109:VAL:O	3:K:112:PRO:HD2	2.21	0.40
3:K:696:ILE:HD11	3:K:732:VAL:HB	2.03	0.40
1:Q:207:ILE:HB	1:Q:212:ARG:NH2	2.36	0.40
1:Q:216:ASP:OD1	1:Q:225:CYS:HA	2.21	0.40
2:R:168:LYS:HA	2:R:171:MET:CE	2.51	0.40
2:R:514:VAL:HG11	2:R:558:THR:HG21	2.03	0.40
2:F:489:THR:HG22	2:F:498:ARG:HA	2.02	0.40
1:A:302:ILE:HG22	1:A:304:LEU:H	1.84	0.40
2:B:714:MET:O	2:B:718:MET:HG2	2.22	0.40
3:C:15:ARG:HA	3:C:18:GLU:OE2	2.21	0.40
4:S:87:LEU:HD13	4:S:99:PHE:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:390:LEU:HB3	2:H:357:PHE:CE2	2.57	0.40
4:V:49:VAL:HA	4:V:52:MET:CE	2.51	0.40
2:R:34:THR:HG22	2:R:36:THR:HG23	2.03	0.40
2:R:742:GLU:O	2:R:746:ILE:HG12	2.21	0.40
3:O:191:GLU:O	3:O:194:GLN:HG2	2.21	0.40
4:X:47:GLU:O	4:X:51:ARG:NH1	2.54	0.40
1:A:633:ILE:O	1:A:636:VAL:HG22	2.22	0.40
1:I:430:GLU:O	2:H:602:ARG:NH2	2.55	0.40
1:L:103:PRO:O	1:L:104:LYS:HB2	2.22	0.40
2:J:40:MET:HE3	2:J:392:ILE:HG21	2.04	0.40
2:J:145:ASN:O	2:J:148:GLU:HG3	2.22	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	708/729 (97%)	668 (94%)	39 (6%)	1 (0%)	51 85
1	E	681/729 (93%)	633 (93%)	48 (7%)	0	100 100
1	I	681/729 (93%)	644 (95%)	36 (5%)	1 (0%)	51 85
1	L	708/729 (97%)	670 (95%)	37 (5%)	1 (0%)	51 85
1	M	708/729 (97%)	670 (95%)	37 (5%)	1 (0%)	51 85
1	Q	681/729 (93%)	642 (94%)	39 (6%)	0	100 100
2	B	676/757 (89%)	642 (95%)	34 (5%)	0	100 100
2	F	658/757 (87%)	624 (95%)	34 (5%)	0	100 100
2	H	658/757 (87%)	630 (96%)	28 (4%)	0	100 100
2	J	676/757 (89%)	648 (96%)	27 (4%)	1 (0%)	51 85
2	N	676/757 (89%)	653 (97%)	22 (3%)	1 (0%)	51 85

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	R	658/757 (87%)	629 (96%)	29 (4%)	0	100	100
3	C	302/792 (38%)	281 (93%)	20 (7%)	1 (0%)	41	76
3	D	227/792 (29%)	209 (92%)	18 (8%)	0	100	100
3	G	332/792 (42%)	309 (93%)	23 (7%)	0	100	100
3	K	302/792 (38%)	283 (94%)	17 (6%)	2 (1%)	22	60
3	O	302/792 (38%)	282 (93%)	18 (6%)	2 (1%)	22	60
3	P	227/792 (29%)	209 (92%)	18 (8%)	0	100	100
4	S	115/121 (95%)	114 (99%)	1 (1%)	0	100	100
4	T	115/121 (95%)	110 (96%)	5 (4%)	0	100	100
4	U	115/121 (95%)	113 (98%)	1 (1%)	1 (1%)	17	55
4	V	115/121 (95%)	112 (97%)	2 (2%)	1 (1%)	17	55
4	W	115/121 (95%)	111 (96%)	3 (3%)	1 (1%)	17	55
4	X	115/121 (95%)	111 (96%)	4 (4%)	0	100	100
All	All	10551/14394 (73%)	9997 (95%)	540 (5%)	14 (0%)	54	85

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	LYS
3	C	176	ILE
1	L	104	LYS
1	M	104	LYS
2	J	662	THR
3	K	176	ILE
4	V	52	MET
3	O	176	ILE
4	U	64	LYS
4	W	61	ARG
1	I	201	ILE
2	N	411	MET
3	O	716	LEU
3	K	174	ALA

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	636/655 (97%)	636 (100%)	0	100	100
1	E	607/655 (93%)	607 (100%)	0	100	100
1	I	608/655 (93%)	608 (100%)	0	100	100
1	L	636/655 (97%)	635 (100%)	1 (0%)	93	98
1	M	636/655 (97%)	635 (100%)	1 (0%)	93	98
1	Q	608/655 (93%)	608 (100%)	0	100	100
2	B	601/669 (90%)	601 (100%)	0	100	100
2	F	582/669 (87%)	582 (100%)	0	100	100
2	H	582/669 (87%)	582 (100%)	0	100	100
2	J	601/669 (90%)	598 (100%)	3 (0%)	88	96
2	N	601/669 (90%)	599 (100%)	2 (0%)	92	97
2	R	582/669 (87%)	579 (100%)	3 (0%)	88	96
3	C	272/691 (39%)	270 (99%)	2 (1%)	84	94
3	D	215/691 (31%)	215 (100%)	0	100	100
3	G	300/691 (43%)	297 (99%)	3 (1%)	76	91
3	K	272/691 (39%)	270 (99%)	2 (1%)	84	94
3	O	272/691 (39%)	270 (99%)	2 (1%)	84	94
3	P	215/691 (31%)	214 (100%)	1 (0%)	88	96
4	S	109/113 (96%)	109 (100%)	0	100	100
4	T	108/113 (96%)	107 (99%)	1 (1%)	78	92
4	U	109/113 (96%)	107 (98%)	2 (2%)	59	85
4	V	108/113 (96%)	107 (99%)	1 (1%)	78	92
4	W	109/113 (96%)	108 (99%)	1 (1%)	78	92
4	X	108/113 (96%)	106 (98%)	2 (2%)	57	84
All	All	9477/12768 (74%)	9450 (100%)	27 (0%)	92	97

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	126	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	143	ARG
4	T	77	ARG
1	L	172	LYS
2	J	1	MET
2	J	126	ARG
2	J	379	LYS
3	K	8	ARG
3	K	175	ARG
4	U	61	ARG
4	U	114	ARG
4	V	77	ARG
2	R	61	THR
2	R	379	LYS
2	R	723	ARG
1	M	551	ARG
2	N	126	ARG
2	N	723	ARG
3	O	175	ARG
3	O	703	ARG
4	W	64	LYS
4	X	77	ARG
4	X	111	GLN
3	G	136	ARG
3	G	175	ARG
3	G	736	LYS
3	P	187	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	425	ASN
2	B	621	GLN
4	S	34	GLN
2	J	145	ASN
2	J	158	ASN
2	J	690	GLN
4	U	62	ASN
2	N	210	GLN
3	G	728	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.

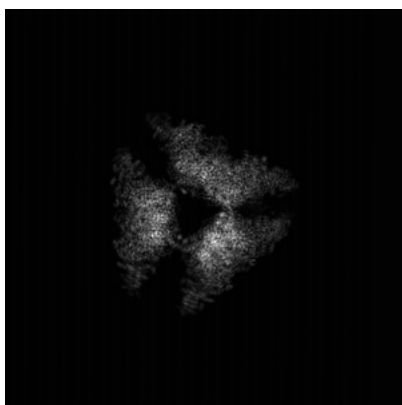
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39022. These allow visual inspection of the internal detail of the map and identification of artifacts.

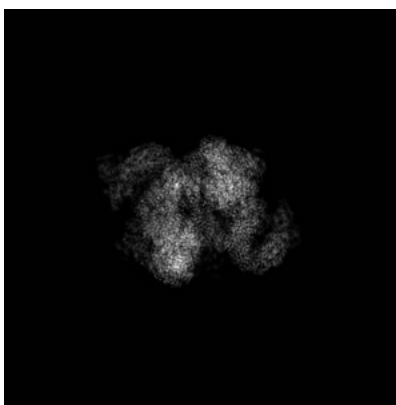
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

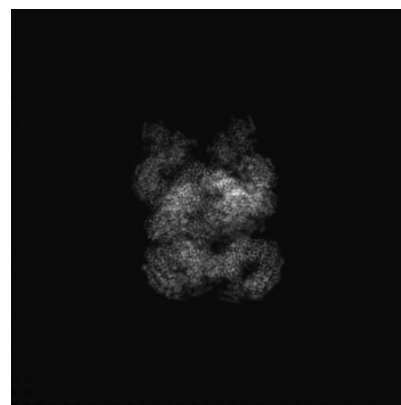
6.1.1 Primary map



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: 280



Y Index: 280



Z Index: 280

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: 312



Y Index: 301

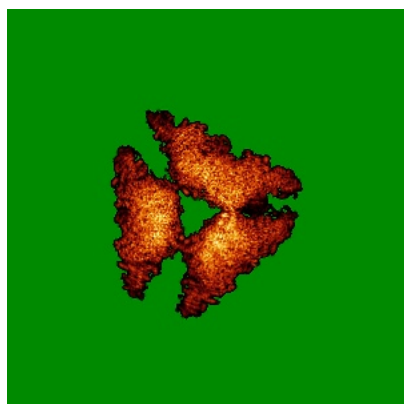


Z Index: 241

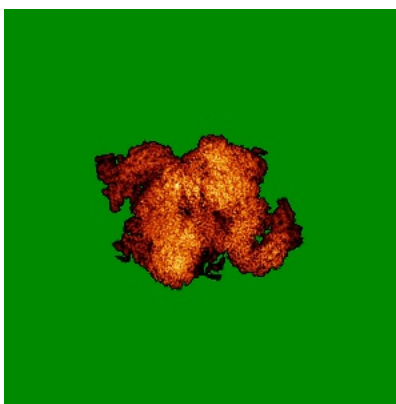
The images above show the largest variance slices of the map in three orthogonal directions.

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

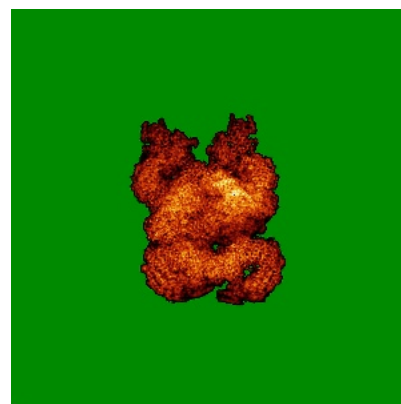
6.4.1 Primary map



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 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

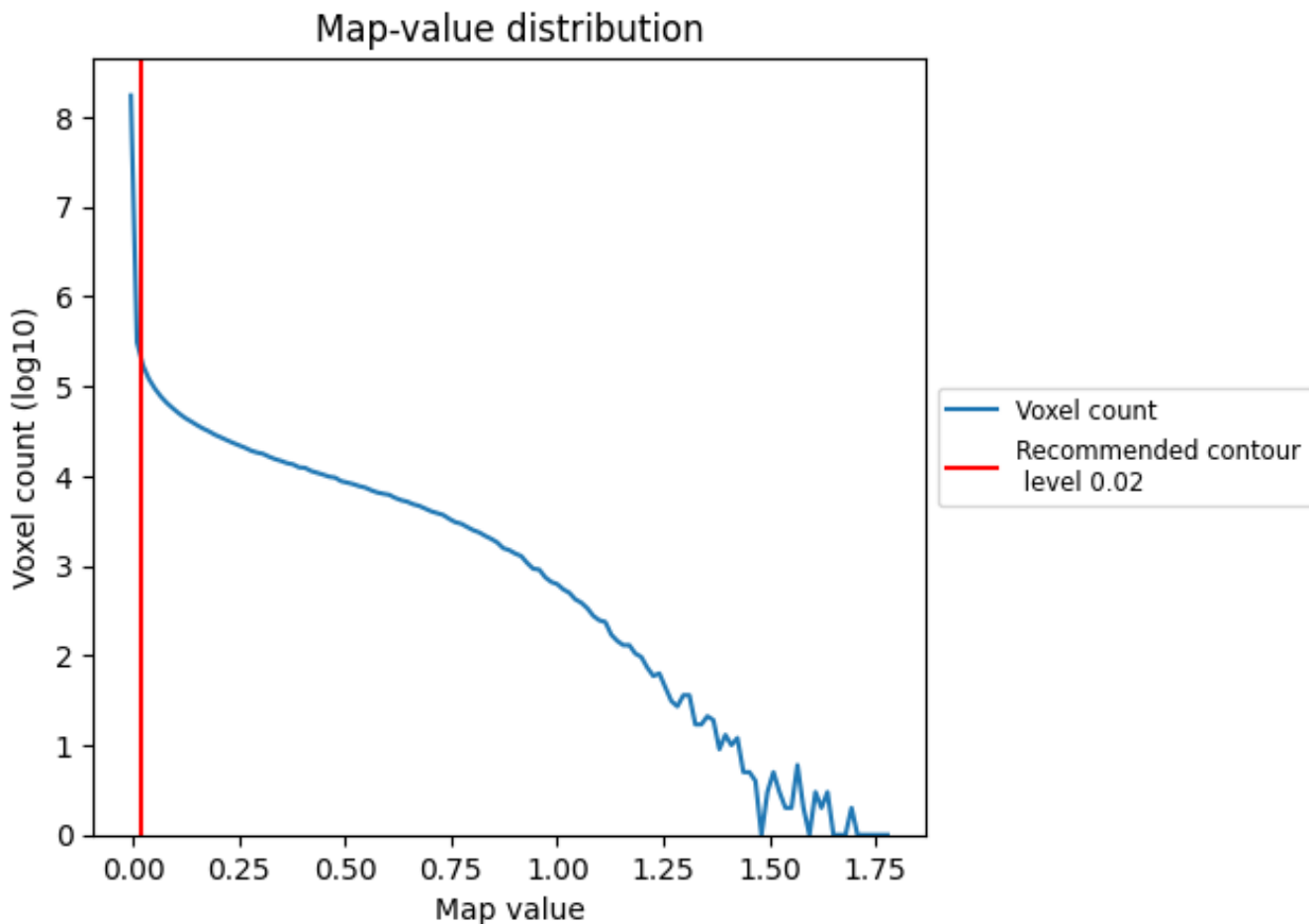
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

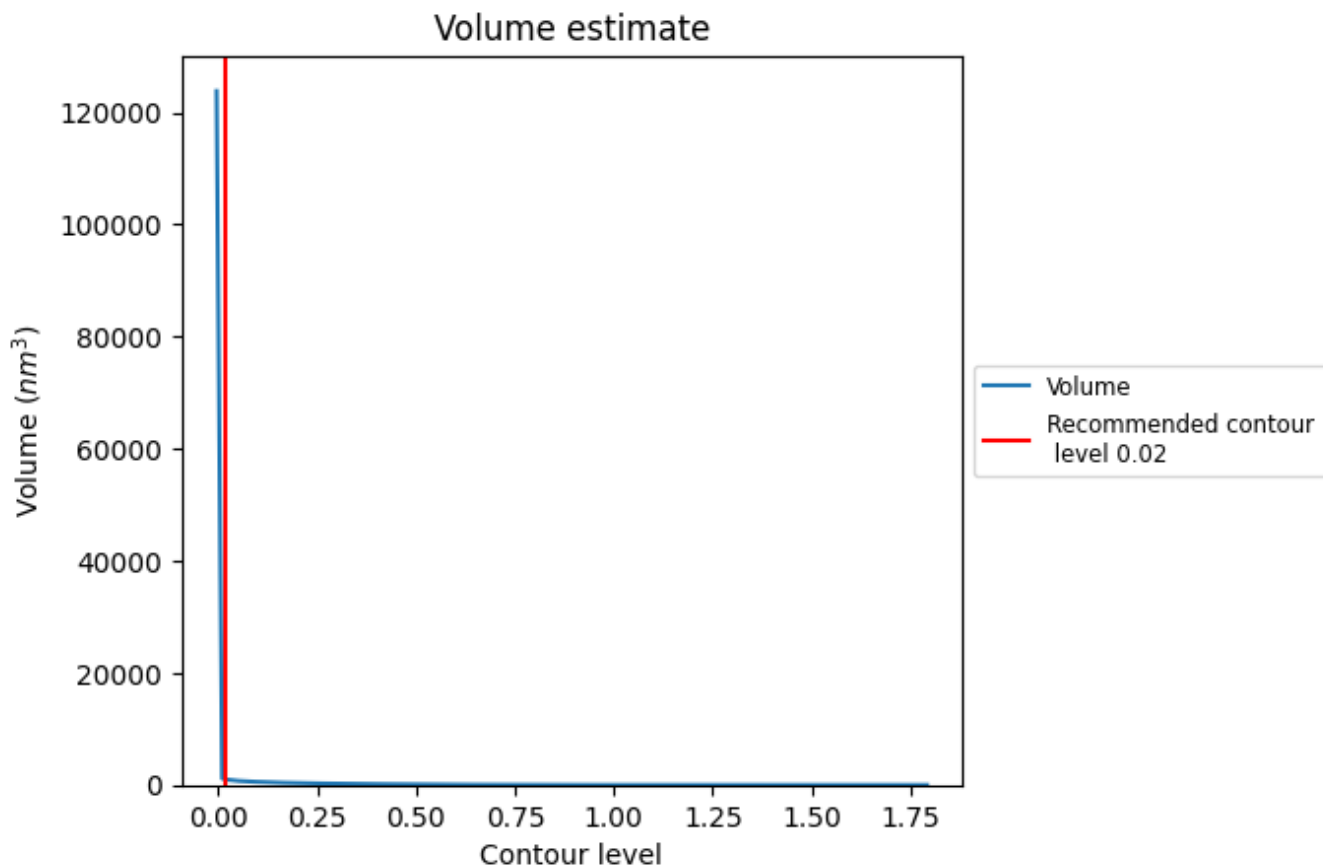
This section contains the results of statistical analysis of the map.

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.

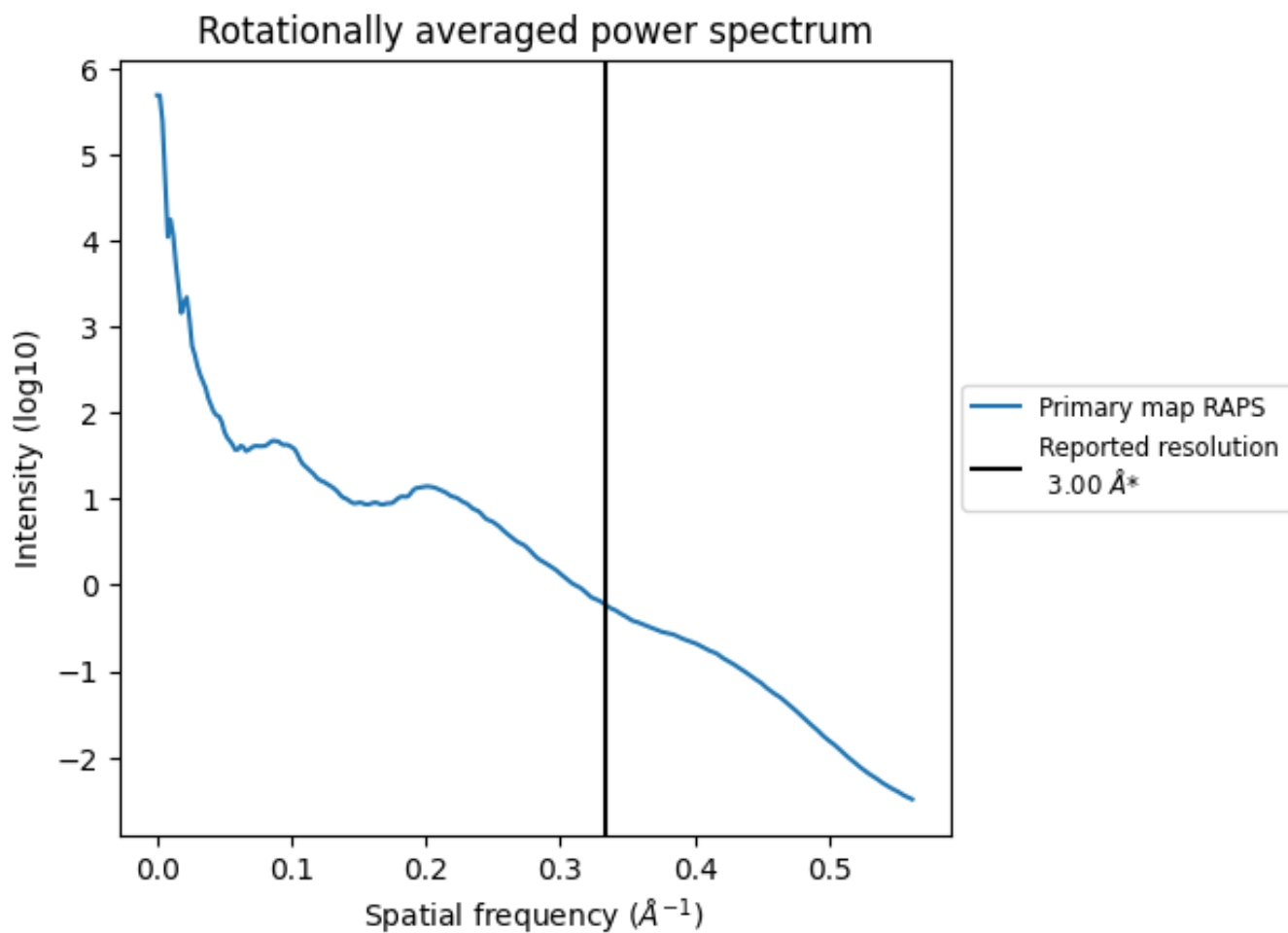
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 986 nm^3 ; this corresponds to an approximate mass of 891 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

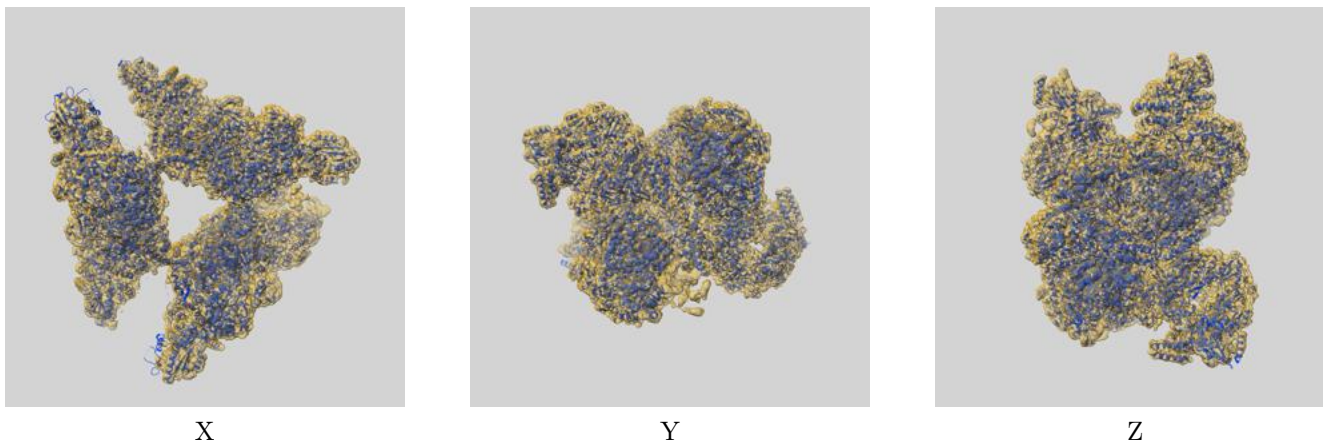
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

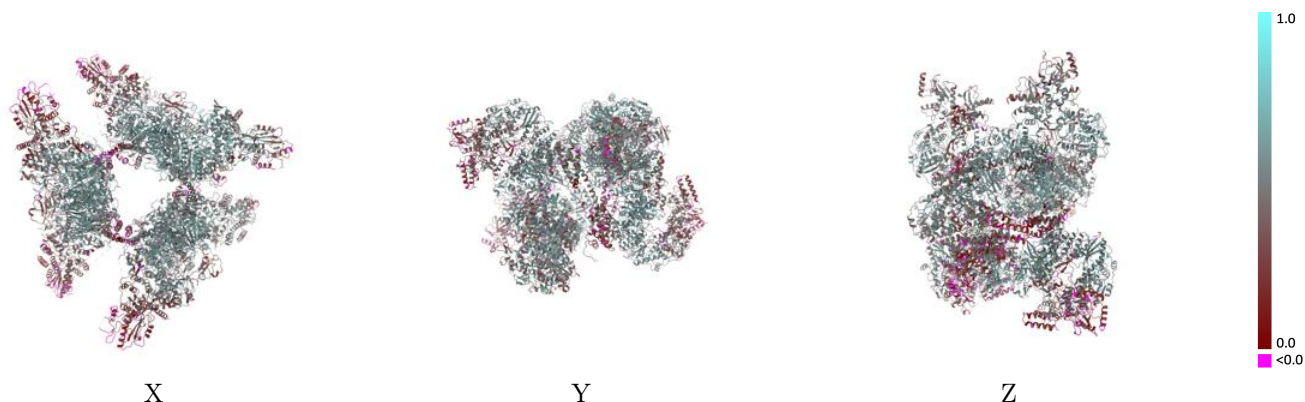
This section contains information regarding the fit between EMDB map EMD-39022 and PDB model 8Y7O. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



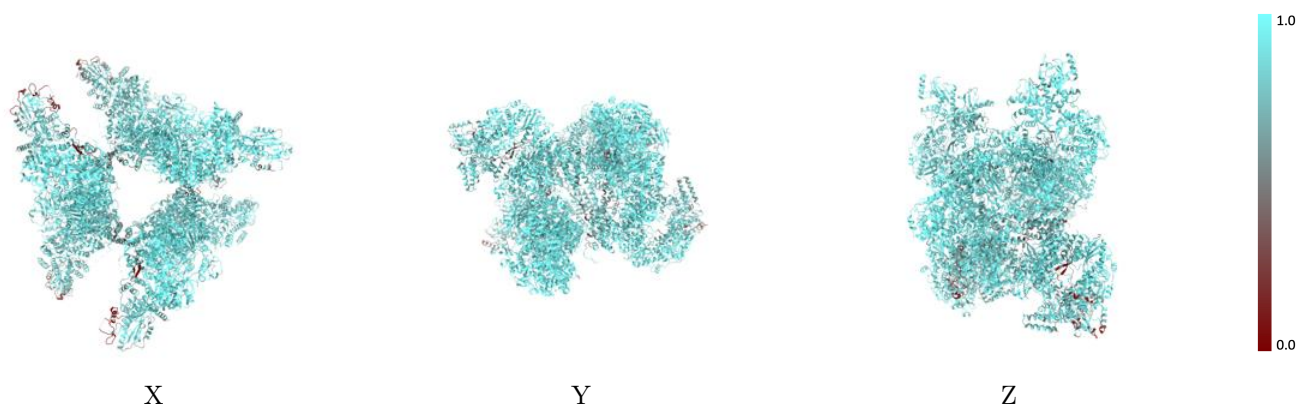
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



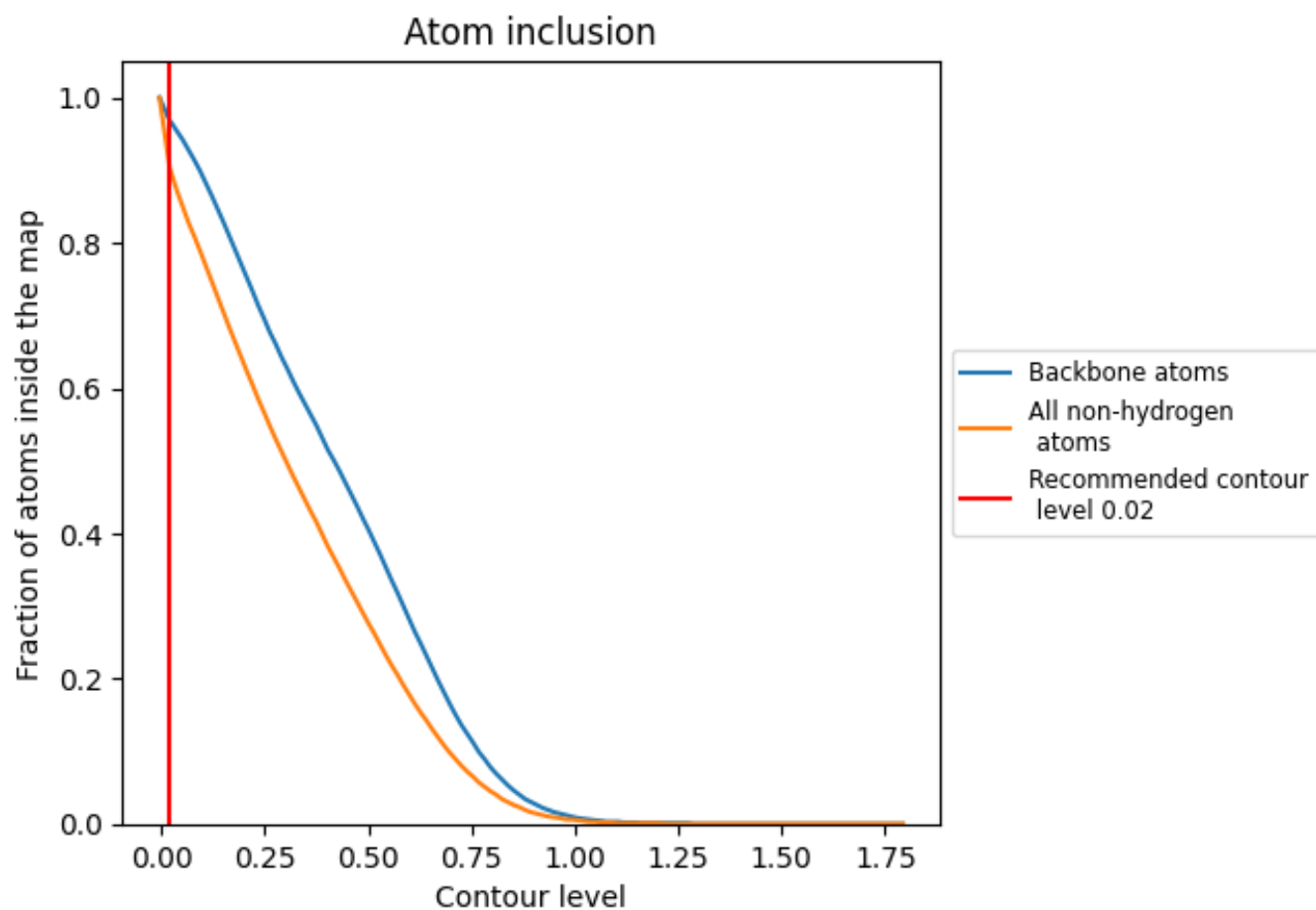
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9030	 0.4470
A	 0.9430	 0.5070
B	 0.9580	 0.5430
C	 0.9020	 0.4690
D	 0.8510	 0.3810
E	 0.8690	 0.4250
F	 0.9290	 0.4610
G	 0.8940	 0.4250
H	 0.9560	 0.5110
I	 0.9520	 0.5010
J	 0.9480	 0.4740
K	 0.7740	 0.3510
L	 0.9000	 0.4340
M	 0.8810	 0.4390
N	 0.9380	 0.4860
O	 0.7700	 0.3570
P	 0.8760	 0.3830
Q	 0.8770	 0.4300
R	 0.9350	 0.4530
S	 0.9130	 0.3860
T	 0.8260	 0.3210
U	 0.8180	 0.2850
V	 0.7730	 0.2550
W	 0.7880	 0.2850
X	 0.7650	 0.2480

