



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 03:50 PM UTC

PDB ID : 8JMW / pdb_00008jmw
EMDB ID : EMD-36428
Title : Fibril form of serine peptidase Vpr
Authors : Cao, Q.; Cheng, Y.
Deposited on : 2023-06-05
Resolution : 2.90 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

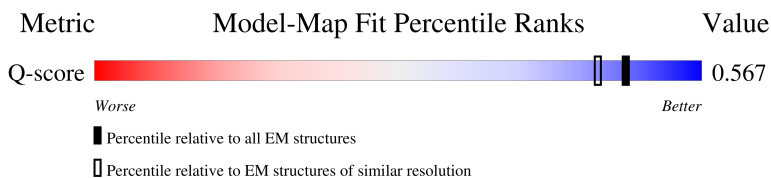
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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	803	 51% 13% 36%
1	B	803	 52% 13% 36%
1	C	803	 51% 13% 36%
1	D	803	 52% 12% 36%

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Mol	Chain	Length	Quality of chain
1	E	803	
1	F	803	
1	G	803	
1	H	803	
1	I	803	
1	J	803	
1	K	803	
1	L	803	
1	M	803	
1	N	803	
1	O	803	
1	P	803	
1	Q	803	
1	R	803	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 69552 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 S8 family serine peptidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	517	Total	C	N	O	S	0	0
			3864	2423	650	780	11		
1	B	517	Total	C	N	O	S	0	0
			3864	2423	650	780	11		
1	C	517	Total	C	N	O	S	0	0
			3864	2423	650	780	11		
1	D	517	Total	C	N	O	S	0	0
			3864	2423	650	780	11		
1	E	517	Total	C	N	O	S	0	0
			3864	2423	650	780	11		
1	F	517	Total	C	N	O	S	0	0
			3864	2423	650	780	11		
1	G	517	Total	C	N	O	S	0	0
			3864	2423	650	780	11		
1	H	517	Total	C	N	O	S	0	0
			3864	2423	650	780	11		
1	I	517	Total	C	N	O	S	0	0
			3864	2423	650	780	11		
1	J	517	Total	C	N	O	S	0	0
			3864	2423	650	780	11		
1	K	517	Total	C	N	O	S	0	0
			3864	2423	650	780	11		
1	L	517	Total	C	N	O	S	0	0
			3864	2423	650	780	11		
1	M	517	Total	C	N	O	S	0	0
			3864	2423	650	780	11		
1	N	517	Total	C	N	O	S	0	0
			3864	2423	650	780	11		
1	O	517	Total	C	N	O	S	0	0
			3864	2423	650	780	11		
1	P	517	Total	C	N	O	S	0	0
			3864	2423	650	780	11		
1	Q	517	Total	C	N	O	S	0	0
			3864	2423	650	780	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	517	Total	C	N	O	S	0	0
			3864	2423	650	780	11		

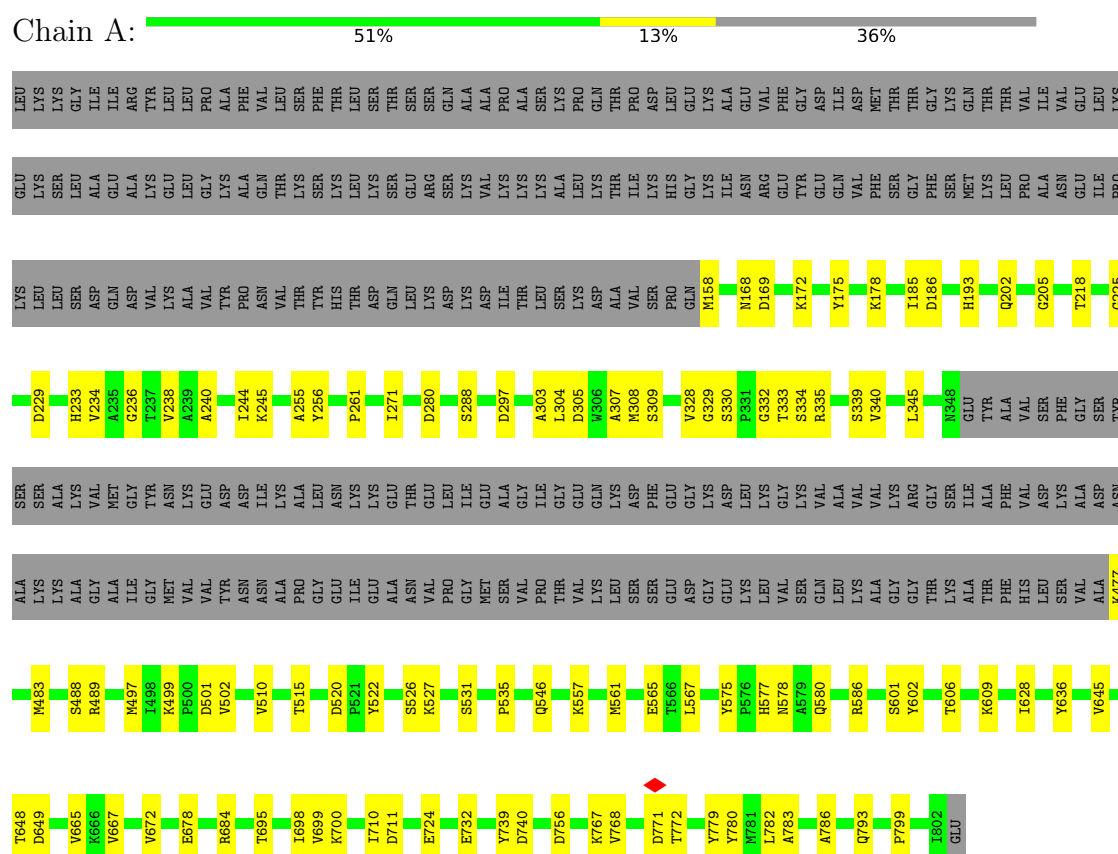
There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	LEU	MET	conflict	UNP A0A6A8LCF5
A	333	THR	ALA	conflict	UNP A0A6A8LCF5
B	1	LEU	MET	conflict	UNP A0A6A8LCF5
B	333	THR	ALA	conflict	UNP A0A6A8LCF5
C	1	LEU	MET	conflict	UNP A0A6A8LCF5
C	333	THR	ALA	conflict	UNP A0A6A8LCF5
D	1	LEU	MET	conflict	UNP A0A6A8LCF5
D	333	THR	ALA	conflict	UNP A0A6A8LCF5
E	1	LEU	MET	conflict	UNP A0A6A8LCF5
E	333	THR	ALA	conflict	UNP A0A6A8LCF5
F	1	LEU	MET	conflict	UNP A0A6A8LCF5
F	333	THR	ALA	conflict	UNP A0A6A8LCF5
G	1	LEU	MET	conflict	UNP A0A6A8LCF5
G	333	THR	ALA	conflict	UNP A0A6A8LCF5
H	1	LEU	MET	conflict	UNP A0A6A8LCF5
H	333	THR	ALA	conflict	UNP A0A6A8LCF5
I	1	LEU	MET	conflict	UNP A0A6A8LCF5
I	333	THR	ALA	conflict	UNP A0A6A8LCF5
J	1	LEU	MET	conflict	UNP A0A6A8LCF5
J	333	THR	ALA	conflict	UNP A0A6A8LCF5
K	1	LEU	MET	conflict	UNP A0A6A8LCF5
K	333	THR	ALA	conflict	UNP A0A6A8LCF5
L	1	LEU	MET	conflict	UNP A0A6A8LCF5
L	333	THR	ALA	conflict	UNP A0A6A8LCF5
M	1	LEU	MET	conflict	UNP A0A6A8LCF5
M	333	THR	ALA	conflict	UNP A0A6A8LCF5
N	1	LEU	MET	conflict	UNP A0A6A8LCF5
N	333	THR	ALA	conflict	UNP A0A6A8LCF5
O	1	LEU	MET	conflict	UNP A0A6A8LCF5
O	333	THR	ALA	conflict	UNP A0A6A8LCF5
P	1	LEU	MET	conflict	UNP A0A6A8LCF5
P	333	THR	ALA	conflict	UNP A0A6A8LCF5
Q	1	LEU	MET	conflict	UNP A0A6A8LCF5
Q	333	THR	ALA	conflict	UNP A0A6A8LCF5
R	1	LEU	MET	conflict	UNP A0A6A8LCF5
R	333	THR	ALA	conflict	UNP A0A6A8LCF5

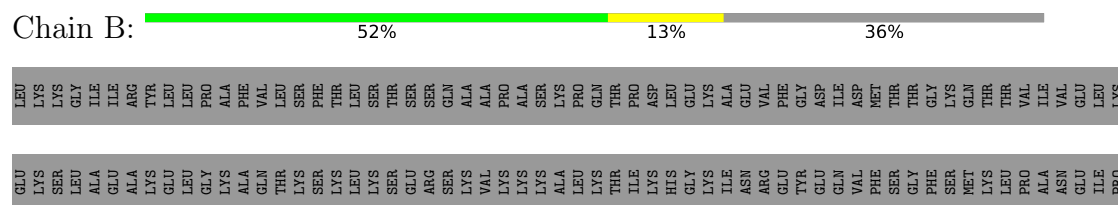
3 Residue-property plots

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

• Molecule 1: S8 family serine peptidase



• Molecule 1: S8 family serine peptidase



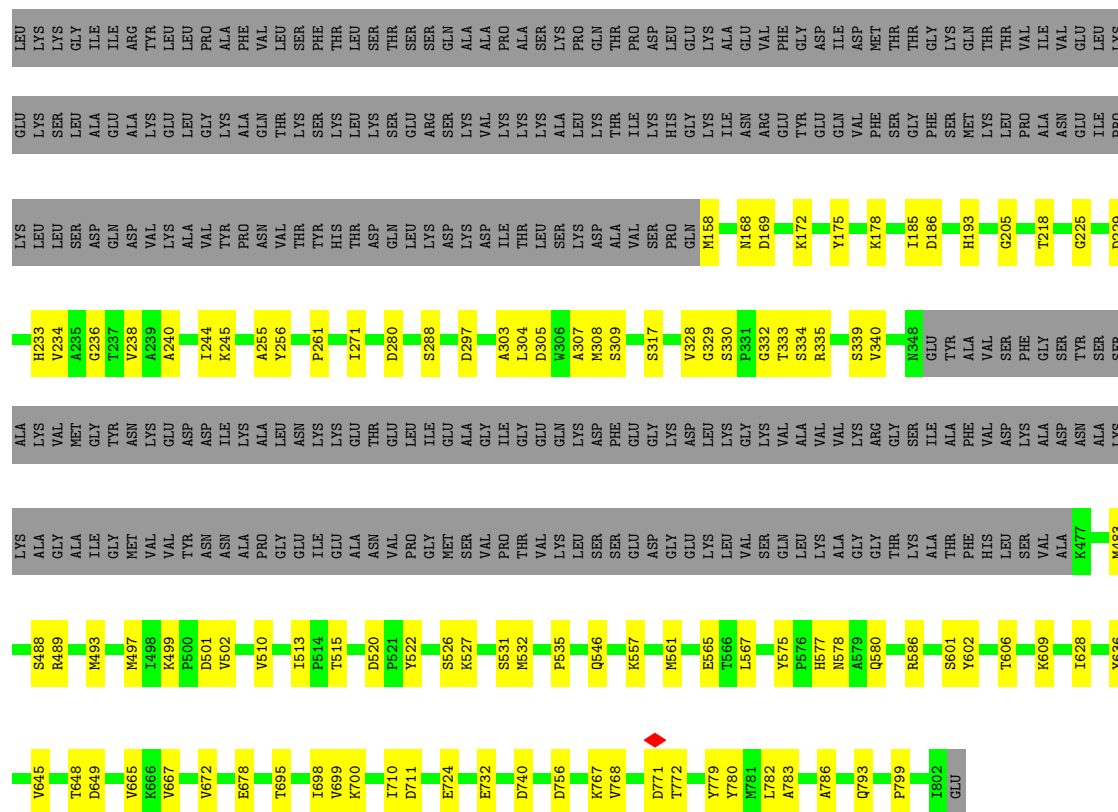






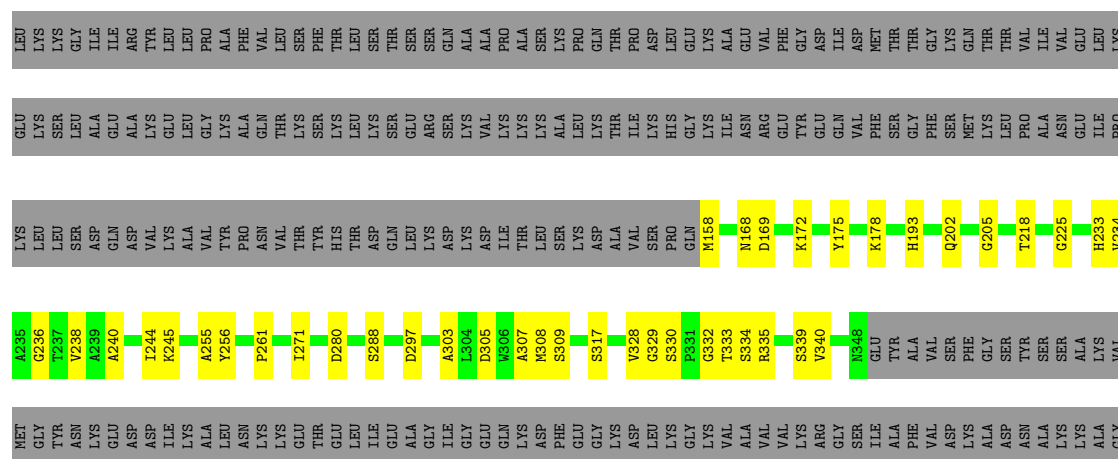
- Molecule 1: S8 family serine peptidase

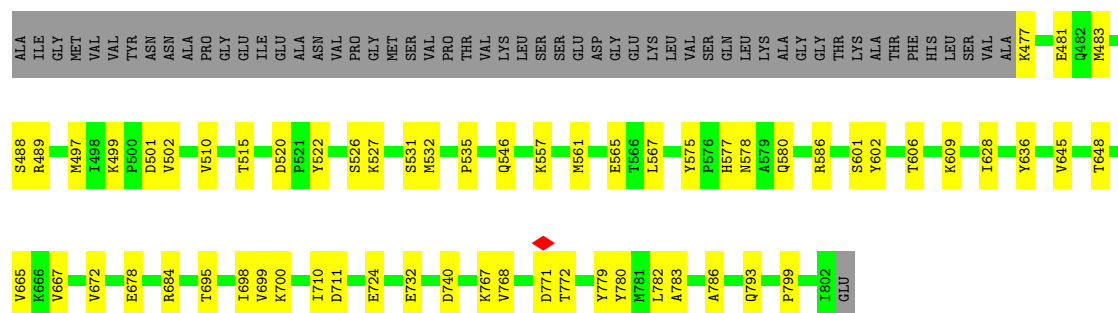
Chain F: 51% 13% 36%



- Molecule 1: S8 family serine peptidase

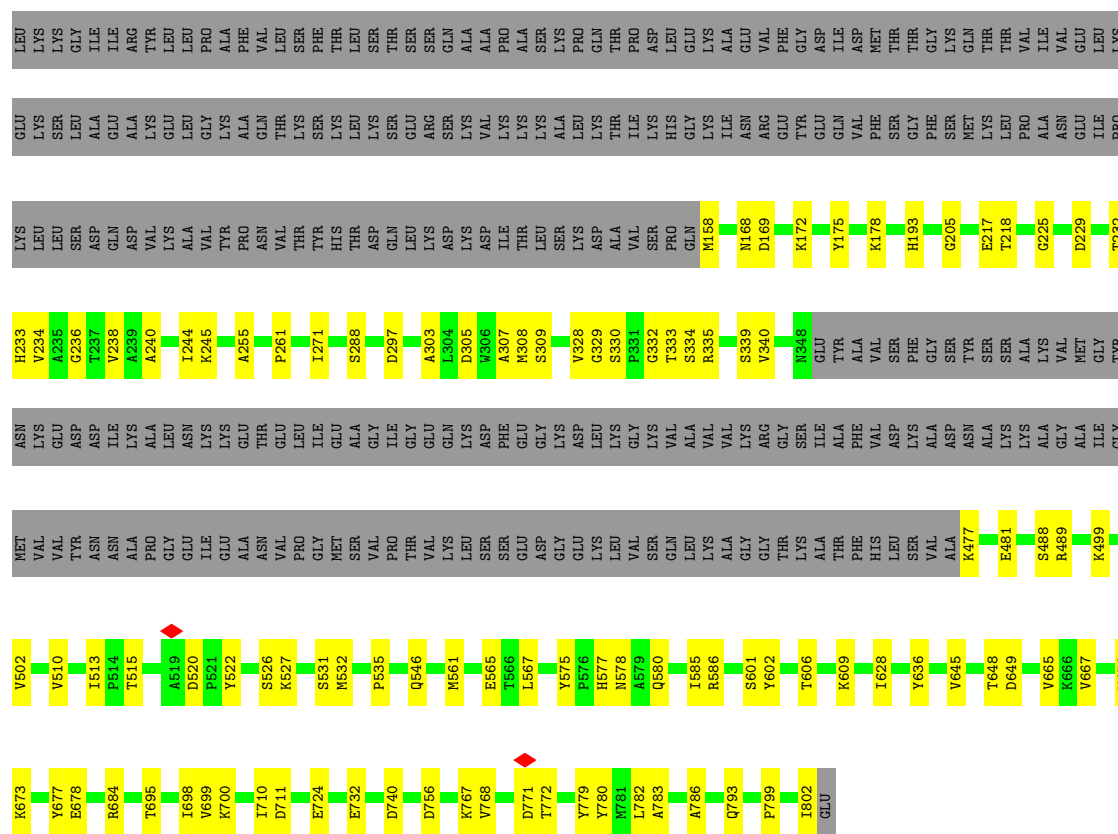
Chain G: 52% 13% 36%





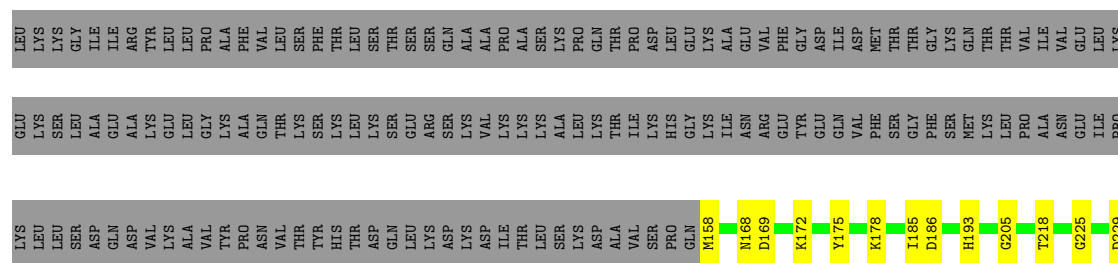
• Molecule 1: S8 family serine peptidase

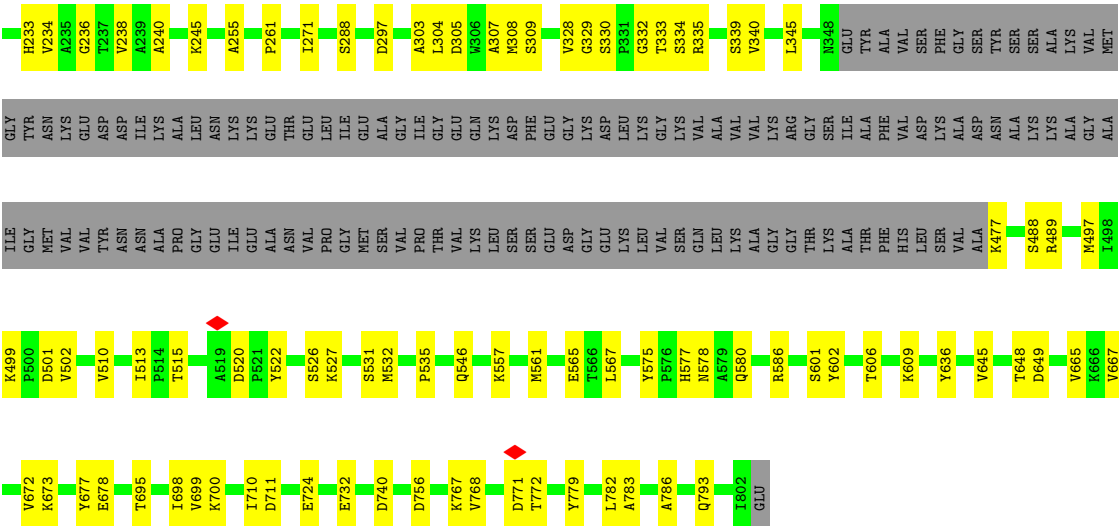
Chain H: 52% 13% 36%



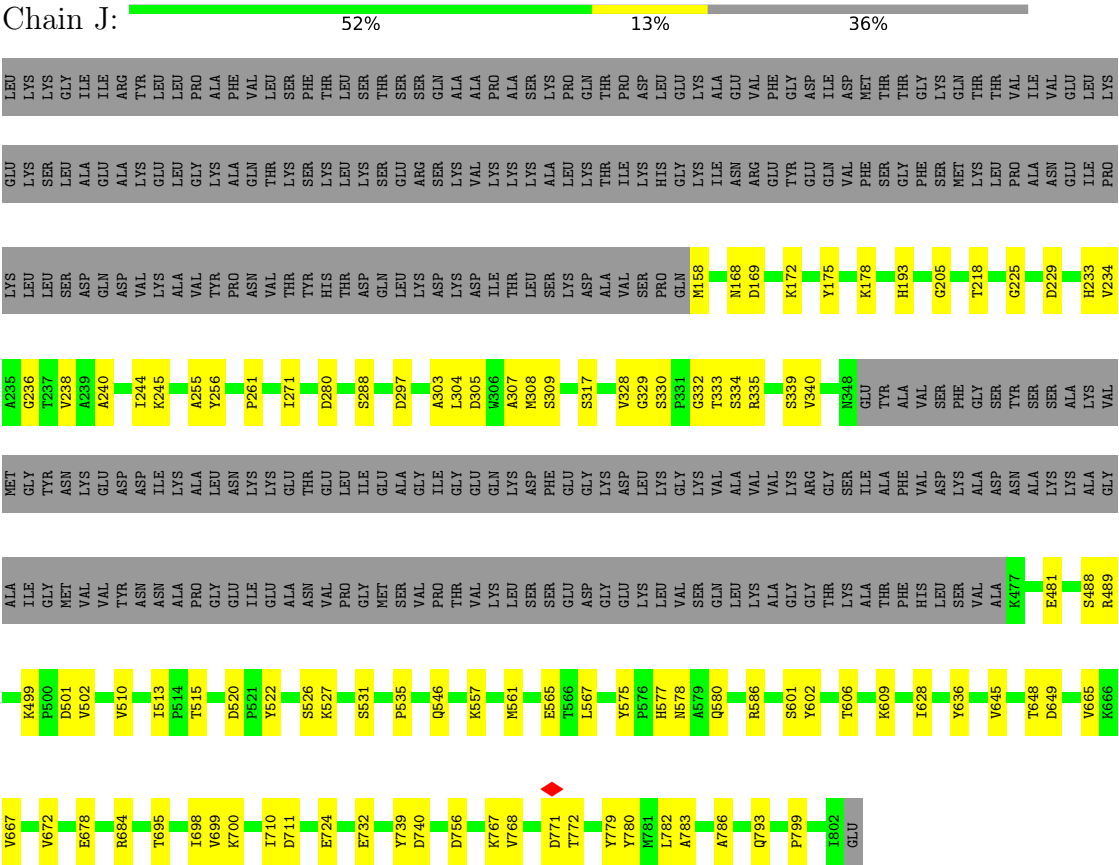
• Molecule 1: S8 family serine peptidase

Chain I: 52% 12% 36%

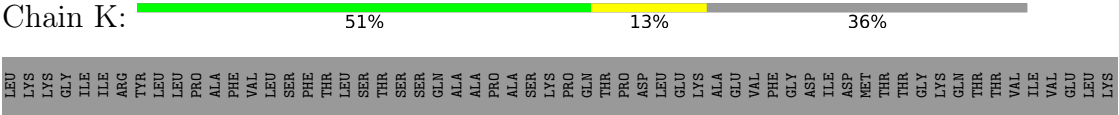


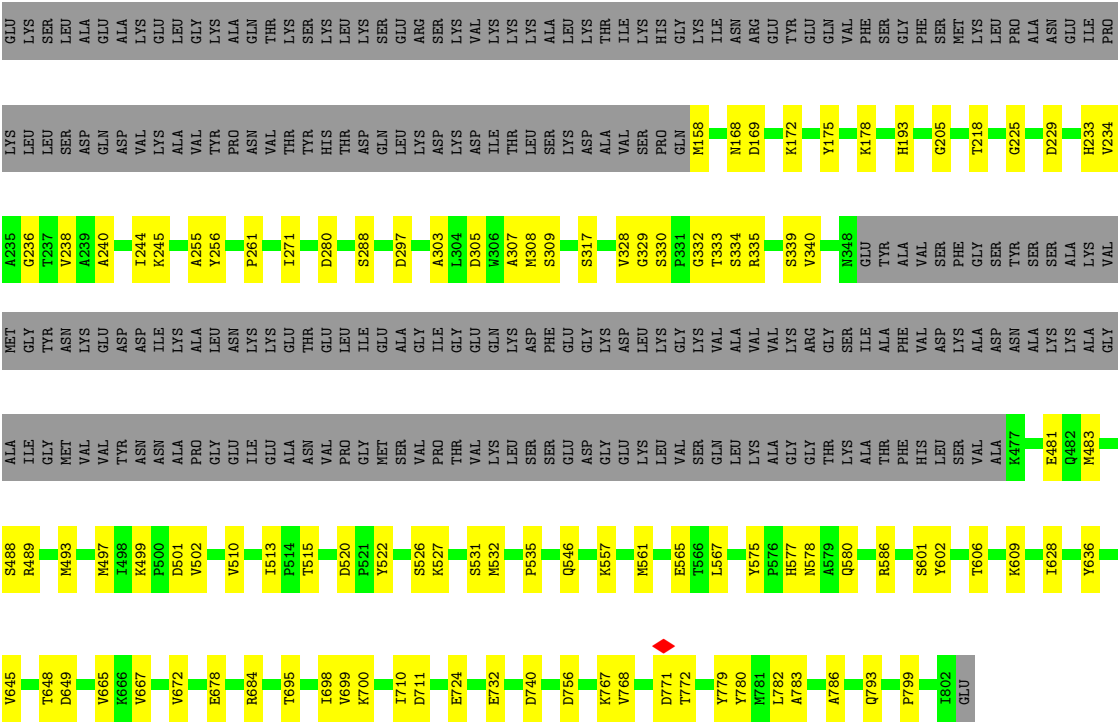


● Molecule 1: S8 family serine peptidase

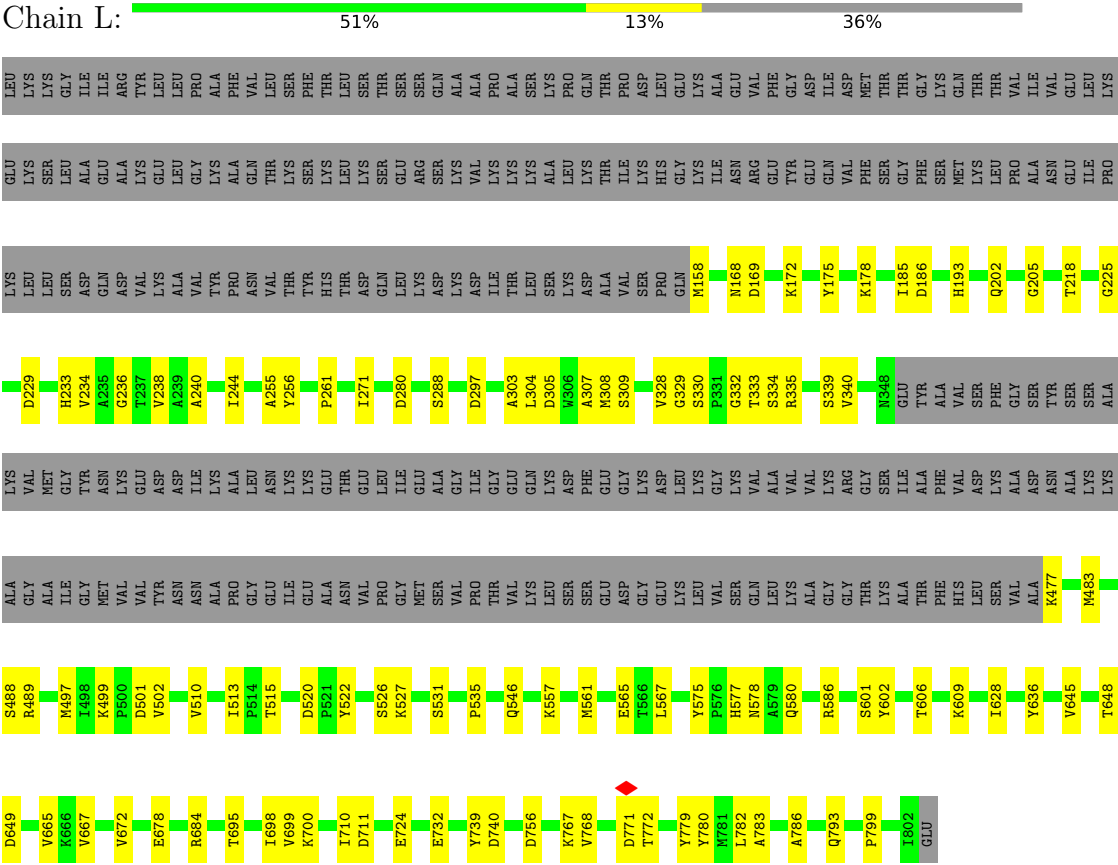


● Molecule 1: S8 family serine peptidase

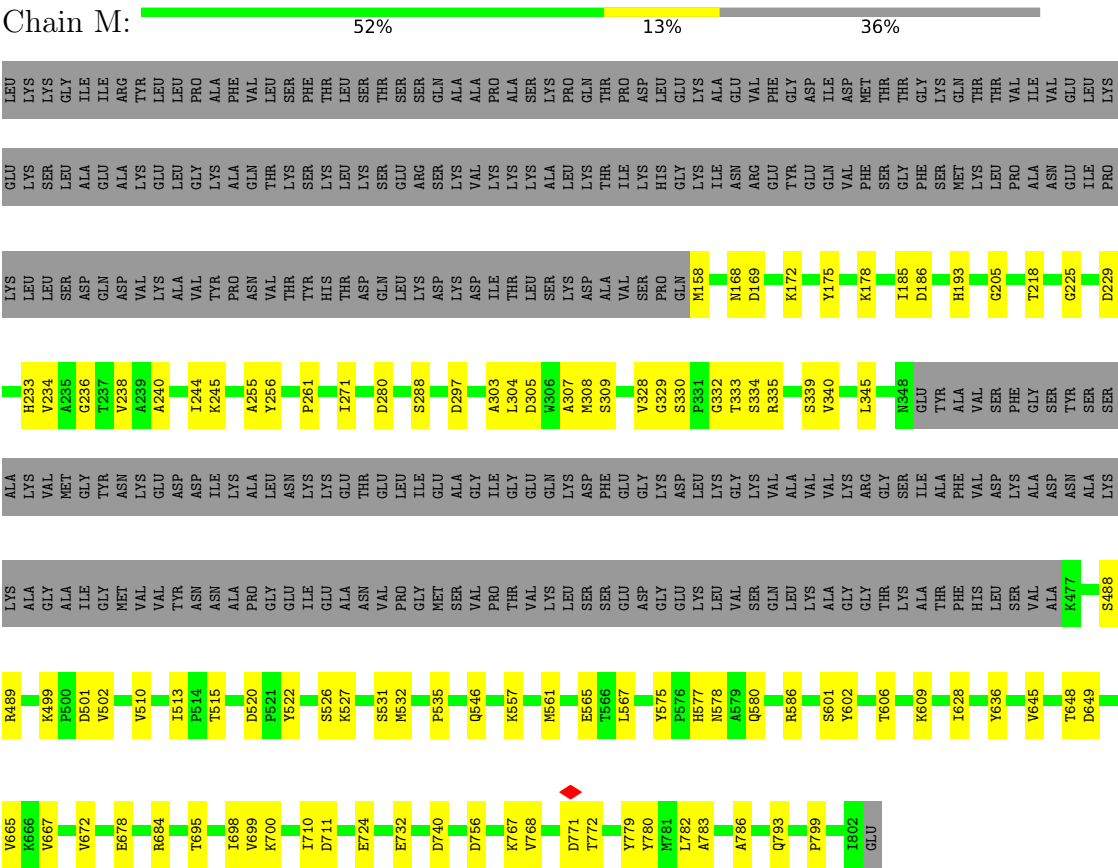




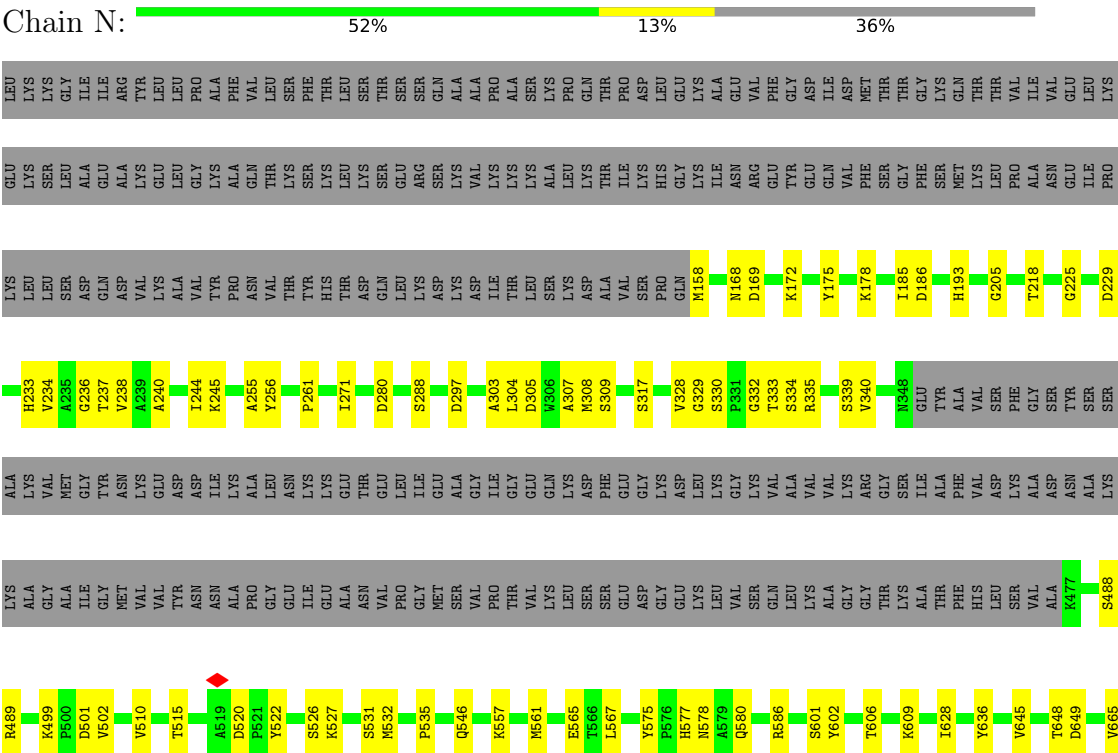
● Molecule 1: S8 family serine peptidase



● Molecule 1: S8 family serine peptidase



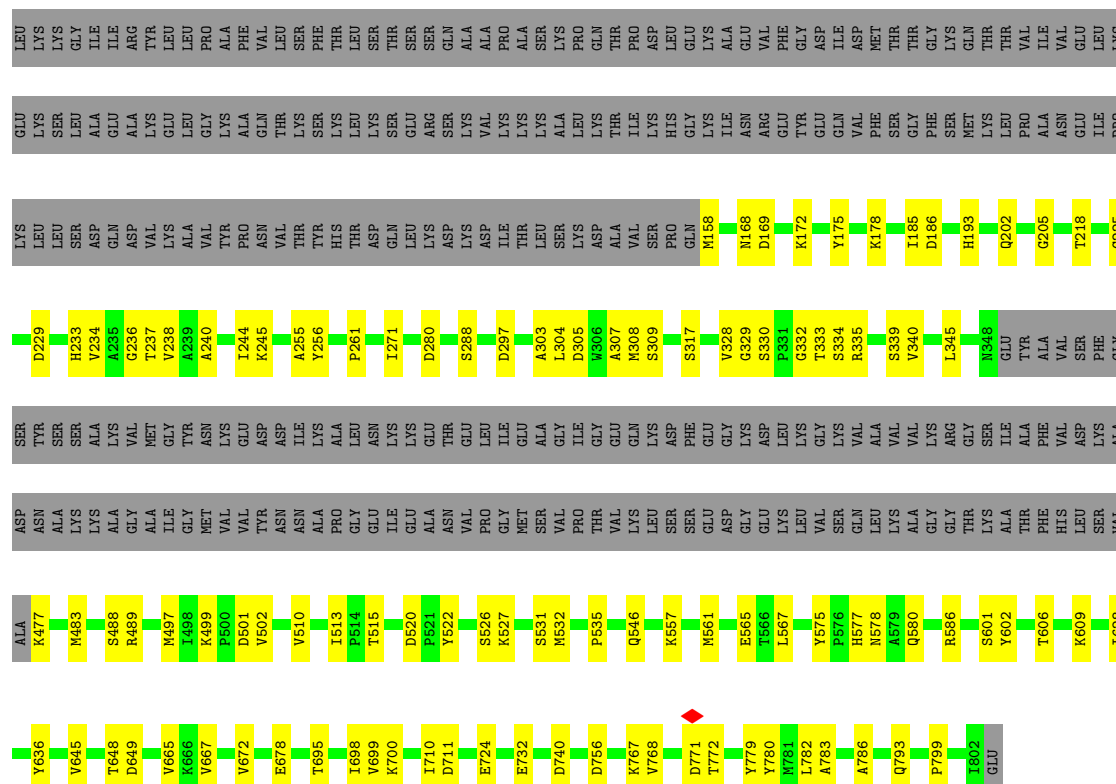
● Molecule 1: S8 family serine peptidase





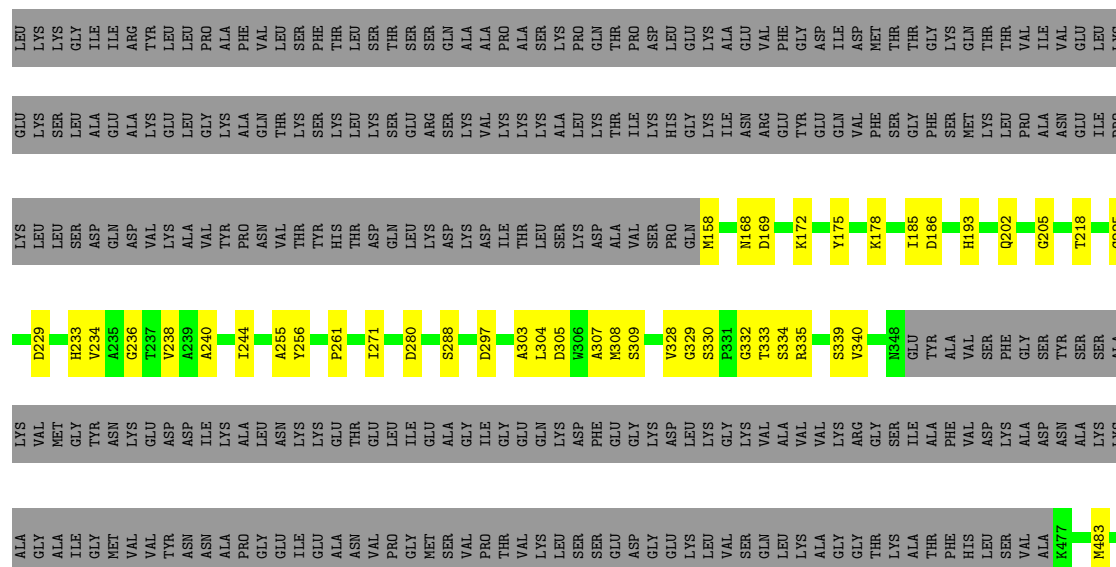
- Molecule 1: S8 family serine peptidase

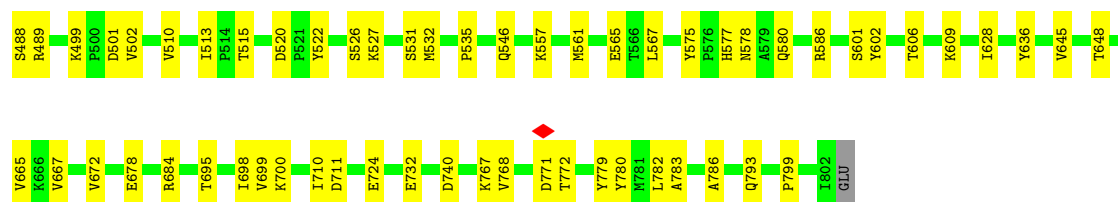
Chain O: 51% 13% 36%



- Molecule 1: S8 family serine peptidase

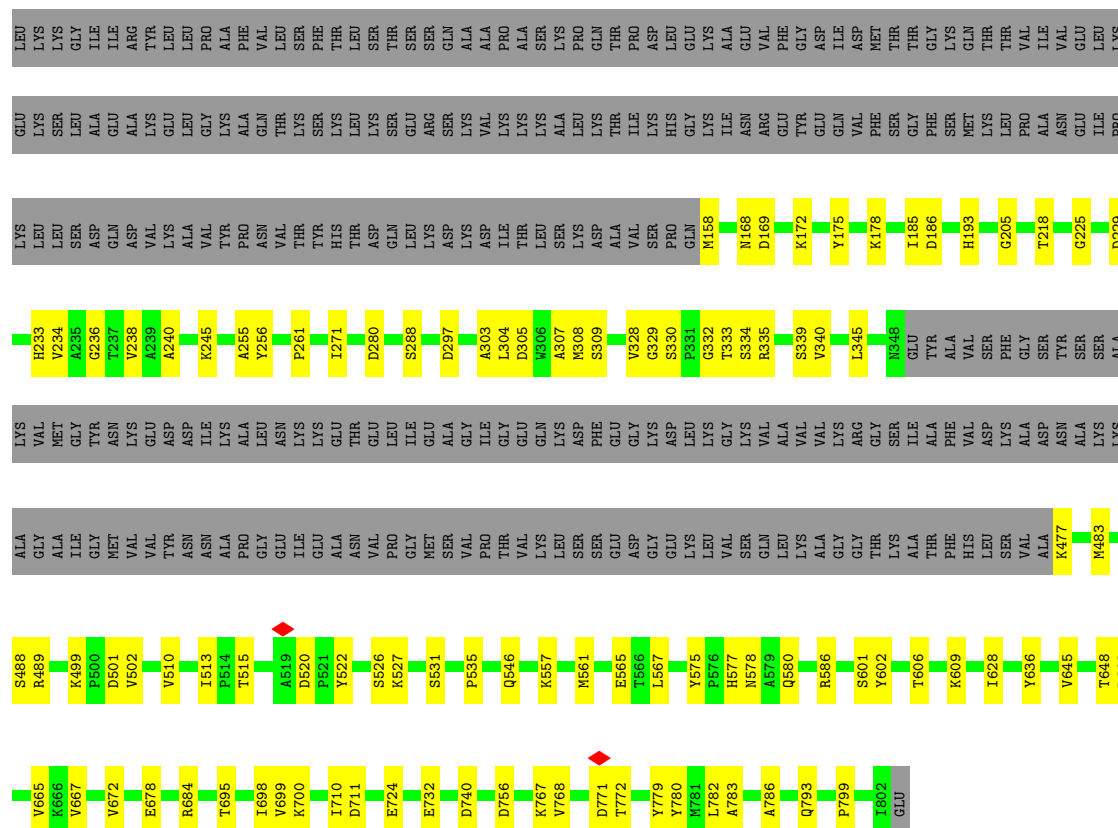
Chain P: 52% 13% 36%





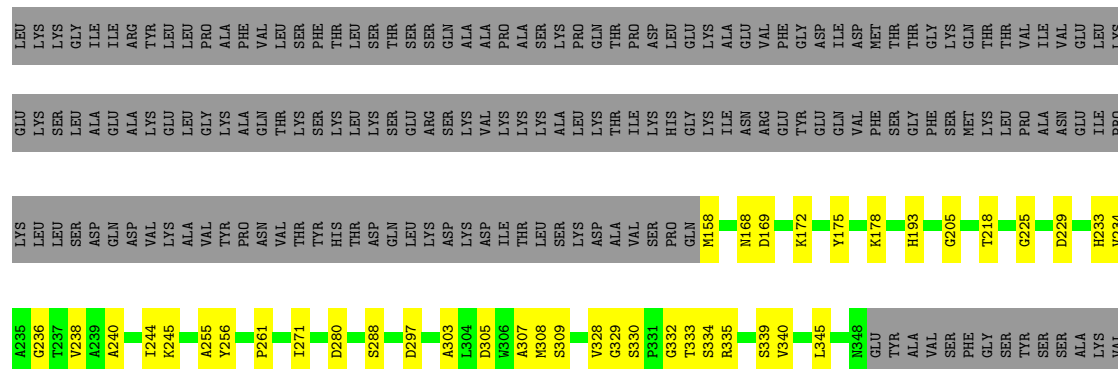
• Molecule 1: S8 family serine peptidase

Chain Q: 52% 13% 36%



• Molecule 1: S8 family serine peptidase

Chain R: 52% 12% 36%



V687	K499	ALA	GLY	MET
V672	P500	GLY	TYR	TYR
E678	D501	MET	ASN	ASN
T695	V502	VAL	LYS	GLY
	V510	TYR	ASP	ASP
	I513	ASN	LYS	LYS
I698	P514	ALA	ILE	ILE
V699	T515	PRO	ALA	ALA
K700		GLY	LEU	LEU
I710	A519	GLY	ASN	ASN
D711	D520	ILE	LYS	LYS
E724	P521	GLU	GLY	LYS
	Y522	ALA	THR	THR
		ASN	GLU	GLU
E732	S526	VAL	LEU	LEU
	K527	PRO	ILE	ILE
D740		GLY	GLY	GLY
	S531	MET	GLU	GLU
D756	M532	SER	ALA	ALA
		VAL	GLY	GLY
K767	P535	PRO	ILE	ILE
V768		THR	GLY	GLY
	Q546	VAL	GLN	GLN
D771		LYS	LYS	LYS
T772	K557	LEU	ASP	ASP
		SER	PHE	PHE
Y779	M561	SER	GLU	GLY
K781	E565	ASP	GLY	GLY
L782	T566	GLY	LYS	LYS
A783	L567	GLU	ASP	ASP
		LEU	LEU	LEU
A786	Y575	LEU	LYS	LYS
	P576	VAL	GLY	GLY
Q793	H577	SER	LYS	LYS
	N578	GLN	VAL	VAL
P799	A579	LEU	ALA	ALA
	Q580	LYS	VAL	VAL
T802		ALA	VAL	VAL
GLU	R586	GLY	LYS	LYS
		GLY	ARG	ARG
	S601	THR	GLY	GLY
	Y602	LYS	SER	SER
		ALA	ILE	ILE
	T606	THR	ALA	ALA
	K609	PHE	PHE	PHE
		HIS	VAL	VAL
		LEU	ASP	ASP
	Y636	SER	LYS	LYS
	V645	VAL	ALA	ALA
		ASP	ASN	ASN
		ALA	ALA	ALA
		K477	LYS	LYS
	T648	M483	LYS	LYS
	D649		GLY	GLY
	V665	S488	ALA	ALA

4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-68.75°, rise=20.46 Å, axial sym=C2	Depositor
Number of segments used	76671	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	4600	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	15.581	Depositor
Minimum map value	-4.358	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.4	Depositor
Map size (Å)	336.0, 336.0, 336.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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	0.33	0/3947	0.37	0/5370
1	B	0.33	0/3947	0.37	0/5370
1	C	0.33	0/3947	0.37	0/5370
1	D	0.33	0/3947	0.37	0/5370
1	E	0.33	0/3947	0.37	0/5370
1	F	0.33	0/3947	0.37	0/5370
1	G	0.33	0/3947	0.37	0/5370
1	H	0.33	0/3947	0.37	0/5370
1	I	0.33	0/3947	0.37	0/5370
1	J	0.33	0/3947	0.37	0/5370
1	K	0.33	0/3947	0.37	0/5370
1	L	0.33	0/3947	0.37	0/5370
1	M	0.33	0/3947	0.37	0/5370
1	N	0.33	0/3947	0.37	0/5370
1	O	0.33	0/3947	0.37	0/5370
1	P	0.33	0/3947	0.37	0/5370
1	Q	0.33	0/3947	0.37	0/5370
1	R	0.33	0/3947	0.37	0/5370
All	All	0.33	0/71046	0.37	0/96660

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	3864	0	3765	76	0
1	B	3864	0	3765	73	0
1	C	3864	0	3765	77	0
1	D	3864	0	3765	69	0
1	E	3864	0	3765	70	0
1	F	3864	0	3765	73	0
1	G	3864	0	3765	72	0
1	H	3864	0	3765	76	0
1	I	3864	0	3765	73	0
1	J	3864	0	3765	73	0
1	K	3864	0	3765	73	0
1	L	3864	0	3765	74	0
1	M	3864	0	3765	72	0
1	N	3864	0	3765	72	0
1	O	3864	0	3765	79	0
1	P	3864	0	3765	73	0
1	Q	3864	0	3765	74	0
1	R	3864	0	3765	69	0
All	All	69552	0	67770	1276	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 9.

All (1276) 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:M:732:GLU:HG2	1:M:786:ALA:O	1.50	1.11
1:Q:732:GLU:HG2	1:Q:786:ALA:O	1.50	1.11
1:A:732:GLU:HG2	1:A:786:ALA:O	1.50	1.11
1:B:732:GLU:HG2	1:B:786:ALA:O	1.50	1.10
1:D:732:GLU:HG2	1:D:786:ALA:O	1.50	1.09
1:G:732:GLU:HG2	1:G:786:ALA:O	1.50	1.09
1:I:732:GLU:HG2	1:I:786:ALA:O	1.50	1.09
1:L:732:GLU:HG2	1:L:786:ALA:O	1.50	1.09
1:F:732:GLU:HG2	1:F:786:ALA:O	1.50	1.09
1:N:732:GLU:HG2	1:N:786:ALA:O	1.50	1.09
1:P:732:GLU:HG2	1:P:786:ALA:O	1.50	1.09
1:O:732:GLU:HG2	1:O:786:ALA:O	1.50	1.09
1:J:732:GLU:HG2	1:J:786:ALA:O	1.50	1.08
1:K:732:GLU:HG2	1:K:786:ALA:O	1.50	1.08
1:C:732:GLU:HG2	1:C:786:ALA:O	1.50	1.08
1:H:732:GLU:HG2	1:H:786:ALA:O	1.50	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:732:GLU:HG2	1:R:786:ALA:O	1.50	1.07
1:E:732:GLU:HG2	1:E:786:ALA:O	1.50	1.07
1:A:297:ASP:OD1	1:A:335:ARG:NH2	2.25	0.70
1:B:297:ASP:OD1	1:B:335:ARG:NH2	2.25	0.70
1:F:297:ASP:OD1	1:F:335:ARG:NH2	2.25	0.70
1:G:297:ASP:OD1	1:G:335:ARG:NH2	2.25	0.70
1:P:297:ASP:OD1	1:P:335:ARG:NH2	2.25	0.70
1:K:297:ASP:OD1	1:K:335:ARG:NH2	2.25	0.70
1:L:297:ASP:OD1	1:L:335:ARG:NH2	2.25	0.69
1:N:297:ASP:OD1	1:N:335:ARG:NH2	2.25	0.69
1:Q:297:ASP:OD1	1:Q:335:ARG:NH2	2.25	0.69
1:R:297:ASP:OD1	1:R:335:ARG:NH2	2.25	0.69
1:M:297:ASP:OD1	1:M:335:ARG:NH2	2.25	0.69
1:C:297:ASP:OD1	1:C:335:ARG:NH2	2.25	0.69
1:H:297:ASP:OD1	1:H:335:ARG:NH2	2.25	0.69
1:D:297:ASP:OD1	1:D:335:ARG:NH2	2.25	0.69
1:I:297:ASP:OD1	1:I:335:ARG:NH2	2.25	0.69
1:E:297:ASP:OD1	1:E:335:ARG:NH2	2.25	0.69
1:O:297:ASP:OD1	1:O:335:ARG:NH2	2.25	0.69
1:J:297:ASP:OD1	1:J:335:ARG:NH2	2.25	0.69
1:J:767:LYS:HE3	1:J:771:ASP:HA	1.75	0.68
1:K:767:LYS:HE3	1:K:771:ASP:HA	1.75	0.68
1:R:767:LYS:HE3	1:R:771:ASP:HA	1.75	0.68
1:Q:732:GLU:CG	1:Q:786:ALA:O	2.38	0.68
1:F:628:ILE:HG13	1:G:271:ILE:HG21	1.76	0.68
1:J:732:GLU:CG	1:J:786:ALA:O	2.38	0.68
1:L:767:LYS:HE3	1:L:771:ASP:HA	1.75	0.68
1:M:767:LYS:HE3	1:M:771:ASP:HA	1.75	0.67
1:O:767:LYS:HE3	1:O:771:ASP:HA	1.75	0.67
1:Q:767:LYS:HE3	1:Q:771:ASP:HA	1.75	0.67
1:D:767:LYS:HE3	1:D:771:ASP:HA	1.75	0.67
1:C:732:GLU:CG	1:C:786:ALA:O	2.38	0.67
1:E:767:LYS:HE3	1:E:771:ASP:HA	1.75	0.67
1:F:732:GLU:CG	1:F:786:ALA:O	2.38	0.67
1:H:767:LYS:HE3	1:H:771:ASP:HA	1.75	0.67
1:B:767:LYS:HE3	1:B:771:ASP:HA	1.75	0.67
1:G:767:LYS:HE3	1:G:771:ASP:HA	1.75	0.67
1:N:767:LYS:HE3	1:N:771:ASP:HA	1.75	0.67
1:F:767:LYS:HE3	1:F:771:ASP:HA	1.75	0.67
1:P:767:LYS:HE3	1:P:771:ASP:HA	1.75	0.67
1:A:767:LYS:HE3	1:A:771:ASP:HA	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:767:LYS:HE3	1:C:771:ASP:HA	1.75	0.66
1:I:767:LYS:HE3	1:I:771:ASP:HA	1.75	0.66
1:N:510:VAL:HG12	1:N:526:SER:HB2	1.78	0.66
1:B:510:VAL:HG12	1:B:526:SER:HB2	1.78	0.66
1:I:510:VAL:HG12	1:I:526:SER:HB2	1.78	0.66
1:O:628:ILE:HG13	1:P:271:ILE:HG21	1.76	0.66
1:N:732:GLU:CG	1:N:786:ALA:O	2.38	0.66
1:P:510:VAL:HG12	1:P:526:SER:HB2	1.78	0.66
1:O:510:VAL:HG12	1:O:526:SER:HB2	1.78	0.65
1:C:510:VAL:HG12	1:C:526:SER:HB2	1.78	0.65
1:K:732:GLU:CG	1:K:786:ALA:O	2.38	0.65
1:H:510:VAL:HG12	1:H:526:SER:HB2	1.78	0.65
1:I:732:GLU:CG	1:I:786:ALA:O	2.38	0.65
1:E:732:GLU:CG	1:E:786:ALA:O	2.38	0.65
1:G:510:VAL:HG12	1:G:526:SER:HB2	1.78	0.65
1:G:732:GLU:CG	1:G:786:ALA:O	2.38	0.65
1:J:510:VAL:HG12	1:J:526:SER:HB2	1.78	0.65
1:F:510:VAL:HG12	1:F:526:SER:HB2	1.78	0.65
1:R:510:VAL:HG12	1:R:526:SER:HB2	1.78	0.65
1:L:510:VAL:HG12	1:L:526:SER:HB2	1.78	0.64
1:R:732:GLU:CG	1:R:786:ALA:O	2.38	0.64
1:D:510:VAL:HG12	1:D:526:SER:HB2	1.78	0.64
1:Q:510:VAL:HG12	1:Q:526:SER:HB2	1.78	0.64
1:E:510:VAL:HG12	1:E:526:SER:HB2	1.78	0.64
1:K:271:ILE:HG21	1:L:628:ILE:HG13	1.80	0.64
1:K:510:VAL:HG12	1:K:526:SER:HB2	1.78	0.64
1:M:510:VAL:HG12	1:M:526:SER:HB2	1.78	0.64
1:O:732:GLU:CG	1:O:786:ALA:O	2.38	0.64
1:P:732:GLU:CG	1:P:786:ALA:O	2.38	0.64
1:L:732:GLU:CG	1:L:786:ALA:O	2.38	0.64
1:A:510:VAL:HG12	1:A:526:SER:HB2	1.78	0.63
1:G:684:ARG:NH2	1:H:756:ASP:OD1	2.31	0.63
1:A:732:GLU:CG	1:A:786:ALA:O	2.38	0.63
1:D:732:GLU:CG	1:D:786:ALA:O	2.38	0.63
1:P:684:ARG:NH2	1:Q:756:ASP:OD1	2.31	0.63
1:B:732:GLU:CG	1:B:786:ALA:O	2.38	0.63
1:A:628:ILE:HG13	1:F:271:ILE:HG21	1.81	0.63
1:B:271:ILE:HG21	1:C:628:ILE:HG13	1.80	0.62
1:Q:628:ILE:HG13	1:R:271:ILE:HG21	1.81	0.62
1:D:271:ILE:HG21	1:E:628:ILE:HG13	1.81	0.62
1:B:218:THR:HG21	1:B:261:PRO:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:THR:HG21	1:C:261:PRO:HB3	1.82	0.62
1:O:218:THR:HG21	1:O:261:PRO:HB3	1.82	0.62
1:A:218:THR:HG21	1:A:261:PRO:HB3	1.82	0.62
1:P:218:THR:HG21	1:P:261:PRO:HB3	1.82	0.62
1:I:218:THR:HG21	1:I:261:PRO:HB3	1.82	0.62
1:J:271:ILE:HG21	1:K:628:ILE:HG13	1.82	0.62
1:M:218:THR:HG21	1:M:261:PRO:HB3	1.82	0.62
1:H:218:THR:HG21	1:H:261:PRO:HB3	1.82	0.62
1:Q:218:THR:HG21	1:Q:261:PRO:HB3	1.82	0.62
1:J:218:THR:HG21	1:J:261:PRO:HB3	1.82	0.62
1:N:218:THR:HG21	1:N:261:PRO:HB3	1.82	0.62
1:L:218:THR:HG21	1:L:261:PRO:HB3	1.82	0.62
1:F:218:THR:HG21	1:F:261:PRO:HB3	1.82	0.61
1:A:271:ILE:HG21	1:B:628:ILE:HG13	1.82	0.61
1:D:218:THR:HG21	1:D:261:PRO:HB3	1.82	0.61
1:M:271:ILE:HG21	1:N:628:ILE:HG13	1.81	0.61
1:G:218:THR:HG21	1:G:261:PRO:HB3	1.82	0.61
1:K:218:THR:HG21	1:K:261:PRO:HB3	1.82	0.61
1:J:628:ILE:HG13	1:O:271:ILE:HG21	1.81	0.61
1:R:218:THR:HG21	1:R:261:PRO:HB3	1.82	0.61
1:E:218:THR:HG21	1:E:261:PRO:HB3	1.82	0.61
1:H:628:ILE:HG13	1:I:271:ILE:HG21	1.81	0.61
1:H:732:GLU:CG	1:H:786:ALA:O	2.38	0.60
1:K:575:TYR:HB2	1:K:580:GLN:HE21	1.67	0.60
1:R:575:TYR:HB2	1:R:580:GLN:HE21	1.67	0.60
1:O:575:TYR:HB2	1:O:580:GLN:HE21	1.67	0.60
1:M:732:GLU:CG	1:M:786:ALA:O	2.38	0.60
1:B:575:TYR:HB2	1:B:580:GLN:HE21	1.67	0.59
1:I:575:TYR:HB2	1:I:580:GLN:HE21	1.67	0.59
1:G:575:TYR:HB2	1:G:580:GLN:HE21	1.67	0.59
1:N:575:TYR:HB2	1:N:580:GLN:HE21	1.67	0.59
1:D:575:TYR:HB2	1:D:580:GLN:HE21	1.67	0.59
1:F:575:TYR:HB2	1:F:580:GLN:HE21	1.67	0.59
1:H:575:TYR:HB2	1:H:580:GLN:HE21	1.67	0.59
1:C:575:TYR:HB2	1:C:580:GLN:HE21	1.67	0.59
1:A:575:TYR:HB2	1:A:580:GLN:HE21	1.67	0.59
1:P:575:TYR:HB2	1:P:580:GLN:HE21	1.67	0.59
1:E:575:TYR:HB2	1:E:580:GLN:HE21	1.67	0.59
1:M:575:TYR:HB2	1:M:580:GLN:HE21	1.67	0.59
1:G:732:GLU:HG2	1:G:786:ALA:C	2.28	0.59
1:K:732:GLU:HG2	1:K:786:ALA:C	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:575:TYR:HB2	1:J:580:GLN:HE21	1.67	0.58
1:L:575:TYR:HB2	1:L:580:GLN:HE21	1.67	0.58
1:E:732:GLU:HG2	1:E:786:ALA:C	2.28	0.58
1:Q:575:TYR:HB2	1:Q:580:GLN:HE21	1.67	0.58
1:R:732:GLU:HG2	1:R:786:ALA:C	2.28	0.58
1:C:732:GLU:HG2	1:C:786:ALA:C	2.28	0.57
1:F:732:GLU:HG2	1:F:786:ALA:C	2.28	0.57
1:M:234:VAL:HG13	1:M:535:PRO:HG3	1.87	0.57
1:A:234:VAL:HG13	1:A:535:PRO:HG3	1.87	0.57
1:E:234:VAL:HG13	1:E:535:PRO:HG3	1.87	0.57
1:Q:234:VAL:HG13	1:Q:535:PRO:HG3	1.87	0.57
1:B:740:ASP:HA	1:B:779:TYR:HD1	1.70	0.57
1:G:710:ILE:HD12	1:G:783:ALA:HB2	1.87	0.57
1:I:234:VAL:HG13	1:I:535:PRO:HG3	1.87	0.57
1:N:732:GLU:HG2	1:N:786:ALA:C	2.28	0.57
1:A:740:ASP:HA	1:A:779:TYR:HD1	1.70	0.57
1:Q:732:GLU:HG2	1:Q:786:ALA:C	2.28	0.57
1:B:710:ILE:HD12	1:B:783:ALA:HB2	1.87	0.57
1:E:710:ILE:HD12	1:E:783:ALA:HB2	1.87	0.57
1:O:234:VAL:HG13	1:O:535:PRO:HG3	1.87	0.57
1:O:710:ILE:HD12	1:O:783:ALA:HB2	1.87	0.57
1:A:288:SER:HB3	1:A:531:SER:HB2	1.87	0.56
1:H:710:ILE:HD12	1:H:783:ALA:HB2	1.87	0.56
1:I:710:ILE:HD12	1:I:783:ALA:HB2	1.87	0.56
1:L:288:SER:HB3	1:L:531:SER:HB2	1.87	0.56
1:O:732:GLU:HG2	1:O:786:ALA:C	2.28	0.56
1:P:740:ASP:HA	1:P:779:TYR:HD1	1.70	0.56
1:Q:740:ASP:HA	1:Q:779:TYR:HD1	1.70	0.56
1:R:710:ILE:HD12	1:R:783:ALA:HB2	1.87	0.56
1:B:732:GLU:HG2	1:B:786:ALA:C	2.28	0.56
1:F:288:SER:HB3	1:F:531:SER:HB2	1.87	0.56
1:J:710:ILE:HD12	1:J:783:ALA:HB2	1.87	0.56
1:K:234:VAL:HG13	1:K:535:PRO:HG3	1.87	0.56
1:M:288:SER:HB3	1:M:531:SER:HB2	1.87	0.56
1:P:710:ILE:HD12	1:P:783:ALA:HB2	1.87	0.56
1:C:710:ILE:HD12	1:C:783:ALA:HB2	1.87	0.56
1:D:234:VAL:HG13	1:D:535:PRO:HG3	1.87	0.56
1:D:710:ILE:HD12	1:D:783:ALA:HB2	1.87	0.56
1:E:288:SER:HB3	1:E:531:SER:HB2	1.87	0.56
1:L:710:ILE:HD12	1:L:783:ALA:HB2	1.87	0.56
1:L:732:GLU:HG2	1:L:786:ALA:C	2.28	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:710:ILE:HD12	1:M:783:ALA:HB2	1.87	0.56
1:N:710:ILE:HD12	1:N:783:ALA:HB2	1.87	0.56
1:N:740:ASP:HA	1:N:779:TYR:HD1	1.70	0.56
1:P:732:GLU:HG2	1:P:786:ALA:C	2.28	0.56
1:Q:288:SER:HB3	1:Q:531:SER:HB2	1.87	0.56
1:A:732:GLU:HG2	1:A:786:ALA:C	2.28	0.56
1:I:732:GLU:HG2	1:I:786:ALA:C	2.28	0.56
1:J:234:VAL:HG13	1:J:535:PRO:HG3	1.87	0.56
1:K:710:ILE:HD12	1:K:783:ALA:HB2	1.87	0.56
1:P:288:SER:HB3	1:P:531:SER:HB2	1.87	0.56
1:R:234:VAL:HG13	1:R:535:PRO:HG3	1.87	0.56
1:C:740:ASP:HA	1:C:779:TYR:HD1	1.70	0.56
1:F:710:ILE:HD12	1:F:783:ALA:HB2	1.87	0.56
1:K:288:SER:HB3	1:K:531:SER:HB2	1.87	0.56
1:M:740:ASP:HA	1:M:779:TYR:HD1	1.70	0.56
1:Q:710:ILE:HD12	1:Q:783:ALA:HB2	1.87	0.56
1:K:740:ASP:HA	1:K:779:TYR:HD1	1.70	0.56
1:M:732:GLU:HG2	1:M:786:ALA:C	2.28	0.56
1:R:288:SER:HB3	1:R:531:SER:HB2	1.87	0.56
1:A:710:ILE:HD12	1:A:783:ALA:HB2	1.87	0.56
1:B:288:SER:HB3	1:B:531:SER:HB2	1.87	0.56
1:C:234:VAL:HG13	1:C:535:PRO:HG3	1.87	0.56
1:H:234:VAL:HG13	1:H:535:PRO:HG3	1.87	0.56
1:O:740:ASP:HA	1:O:779:TYR:HD1	1.70	0.56
1:F:234:VAL:HG13	1:F:535:PRO:HG3	1.87	0.56
1:H:732:GLU:HG2	1:H:786:ALA:C	2.28	0.56
1:P:234:VAL:HG13	1:P:535:PRO:HG3	1.87	0.56
1:J:732:GLU:HG2	1:J:786:ALA:C	2.28	0.56
1:J:740:ASP:HA	1:J:779:TYR:HD1	1.70	0.56
1:N:234:VAL:HG13	1:N:535:PRO:HG3	1.87	0.56
1:D:307:ALA:C	1:D:309:SER:H	2.14	0.56
1:E:740:ASP:HA	1:E:779:TYR:HD1	1.70	0.55
1:D:732:GLU:HG2	1:D:786:ALA:C	2.28	0.55
1:F:740:ASP:HA	1:F:779:TYR:HD1	1.70	0.55
1:G:234:VAL:HG13	1:G:535:PRO:HG3	1.87	0.55
1:I:288:SER:HB3	1:I:531:SER:HB2	1.87	0.55
1:J:307:ALA:C	1:J:309:SER:H	2.14	0.55
1:D:288:SER:HB3	1:D:531:SER:HB2	1.87	0.55
1:H:288:SER:HB3	1:H:531:SER:HB2	1.87	0.55
1:L:234:VAL:HG13	1:L:535:PRO:HG3	1.87	0.55
1:B:234:VAL:HG13	1:B:535:PRO:HG3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:740:ASP:HA	1:D:779:TYR:HD1	1.70	0.55
1:G:288:SER:HB3	1:G:531:SER:HB2	1.87	0.55
1:N:288:SER:HB3	1:N:531:SER:HB2	1.87	0.55
1:O:307:ALA:C	1:O:309:SER:H	2.14	0.55
1:R:740:ASP:HA	1:R:779:TYR:HD1	1.70	0.55
1:H:740:ASP:HA	1:H:779:TYR:HD1	1.70	0.55
1:J:288:SER:HB3	1:J:531:SER:HB2	1.87	0.55
1:L:740:ASP:HA	1:L:779:TYR:HD1	1.70	0.55
1:N:307:ALA:C	1:N:309:SER:H	2.14	0.55
1:I:307:ALA:C	1:I:309:SER:H	2.14	0.55
1:I:740:ASP:HA	1:I:779:TYR:HD1	1.70	0.55
1:O:288:SER:HB3	1:O:531:SER:HB2	1.87	0.55
1:G:307:ALA:C	1:G:309:SER:H	2.14	0.55
1:C:288:SER:HB3	1:C:531:SER:HB2	1.87	0.55
1:G:740:ASP:HA	1:G:779:TYR:HD1	1.70	0.55
1:Q:307:ALA:C	1:Q:309:SER:H	2.14	0.55
1:C:307:ALA:C	1:C:309:SER:H	2.14	0.54
1:H:307:ALA:C	1:H:309:SER:H	2.14	0.54
1:L:307:ALA:C	1:L:309:SER:H	2.14	0.54
1:A:307:ALA:C	1:A:309:SER:H	2.14	0.54
1:K:307:ALA:C	1:K:309:SER:H	2.14	0.54
1:B:307:ALA:C	1:B:309:SER:H	2.14	0.54
1:R:307:ALA:C	1:R:309:SER:H	2.14	0.54
1:A:178:LYS:N	1:A:546:GLN:OE1	2.41	0.54
1:M:178:LYS:N	1:M:546:GLN:OE1	2.42	0.54
1:M:307:ALA:C	1:M:309:SER:H	2.14	0.54
1:Q:178:LYS:N	1:Q:546:GLN:OE1	2.42	0.54
1:F:307:ALA:C	1:F:309:SER:H	2.14	0.53
1:E:307:ALA:C	1:E:309:SER:H	2.14	0.53
1:B:178:LYS:N	1:B:546:GLN:OE1	2.42	0.53
1:F:178:LYS:N	1:F:546:GLN:OE1	2.42	0.53
1:L:178:LYS:N	1:L:546:GLN:OE1	2.42	0.53
1:R:178:LYS:N	1:R:546:GLN:OE1	2.42	0.53
1:D:178:LYS:N	1:D:546:GLN:OE1	2.42	0.53
1:N:178:LYS:N	1:N:546:GLN:OE1	2.42	0.53
1:I:340:VAL:HA	1:I:502:VAL:O	2.09	0.53
1:P:340:VAL:HA	1:P:502:VAL:O	2.09	0.53
1:A:256:TYR:OH	1:A:280:ASP:OD2	2.26	0.52
1:C:178:LYS:N	1:C:546:GLN:OE1	2.42	0.52
1:E:305:ASP:OD1	1:E:334:SER:HB2	2.10	0.52
1:D:340:VAL:HA	1:D:502:VAL:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:305:ASP:OD1	1:I:334:SER:HB2	2.10	0.52
1:J:178:LYS:N	1:J:546:GLN:OE1	2.41	0.52
1:B:305:ASP:OD1	1:B:334:SER:HB2	2.10	0.52
1:F:305:ASP:OD1	1:F:334:SER:HB2	2.10	0.52
1:H:340:VAL:HA	1:H:502:VAL:O	2.09	0.52
1:K:340:VAL:HA	1:K:502:VAL:O	2.09	0.52
1:O:178:LYS:N	1:O:546:GLN:OE1	2.42	0.52
1:P:307:ALA:C	1:P:309:SER:H	2.14	0.52
1:A:305:ASP:OD1	1:A:334:SER:HB2	2.10	0.52
1:G:305:ASP:OD1	1:G:334:SER:HB2	2.10	0.52
1:M:340:VAL:HA	1:M:502:VAL:O	2.09	0.52
1:N:305:ASP:OD1	1:N:334:SER:HB2	2.10	0.52
1:D:305:ASP:OD1	1:D:334:SER:HB2	2.10	0.52
1:J:305:ASP:OD1	1:J:334:SER:HB2	2.10	0.52
1:O:305:ASP:OD1	1:O:334:SER:HB2	2.10	0.52
1:B:340:VAL:HA	1:B:502:VAL:O	2.09	0.52
1:L:340:VAL:HA	1:L:502:VAL:O	2.09	0.52
1:O:340:VAL:HA	1:O:502:VAL:O	2.10	0.52
1:A:340:VAL:HA	1:A:502:VAL:O	2.09	0.52
1:J:340:VAL:HA	1:J:502:VAL:O	2.09	0.52
1:F:340:VAL:HA	1:F:502:VAL:O	2.10	0.52
1:G:178:LYS:N	1:G:546:GLN:OE1	2.41	0.52
1:C:305:ASP:OD1	1:C:334:SER:HB2	2.10	0.52
1:C:340:VAL:HA	1:C:502:VAL:O	2.09	0.52
1:E:178:LYS:N	1:E:546:GLN:OE1	2.42	0.52
1:H:305:ASP:OD1	1:H:334:SER:HB2	2.10	0.52
1:K:178:LYS:N	1:K:546:GLN:OE1	2.42	0.52
1:R:340:VAL:HA	1:R:502:VAL:O	2.09	0.52
1:E:340:VAL:HA	1:E:502:VAL:O	2.09	0.52
1:G:340:VAL:HA	1:G:502:VAL:O	2.09	0.51
1:K:636:TYR:OH	1:K:648:THR:O	2.28	0.51
1:E:575:TYR:HB2	1:E:580:GLN:NE2	2.26	0.51
1:K:575:TYR:HB2	1:K:580:GLN:NE2	2.26	0.51
1:M:305:ASP:OD1	1:M:334:SER:HB2	2.10	0.51
1:P:305:ASP:OD1	1:P:334:SER:HB2	2.10	0.51
1:R:305:ASP:OD1	1:R:334:SER:HB2	2.10	0.51
1:K:305:ASP:OD1	1:K:334:SER:HB2	2.10	0.51
1:F:168:ASN:O	1:F:172:LYS:HG3	2.11	0.51
1:G:575:TYR:HB2	1:G:580:GLN:NE2	2.26	0.51
1:L:168:ASN:O	1:L:172:LYS:HG3	2.11	0.51
1:L:305:ASP:OD1	1:L:334:SER:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:340:VAL:HA	1:N:502:VAL:O	2.09	0.51
1:R:168:ASN:O	1:R:172:LYS:HG3	2.11	0.51
1:E:168:ASN:O	1:E:172:LYS:HG3	2.11	0.51
1:E:489:ARG:HB3	1:E:578:ASN:O	2.11	0.51
1:M:489:ARG:HB3	1:M:578:ASN:O	2.11	0.51
1:G:168:ASN:O	1:G:172:LYS:HG3	2.11	0.51
1:G:489:ARG:HB3	1:G:578:ASN:O	2.11	0.51
1:I:178:LYS:N	1:I:546:GLN:OE1	2.42	0.51
1:J:489:ARG:HB3	1:J:578:ASN:O	2.11	0.51
1:K:489:ARG:HB3	1:K:578:ASN:O	2.11	0.51
1:P:489:ARG:HB3	1:P:578:ASN:O	2.11	0.51
1:P:575:TYR:HB2	1:P:580:GLN:NE2	2.26	0.51
1:Q:305:ASP:OD1	1:Q:334:SER:HB2	2.10	0.51
1:R:489:ARG:HB3	1:R:578:ASN:O	2.11	0.51
1:B:489:ARG:HB3	1:B:578:ASN:O	2.11	0.51
1:F:575:TYR:HB2	1:F:580:GLN:NE2	2.26	0.51
1:L:575:TYR:HB2	1:L:580:GLN:NE2	2.26	0.51
1:Q:340:VAL:HA	1:Q:502:VAL:O	2.09	0.51
1:B:575:TYR:HB2	1:B:580:GLN:NE2	2.26	0.51
1:C:489:ARG:HB3	1:C:578:ASN:O	2.11	0.51
1:D:575:TYR:HB2	1:D:580:GLN:NE2	2.26	0.51
1:F:489:ARG:HB3	1:F:578:ASN:O	2.11	0.51
1:H:575:TYR:HB2	1:H:580:GLN:NE2	2.26	0.51
1:J:168:ASN:O	1:J:172:LYS:HG3	2.11	0.51
1:R:575:TYR:HB2	1:R:580:GLN:NE2	2.26	0.51
1:A:168:ASN:O	1:A:172:LYS:HG3	2.11	0.51
1:D:168:ASN:O	1:D:172:LYS:HG3	2.11	0.51
1:H:178:LYS:N	1:H:546:GLN:OE1	2.42	0.51
1:L:489:ARG:HB3	1:L:578:ASN:O	2.11	0.51
1:E:175:TYR:HA	1:E:546:GLN:NE2	2.26	0.50
1:O:575:TYR:HB2	1:O:580:GLN:NE2	2.26	0.50
1:Q:489:ARG:HB3	1:Q:578:ASN:O	2.11	0.50
1:C:175:TYR:HA	1:C:546:GLN:NE2	2.27	0.50
1:G:740:ASP:HA	1:G:779:TYR:CD1	2.47	0.50
1:H:168:ASN:O	1:H:172:LYS:HG3	2.11	0.50
1:K:740:ASP:HA	1:K:779:TYR:CD1	2.47	0.50
1:N:489:ARG:HB3	1:N:578:ASN:O	2.11	0.50
1:N:575:TYR:HB2	1:N:580:GLN:NE2	2.26	0.50
1:A:575:TYR:HB2	1:A:580:GLN:NE2	2.26	0.50
1:E:740:ASP:HA	1:E:779:TYR:CD1	2.47	0.50
1:J:575:TYR:HB2	1:J:580:GLN:NE2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:168:ASN:O	1:K:172:LYS:HG3	2.11	0.50
1:O:175:TYR:HA	1:O:546:GLN:NE2	2.27	0.50
1:P:175:TYR:HA	1:P:546:GLN:NE2	2.27	0.50
1:P:178:LYS:N	1:P:546:GLN:OE1	2.41	0.50
1:Q:168:ASN:O	1:Q:172:LYS:HG3	2.11	0.50
1:Q:175:TYR:HA	1:Q:546:GLN:NE2	2.27	0.50
1:Q:575:TYR:HB2	1:Q:580:GLN:NE2	2.26	0.50
1:A:489:ARG:HB3	1:A:578:ASN:O	2.11	0.50
1:D:489:ARG:HB3	1:D:578:ASN:O	2.11	0.50
1:I:575:TYR:HB2	1:I:580:GLN:NE2	2.26	0.50
1:K:175:TYR:HA	1:K:546:GLN:NE2	2.27	0.50
1:M:575:TYR:HB2	1:M:580:GLN:NE2	2.26	0.50
1:O:489:ARG:HB3	1:O:578:ASN:O	2.11	0.50
1:O:628:ILE:HD11	1:P:271:ILE:HG12	1.94	0.50
1:R:175:TYR:HA	1:R:546:GLN:NE2	2.27	0.50
1:A:175:TYR:HA	1:A:546:GLN:NE2	2.27	0.50
1:C:168:ASN:O	1:C:172:LYS:HG3	2.11	0.50
1:I:489:ARG:HB3	1:I:578:ASN:O	2.11	0.50
1:Q:740:ASP:HA	1:Q:779:TYR:CD1	2.47	0.50
1:B:175:TYR:HA	1:B:546:GLN:NE2	2.27	0.50
1:B:756:ASP:OD1	1:C:684:ARG:NH2	2.45	0.50
1:C:740:ASP:HA	1:C:779:TYR:CD1	2.47	0.50
1:P:168:ASN:O	1:P:172:LYS:HG3	2.11	0.50
1:F:628:ILE:HD11	1:G:271:ILE:HG12	1.94	0.50
1:G:175:TYR:HA	1:G:546:GLN:NE2	2.27	0.50
1:J:256:TYR:OH	1:J:280:ASP:OD2	2.26	0.50
1:A:739:TYR:OH	1:P:202:GLN:O	2.20	0.50
1:G:158:MET:HE3	1:G:158:MET:HA	1.94	0.50
1:J:740:ASP:HA	1:J:779:TYR:CD1	2.47	0.50
1:M:168:ASN:O	1:M:172:LYS:HG3	2.11	0.50
1:O:330:SER:O	1:O:333:THR:OG1	2.30	0.50
1:B:168:ASN:O	1:B:172:LYS:HG3	2.11	0.50
1:F:330:SER:O	1:F:333:THR:OG1	2.30	0.50
1:H:175:TYR:HA	1:H:546:GLN:NE2	2.27	0.50
1:I:175:TYR:HA	1:I:546:GLN:NE2	2.27	0.50
1:N:330:SER:O	1:N:333:THR:OG1	2.30	0.50
1:R:330:SER:O	1:R:333:THR:OG1	2.30	0.50
1:C:575:TYR:HB2	1:C:580:GLN:NE2	2.26	0.49
1:D:175:TYR:HA	1:D:546:GLN:NE2	2.27	0.49
1:D:740:ASP:HA	1:D:779:TYR:CD1	2.47	0.49
1:E:330:SER:O	1:E:333:THR:OG1	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:175:TYR:HA	1:J:546:GLN:NE2	2.27	0.49
1:K:330:SER:O	1:K:333:THR:OG1	2.30	0.49
1:L:740:ASP:HA	1:L:779:TYR:CD1	2.47	0.49
1:N:158:MET:HA	1:N:158:MET:HE3	1.94	0.49
1:N:175:TYR:HA	1:N:546:GLN:NE2	2.26	0.49
1:Q:330:SER:O	1:Q:333:THR:OG1	2.30	0.49
1:B:740:ASP:HA	1:B:779:TYR:CD1	2.47	0.49
1:I:330:SER:O	1:I:333:THR:OG1	2.30	0.49
1:K:158:MET:HE3	1:K:158:MET:HA	1.94	0.49
1:L:330:SER:O	1:L:333:THR:OG1	2.30	0.49
1:M:330:SER:O	1:M:333:THR:OG1	2.30	0.49
1:N:168:ASN:O	1:N:172:LYS:HG3	2.11	0.49
1:P:256:TYR:OH	1:P:280:ASP:OD2	2.26	0.49
1:P:330:SER:O	1:P:333:THR:OG1	2.30	0.49
1:P:636:TYR:OH	1:P:648:THR:O	2.28	0.49
1:P:740:ASP:HA	1:P:779:TYR:CD1	2.47	0.49
1:Q:256:TYR:OH	1:Q:280:ASP:OD2	2.26	0.49
1:B:330:SER:O	1:B:333:THR:OG1	2.30	0.49
1:C:158:MET:HE3	1:C:158:MET:HA	1.94	0.49
1:C:330:SER:O	1:C:333:THR:OG1	2.30	0.49
1:F:175:TYR:HA	1:F:546:GLN:NE2	2.27	0.49
1:H:489:ARG:HB3	1:H:578:ASN:O	2.11	0.49
1:I:168:ASN:O	1:I:172:LYS:HG3	2.11	0.49
1:O:158:MET:HE3	1:O:158:MET:HA	1.94	0.49
1:D:256:TYR:OH	1:D:280:ASP:OD2	2.26	0.49
1:D:330:SER:O	1:D:333:THR:OG1	2.30	0.49
1:F:740:ASP:HA	1:F:779:TYR:CD1	2.47	0.49
1:I:636:TYR:OH	1:I:648:THR:O	2.28	0.49
1:K:756:ASP:OD1	1:L:684:ARG:NH2	2.45	0.49
1:O:740:ASP:HA	1:O:779:TYR:CD1	2.47	0.49
1:E:158:MET:HE3	1:E:158:MET:HA	1.94	0.49
1:G:330:SER:O	1:G:333:THR:OG1	2.30	0.49
1:I:158:MET:HE3	1:I:158:MET:HA	1.94	0.49
1:I:515:THR:OG1	1:I:520:ASP:O	2.31	0.49
1:L:515:THR:OG1	1:L:520:ASP:O	2.31	0.49
1:M:175:TYR:HA	1:M:546:GLN:NE2	2.27	0.49
1:A:636:TYR:OH	1:A:648:THR:O	2.28	0.49
1:B:158:MET:HA	1:B:158:MET:HE3	1.94	0.49
1:D:158:MET:HE3	1:D:158:MET:HA	1.94	0.49
1:J:330:SER:O	1:J:333:THR:OG1	2.30	0.49
1:L:175:TYR:HA	1:L:546:GLN:NE2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:636:TYR:OH	1:R:648:THR:O	2.28	0.49
1:R:740:ASP:HA	1:R:779:TYR:CD1	2.47	0.49
1:H:330:SER:O	1:H:333:THR:OG1	2.30	0.49
1:J:636:TYR:OH	1:J:648:THR:O	2.28	0.49
1:K:515:THR:OG1	1:K:520:ASP:O	2.31	0.49
1:O:168:ASN:O	1:O:172:LYS:HG3	2.11	0.49
1:J:158:MET:HE3	1:J:158:MET:HA	1.94	0.49
1:N:636:TYR:OH	1:N:648:THR:O	2.28	0.49
1:O:609:LYS:O	1:O:700:LYS:NZ	2.46	0.49
1:P:158:MET:HE3	1:P:158:MET:HA	1.94	0.49
1:R:158:MET:HE3	1:R:158:MET:HA	1.94	0.49
1:D:667:VAL:HG13	1:D:672:VAL:HG21	1.95	0.48
1:H:667:VAL:HG13	1:H:672:VAL:HG21	1.95	0.48
1:I:205:GLY:HA3	1:I:255:ALA:O	2.13	0.48
1:B:205:GLY:HA3	1:B:255:ALA:O	2.13	0.48
1:C:636:TYR:OH	1:C:648:THR:O	2.28	0.48
1:E:205:GLY:HA3	1:E:255:ALA:O	2.13	0.48
1:E:636:TYR:OH	1:E:648:THR:O	2.28	0.48
1:F:205:GLY:HA3	1:F:255:ALA:O	2.13	0.48
1:L:636:TYR:OH	1:L:648:THR:O	2.28	0.48
1:P:205:GLY:HA3	1:P:255:ALA:O	2.13	0.48
1:R:602:TYR:O	1:R:695:THR:HA	2.14	0.48
1:H:158:MET:HE3	1:H:158:MET:HA	1.94	0.48
1:I:602:TYR:O	1:I:695:THR:HA	2.14	0.48
1:I:740:ASP:HA	1:I:779:TYR:CD1	2.47	0.48
1:K:602:TYR:O	1:K:695:THR:HA	2.14	0.48
1:O:515:THR:OG1	1:O:520:ASP:O	2.31	0.48
1:F:158:MET:HE3	1:F:158:MET:HA	1.94	0.48
1:G:609:LYS:O	1:G:700:LYS:NZ	2.46	0.48
1:M:205:GLY:HA3	1:M:255:ALA:O	2.14	0.48
1:N:740:ASP:HA	1:N:779:TYR:CD1	2.47	0.48
1:C:756:ASP:OD1	1:D:684:ARG:NH2	2.46	0.48
1:D:602:TYR:O	1:D:695:THR:HA	2.14	0.48
1:A:205:GLY:HA3	1:A:255:ALA:O	2.13	0.48
1:F:577:HIS:H	1:F:678:GLU:CD	2.22	0.48
1:O:205:GLY:HA3	1:O:255:ALA:O	2.13	0.48
1:P:602:TYR:O	1:P:695:THR:HA	2.14	0.48
1:Q:602:TYR:O	1:Q:695:THR:HA	2.14	0.48
1:D:205:GLY:HA3	1:D:255:ALA:O	2.14	0.48
1:H:602:TYR:O	1:H:695:THR:HA	2.14	0.48
1:H:740:ASP:HA	1:H:779:TYR:CD1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:609:LYS:O	1:I:700:LYS:NZ	2.46	0.48
1:M:740:ASP:HA	1:M:779:TYR:CD1	2.47	0.48
1:A:602:TYR:O	1:A:695:THR:HA	2.14	0.48
1:A:667:VAL:HG13	1:A:672:VAL:HG21	1.95	0.48
1:C:577:HIS:H	1:C:678:GLU:CD	2.22	0.48
1:G:205:GLY:HA3	1:G:255:ALA:O	2.13	0.48
1:G:602:TYR:O	1:G:695:THR:HA	2.14	0.48
1:J:577:HIS:H	1:J:678:GLU:CD	2.22	0.48
1:K:205:GLY:HA3	1:K:255:ALA:O	2.13	0.48
1:N:609:LYS:O	1:N:700:LYS:NZ	2.46	0.48
1:O:602:TYR:O	1:O:695:THR:HA	2.14	0.48
1:R:205:GLY:HA3	1:R:255:ALA:O	2.13	0.48
1:A:158:MET:HE3	1:A:158:MET:HA	1.94	0.48
1:D:606:THR:HG22	1:D:698:ILE:HB	1.96	0.48
1:F:602:TYR:O	1:F:695:THR:HA	2.14	0.48
1:G:667:VAL:HG13	1:G:672:VAL:HG21	1.95	0.48
1:L:158:MET:HE3	1:L:158:MET:HA	1.94	0.48
1:L:602:TYR:O	1:L:695:THR:HA	2.14	0.48
1:N:256:TYR:OH	1:N:280:ASP:OD2	2.26	0.48
1:O:577:HIS:H	1:O:678:GLU:CD	2.22	0.48
1:Q:667:VAL:HG13	1:Q:672:VAL:HG21	1.95	0.48
1:G:606:THR:HG22	1:G:698:ILE:HB	1.96	0.48
1:I:307:ALA:O	1:I:308:MET:HB2	2.14	0.48
1:L:606:THR:HG22	1:L:698:ILE:HB	1.96	0.48
1:O:667:VAL:HG13	1:O:672:VAL:HG21	1.95	0.48
1:Q:577:HIS:H	1:Q:678:GLU:CD	2.22	0.48
1:Q:606:THR:HG22	1:Q:698:ILE:HB	1.96	0.48
1:R:667:VAL:HG13	1:R:672:VAL:HG21	1.95	0.48
1:A:577:HIS:H	1:A:678:GLU:CD	2.22	0.47
1:D:577:HIS:H	1:D:678:GLU:CD	2.22	0.47
1:E:602:TYR:O	1:E:695:THR:HA	2.14	0.47
1:G:577:HIS:H	1:G:678:GLU:CD	2.22	0.47
1:J:205:GLY:HA3	1:J:255:ALA:O	2.14	0.47
1:L:205:GLY:HA3	1:L:255:ALA:O	2.13	0.47
1:M:158:MET:HE3	1:M:158:MET:HA	1.94	0.47
1:M:609:LYS:O	1:M:700:LYS:NZ	2.46	0.47
1:B:577:HIS:H	1:B:678:GLU:CD	2.22	0.47
1:B:602:TYR:O	1:B:695:THR:HA	2.14	0.47
1:C:205:GLY:HA3	1:C:255:ALA:O	2.13	0.47
1:H:205:GLY:HA3	1:H:255:ALA:O	2.13	0.47
1:K:256:TYR:OH	1:K:280:ASP:OD2	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:577:HIS:H	1:K:678:GLU:CD	2.22	0.47
1:N:667:VAL:HG13	1:N:672:VAL:HG21	1.95	0.47
1:P:307:ALA:O	1:P:308:MET:HB2	2.14	0.47
1:Q:158:MET:HE3	1:Q:158:MET:HA	1.94	0.47
1:R:577:HIS:H	1:R:678:GLU:CD	2.22	0.47
1:R:606:THR:HG22	1:R:698:ILE:HB	1.96	0.47
1:H:606:THR:HG22	1:H:698:ILE:HB	1.96	0.47
1:K:606:THR:HG22	1:K:698:ILE:HB	1.96	0.47
1:L:756:ASP:OD1	1:M:684:ARG:NH2	2.46	0.47
1:M:667:VAL:HG13	1:M:672:VAL:HG21	1.95	0.47
1:P:667:VAL:HG13	1:P:672:VAL:HG21	1.95	0.47
1:A:330:SER:O	1:A:333:THR:OG1	2.30	0.47
1:D:515:THR:OG1	1:D:520:ASP:O	2.31	0.47
1:E:667:VAL:HG13	1:E:672:VAL:HG21	1.95	0.47
1:K:667:VAL:HG13	1:K:672:VAL:HG21	1.95	0.47
1:M:577:HIS:H	1:M:678:GLU:CD	2.22	0.47
1:P:577:HIS:H	1:P:678:GLU:CD	2.22	0.47
1:R:609:LYS:O	1:R:700:LYS:NZ	2.46	0.47
1:A:307:ALA:O	1:A:308:MET:HB2	2.14	0.47
1:B:307:ALA:O	1:B:308:MET:HB2	2.14	0.47
1:C:602:TYR:O	1:C:695:THR:HA	2.14	0.47
1:H:307:ALA:O	1:H:308:MET:HB2	2.14	0.47
1:L:768:VAL:O	1:L:772:THR:HB	2.15	0.47
1:M:602:TYR:O	1:M:695:THR:HA	2.14	0.47
1:O:307:ALA:O	1:O:308:MET:HB2	2.14	0.47
1:B:609:LYS:O	1:B:700:LYS:NZ	2.46	0.47
1:B:667:VAL:HG13	1:B:672:VAL:HG21	1.95	0.47
1:C:606:THR:HG22	1:C:698:ILE:HB	1.96	0.47
1:E:609:LYS:O	1:E:700:LYS:NZ	2.46	0.47
1:F:636:TYR:OH	1:F:648:THR:O	2.28	0.47
1:M:307:ALA:O	1:M:308:MET:HB2	2.14	0.47
1:N:205:GLY:HA3	1:N:255:ALA:O	2.13	0.47
1:N:602:TYR:O	1:N:695:THR:HA	2.14	0.47
1:A:740:ASP:HA	1:A:779:TYR:CD1	2.47	0.47
1:C:667:VAL:HG13	1:C:672:VAL:HG21	1.95	0.47
1:E:577:HIS:H	1:E:678:GLU:CD	2.22	0.47
1:F:667:VAL:HG13	1:F:672:VAL:HG21	1.95	0.47
1:F:768:VAL:O	1:F:772:THR:HB	2.15	0.47
1:J:602:TYR:O	1:J:695:THR:HA	2.14	0.47
1:J:667:VAL:HG13	1:J:672:VAL:HG21	1.95	0.47
1:L:667:VAL:HG13	1:L:672:VAL:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:577:HIS:H	1:N:678:GLU:CD	2.22	0.47
1:Q:205:GLY:HA3	1:Q:255:ALA:O	2.13	0.47
1:C:768:VAL:O	1:C:772:THR:HB	2.15	0.47
1:D:307:ALA:O	1:D:308:MET:HB2	2.14	0.47
1:C:609:LYS:O	1:C:700:LYS:NZ	2.46	0.47
1:E:606:THR:HG22	1:E:698:ILE:HB	1.96	0.47
1:I:667:VAL:HG13	1:I:672:VAL:HG21	1.95	0.47
1:J:606:THR:HG22	1:J:698:ILE:HB	1.96	0.47
1:L:577:HIS:H	1:L:678:GLU:CD	2.22	0.47
1:O:606:THR:HG22	1:O:698:ILE:HB	1.96	0.47
1:Q:636:TYR:OH	1:Q:648:THR:O	2.28	0.47
1:R:256:TYR:OH	1:R:280:ASP:OD2	2.26	0.47
1:D:609:LYS:O	1:D:700:LYS:NZ	2.46	0.47
1:F:606:THR:HG22	1:F:698:ILE:HB	1.96	0.47
1:H:577:HIS:H	1:H:678:GLU:CD	2.22	0.47
1:J:768:VAL:O	1:J:772:THR:HB	2.15	0.47
1:L:609:LYS:O	1:L:700:LYS:NZ	2.46	0.47
1:M:606:THR:HG22	1:M:698:ILE:HB	1.96	0.47
1:P:606:THR:HG22	1:P:698:ILE:HB	1.96	0.47
1:Q:768:VAL:O	1:Q:772:THR:HB	2.15	0.47
1:R:768:VAL:O	1:R:772:THR:HB	2.15	0.47
1:B:256:TYR:OH	1:B:280:ASP:OD2	2.26	0.46
1:D:782:LEU:HD11	1:D:793:GLN:HB2	1.97	0.46
1:F:609:LYS:O	1:F:700:LYS:NZ	2.46	0.46
1:P:768:VAL:O	1:P:772:THR:HB	2.15	0.46
1:R:307:ALA:O	1:R:308:MET:HB2	2.14	0.46
1:A:565:GLU:HG3	1:A:586:ARG:NE	2.31	0.46
1:A:606:THR:HG22	1:A:698:ILE:HB	1.96	0.46
1:I:565:GLU:HG3	1:I:586:ARG:NE	2.31	0.46
1:I:577:HIS:H	1:I:678:GLU:CD	2.22	0.46
1:L:565:GLU:HG3	1:L:586:ARG:NE	2.31	0.46
1:M:256:TYR:OH	1:M:280:ASP:OD2	2.26	0.46
1:N:307:ALA:O	1:N:308:MET:HB2	2.14	0.46
1:P:565:GLU:HG3	1:P:586:ARG:NE	2.31	0.46
1:Q:565:GLU:HG3	1:Q:586:ARG:NE	2.31	0.46
1:C:782:LEU:HD11	1:C:793:GLN:HB2	1.98	0.46
1:J:782:LEU:HD11	1:J:793:GLN:HB2	1.97	0.46
1:N:606:THR:HG22	1:N:698:ILE:HB	1.96	0.46
1:N:768:VAL:O	1:N:772:THR:HB	2.15	0.46
1:B:565:GLU:HG3	1:B:586:ARG:NE	2.31	0.46
1:B:606:THR:HG22	1:B:698:ILE:HB	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:768:VAL:O	1:B:772:THR:HB	2.15	0.46
1:C:307:ALA:O	1:C:308:MET:HB2	2.14	0.46
1:E:565:GLU:HG3	1:E:586:ARG:NE	2.31	0.46
1:F:565:GLU:HG3	1:F:586:ARG:NE	2.31	0.46
1:K:307:ALA:O	1:K:308:MET:HB2	2.14	0.46
1:L:649:ASP:OD2	1:L:649:ASP:N	2.49	0.46
1:M:565:GLU:HG3	1:M:586:ARG:NE	2.31	0.46
1:M:768:VAL:O	1:M:772:THR:HB	2.15	0.46
1:O:565:GLU:HG3	1:O:586:ARG:NE	2.31	0.46
1:F:307:ALA:O	1:F:308:MET:HB2	2.14	0.46
1:H:782:LEU:HD11	1:H:793:GLN:HB2	1.98	0.46
1:I:606:THR:HG22	1:I:698:ILE:HB	1.96	0.46
1:I:768:VAL:O	1:I:772:THR:HB	2.15	0.46
1:K:649:ASP:OD2	1:K:649:ASP:N	2.49	0.46
1:L:307:ALA:O	1:L:308:MET:HB2	2.14	0.46
1:M:649:ASP:OD2	1:M:649:ASP:N	2.49	0.46
1:N:782:LEU:HD11	1:N:793:GLN:HB2	1.98	0.46
1:R:515:THR:OG1	1:R:520:ASP:O	2.31	0.46
1:E:307:ALA:O	1:E:308:MET:HB2	2.14	0.46
1:E:515:THR:OG1	1:E:520:ASP:O	2.31	0.46
1:E:768:VAL:O	1:E:772:THR:HB	2.15	0.46
1:F:515:THR:OG1	1:F:520:ASP:O	2.31	0.46
1:G:307:ALA:O	1:G:308:MET:HB2	2.14	0.46
1:G:782:LEU:HD11	1:G:793:GLN:HB2	1.97	0.46
1:A:768:VAL:O	1:A:772:THR:HB	2.15	0.46
1:D:565:GLU:HG3	1:D:586:ARG:NE	2.31	0.46
1:G:202:GLN:O	1:J:739:TYR:OH	2.20	0.46
1:H:565:GLU:HG3	1:H:586:ARG:NE	2.31	0.46
1:J:307:ALA:O	1:J:308:MET:HB2	2.14	0.46
1:K:782:LEU:HD11	1:K:793:GLN:HB2	1.97	0.46
1:N:565:GLU:HG3	1:N:586:ARG:NE	2.31	0.46
1:O:782:LEU:HD11	1:O:793:GLN:HB2	1.98	0.46
1:P:684:ARG:HH21	1:Q:756:ASP:CG	2.24	0.46
1:Q:307:ALA:O	1:Q:308:MET:HB2	2.14	0.46
1:A:202:GLN:O	1:L:739:TYR:OH	2.23	0.46
1:I:649:ASP:OD2	1:I:649:ASP:N	2.49	0.46
1:R:782:LEU:HD11	1:R:793:GLN:HB2	1.97	0.46
1:B:782:LEU:HD11	1:B:793:GLN:HB2	1.97	0.46
1:C:567:LEU:H	1:C:580:GLN:NE2	2.14	0.46
1:D:768:VAL:O	1:D:772:THR:HB	2.15	0.46
1:G:768:VAL:O	1:G:772:THR:HB	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:565:GLU:HG3	1:K:586:ARG:NE	2.31	0.46
1:K:768:VAL:O	1:K:772:THR:HB	2.15	0.46
1:E:782:LEU:HD11	1:E:793:GLN:HB2	1.98	0.46
1:I:782:LEU:HD11	1:I:793:GLN:HB2	1.97	0.46
1:N:567:LEU:H	1:N:580:GLN:NE2	2.14	0.46
1:N:649:ASP:OD2	1:N:649:ASP:N	2.49	0.46
1:O:567:LEU:H	1:O:580:GLN:NE2	2.14	0.46
1:B:567:LEU:H	1:B:580:GLN:NE2	2.14	0.45
1:C:565:GLU:HG3	1:C:586:ARG:NE	2.31	0.45
1:F:256:TYR:OH	1:F:280:ASP:OD2	2.26	0.45
1:G:515:THR:OG1	1:G:520:ASP:O	2.31	0.45
1:J:649:ASP:OD2	1:J:649:ASP:N	2.49	0.45
1:J:756:ASP:OD1	1:K:684:ARG:NH2	2.49	0.45
1:O:768:VAL:O	1:O:772:THR:HB	2.15	0.45
1:P:567:LEU:H	1:P:580:GLN:NE2	2.14	0.45
1:A:756:ASP:OD1	1:B:684:ARG:NH2	2.49	0.45
1:H:567:LEU:H	1:H:580:GLN:NE2	2.14	0.45
1:H:684:ARG:NH2	1:I:756:ASP:OD1	2.50	0.45
1:Q:483:MET:HB3	1:Q:483:MET:HE3	1.64	0.45
1:R:236:GLY:HA2	1:R:240:ALA:HB2	1.99	0.45
1:R:565:GLU:HG3	1:R:586:ARG:NE	2.31	0.45
1:A:609:LYS:O	1:A:700:LYS:NZ	2.46	0.45
1:G:497:MET:HE3	1:G:497:MET:HB2	1.84	0.45
1:G:684:ARG:HH21	1:H:756:ASP:CG	2.24	0.45
1:H:768:VAL:O	1:H:772:THR:HB	2.15	0.45
1:I:567:LEU:H	1:I:580:GLN:NE2	2.14	0.45
1:J:684:ARG:NH2	1:O:756:ASP:OD1	2.50	0.45
1:K:236:GLY:HA2	1:K:240:ALA:HB2	1.99	0.45
1:L:256:TYR:OH	1:L:280:ASP:OD2	2.26	0.45
1:E:332:GLY:O	1:E:499:LYS:HD2	2.17	0.45
1:E:483:MET:HE3	1:E:483:MET:HB3	1.64	0.45
1:F:332:GLY:O	1:F:499:LYS:HD2	2.17	0.45
1:G:236:GLY:HA2	1:G:240:ALA:HB2	1.99	0.45
1:H:649:ASP:OD2	1:H:649:ASP:N	2.49	0.45
1:L:233:HIS:CD2	1:L:527:LYS:HG3	2.52	0.45
1:M:332:GLY:O	1:M:499:LYS:HD2	2.17	0.45
1:O:233:HIS:CD2	1:O:527:LYS:HG3	2.52	0.45
1:O:649:ASP:OD2	1:O:649:ASP:N	2.49	0.45
1:Q:236:GLY:HA2	1:Q:240:ALA:HB2	1.99	0.45
1:B:497:MET:HB2	1:B:497:MET:HE3	1.84	0.45
1:C:304:LEU:HD12	1:C:304:LEU:HA	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:236:GLY:HA2	1:F:240:ALA:HB2	1.99	0.45
1:H:332:GLY:O	1:H:499:LYS:HD2	2.17	0.45
1:K:233:HIS:CD2	1:K:527:LYS:HG3	2.52	0.45
1:M:567:LEU:H	1:M:580:GLN:NE2	2.14	0.45
1:P:332:GLY:O	1:P:499:LYS:HD2	2.17	0.45
1:Q:233:HIS:CD2	1:Q:527:LYS:HG3	2.52	0.45
1:C:233:HIS:CD2	1:C:527:LYS:HG3	2.52	0.45
1:D:756:ASP:OD1	1:E:684:ARG:NH2	2.50	0.45
1:F:782:LEU:HD11	1:F:793:GLN:HB2	1.98	0.45
1:J:236:GLY:HA2	1:J:240:ALA:HB2	1.99	0.45
1:L:236:GLY:HA2	1:L:240:ALA:HB2	1.99	0.45
1:L:271:ILE:HG21	1:M:628:ILE:HG13	1.99	0.45
1:M:782:LEU:HD11	1:M:793:GLN:HB2	1.97	0.45
1:N:532:MET:HB3	1:N:532:MET:HE3	1.45	0.45
1:P:782:LEU:HD11	1:P:793:GLN:HB2	1.97	0.45
1:R:233:HIS:CD2	1:R:527:LYS:HG3	2.52	0.45
1:R:567:LEU:H	1:R:580:GLN:NE2	2.14	0.45
1:D:236:GLY:HA2	1:D:240:ALA:HB2	1.99	0.45
1:D:636:TYR:OH	1:D:648:THR:O	2.28	0.45
1:E:236:GLY:HA2	1:E:240:ALA:HB2	1.99	0.45
1:E:567:LEU:H	1:E:580:GLN:NE2	2.14	0.45
1:I:233:HIS:CD2	1:I:527:LYS:HG3	2.52	0.45
1:J:332:GLY:O	1:J:499:LYS:HD2	2.17	0.45
1:M:233:HIS:CD2	1:M:527:LYS:HG3	2.52	0.45
1:Q:332:GLY:O	1:Q:499:LYS:HD2	2.17	0.45
1:D:332:GLY:O	1:D:499:LYS:HD2	2.17	0.45
1:F:532:MET:HE3	1:F:532:MET:HB3	1.45	0.45
1:G:332:GLY:O	1:G:499:LYS:HD2	2.17	0.45
1:H:236:GLY:HA2	1:H:240:ALA:HB2	1.99	0.45
1:J:565:GLU:HG3	1:J:586:ARG:NE	2.31	0.45
1:J:567:LEU:H	1:J:580:GLN:NE2	2.14	0.45
1:L:332:GLY:O	1:L:499:LYS:HD2	2.17	0.45
1:L:782:LEU:HD11	1:L:793:GLN:HB2	1.98	0.45
1:O:332:GLY:O	1:O:499:LYS:HD2	2.17	0.45
1:P:233:HIS:CD2	1:P:527:LYS:HG3	2.52	0.45
1:A:236:GLY:HA2	1:A:240:ALA:HB2	1.99	0.45
1:B:332:GLY:O	1:B:499:LYS:HD2	2.17	0.45
1:C:271:ILE:HG21	1:D:628:ILE:HG13	1.99	0.45
1:C:332:GLY:O	1:C:499:LYS:HD2	2.17	0.45
1:D:193:HIS:CD2	1:D:522:TYR:HB3	2.52	0.45
1:G:233:HIS:CD2	1:G:527:LYS:HG3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:756:ASP:OD1	1:N:684:ARG:NH2	2.50	0.45
1:O:256:TYR:OH	1:O:280:ASP:OD2	2.26	0.45
1:P:328:VAL:HA	1:P:488:SER:HB3	1.99	0.45
1:F:699:VAL:HG12	1:F:700:LYS:HG2	2.00	0.45
1:G:565:GLU:HG3	1:G:586:ARG:NE	2.31	0.45
1:G:567:LEU:H	1:G:580:GLN:NE2	2.14	0.45
1:H:233:HIS:CD2	1:H:527:LYS:HG3	2.52	0.45
1:I:332:GLY:O	1:I:499:LYS:HD2	2.17	0.45
1:J:193:HIS:CD2	1:J:522:TYR:HB3	2.52	0.45
1:J:233:HIS:CD2	1:J:527:LYS:HG3	2.52	0.45
1:M:328:VAL:HA	1:M:488:SER:HB3	1.99	0.45
1:M:515:THR:OG1	1:M:520:ASP:O	2.31	0.45
1:Q:328:VAL:HA	1:Q:488:SER:HB3	1.99	0.45
1:A:782:LEU:HD11	1:A:793:GLN:HB2	1.97	0.44
1:D:233:HIS:CD2	1:D:527:LYS:HG3	2.52	0.44
1:F:233:HIS:CD2	1:F:527:LYS:HG3	2.52	0.44
1:H:193:HIS:CD2	1:H:522:TYR:HB3	2.52	0.44
1:H:532:MET:HE3	1:H:532:MET:HB3	1.45	0.44
1:I:501:ASP:OD2	1:I:557:LYS:NZ	2.51	0.44
1:J:609:LYS:O	1:J:700:LYS:NZ	2.46	0.44
1:K:483:MET:HE3	1:K:483:MET:HB3	1.64	0.44
1:K:699:VAL:HG12	1:K:700:LYS:HG2	1.99	0.44
1:L:328:VAL:HA	1:L:488:SER:HB3	2.00	0.44
1:O:328:VAL:HA	1:O:488:SER:HB3	1.99	0.44
1:Q:699:VAL:HG12	1:Q:700:LYS:HG2	2.00	0.44
1:E:233:HIS:CD2	1:E:527:LYS:HG3	2.52	0.44
1:F:567:LEU:H	1:F:580:GLN:NE2	2.14	0.44
1:F:567:LEU:O	1:F:580:GLN:NE2	2.51	0.44
1:G:699:VAL:HG12	1:G:700:LYS:HG2	2.00	0.44
1:J:567:LEU:O	1:J:580:GLN:NE2	2.51	0.44
1:K:332:GLY:O	1:K:499:LYS:HD2	2.17	0.44
1:L:699:VAL:HG12	1:L:700:LYS:HG2	2.00	0.44
1:N:328:VAL:HA	1:N:488:SER:HB3	2.00	0.44
1:N:332:GLY:O	1:N:499:LYS:HD2	2.17	0.44
1:N:567:LEU:O	1:N:580:GLN:NE2	2.51	0.44
1:Q:567:LEU:O	1:Q:580:GLN:NE2	2.51	0.44
1:Q:782:LEU:HD11	1:Q:793:GLN:HB2	1.98	0.44
1:R:699:VAL:HG12	1:R:700:LYS:HG2	2.00	0.44
1:A:567:LEU:H	1:A:580:GLN:NE2	2.14	0.44
1:A:699:VAL:HG12	1:A:700:LYS:HG2	1.99	0.44
1:B:561:MET:HE2	1:B:561:MET:HB3	1.87	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:GLY:HA2	1:C:240:ALA:HB2	1.99	0.44
1:C:567:LEU:O	1:C:580:GLN:NE2	2.51	0.44
1:E:567:LEU:O	1:E:580:GLN:NE2	2.51	0.44
1:H:673:LYS:O	1:H:677:TYR:OH	2.26	0.44
1:K:501:ASP:OD2	1:K:557:LYS:NZ	2.51	0.44
1:K:567:LEU:O	1:K:580:GLN:NE2	2.51	0.44
1:L:497:MET:HE3	1:L:497:MET:HB2	1.84	0.44
1:L:501:ASP:OD2	1:L:557:LYS:NZ	2.51	0.44
1:N:233:HIS:CD2	1:N:527:LYS:HG3	2.52	0.44
1:O:501:ASP:OD2	1:O:557:LYS:NZ	2.51	0.44
1:P:236:GLY:HA2	1:P:240:ALA:HB2	1.99	0.44
1:A:684:ARG:NH2	1:F:756:ASP:OD1	2.50	0.44
1:D:567:LEU:H	1:D:580:GLN:NE2	2.14	0.44
1:D:699:VAL:HG12	1:D:700:LYS:HG2	2.00	0.44
1:E:699:VAL:HG12	1:E:700:LYS:HG2	1.99	0.44
1:I:497:MET:HE3	1:I:497:MET:HB2	1.84	0.44
1:M:193:HIS:CD2	1:M:522:TYR:HB3	2.52	0.44
1:M:236:GLY:HA2	1:M:240:ALA:HB2	1.99	0.44
1:O:532:MET:HB3	1:O:532:MET:HE3	1.45	0.44
1:R:332:GLY:O	1:R:499:LYS:HD2	2.17	0.44
1:A:233:HIS:CD2	1:A:527:LYS:HG3	2.52	0.44
1:B:233:HIS:CD2	1:B:527:LYS:HG3	2.52	0.44
1:C:193:HIS:CD2	1:C:522:TYR:HB3	2.52	0.44
1:G:193:HIS:CD2	1:G:522:TYR:HB3	2.52	0.44
1:H:567:LEU:O	1:H:580:GLN:NE2	2.51	0.44
1:I:236:GLY:HA2	1:I:240:ALA:HB2	1.99	0.44
1:J:699:VAL:HG12	1:J:700:LYS:HG2	1.99	0.44
1:K:532:MET:HB3	1:K:532:MET:HE3	1.45	0.44
1:K:567:LEU:H	1:K:580:GLN:NE2	2.14	0.44
1:N:515:THR:OG1	1:N:520:ASP:O	2.31	0.44
1:O:236:GLY:HA2	1:O:240:ALA:HB2	1.99	0.44
1:P:483:MET:HB3	1:P:483:MET:HE3	1.65	0.44
1:P:501:ASP:OD2	1:P:557:LYS:NZ	2.51	0.44
1:Q:567:LEU:H	1:Q:580:GLN:NE2	2.14	0.44
1:A:193:HIS:CD2	1:A:522:TYR:HB3	2.52	0.44
1:A:332:GLY:O	1:A:499:LYS:HD2	2.17	0.44
1:B:236:GLY:HA2	1:B:240:ALA:HB2	1.99	0.44
1:B:477:LYS:HD2	1:B:477:LYS:HA	1.85	0.44
1:B:636:TYR:OH	1:B:648:THR:O	2.28	0.44
1:H:515:THR:OG1	1:H:520:ASP:O	2.31	0.44
1:R:567:LEU:O	1:R:580:GLN:NE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:HIS:CD2	1:B:522:TYR:HB3	2.52	0.44
1:E:304:LEU:HD12	1:E:304:LEU:HA	1.80	0.44
1:F:304:LEU:HD12	1:F:304:LEU:HA	1.80	0.44
1:J:501:ASP:OD2	1:J:557:LYS:NZ	2.51	0.44
1:L:193:HIS:CD2	1:L:522:TYR:HB3	2.52	0.44
1:M:636:TYR:OH	1:M:648:THR:O	2.28	0.44
1:P:193:HIS:CD2	1:P:522:TYR:HB3	2.52	0.44
1:Q:684:ARG:NH2	1:R:756:ASP:OD1	2.50	0.44
1:F:328:VAL:HA	1:F:488:SER:HB3	1.99	0.44
1:H:609:LYS:O	1:H:700:LYS:NZ	2.46	0.44
1:H:636:TYR:OH	1:H:648:THR:O	2.28	0.44
1:I:567:LEU:O	1:I:580:GLN:NE2	2.51	0.44
1:J:515:THR:OG1	1:J:520:ASP:O	2.31	0.44
1:K:609:LYS:O	1:K:700:LYS:NZ	2.46	0.44
1:L:567:LEU:H	1:L:580:GLN:NE2	2.14	0.44
1:L:567:LEU:O	1:L:580:GLN:NE2	2.51	0.44
1:O:567:LEU:O	1:O:580:GLN:NE2	2.51	0.44
1:P:699:VAL:HG12	1:P:700:LYS:HG2	2.00	0.44
1:R:193:HIS:CD2	1:R:522:TYR:HB3	2.52	0.44
1:R:328:VAL:HA	1:R:488:SER:HB3	1.99	0.44
1:B:567:LEU:O	1:B:580:GLN:NE2	2.51	0.44
1:G:328:VAL:HA	1:G:488:SER:HB3	1.99	0.44
1:H:699:VAL:HG12	1:H:700:LYS:HG2	2.00	0.44
1:M:567:LEU:O	1:M:580:GLN:NE2	2.51	0.44
1:M:699:VAL:HG12	1:M:700:LYS:HG2	2.00	0.44
1:O:636:TYR:OH	1:O:648:THR:O	2.28	0.44
1:P:304:LEU:HD12	1:P:304:LEU:HA	1.80	0.44
1:P:609:LYS:O	1:P:700:LYS:NZ	2.46	0.44
1:Q:609:LYS:O	1:Q:700:LYS:NZ	2.46	0.44
1:A:567:LEU:O	1:A:580:GLN:NE2	2.51	0.43
1:D:328:VAL:HA	1:D:488:SER:HB3	1.99	0.43
1:N:236:GLY:HA2	1:N:240:ALA:HB2	1.99	0.43
1:O:193:HIS:CD2	1:O:522:TYR:HB3	2.52	0.43
1:O:308:MET:HE3	1:O:308:MET:HB3	1.94	0.43
1:Q:193:HIS:CD2	1:Q:522:TYR:HB3	2.52	0.43
1:B:699:VAL:HG12	1:B:700:LYS:HG2	1.99	0.43
1:F:193:HIS:CD2	1:F:522:TYR:HB3	2.52	0.43
1:G:567:LEU:O	1:G:580:GLN:NE2	2.51	0.43
1:I:193:HIS:CD2	1:I:522:TYR:HB3	2.52	0.43
1:K:328:VAL:HA	1:K:488:SER:HB3	1.99	0.43
1:N:193:HIS:CD2	1:N:522:TYR:HB3	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:304:LEU:HD12	1:O:304:LEU:HA	1.80	0.43
1:P:567:LEU:O	1:P:580:GLN:NE2	2.51	0.43
1:R:477:LYS:HD2	1:R:477:LYS:HA	1.85	0.43
1:A:328:VAL:HA	1:A:488:SER:HB3	1.99	0.43
1:A:711:ASP:OD1	1:A:724:GLU:HB3	2.19	0.43
1:E:328:VAL:HA	1:E:488:SER:HB3	2.00	0.43
1:E:501:ASP:OD2	1:E:557:LYS:NZ	2.51	0.43
1:H:711:ASP:OD1	1:H:724:GLU:HB3	2.19	0.43
1:I:304:LEU:HD12	1:I:304:LEU:HA	1.80	0.43
1:K:193:HIS:CD2	1:K:522:TYR:HB3	2.52	0.43
1:N:561:MET:HE2	1:N:561:MET:HB3	1.87	0.43
1:N:711:ASP:OD1	1:N:724:GLU:HB3	2.19	0.43
1:O:497:MET:HE3	1:O:497:MET:HB2	1.84	0.43
1:C:328:VAL:HA	1:C:488:SER:HB3	2.00	0.43
1:C:699:VAL:HG12	1:C:700:LYS:HG2	2.00	0.43
1:D:567:LEU:O	1:D:580:GLN:NE2	2.51	0.43
1:H:328:VAL:HA	1:H:488:SER:HB3	1.99	0.43
1:I:328:VAL:HA	1:I:488:SER:HB3	1.99	0.43
1:I:532:MET:HE3	1:I:532:MET:HB3	1.45	0.43
1:I:711:ASP:OD1	1:I:724:GLU:HB3	2.19	0.43
1:M:711:ASP:OD1	1:M:724:GLU:HB3	2.19	0.43
1:O:699:VAL:HG12	1:O:700:LYS:HG2	2.00	0.43
1:Q:515:THR:OG1	1:Q:520:ASP:O	2.31	0.43
1:B:501:ASP:OD2	1:B:557:LYS:NZ	2.51	0.43
1:F:711:ASP:OD1	1:F:724:GLU:HB3	2.19	0.43
1:G:636:TYR:OH	1:G:648:THR:O	2.28	0.43
1:H:477:LYS:HD2	1:H:477:LYS:HA	1.85	0.43
1:I:699:VAL:HG12	1:I:700:LYS:HG2	2.00	0.43
1:K:169:ASP:HA	1:K:172:LYS:HE2	2.00	0.43
1:O:711:ASP:OD1	1:O:724:GLU:HB3	2.19	0.43
1:Q:501:ASP:OD2	1:Q:557:LYS:NZ	2.51	0.43
1:B:328:VAL:HA	1:B:488:SER:HB3	1.99	0.43
1:B:532:MET:HE3	1:B:532:MET:HB3	1.45	0.43
1:C:497:MET:HE3	1:C:497:MET:HB2	1.84	0.43
1:C:501:ASP:OD2	1:C:557:LYS:NZ	2.51	0.43
1:E:193:HIS:CD2	1:E:522:TYR:HB3	2.52	0.43
1:F:169:ASP:HA	1:F:172:LYS:HE2	2.01	0.43
1:G:169:ASP:HA	1:G:172:LYS:HE2	2.01	0.43
1:G:483:MET:HE3	1:G:483:MET:HB3	1.65	0.43
1:G:711:ASP:OD1	1:G:724:GLU:HB3	2.19	0.43
1:J:229:ASP:OD1	1:J:229:ASP:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:711:ASP:OD1	1:J:724:GLU:HB3	2.19	0.43
1:K:497:MET:HE3	1:K:497:MET:HB2	1.84	0.43
1:R:169:ASP:HA	1:R:172:LYS:HE2	2.01	0.43
1:R:711:ASP:OD1	1:R:724:GLU:HB3	2.19	0.43
1:E:169:ASP:HA	1:E:172:LYS:HE2	2.01	0.43
1:I:345:LEU:HD23	1:I:345:LEU:HA	1.88	0.43
1:J:304:LEU:HD12	1:J:304:LEU:HA	1.80	0.43
1:N:699:VAL:HG12	1:N:700:LYS:HG2	1.99	0.43
1:R:532:MET:HB3	1:R:532:MET:HE3	1.45	0.43
1:B:711:ASP:OD1	1:B:724:GLU:HB3	2.19	0.43
1:C:339:SER:OG	1:C:499:LYS:HD3	2.19	0.43
1:C:711:ASP:OD1	1:C:724:GLU:HB3	2.19	0.43
1:D:339:SER:OG	1:D:499:LYS:HD3	2.19	0.43
1:D:501:ASP:OD2	1:D:557:LYS:NZ	2.51	0.43
1:E:493:MET:HE3	1:E:493:MET:HB3	1.91	0.43
1:J:328:VAL:HA	1:J:488:SER:HB3	1.99	0.43
1:K:339:SER:OG	1:K:499:LYS:HD3	2.19	0.43
1:L:711:ASP:OD1	1:L:724:GLU:HB3	2.19	0.43
1:O:477:LYS:HD2	1:O:477:LYS:HA	1.85	0.43
1:Q:339:SER:OG	1:Q:499:LYS:HD3	2.19	0.43
1:L:339:SER:OG	1:L:499:LYS:HD3	2.19	0.43
1:O:339:SER:OG	1:O:499:LYS:HD3	2.19	0.43
1:O:483:MET:HE3	1:O:483:MET:HB3	1.64	0.43
1:P:308:MET:HE3	1:P:308:MET:HB3	1.94	0.43
1:A:339:SER:OG	1:A:499:LYS:HD3	2.19	0.43
1:A:477:LYS:HA	1:A:477:LYS:HD2	1.85	0.43
1:B:169:ASP:HA	1:B:172:LYS:HE2	2.00	0.43
1:C:238:VAL:HG23	1:C:535:PRO:HB3	2.01	0.43
1:E:743:LEU:HD23	1:L:202:GLN:HE22	1.84	0.43
1:E:783:ALA:O	1:E:793:GLN:HA	2.19	0.43
1:F:339:SER:OG	1:F:499:LYS:HD3	2.19	0.43
1:K:711:ASP:OD1	1:K:724:GLU:HB3	2.19	0.43
1:L:169:ASP:HA	1:L:172:LYS:HE2	2.01	0.43
1:L:304:LEU:HD12	1:L:304:LEU:HA	1.80	0.43
1:O:238:VAL:HG23	1:O:535:PRO:HB3	2.01	0.43
1:Q:711:ASP:OD1	1:Q:724:GLU:HB3	2.19	0.43
1:R:483:MET:HB3	1:R:483:MET:HE3	1.64	0.43
1:A:483:MET:HE3	1:A:483:MET:HB3	1.64	0.42
1:A:515:THR:OG1	1:A:520:ASP:O	2.31	0.42
1:D:169:ASP:HA	1:D:172:LYS:HE2	2.01	0.42
1:F:238:VAL:HG23	1:F:535:PRO:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:339:SER:OG	1:H:499:LYS:HD3	2.19	0.42
1:I:238:VAL:HG23	1:I:535:PRO:HB3	2.01	0.42
1:I:339:SER:OG	1:I:499:LYS:HD3	2.19	0.42
1:K:238:VAL:HG23	1:K:535:PRO:HB3	2.01	0.42
1:N:783:ALA:O	1:N:793:GLN:HA	2.19	0.42
1:Q:561:MET:HE2	1:Q:561:MET:HB3	1.87	0.42
1:R:339:SER:OG	1:R:499:LYS:HD3	2.19	0.42
1:R:501:ASP:OD2	1:R:557:LYS:NZ	2.51	0.42
1:B:561:MET:HE1	1:B:601:SER:HB3	2.01	0.42
1:C:515:THR:OG1	1:C:520:ASP:O	2.31	0.42
1:F:783:ALA:O	1:F:793:GLN:HA	2.19	0.42
1:I:169:ASP:HA	1:I:172:LYS:HE2	2.01	0.42
1:J:339:SER:OG	1:J:499:LYS:HD3	2.19	0.42
1:L:238:VAL:HG23	1:L:535:PRO:HB3	2.01	0.42
1:O:169:ASP:HA	1:O:172:LYS:HE2	2.01	0.42
1:O:345:LEU:HD23	1:O:345:LEU:HA	1.88	0.42
1:Q:783:ALA:O	1:Q:793:GLN:HA	2.19	0.42
1:D:711:ASP:OD1	1:D:724:GLU:HB3	2.19	0.42
1:G:532:MET:HE3	1:G:532:MET:HB3	1.45	0.42
1:G:783:ALA:O	1:G:793:GLN:HA	2.19	0.42
1:J:169:ASP:HA	1:J:172:LYS:HE2	2.01	0.42
1:L:783:ALA:O	1:L:793:GLN:HA	2.19	0.42
1:M:339:SER:OG	1:M:499:LYS:HD3	2.19	0.42
1:M:783:ALA:O	1:M:793:GLN:HA	2.19	0.42
1:N:169:ASP:HA	1:N:172:LYS:HE2	2.01	0.42
1:O:233:HIS:NE2	1:O:527:LYS:HG3	2.35	0.42
1:P:169:ASP:HA	1:P:172:LYS:HE2	2.01	0.42
1:P:233:HIS:NE2	1:P:527:LYS:HG3	2.35	0.42
1:Q:169:ASP:HA	1:Q:172:LYS:HE2	2.01	0.42
1:A:561:MET:HE1	1:A:601:SER:HB3	2.01	0.42
1:D:229:ASP:OD1	1:D:229:ASP:N	2.52	0.42
1:D:783:ALA:O	1:D:793:GLN:HA	2.19	0.42
1:E:238:VAL:HG23	1:E:535:PRO:HB3	2.01	0.42
1:E:339:SER:OG	1:E:499:LYS:HD3	2.19	0.42
1:F:493:MET:HE3	1:F:493:MET:HB3	1.91	0.42
1:M:561:MET:HE1	1:M:601:SER:HB3	2.01	0.42
1:P:561:MET:HE1	1:P:601:SER:HB3	2.01	0.42
1:P:783:ALA:O	1:P:793:GLN:HA	2.19	0.42
1:R:238:VAL:HG23	1:R:535:PRO:HB3	2.01	0.42
1:A:169:ASP:HA	1:A:172:LYS:HE2	2.01	0.42
1:B:783:ALA:O	1:B:793:GLN:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:ASP:OD1	1:C:229:ASP:N	2.52	0.42
1:C:783:ALA:O	1:C:793:GLN:HA	2.19	0.42
1:E:711:ASP:OD1	1:E:724:GLU:HB3	2.19	0.42
1:J:233:HIS:NE2	1:J:527:LYS:HG3	2.35	0.42
1:J:271:ILE:HG13	1:J:303:ALA:HB2	2.02	0.42
1:N:225:GLY:HA3	1:N:261:PRO:HB2	2.02	0.42
1:N:304:LEU:HD12	1:N:304:LEU:HA	1.80	0.42
1:O:561:MET:HE1	1:O:601:SER:HB3	2.01	0.42
1:P:645:VAL:HG22	1:P:665:VAL:HG23	2.02	0.42
1:P:711:ASP:OD1	1:P:724:GLU:HB3	2.19	0.42
1:A:308:MET:HE3	1:A:308:MET:HB3	1.94	0.42
1:C:202:GLN:HE22	1:N:743:LEU:HD23	1.84	0.42
1:D:329:GLY:O	1:D:333:THR:HG23	2.20	0.42
1:F:229:ASP:OD1	1:F:229:ASP:N	2.52	0.42
1:G:256:TYR:OH	1:G:280:ASP:OD2	2.26	0.42
1:H:271:ILE:HG13	1:H:303:ALA:HB2	2.02	0.42
1:M:229:ASP:OD1	1:M:229:ASP:N	2.52	0.42
1:M:645:VAL:HG22	1:M:665:VAL:HG23	2.02	0.42
1:O:225:GLY:HA3	1:O:261:PRO:HB2	2.02	0.42
1:O:645:VAL:HG22	1:O:665:VAL:HG23	2.02	0.42
1:Q:238:VAL:HG23	1:Q:535:PRO:HB3	2.01	0.42
1:A:501:ASP:OD2	1:A:557:LYS:NZ	2.51	0.42
1:C:169:ASP:HA	1:C:172:LYS:HE2	2.01	0.42
1:D:271:ILE:HG13	1:D:303:ALA:HB2	2.02	0.42
1:E:229:ASP:N	1:E:229:ASP:OD1	2.52	0.42
1:G:238:VAL:HG23	1:G:535:PRO:HB3	2.01	0.42
1:H:225:GLY:HA3	1:H:261:PRO:HB2	2.02	0.42
1:I:561:MET:HE1	1:I:601:SER:HB3	2.01	0.42
1:N:645:VAL:HG22	1:N:665:VAL:HG23	2.02	0.42
1:P:532:MET:HE3	1:P:532:MET:HB3	1.45	0.42
1:R:229:ASP:N	1:R:229:ASP:OD1	2.52	0.42
1:A:229:ASP:OD1	1:A:229:ASP:N	2.52	0.42
1:A:238:VAL:HG23	1:A:535:PRO:HB3	2.01	0.42
1:B:233:HIS:NE2	1:B:527:LYS:HG3	2.35	0.42
1:B:329:GLY:O	1:B:333:THR:HG23	2.20	0.42
1:C:225:GLY:HA3	1:C:261:PRO:HB2	2.02	0.42
1:H:229:ASP:OD1	1:H:229:ASP:N	2.52	0.42
1:H:308:MET:HE3	1:H:308:MET:HB3	1.94	0.42
1:J:783:ALA:O	1:J:793:GLN:HA	2.19	0.42
1:M:169:ASP:HA	1:M:172:LYS:HE2	2.01	0.42
1:M:238:VAL:HG23	1:M:535:PRO:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:329:GLY:O	1:M:333:THR:HG23	2.20	0.42
1:N:329:GLY:O	1:N:333:THR:HG23	2.20	0.42
1:N:339:SER:OG	1:N:499:LYS:HD3	2.19	0.42
1:N:561:MET:HE1	1:N:601:SER:HB3	2.02	0.42
1:O:229:ASP:N	1:O:229:ASP:OD1	2.52	0.42
1:O:329:GLY:O	1:O:333:THR:HG23	2.20	0.42
1:Q:645:VAL:HG22	1:Q:665:VAL:HG23	2.02	0.42
1:R:329:GLY:O	1:R:333:THR:HG23	2.20	0.42
1:A:233:HIS:NE2	1:A:527:LYS:HG3	2.35	0.42
1:B:238:VAL:HG23	1:B:535:PRO:HB3	2.01	0.42
1:C:645:VAL:HG22	1:C:665:VAL:HG23	2.02	0.42
1:D:645:VAL:HG22	1:D:665:VAL:HG23	2.02	0.42
1:F:483:MET:HB3	1:F:483:MET:HE3	1.64	0.42
1:H:238:VAL:HG23	1:H:535:PRO:HB3	2.01	0.42
1:I:229:ASP:OD1	1:I:229:ASP:N	2.52	0.42
1:I:308:MET:HE3	1:I:308:MET:HB3	1.94	0.42
1:J:329:GLY:O	1:J:333:THR:HG23	2.20	0.42
1:L:645:VAL:HG22	1:L:665:VAL:HG23	2.02	0.42
1:O:271:ILE:HG13	1:O:303:ALA:HB2	2.02	0.42
1:O:783:ALA:O	1:O:793:GLN:HA	2.19	0.42
1:P:225:GLY:HA3	1:P:261:PRO:HB2	2.02	0.42
1:P:238:VAL:HG23	1:P:535:PRO:HB3	2.01	0.42
1:C:233:HIS:NE2	1:C:527:LYS:HG3	2.35	0.42
1:C:271:ILE:HG13	1:C:303:ALA:HB2	2.02	0.42
1:C:329:GLY:O	1:C:333:THR:HG23	2.20	0.42
1:C:561:MET:HE1	1:C:601:SER:HB3	2.01	0.42
1:D:225:GLY:HA3	1:D:261:PRO:HB2	2.02	0.42
1:D:238:VAL:HG23	1:D:535:PRO:HB3	2.01	0.42
1:F:158:MET:HB3	1:F:244:ILE:HG23	2.02	0.42
1:G:645:VAL:HG22	1:G:665:VAL:HG23	2.02	0.42
1:H:169:ASP:HA	1:H:172:LYS:HE2	2.01	0.42
1:H:233:HIS:NE2	1:H:527:LYS:HG3	2.35	0.42
1:I:271:ILE:HG13	1:I:303:ALA:HB2	2.02	0.42
1:J:645:VAL:HG22	1:J:665:VAL:HG23	2.02	0.42
1:B:645:VAL:HG22	1:B:665:VAL:HG23	2.02	0.41
1:C:345:LEU:HD23	1:C:345:LEU:HA	1.88	0.41
1:D:158:MET:HB3	1:D:244:ILE:HG23	2.02	0.41
1:E:158:MET:HB3	1:E:244:ILE:HG23	2.02	0.41
1:E:240:ALA:O	1:E:245:LYS:HA	2.20	0.41
1:G:271:ILE:HG13	1:G:303:ALA:HB2	2.02	0.41
1:G:339:SER:OG	1:G:499:LYS:HD3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:645:VAL:HG22	1:H:665:VAL:HG23	2.02	0.41
1:I:233:HIS:NE2	1:I:527:LYS:HG3	2.35	0.41
1:I:329:GLY:O	1:I:333:THR:HG23	2.20	0.41
1:K:233:HIS:NE2	1:K:527:LYS:HG3	2.35	0.41
1:L:229:ASP:N	1:L:229:ASP:OD1	2.52	0.41
1:L:329:GLY:O	1:L:333:THR:HG23	2.20	0.41
1:L:477:LYS:HD2	1:L:477:LYS:HA	1.85	0.41
1:L:561:MET:HE1	1:L:601:SER:HB3	2.01	0.41
1:Q:561:MET:HE1	1:Q:601:SER:HB3	2.01	0.41
1:A:271:ILE:HG13	1:A:303:ALA:HB2	2.02	0.41
1:A:329:GLY:O	1:A:333:THR:HG23	2.20	0.41
1:A:783:ALA:O	1:A:793:GLN:HA	2.19	0.41
1:B:229:ASP:OD1	1:B:229:ASP:N	2.52	0.41
1:B:339:SER:OG	1:B:499:LYS:HD3	2.19	0.41
1:E:233:HIS:NE2	1:E:527:LYS:HG3	2.35	0.41
1:E:329:GLY:O	1:E:333:THR:HG23	2.20	0.41
1:G:225:GLY:HA3	1:G:261:PRO:HB2	2.02	0.41
1:G:233:HIS:NE2	1:G:527:LYS:HG3	2.35	0.41
1:G:561:MET:HE1	1:G:601:SER:HB3	2.01	0.41
1:H:561:MET:HE1	1:H:601:SER:HB3	2.01	0.41
1:I:673:LYS:O	1:I:677:TYR:OH	2.26	0.41
1:M:225:GLY:HA3	1:M:261:PRO:HB2	2.02	0.41
1:M:271:ILE:HG13	1:M:303:ALA:HB2	2.02	0.41
1:N:233:HIS:NE2	1:N:527:LYS:HG3	2.35	0.41
1:N:501:ASP:OD2	1:N:557:LYS:NZ	2.51	0.41
1:P:329:GLY:O	1:P:333:THR:HG23	2.20	0.41
1:P:339:SER:OG	1:P:499:LYS:HD3	2.19	0.41
1:Q:233:HIS:NE2	1:Q:527:LYS:HG3	2.35	0.41
1:Q:304:LEU:HD12	1:Q:304:LEU:HA	1.80	0.41
1:D:561:MET:HE1	1:D:601:SER:HB3	2.01	0.41
1:G:158:MET:HB3	1:G:244:ILE:HG23	2.02	0.41
1:H:329:GLY:O	1:H:333:THR:HG23	2.20	0.41
1:I:645:VAL:HG22	1:I:665:VAL:HG23	2.02	0.41
1:I:783:ALA:O	1:I:793:GLN:HA	2.19	0.41
1:K:271:ILE:HG13	1:K:303:ALA:HB2	2.02	0.41
1:K:783:ALA:O	1:K:793:GLN:HA	2.19	0.41
1:N:238:VAL:HG23	1:N:535:PRO:HB3	2.01	0.41
1:N:240:ALA:O	1:N:245:LYS:HA	2.20	0.41
1:O:158:MET:HB3	1:O:244:ILE:HG23	2.02	0.41
1:Q:271:ILE:HG13	1:Q:303:ALA:HB2	2.02	0.41
1:A:158:MET:HB3	1:A:244:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:MET:HB3	1:C:244:ILE:HG23	2.02	0.41
1:E:256:TYR:OH	1:E:280:ASP:OD2	2.26	0.41
1:H:527:LYS:HE2	1:H:527:LYS:HB3	1.87	0.41
1:H:783:ALA:O	1:H:793:GLN:HA	2.19	0.41
1:K:229:ASP:OD1	1:K:229:ASP:N	2.52	0.41
1:K:240:ALA:O	1:K:245:LYS:HA	2.21	0.41
1:L:158:MET:HB2	1:L:510:VAL:O	2.21	0.41
1:M:233:HIS:NE2	1:M:527:LYS:HG3	2.35	0.41
1:Q:345:LEU:HD23	1:Q:345:LEU:HA	1.88	0.41
1:R:783:ALA:O	1:R:793:GLN:HA	2.19	0.41
1:F:649:ASP:OD2	1:F:649:ASP:N	2.49	0.41
1:G:240:ALA:O	1:G:245:LYS:HA	2.21	0.41
1:G:329:GLY:O	1:G:333:THR:HG23	2.20	0.41
1:G:477:LYS:HD2	1:G:477:LYS:HA	1.85	0.41
1:H:158:MET:HB3	1:H:244:ILE:HG23	2.02	0.41
1:H:780:TYR:CZ	1:H:799:PRO:HG3	2.56	0.41
1:N:158:MET:HB3	1:N:244:ILE:HG23	2.02	0.41
1:P:515:THR:OG1	1:P:520:ASP:O	2.31	0.41
1:Q:649:ASP:OD2	1:Q:649:ASP:N	2.49	0.41
1:A:645:VAL:HG22	1:A:665:VAL:HG23	2.02	0.41
1:B:233:HIS:HD2	1:B:513:ILE:HG23	1.86	0.41
1:E:158:MET:HB2	1:E:510:VAL:O	2.21	0.41
1:E:271:ILE:HG13	1:E:303:ALA:HB2	2.02	0.41
1:E:561:MET:HE1	1:E:601:SER:HB3	2.02	0.41
1:I:233:HIS:HD2	1:I:513:ILE:HG23	1.86	0.41
1:J:158:MET:HB3	1:J:244:ILE:HG23	2.02	0.41
1:L:233:HIS:HD2	1:L:513:ILE:HG23	1.86	0.41
1:M:532:MET:HE3	1:M:532:MET:HB3	1.45	0.41
1:N:229:ASP:OD1	1:N:229:ASP:N	2.52	0.41
1:Q:233:HIS:HD2	1:Q:513:ILE:HG23	1.86	0.41
1:R:240:ALA:O	1:R:245:LYS:HA	2.20	0.41
1:A:780:TYR:CZ	1:A:799:PRO:HG3	2.56	0.41
1:B:304:LEU:HD12	1:B:304:LEU:HA	1.80	0.41
1:B:515:THR:OG1	1:B:520:ASP:O	2.31	0.41
1:C:780:TYR:CZ	1:C:799:PRO:HG3	2.56	0.41
1:E:645:VAL:HG22	1:E:665:VAL:HG23	2.02	0.41
1:F:233:HIS:NE2	1:F:527:LYS:HG3	2.35	0.41
1:F:645:VAL:HG22	1:F:665:VAL:HG23	2.02	0.41
1:J:238:VAL:HG23	1:J:535:PRO:HB3	2.01	0.41
1:K:329:GLY:O	1:K:333:THR:HG23	2.20	0.41
1:Q:158:MET:HB2	1:Q:510:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:158:MET:HB3	1:R:244:ILE:HG23	2.02	0.41
1:R:158:MET:HB2	1:R:510:VAL:O	2.21	0.41
1:A:158:MET:HB2	1:A:510:VAL:O	2.21	0.41
1:A:225:GLY:HA3	1:A:261:PRO:HB2	2.02	0.41
1:D:233:HIS:NE2	1:D:527:LYS:HG3	2.35	0.41
1:D:304:LEU:HA	1:D:304:LEU:HD12	1.80	0.41
1:D:780:TYR:CZ	1:D:799:PRO:HG3	2.56	0.41
1:F:271:ILE:HG13	1:F:303:ALA:HB2	2.02	0.41
1:F:329:GLY:O	1:F:333:THR:HG23	2.20	0.41
1:F:497:MET:HE3	1:F:497:MET:HB2	1.84	0.41
1:F:561:MET:HE1	1:F:601:SER:HB3	2.01	0.41
1:J:561:MET:HE1	1:J:601:SER:HB3	2.01	0.41
1:K:158:MET:HB3	1:K:244:ILE:HG23	2.02	0.41
1:L:233:HIS:NE2	1:L:527:LYS:HG3	2.35	0.41
1:L:271:ILE:HG13	1:L:303:ALA:HB2	2.02	0.41
1:P:628:ILE:HG13	1:Q:271:ILE:HG21	2.03	0.41
1:R:271:ILE:HG13	1:R:303:ALA:HB2	2.02	0.41
1:R:561:MET:HE1	1:R:601:SER:HB3	2.01	0.41
1:A:240:ALA:O	1:A:245:LYS:HA	2.21	0.41
1:A:345:LEU:HD23	1:A:345:LEU:HA	1.88	0.41
1:A:497:MET:HE3	1:A:497:MET:HB2	1.84	0.41
1:A:649:ASP:OD2	1:A:649:ASP:N	2.49	0.41
1:B:225:GLY:HA3	1:B:261:PRO:HB2	2.02	0.41
1:B:240:ALA:O	1:B:245:LYS:HA	2.21	0.41
1:B:271:ILE:HG13	1:B:303:ALA:HB2	2.02	0.41
1:B:345:LEU:HD23	1:B:345:LEU:HA	1.88	0.41
1:B:739:TYR:OH	1:O:202:GLN:O	2.27	0.41
1:C:158:MET:HB2	1:C:510:VAL:O	2.21	0.41
1:C:240:ALA:O	1:C:245:LYS:HA	2.21	0.41
1:F:240:ALA:O	1:F:245:LYS:HA	2.21	0.41
1:F:501:ASP:OD2	1:F:557:LYS:NZ	2.51	0.41
1:G:780:TYR:CZ	1:G:799:PRO:HG3	2.56	0.41
1:I:561:MET:HE2	1:I:561:MET:HB3	1.87	0.41
1:J:240:ALA:O	1:J:245:LYS:HA	2.20	0.41
1:K:158:MET:HB2	1:K:510:VAL:O	2.21	0.41
1:K:561:MET:HE1	1:K:601:SER:HB3	2.01	0.41
1:M:158:MET:HB3	1:M:244:ILE:HG23	2.02	0.41
1:N:271:ILE:HG13	1:N:303:ALA:HB2	2.02	0.41
1:N:527:LYS:HE2	1:N:527:LYS:HB3	1.87	0.41
1:P:158:MET:HB3	1:P:244:ILE:HG23	2.02	0.41
1:P:271:ILE:HG13	1:P:303:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:307:ALA:C	1:P:309:SER:N	2.79	0.41
1:Q:240:ALA:O	1:Q:245:LYS:HA	2.21	0.41
1:Q:329:GLY:O	1:Q:333:THR:HG23	2.20	0.41
1:Q:477:LYS:HD2	1:Q:477:LYS:HA	1.85	0.41
1:R:645:VAL:HG22	1:R:665:VAL:HG23	2.02	0.41
1:A:304:LEU:HA	1:A:304:LEU:HD12	1.80	0.41
1:A:307:ALA:C	1:A:309:SER:N	2.79	0.41
1:C:256:TYR:OH	1:C:280:ASP:OD2	2.26	0.41
1:C:483:MET:HE3	1:C:483:MET:HB3	1.65	0.41
1:F:225:GLY:HA3	1:F:261:PRO:HB2	2.02	0.41
1:G:628:ILE:HG13	1:H:271:ILE:HG21	2.03	0.41
1:H:481:GLU:HB3	1:H:567:LEU:HD22	2.03	0.41
1:I:225:GLY:HA3	1:I:261:PRO:HB2	2.02	0.41
1:J:225:GLY:HA3	1:J:261:PRO:HB2	2.02	0.41
1:J:233:HIS:HD2	1:J:513:ILE:HG23	1.86	0.41
1:L:225:GLY:HA3	1:L:261:PRO:HB2	2.02	0.41
1:L:483:MET:HB3	1:L:483:MET:HE3	1.65	0.41
1:M:240:ALA:O	1:M:245:LYS:HA	2.21	0.41
1:M:307:ALA:C	1:M:309:SER:N	2.79	0.41
1:N:158:MET:HB2	1:N:510:VAL:O	2.21	0.41
1:O:158:MET:HB2	1:O:510:VAL:O	2.21	0.41
1:Q:307:ALA:C	1:Q:309:SER:N	2.79	0.41
1:R:233:HIS:NE2	1:R:527:LYS:HG3	2.35	0.41
1:R:345:LEU:HD23	1:R:345:LEU:HA	1.88	0.41
1:A:185:ILE:O	1:A:186:ASP:OD1	2.40	0.40
1:C:233:HIS:HD2	1:C:513:ILE:HG23	1.86	0.40
1:C:308:MET:HE3	1:C:308:MET:HB3	1.94	0.40
1:E:225:GLY:HA3	1:E:261:PRO:HB2	2.02	0.40
1:H:217:GLU:OE2	1:H:232:THR:OG1	2.37	0.40
1:H:240:ALA:O	1:H:245:LYS:HA	2.21	0.40
1:H:802:ILE:HD13	1:H:802:ILE:HA	1.98	0.40
1:J:481:GLU:HB3	1:J:567:LEU:HD22	2.03	0.40
1:K:645:VAL:HG22	1:K:665:VAL:HG23	2.02	0.40
1:M:233:HIS:HD2	1:M:513:ILE:HG23	1.86	0.40
1:M:501:ASP:OD2	1:M:557:LYS:NZ	2.51	0.40
1:M:780:TYR:CZ	1:M:799:PRO:HG3	2.56	0.40
1:O:240:ALA:O	1:O:245:LYS:HA	2.21	0.40
1:O:780:TYR:CZ	1:O:799:PRO:HG3	2.56	0.40
1:P:780:TYR:CZ	1:P:799:PRO:HG3	2.56	0.40
1:B:185:ILE:O	1:B:186:ASP:OD1	2.40	0.40
1:B:307:ALA:C	1:B:309:SER:N	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:483:MET:HE3	1:B:483:MET:HB3	1.64	0.40
1:D:481:GLU:HB3	1:D:567:LEU:HD22	2.03	0.40
1:E:307:ALA:C	1:E:309:SER:N	2.79	0.40
1:G:481:GLU:HB3	1:G:567:LEU:HD22	2.03	0.40
1:I:158:MET:HB2	1:I:510:VAL:O	2.21	0.40
1:I:240:ALA:O	1:I:245:LYS:HA	2.20	0.40
1:I:477:LYS:HD2	1:I:477:LYS:HA	1.85	0.40
1:J:780:TYR:CZ	1:J:799:PRO:HG3	2.56	0.40
1:K:233:HIS:HD2	1:K:513:ILE:HG23	1.86	0.40
1:K:780:TYR:CZ	1:K:799:PRO:HG3	2.56	0.40
1:L:780:TYR:CZ	1:L:799:PRO:HG3	2.56	0.40
1:M:185:ILE:O	1:M:186:ASP:OD1	2.40	0.40
1:N:780:TYR:CZ	1:N:799:PRO:HG3	2.56	0.40
1:P:185:ILE:O	1:P:186:ASP:OD1	2.40	0.40
1:P:233:HIS:HD2	1:P:513:ILE:HG23	1.86	0.40
1:Q:229:ASP:N	1:Q:229:ASP:OD1	2.52	0.40
1:R:649:ASP:OD2	1:R:649:ASP:N	2.49	0.40
1:C:672:VAL:HG11	1:C:699:VAL:HG21	2.04	0.40
1:D:240:ALA:O	1:D:245:LYS:HA	2.21	0.40
1:D:672:VAL:HG11	1:D:699:VAL:HG21	2.04	0.40
1:F:233:HIS:HD2	1:F:513:ILE:HG23	1.86	0.40
1:F:780:TYR:CZ	1:F:799:PRO:HG3	2.56	0.40
1:G:158:MET:HB2	1:G:510:VAL:O	2.21	0.40
1:G:501:ASP:OD2	1:G:557:LYS:NZ	2.51	0.40
1:H:233:HIS:HD2	1:H:513:ILE:HG23	1.86	0.40
1:I:185:ILE:O	1:I:186:ASP:OD1	2.40	0.40
1:I:307:ALA:C	1:I:309:SER:N	2.79	0.40
1:J:158:MET:HB2	1:J:510:VAL:O	2.21	0.40
1:M:158:MET:HB2	1:M:510:VAL:O	2.21	0.40
1:Q:185:ILE:O	1:Q:186:ASP:OD1	2.40	0.40
1:Q:780:TYR:CZ	1:Q:799:PRO:HG3	2.56	0.40
1:R:225:GLY:HA3	1:R:261:PRO:HB2	2.02	0.40
1:C:317:SER:HB3	1:C:531:SER:HA	2.04	0.40
1:C:481:GLU:HB3	1:C:567:LEU:HD22	2.03	0.40
1:G:317:SER:HB3	1:G:531:SER:HA	2.04	0.40
1:H:672:VAL:HG11	1:H:699:VAL:HG21	2.04	0.40
1:K:225:GLY:HA3	1:K:261:PRO:HB2	2.02	0.40
1:K:317:SER:HB3	1:K:531:SER:HA	2.04	0.40
1:K:481:GLU:HB3	1:K:567:LEU:HD22	2.03	0.40
1:K:493:MET:HE3	1:K:493:MET:HB3	1.91	0.40
1:L:185:ILE:O	1:L:186:ASP:OD1	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:308:MET:HE3	1:L:308:MET:HB3	1.94	0.40
1:N:158:MET:SD	1:N:237:THR:HG23	2.62	0.40
1:O:158:MET:SD	1:O:237:THR:HG23	2.62	0.40
1:P:158:MET:HB2	1:P:510:VAL:O	2.21	0.40
1:P:229:ASP:N	1:P:229:ASP:OD1	2.52	0.40
1:Q:225:GLY:HA3	1:Q:261:PRO:HB2	2.02	0.40
1:C:185:ILE:O	1:C:186:ASP:OD1	2.40	0.40
1:C:532:MET:HE3	1:C:532:MET:HB3	1.45	0.40
1:D:317:SER:HB3	1:D:531:SER:HA	2.04	0.40
1:D:532:MET:HB3	1:D:532:MET:HE3	1.45	0.40
1:E:233:HIS:HD2	1:E:513:ILE:HG23	1.86	0.40
1:E:317:SER:HB3	1:E:531:SER:HA	2.04	0.40
1:E:780:TYR:CZ	1:E:799:PRO:HG3	2.56	0.40
1:F:185:ILE:O	1:F:186:ASP:OD1	2.40	0.40
1:F:317:SER:HB3	1:F:531:SER:HA	2.04	0.40
1:H:502:VAL:HG11	1:H:585:ILE:CG2	2.52	0.40
1:H:628:ILE:HD11	1:I:271:ILE:HG12	2.04	0.40
1:J:317:SER:HB3	1:J:531:SER:HA	2.04	0.40
1:J:628:ILE:HD11	1:O:271:ILE:HG12	2.04	0.40
1:J:672:VAL:HG11	1:J:699:VAL:HG21	2.04	0.40
1:L:158:MET:HB3	1:L:244:ILE:HG23	2.02	0.40
1:M:304:LEU:HD12	1:M:304:LEU:HA	1.80	0.40
1:M:345:LEU:HD23	1:M:345:LEU:HA	1.88	0.40
1:N:185:ILE:O	1:N:186:ASP:OD1	2.40	0.40
1:N:317:SER:HB3	1:N:531:SER:HA	2.04	0.40
1:O:185:ILE:O	1:O:186:ASP:OD1	2.40	0.40
1:O:233:HIS:HD2	1:O:513:ILE:HG23	1.86	0.40
1:O:317:SER:HB3	1:O:531:SER:HA	2.04	0.40
1:R:233:HIS:HD2	1:R:513:ILE:HG23	1.86	0.40
1:R:780:TYR:CZ	1:R:799:PRO:HG3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	513/803 (64%)	484 (94%)	29 (6%)	0	100	100
1	B	513/803 (64%)	484 (94%)	29 (6%)	0	100	100
1	C	513/803 (64%)	484 (94%)	29 (6%)	0	100	100
1	D	513/803 (64%)	484 (94%)	29 (6%)	0	100	100
1	E	513/803 (64%)	484 (94%)	29 (6%)	0	100	100
1	F	513/803 (64%)	484 (94%)	29 (6%)	0	100	100
1	G	513/803 (64%)	484 (94%)	29 (6%)	0	100	100
1	H	513/803 (64%)	484 (94%)	29 (6%)	0	100	100
1	I	513/803 (64%)	484 (94%)	29 (6%)	0	100	100
1	J	513/803 (64%)	484 (94%)	29 (6%)	0	100	100
1	K	513/803 (64%)	484 (94%)	29 (6%)	0	100	100
1	L	513/803 (64%)	484 (94%)	29 (6%)	0	100	100
1	M	513/803 (64%)	484 (94%)	29 (6%)	0	100	100
1	N	513/803 (64%)	484 (94%)	29 (6%)	0	100	100
1	O	513/803 (64%)	484 (94%)	29 (6%)	0	100	100
1	P	513/803 (64%)	484 (94%)	29 (6%)	0	100	100
1	Q	513/803 (64%)	484 (94%)	29 (6%)	0	100	100
1	R	513/803 (64%)	484 (94%)	29 (6%)	0	100	100
All	All	9234/14454 (64%)	8712 (94%)	522 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	409/648 (63%)	409 (100%)	0	100	100

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	409/648 (63%)	409 (100%)	0	100	100
1	C	409/648 (63%)	409 (100%)	0	100	100
1	D	409/648 (63%)	409 (100%)	0	100	100
1	E	409/648 (63%)	409 (100%)	0	100	100
1	F	409/648 (63%)	409 (100%)	0	100	100
1	G	409/648 (63%)	409 (100%)	0	100	100
1	H	409/648 (63%)	409 (100%)	0	100	100
1	I	409/648 (63%)	409 (100%)	0	100	100
1	J	409/648 (63%)	409 (100%)	0	100	100
1	K	409/648 (63%)	409 (100%)	0	100	100
1	L	409/648 (63%)	409 (100%)	0	100	100
1	M	409/648 (63%)	409 (100%)	0	100	100
1	N	409/648 (63%)	409 (100%)	0	100	100
1	O	409/648 (63%)	409 (100%)	0	100	100
1	P	409/648 (63%)	409 (100%)	0	100	100
1	Q	409/648 (63%)	409 (100%)	0	100	100
1	R	409/648 (63%)	409 (100%)	0	100	100
All	All	7362/11664 (63%)	7362 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	ASN
1	A	325	ASN
1	A	580	GLN
1	B	241	ASN
1	B	580	GLN
1	B	633	GLN
1	C	202	GLN
1	C	241	ASN
1	C	580	GLN
1	D	241	ASN
1	D	580	GLN
1	E	241	ASN

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Mol	Chain	Res	Type
1	E	580	GLN
1	F	241	ASN
1	F	580	GLN
1	G	202	GLN
1	G	241	ASN
1	G	580	GLN
1	G	793	GLN
1	H	241	ASN
1	H	580	GLN
1	I	241	ASN
1	I	580	GLN
1	J	241	ASN
1	J	580	GLN
1	K	241	ASN
1	K	580	GLN
1	L	202	GLN
1	L	241	ASN
1	L	580	GLN
1	M	241	ASN
1	M	580	GLN
1	N	241	ASN
1	N	580	GLN
1	O	241	ASN
1	O	580	GLN
1	P	202	GLN
1	P	241	ASN
1	P	580	GLN
1	P	793	GLN
1	Q	241	ASN
1	Q	580	GLN
1	R	241	ASN
1	R	562	ASN
1	R	580	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

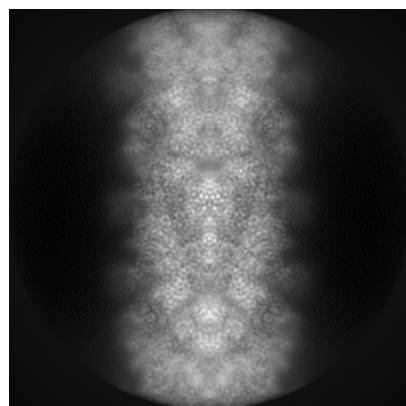
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36428. These allow visual inspection of the internal detail of the map and identification of artifacts.

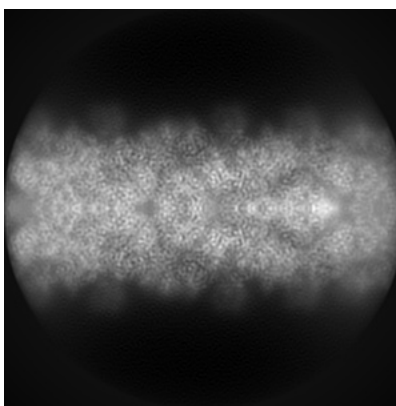
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

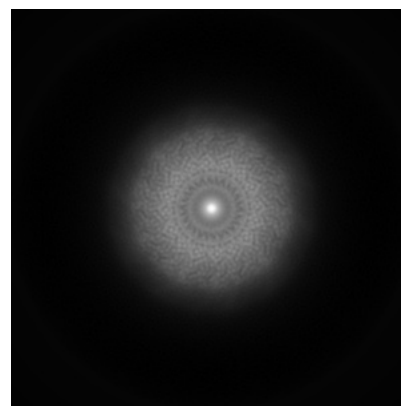
6.1.1 Primary map



X

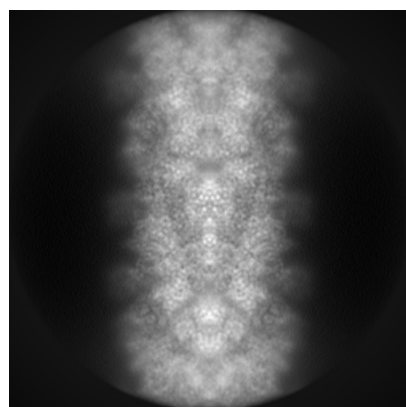


Y

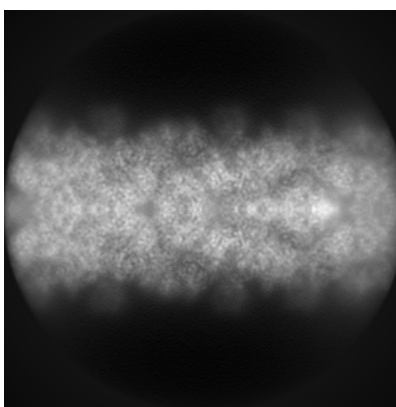


Z

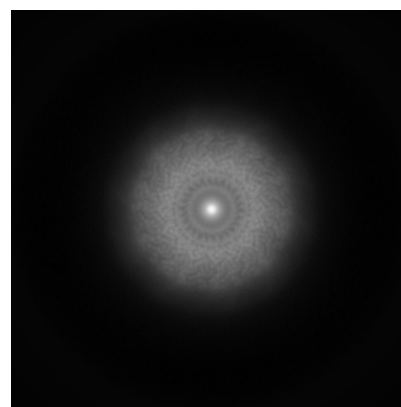
6.1.2 Raw map



X



Y

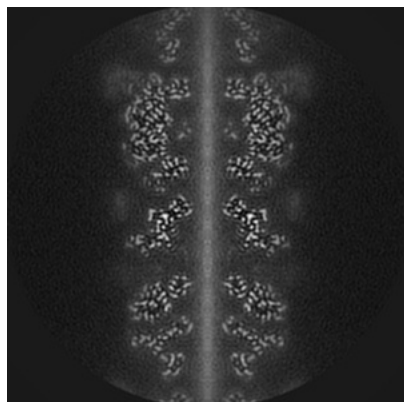


Z

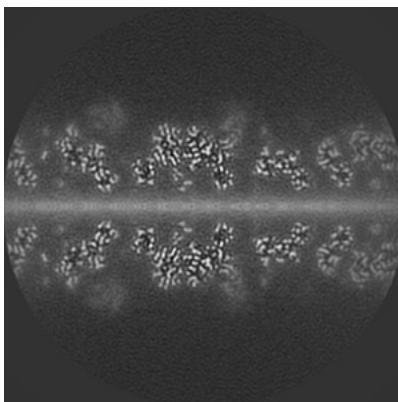
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

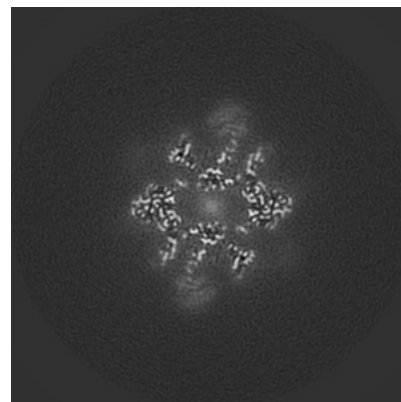
6.2.1 Primary map



X Index: 160

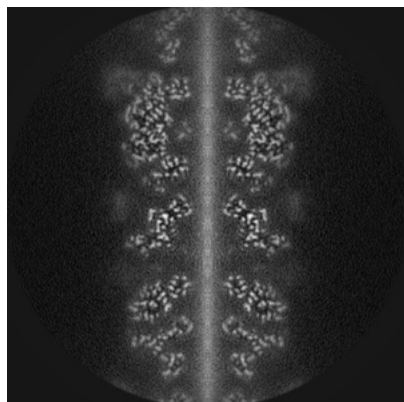


Y Index: 160

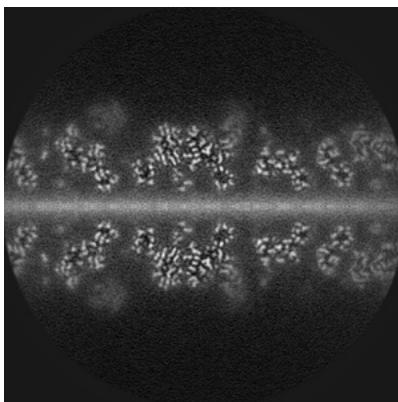


Z Index: 160

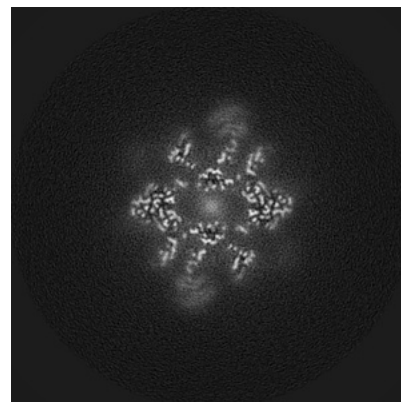
6.2.2 Raw map



X Index: 160



Y Index: 160

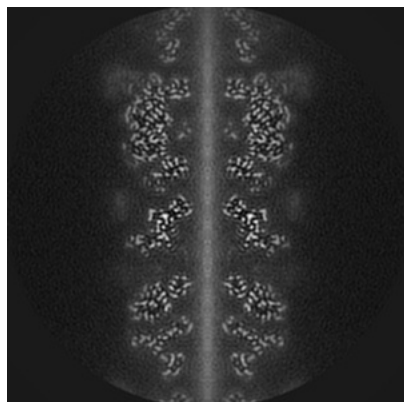


Z Index: 160

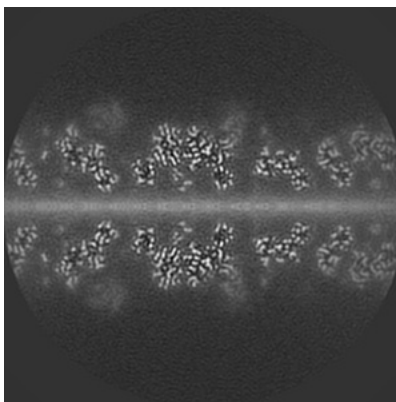
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

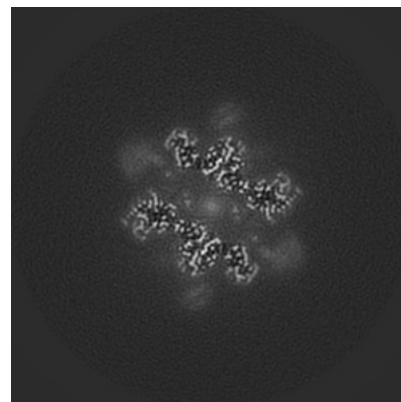
6.3.1 Primary map



X Index: 160

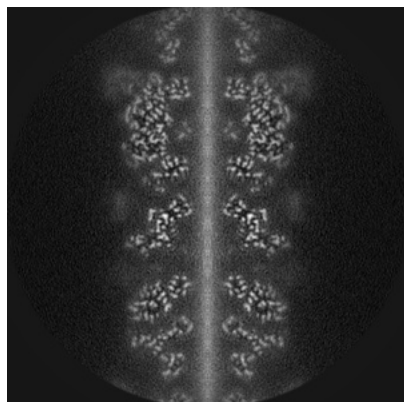


Y Index: 160

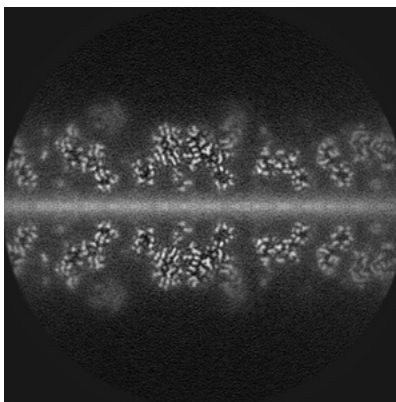


Z Index: 150

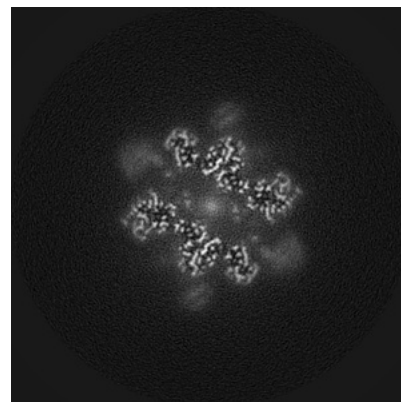
6.3.2 Raw map



X Index: 160



Y Index: 160

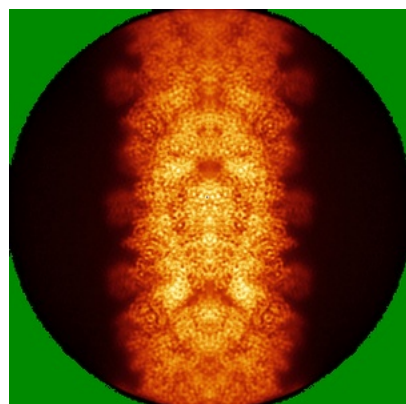


Z Index: 150

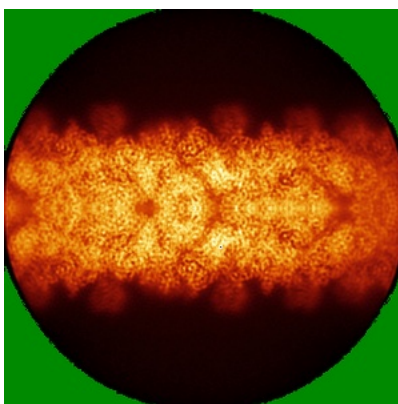
The images above show the largest variance slices of the map in three orthogonal directions.

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

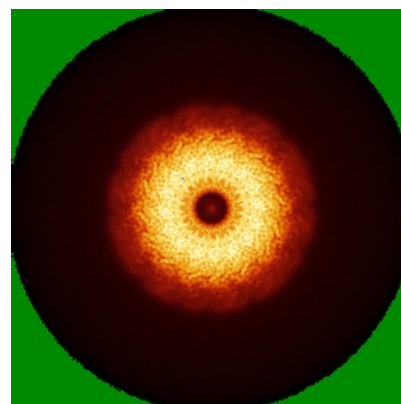
6.4.1 Primary map



X

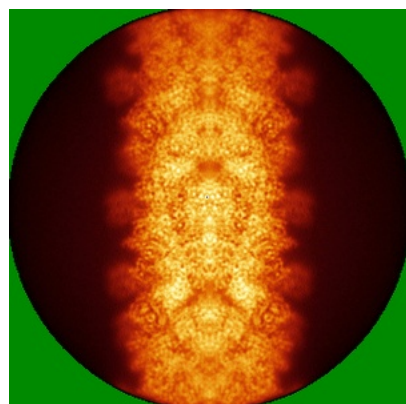


Y

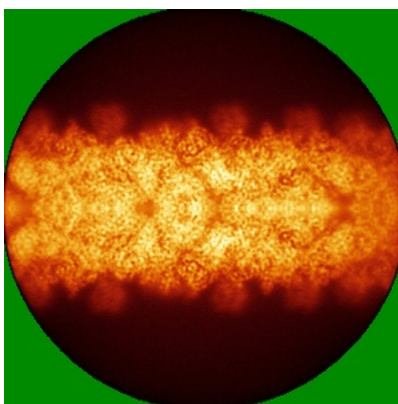


Z

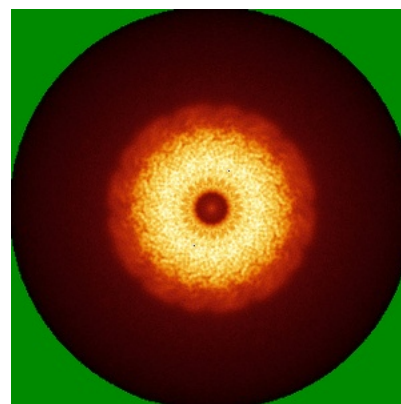
6.4.2 Raw map



X



Y

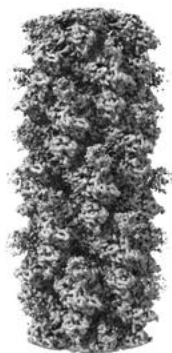


Z

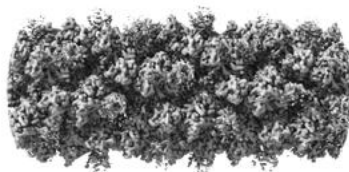
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

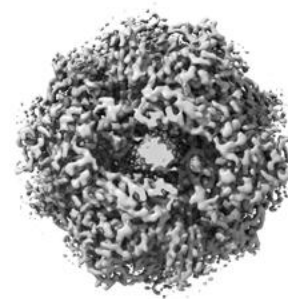
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

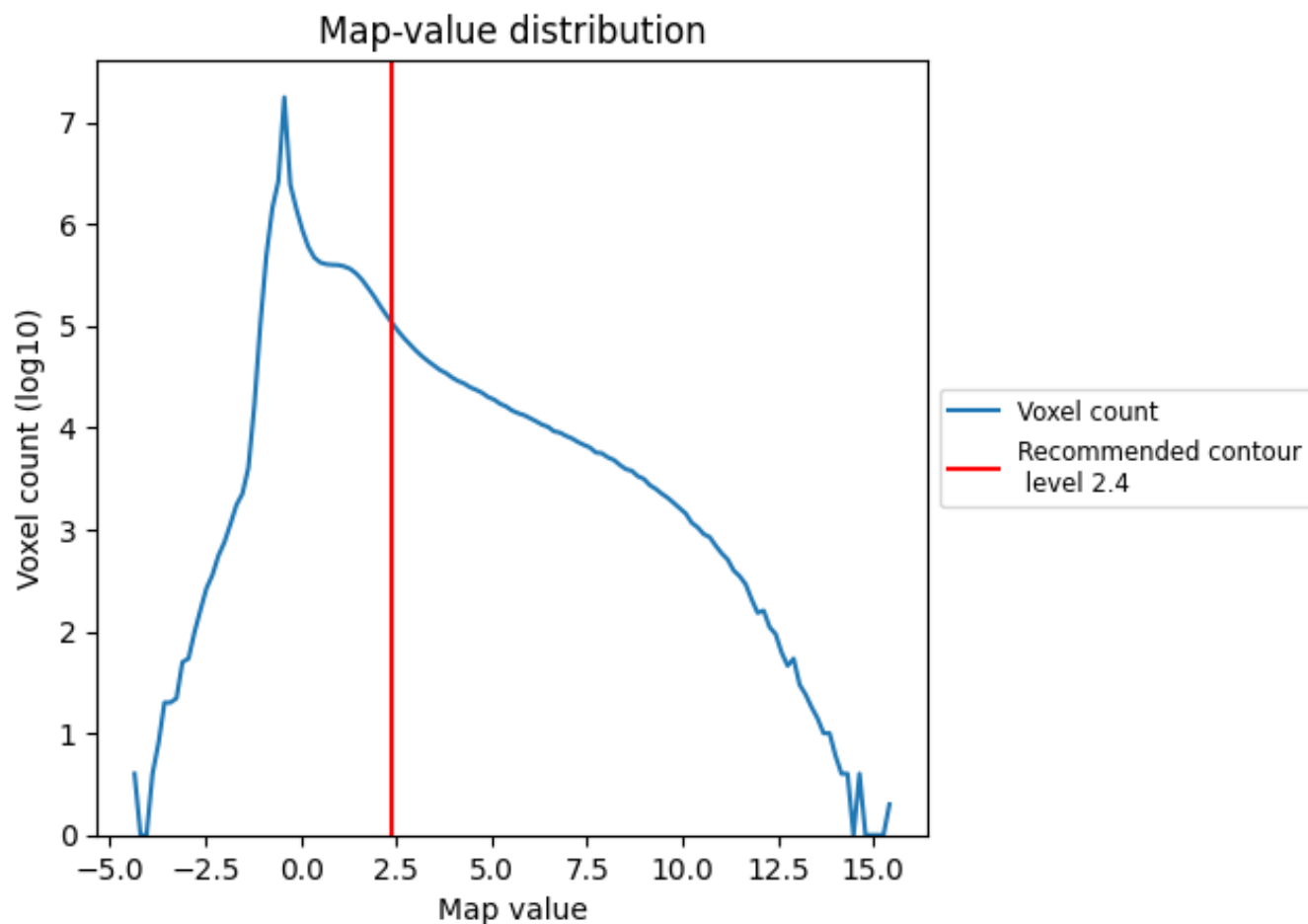
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

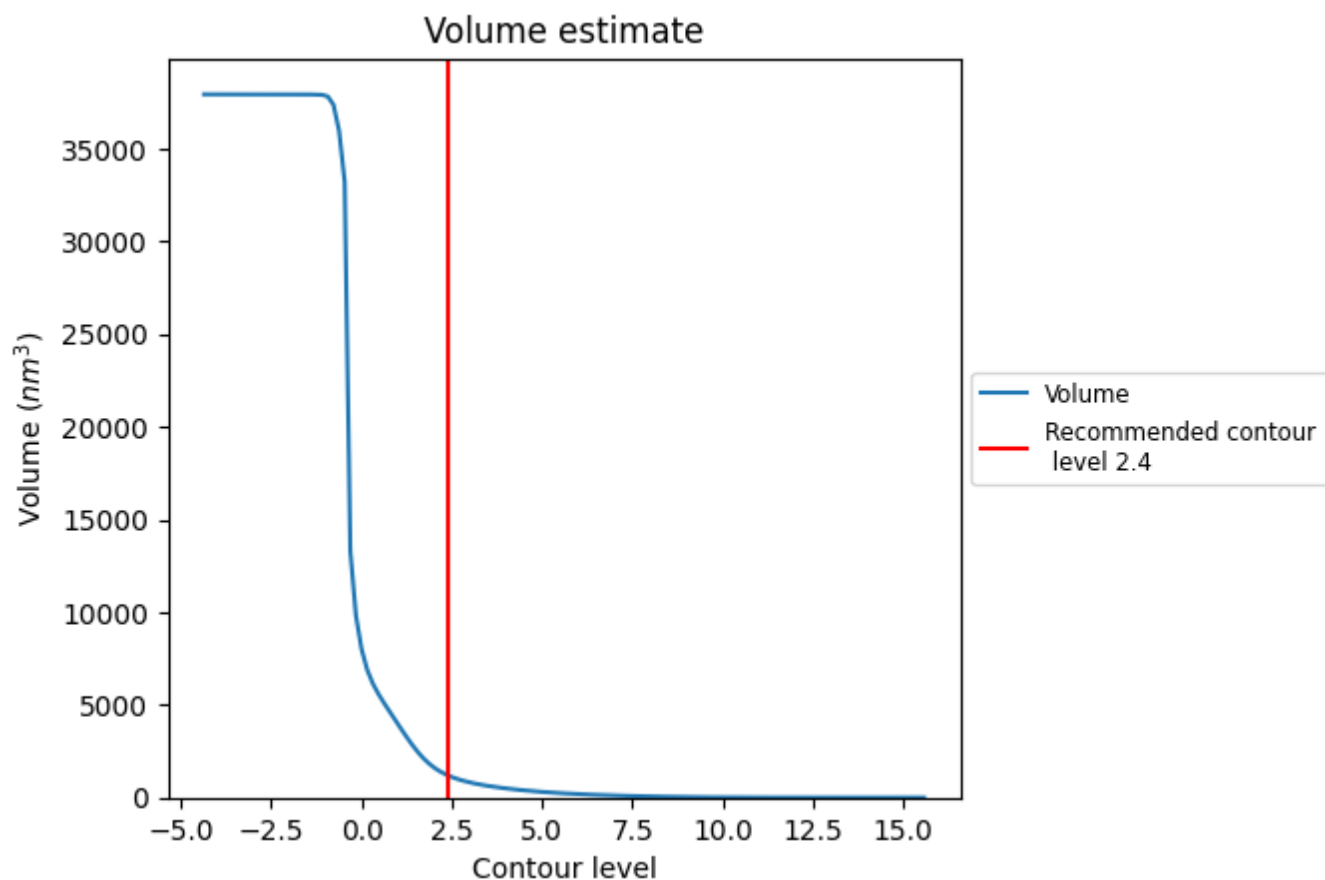
This section contains the results of statistical analysis of the map.

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.

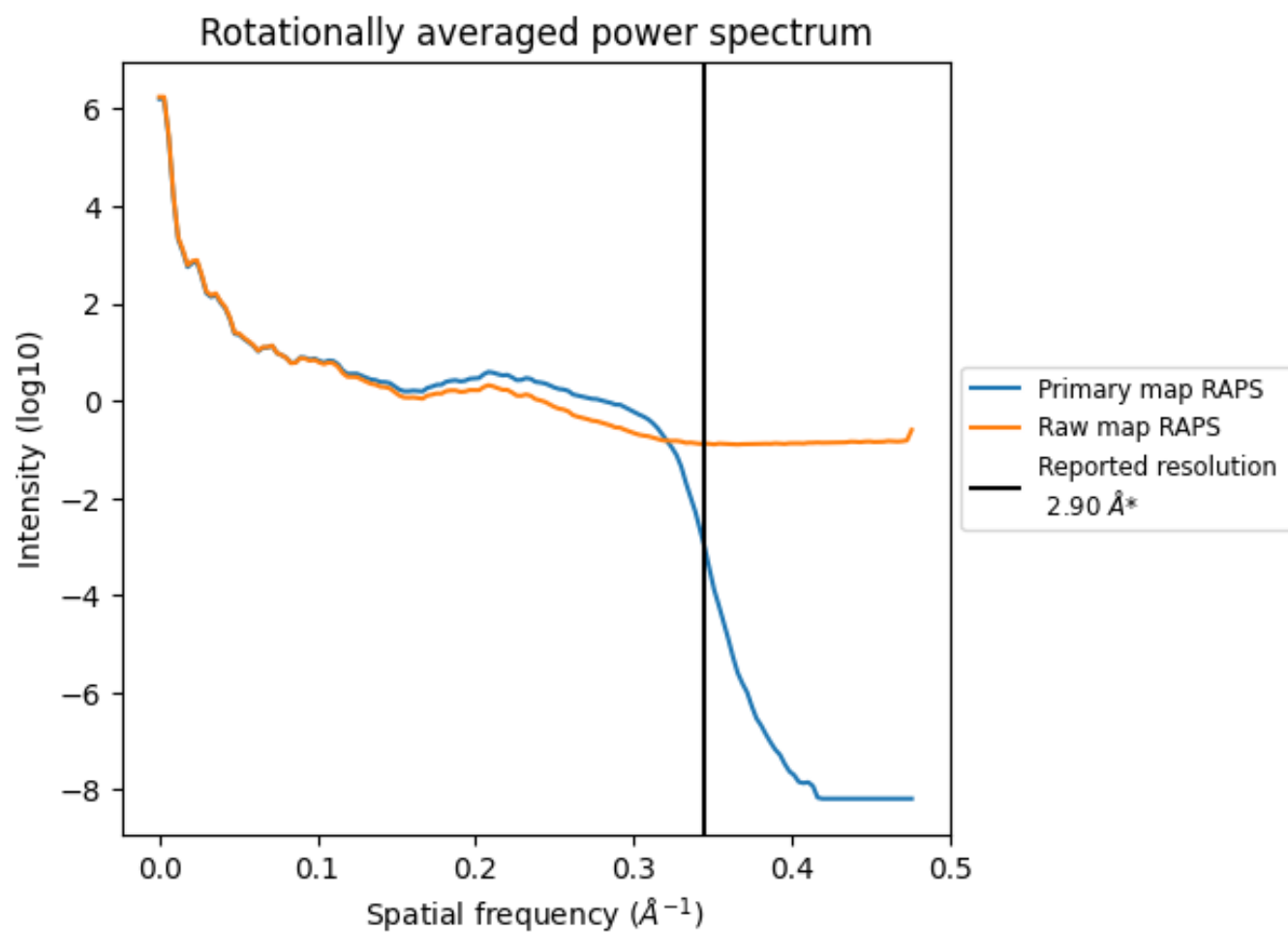
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1194 nm^3 ; this corresponds to an approximate mass of 1078 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 ⓘ

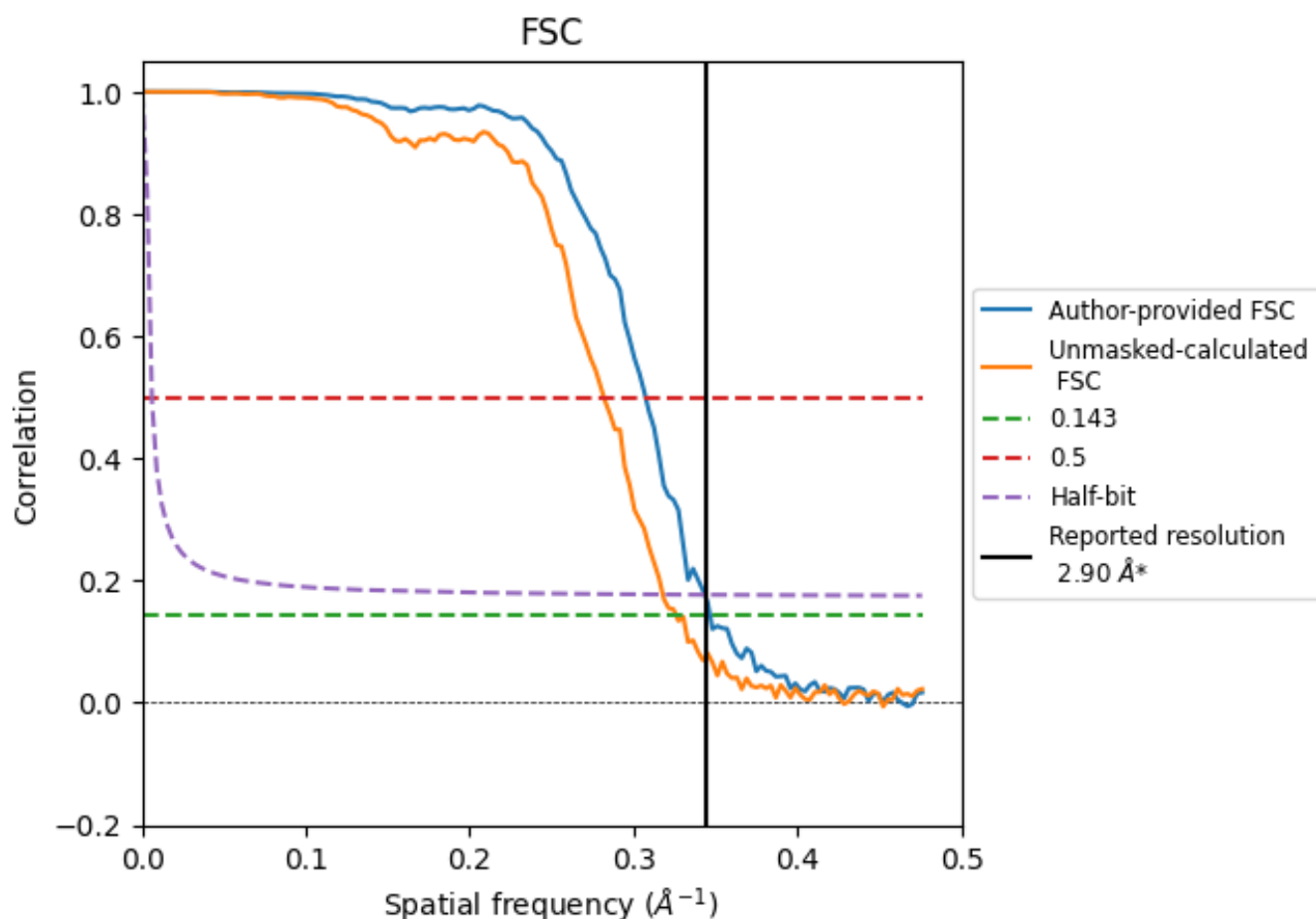


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.88	3.25	2.91
Unmasked-calculated*	3.07	3.55	3.15

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

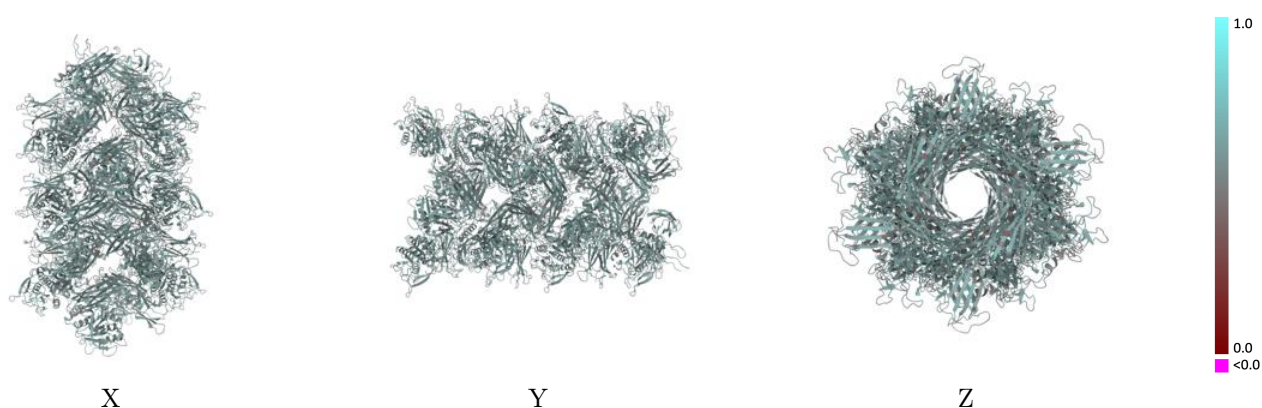
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-36428 and PDB model 8JMW. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

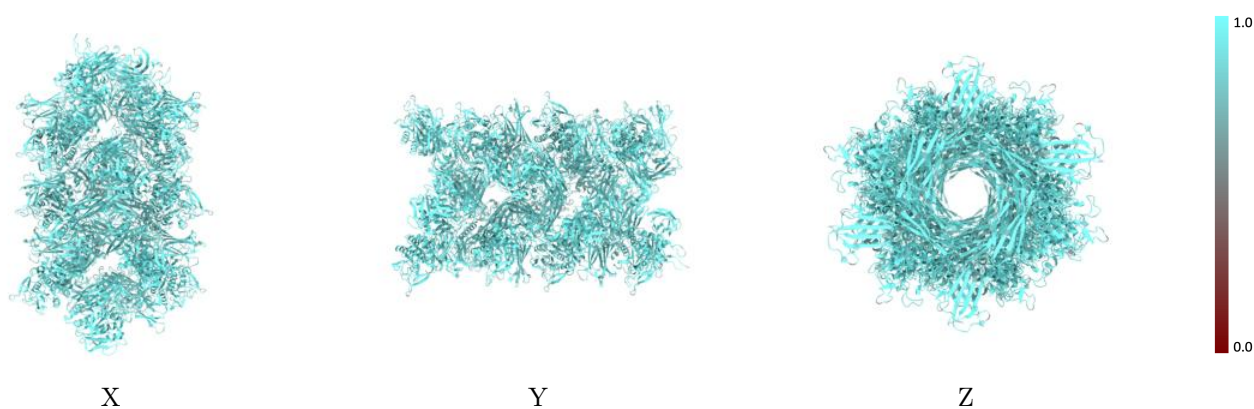
This section was not generated.

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



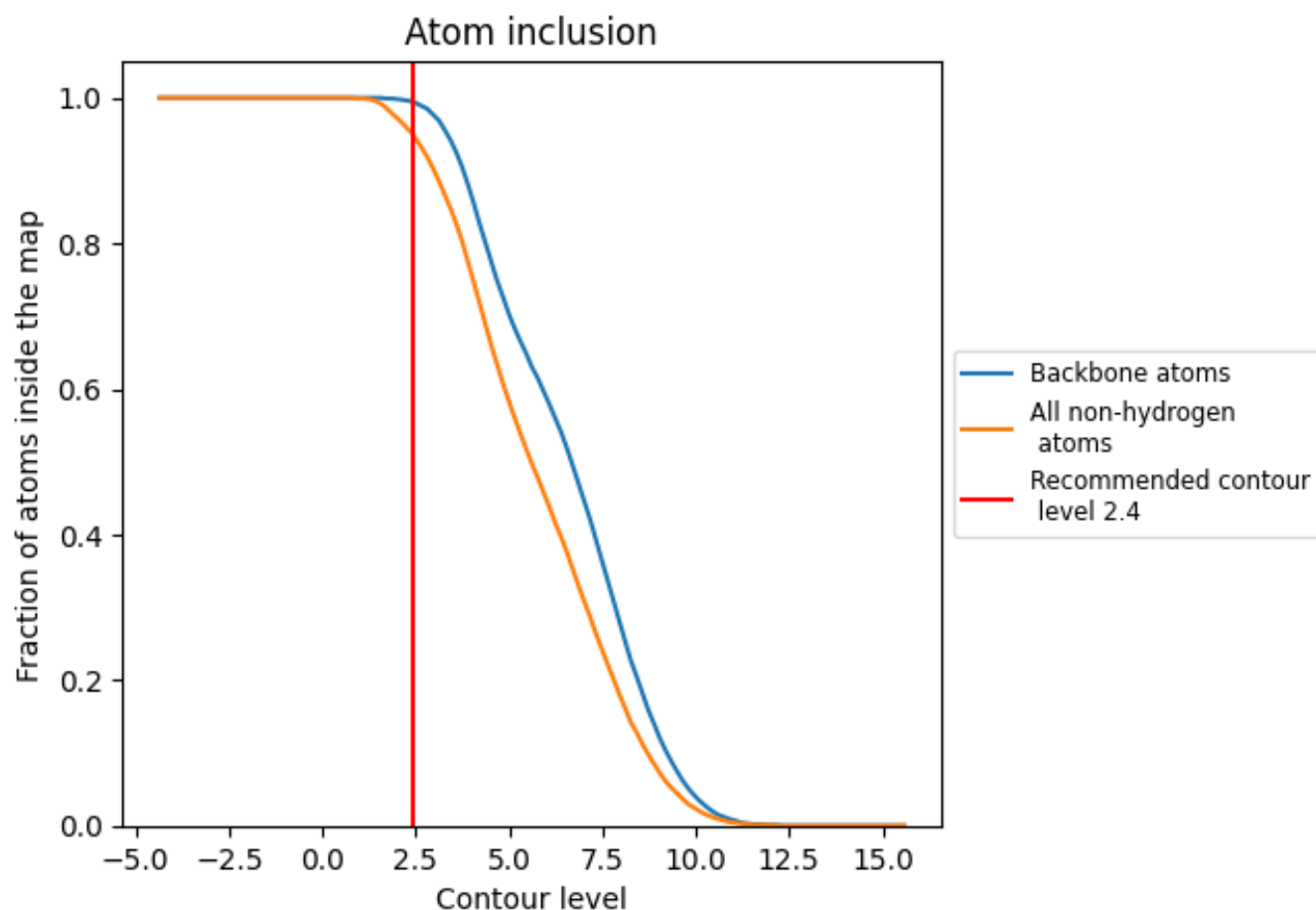
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 95% 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 (2.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9510	 0.5670
A	 0.9550	 0.5720
B	 0.9550	 0.5720
C	 0.9540	 0.5670
D	 0.9530	 0.5660
E	 0.9480	 0.5590
F	 0.9530	 0.5710
G	 0.9490	 0.5640
H	 0.9480	 0.5670
I	 0.9430	 0.5620
J	 0.9550	 0.5730
K	 0.9550	 0.5720
L	 0.9540	 0.5650
M	 0.9530	 0.5670
N	 0.9480	 0.5600
O	 0.9530	 0.5720
P	 0.9490	 0.5670
Q	 0.9480	 0.5660
R	 0.9430	 0.5610

