



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 11:09 PM UTC

PDB ID : 6VZG / pdb_00006vzg
EMDB ID : EMD-21489
Title : Cryo-EM structure of Sth1-Arp7-Arp9-Rtt102
Authors : Leschziner, A.E.; Baker, R.W.
Deposited on : 2020-02-28
Resolution : 4.20 Å(reported)
Based on initial models : 5TGC, 4I6M

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:

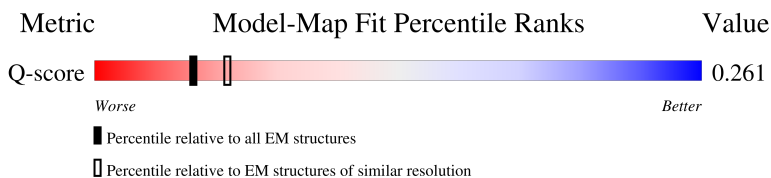
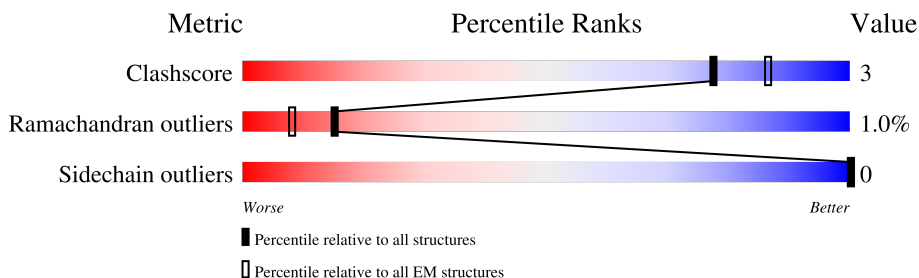
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 4.20 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.



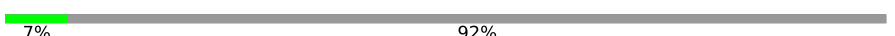
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

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	1-L	477	68% 76% 6% 18%
1	10-L	477	74% 8% 18%
1	2-L	477	76% 6% 18%
1	3-L	477	74% 7% 18%

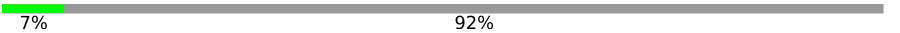
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Mol	Chain	Length	Quality of chain
1	4-L	477	 74%8%18%
1	5-L	477	 75%7%18%
1	6-L	477	 76%6%18%
1	7-L	477	 74%8%18%
1	8-L	477	 74%8%18%
1	9-L	477	 75%7%18%
2	1-M	467	 77%79%6%15%
2	10-M	467	 79%6%15%
2	2-M	467	 78%6%15%
2	3-M	467	 77%7%15%
2	4-M	467	 78%6%15%
2	5-M	467	 78%7%15%
2	6-M	467	 77%7%15%
2	7-M	467	 78%6%15%
2	8-M	467	 79%6%15%
2	9-M	467	 78%6%15%
3	1-K	813	 8%7%92%
3	10-K	813	 7%92%
3	2-K	813	 8%92%
3	3-K	813	 8%92%
3	4-K	813	 7%92%
3	5-K	813	 7%92%
3	6-K	813	 7%92%
3	7-K	813	 7%92%
3	8-K	813	 7%92%

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Mol	Chain	Length	Quality of chain
3	9-K	813	
4	1-N	157	
4	10-N	157	
4	2-N	157	
4	3-N	157	
4	4-N	157	
4	5-N	157	
4	6-N	157	
4	7-N	157	
4	8-N	157	
4	9-N	157	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 74080 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 Actin-related protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1-L	393	Total	C	N	O	S	0	0
			3154	2035	514	590	15		
1	2-L	393	Total	C	N	O	S	0	0
			3154	2035	514	590	15		
1	3-L	393	Total	C	N	O	S	0	0
			3154	2035	514	590	15		
1	4-L	393	Total	C	N	O	S	0	0
			3154	2035	514	590	15		
1	5-L	393	Total	C	N	O	S	0	0
			3154	2035	514	590	15		
1	6-L	393	Total	C	N	O	S	0	0
			3154	2035	514	590	15		
1	7-L	393	Total	C	N	O	S	0	0
			3154	2035	514	590	15		
1	8-L	393	Total	C	N	O	S	0	0
			3154	2035	514	590	15		
1	9-L	393	Total	C	N	O	S	0	0
			3154	2035	514	590	15		
1	10-L	393	Total	C	N	O	S	0	0
			3154	2035	514	590	15		

- Molecule 2 is a protein called Actin-like protein ARP9.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1-M	396	Total	C	N	O	S	0	0
			3192	2048	521	616	7		
2	2-M	396	Total	C	N	O	S	0	0
			3192	2048	521	616	7		
2	3-M	396	Total	C	N	O	S	0	0
			3192	2048	521	616	7		
2	4-M	396	Total	C	N	O	S	0	0
			3192	2048	521	616	7		
2	5-M	396	Total	C	N	O	S	0	0
			3192	2048	521	616	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	6-M	396	Total	C	N	O	S	0	0
			3192	2048	521	616	7		
2	7-M	396	Total	C	N	O	S	0	0
			3192	2048	521	616	7		
2	8-M	396	Total	C	N	O	S	0	0
			3192	2048	521	616	7		
2	9-M	396	Total	C	N	O	S	0	0
			3192	2048	521	616	7		
2	10-M	396	Total	C	N	O	S	0	0
			3192	2048	521	616	7		

- Molecule 3 is a protein called Nuclear protein STH1/NPS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1-K	62	Total	C	N	O	S	0	0
			537	329	110	96	2		
3	2-K	62	Total	C	N	O	S	0	0
			537	329	110	96	2		
3	3-K	62	Total	C	N	O	S	0	0
			537	329	110	96	2		
3	4-K	62	Total	C	N	O	S	0	0
			537	329	110	96	2		
3	5-K	62	Total	C	N	O	S	0	0
			537	329	110	96	2		
3	6-K	62	Total	C	N	O	S	0	0
			537	329	110	96	2		
3	7-K	62	Total	C	N	O	S	0	0
			537	329	110	96	2		
3	8-K	62	Total	C	N	O	S	0	0
			537	329	110	96	2		
3	9-K	62	Total	C	N	O	S	0	0
			537	329	110	96	2		
3	10-K	62	Total	C	N	O	S	0	0
			537	329	110	96	2		

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	285	MET	-	initiating methionine	UNP P32597
K	286	GLY	-	expression tag	UNP P32597
K	287	SER	-	expression tag	UNP P32597
K	288	SER	-	expression tag	UNP P32597

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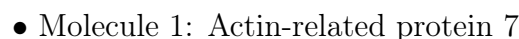
Chain	Residue	Modelled	Actual	Comment	Reference
K	289	HIS	-	expression tag	UNP P32597
K	290	HIS	-	expression tag	UNP P32597
K	291	HIS	-	expression tag	UNP P32597
K	292	HIS	-	expression tag	UNP P32597
K	293	HIS	-	expression tag	UNP P32597
K	294	HIS	-	expression tag	UNP P32597
K	295	SER	-	expression tag	UNP P32597
K	296	GLN	-	expression tag	UNP P32597
K	297	ASP	-	expression tag	UNP P32597
K	298	PRO	-	expression tag	UNP P32597
K	299	ASN	-	expression tag	UNP P32597
K	300	SER	-	expression tag	UNP P32597
K	372	LYS	ARG	conflict	UNP P32597

- Molecule 4 is a protein called Regulator of Ty1 transposition protein 102.

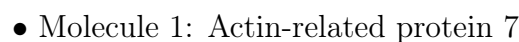
Mol	Chain	Residues	Atoms					AltConf	Trace
4	1-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		
4	2-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		
4	3-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		
4	4-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		
4	5-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		
4	6-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		
4	7-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		
4	8-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		
4	9-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		
4	10-N	55	Total	C	N	O	S	0	0
			494	315	85	92	2		

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

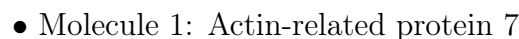
Response	Percentage
Yes	76%
No	6%
Don't know	18%



Category	Percentage
Very good	74%
Good	8%
Not good	18%
Very bad	0%

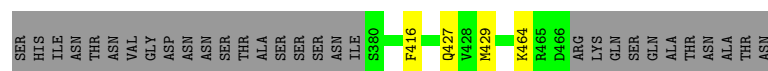


Category	Percentage
Very good	74%
Good	8%
Not good	18%
Very bad	0%

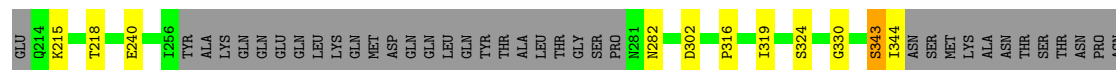
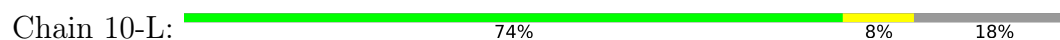


App Type	Percentage
Shopping app	75%
Social media app	7%
Productivity app	18%

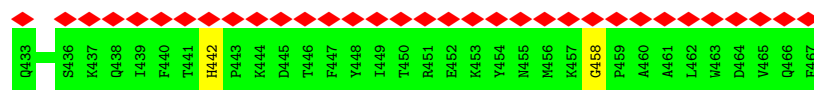
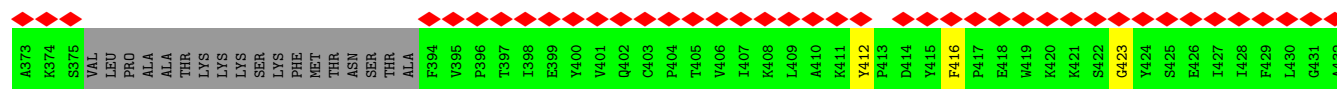
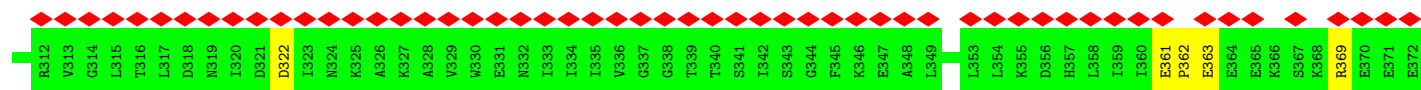
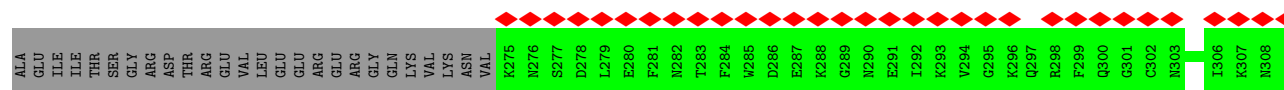
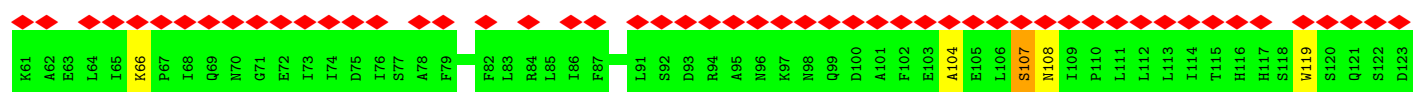
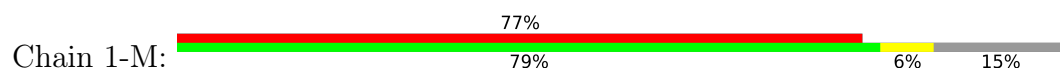




• Molecule 1: Actin-related protein 7

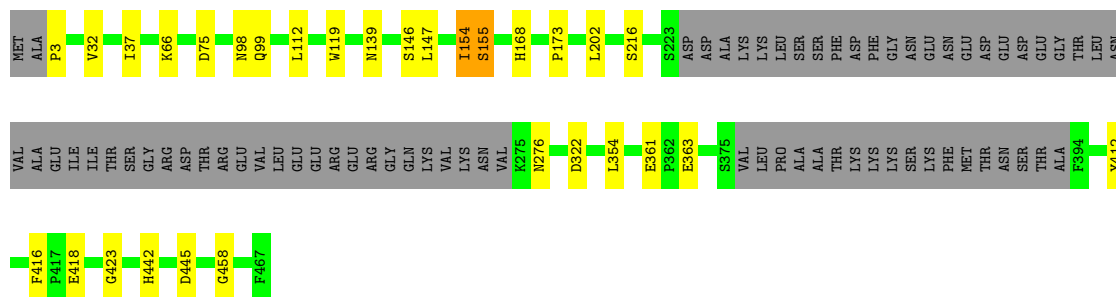


• Molecule 2: Actin-like protein ARP9



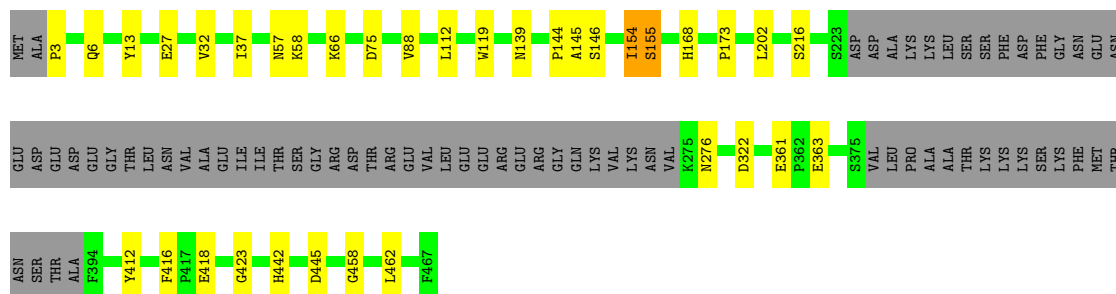
• Molecule 2: Actin-like protein ARP9

Chain 2-M:  78% 6% 15%



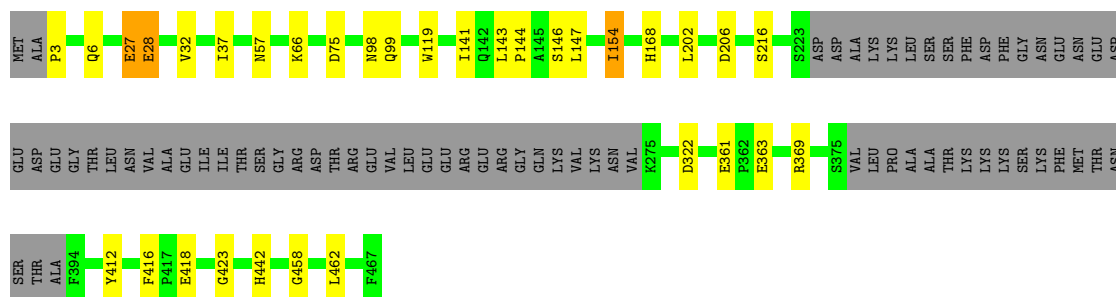
- Molecule 2: Actin-like protein ARP9

Chain 3-M:  77% 7% 15%



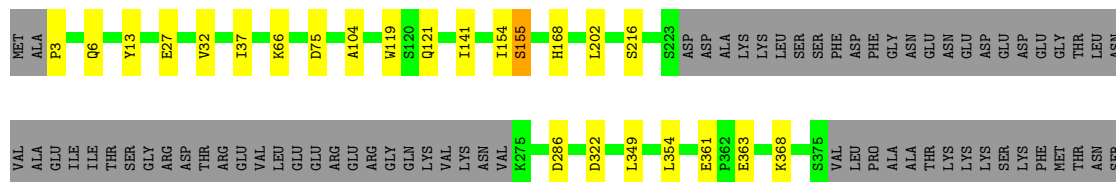
- Molecule 2: Actin-like protein ARP9

Chain 4-M:  78% 6% 15%



- Molecule 2: Actin-like protein ARP9

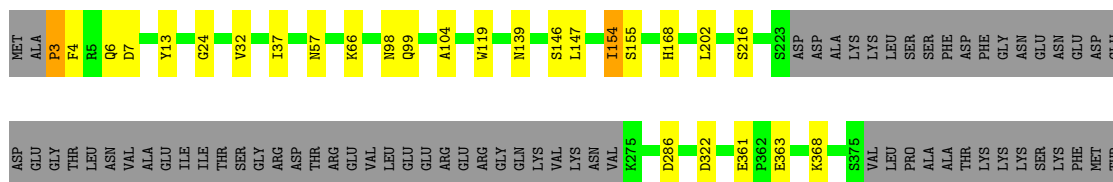
Chain 5-M:  78% 7% 15%





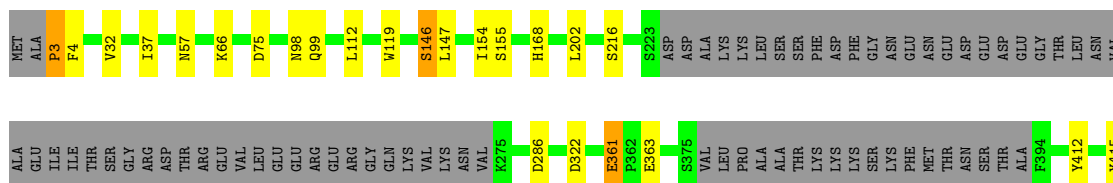
- Molecule 2: Actin-like protein ARP9

Chain 6-M: 77% 7% 15%



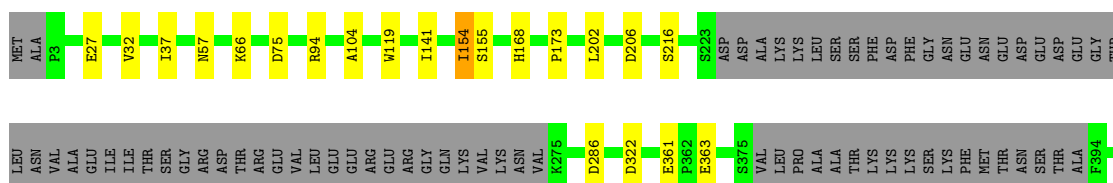
- Molecule 2: Actin-like protein ARP9

Chain 7-M: 78% 6% 15%



- Molecule 2: Actin-like protein ARP9

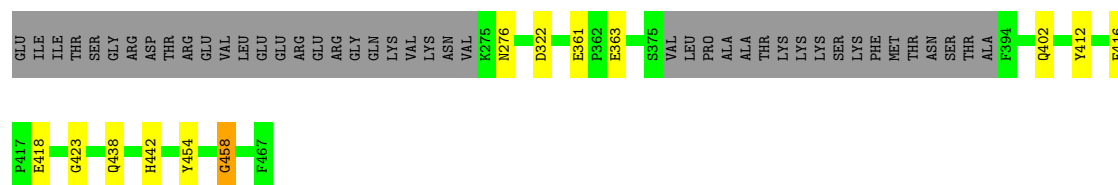
Chain 8-M: 79% 6% 15%



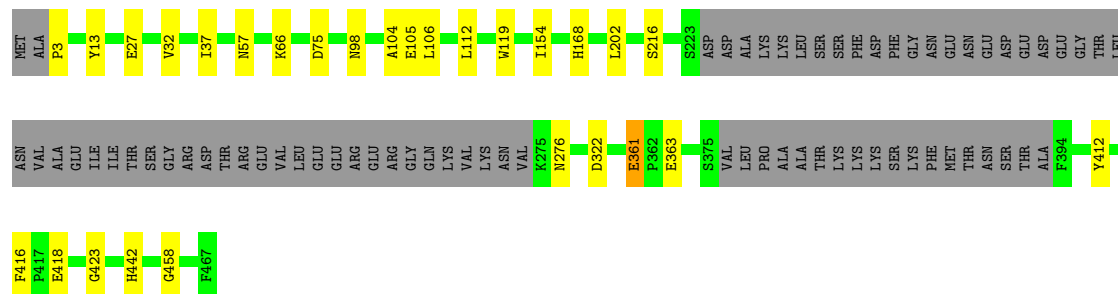
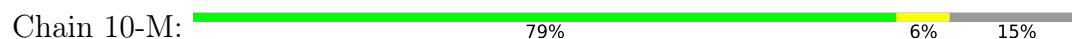
- Molecule 2: Actin-like protein ARP9

Chain 9-M: 78% 6% 15%

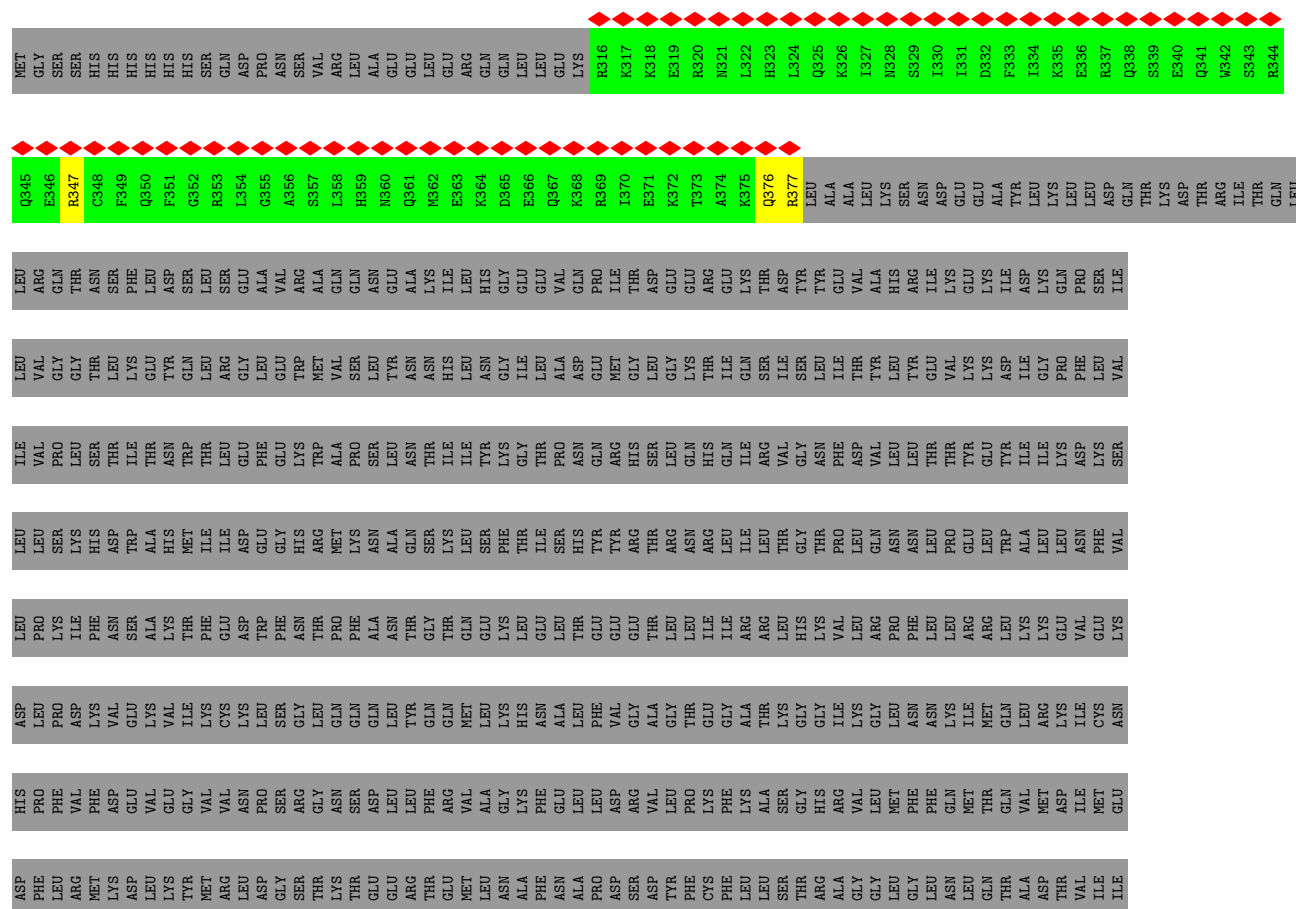




- Molecule 2: Actin-like protein ARP9

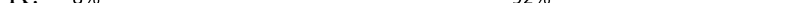


- Molecule 3: Nuclear protein STH1/NPS1



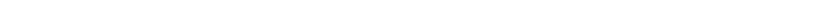
[illegible]

- Molecule 3: Nuclear protein STH1/NPS1

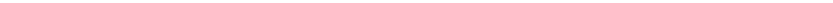
Chain 2-K:  8% 92%

[illegible]

- Molecule 3: Nuclear protein STH1/NPS1

Chain 3-K:  8% 92%

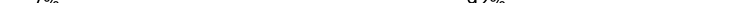
- Molecule 3: Nuclear protein STH1/NPS1

Chain 4-K:  7% 92%

LYS	PRO	GLN	TLE	MET
ASP	PHE	PRO	THR	GLY
LYS	LEU	SER	GLN	SER
SER	SER	ILE	LEU	LEU
LEU	ILE	VAL	ARG	HIS
LEU	VAL	GLY	GLN	HIS
SER	PRO	GLY	THR	HIS
LYS	LEU	GLY	THR	HIS
HIS	SER	THR	ASN	HIS
ASP	THR	LEU	SER	SER
TRP	ILE	LYS	PHE	SER
ALA	THR	GLU	LEU	GLN
HIS	ASN	TRR	ASP	ASP
MET	TRP	GLN	SER	PRO
ILE	THR	LEU	LEU	ASN
ILE	LEU	ARG	SER	VAL
ASP	GLU	GLY	GLU	VAL
GLY	PHE	LEU	ALA	ARG
GLY	GLU	GLU	VAL	LEU
HIS	LYS	TRP	ARG	ALA
ARG	TRP	MET	ALA	GLU
MET	ALA	VAL	GLN	GLU
LYS	PRO	SER	GLN	LEU
ASN	SER	LEU	ASN	GLU
ALA	LEU	TRR	GLU	ARG
GLN	ASN	ASN	ALA	GLN
SER	THR	ASN	LYS	GLN
ILE	ILE	HIS	ILE	LEU
LYS	ILE	LEU	LEU	LEU
SER	TYR	ASN	HIS	LYS
PHE	GLY	GLY	GLY	GLY
THR	LYS	ILE	GLU	RS16
ILE	SER	LEU	GLU	Q341
SER	PRO	ALA	VAL	W342
ARG	ASN	ASP	GLN	W342
ARG	GLN	GLU	PRO	RS17
ASN	GLN	LYS	GLU	LEU
ARG	HIS	THR	ARG	LYS
LEU	GLN	ILE	GLU	SER
ILE	ILE	GLN	LYS	ASN
LEU	ARG	SER	THR	ASP
THR	VAL	ILE	ASP	GLU
GLY	GLY	SER	TYR	GLU
THR	ASN	LEU	TYR	ALA
PRO	PHE	ILE	GLU	TYR
LEU	ASP	THR	VAL	LEU
GLN	VAL	TRR	ALA	LYS
ASN	LEU	LEU	HIS	LEU
ASN	LEU	TYR	ARG	LEU
LEU	THR	GLU	ILE	ASP
PRO	THR	VAL	LYS	GLN
GLU	TYR	GLU	GLU	THR
LEU	GLU	LYS	LYS	LYS
TRP	TYR	ASP	ILE	ASP
ALA	ILE	ILE	ASP	THR
LEU	ILE	GLY	LYS	ASP

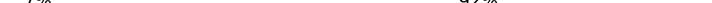
[illegible]

- Molecule 3: Nuclear protein STH1/NPS1

Chain 6-K:  7% 92%

[illegible]

- Molecule 3: Nuclear protein STH1/NPS1

Chain 7-K:  7% 92%

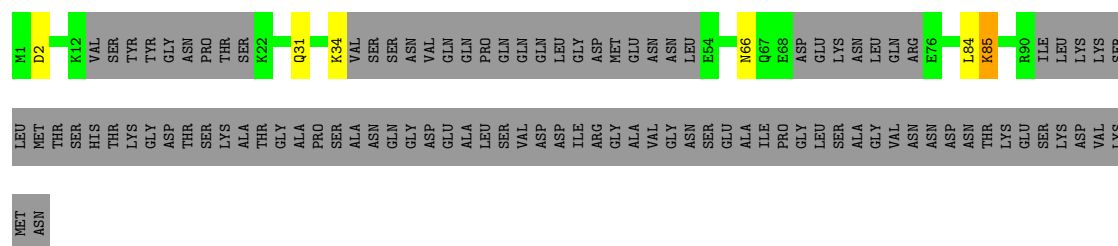
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ILE	THR	GLN	LEU	LEU	ARG	GLN	THR	THR	ASN	SER	PHE	LEU	ASP	SER	LEU	GLU	ALA	VAL	ARG	GLU	GLN	GLN	ASN	GLU	ALA	LYS	ILE	LEU	GLY	GLU	VAL	GLN	PRO	ILE	THR	ASP	GLU	GLU	GLU	ARG	GLU	LYS	VAL	ALA	ALA	HIS	LEU	ILE	LYS	GLU	ILE	ASP	LYS

[illegible]

Chain 1-N:

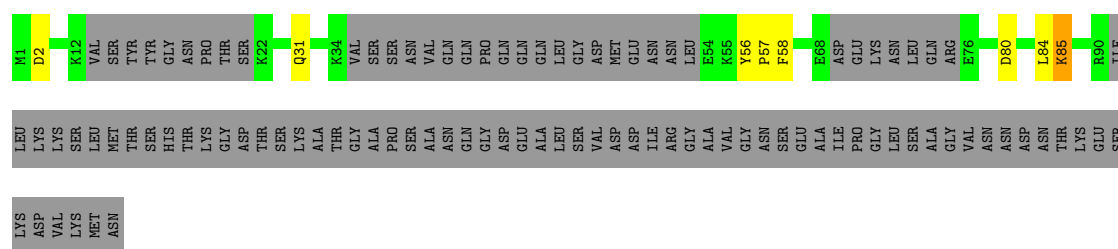
LEU	SER	VAL	ASP	ASP	ILE	ARG	GLY	ALA	VAL	GLY	ASP	ASN	GLU	LYS	ASN	LEU	GLN	ARG	E76	S77	G78	E79	D80	T81	L82	D83	L84	E85	E86	F87	D88	R89	R90	ILE	LEU	LYS	LYS	SER	SER	LEU	MET	THR	SER	SER	HIS	THR	LYS	GLY	ASP	THR	SER	LYS	ALA	THR	GLY	ALA	PRO	SER	ALA	ASN	GLN	GLY	ASP	MET	ASN	GLU	LEU	E54	K55	Y56	P57	F58	R59	Y60
M1	D2	P3	Q4	T5	L6	I7	T8	K9	A10	M11	K12	VAL	SER	TYR	TYR	GLY	ASN	PRO	THR	SER	K22	E23	S24	W25	R26	Y27	D28	W29	Y30	Q31	P32	S33	K34	VAL	SER	SER	ASN	VAL	GLN	GLN	PRO	GLN	GLN	LEU	GLY	ASP	MET	GLU	ASN	ASN	LEU	E54	K55	Y56	P57	F58	R59	Y60																

Chain 2-N: 31% 65%



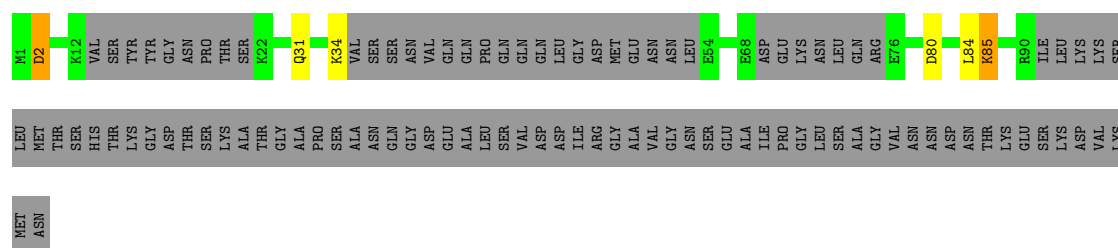
- Molecule 4: Regulator of Ty1 transposition protein 102

Chain 3-N: 30% 65%



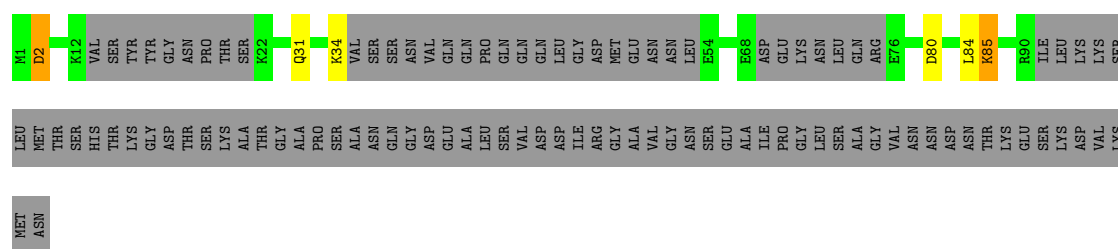
- Molecule 4: Regulator of Ty1 transposition protein 102

Chain 4-N: 31% 65%



- Molecule 4: Regulator of Ty1 transposition protein 102

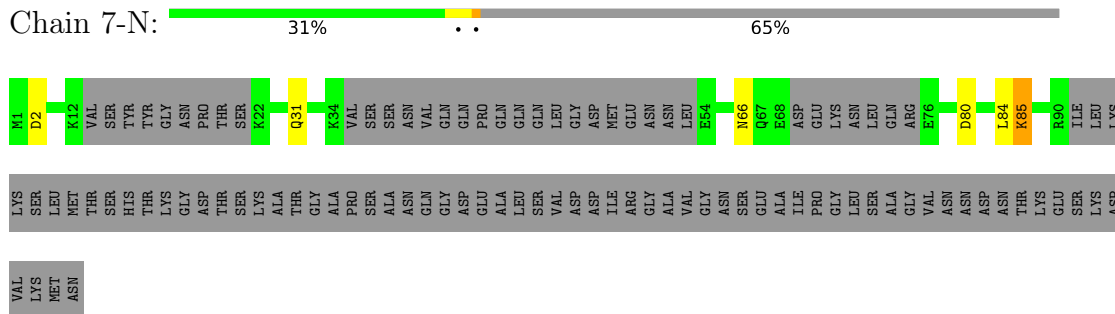
Chain 5-N: 31% 65%



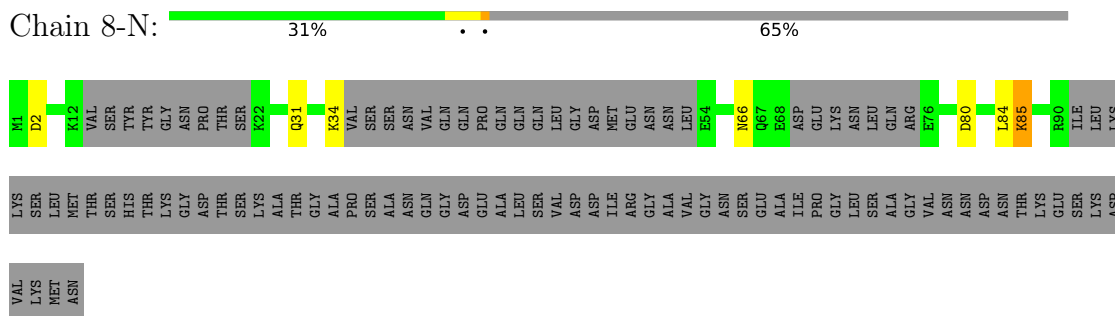
- Molecule 4: Regulator of Ty1 transposition protein 102

Chain 6-N: 32% 65%

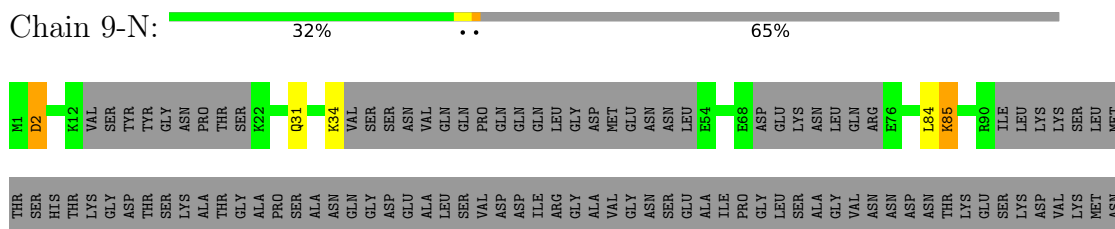
● Molecule 4: Regulator of Ty1 transposition protein 102



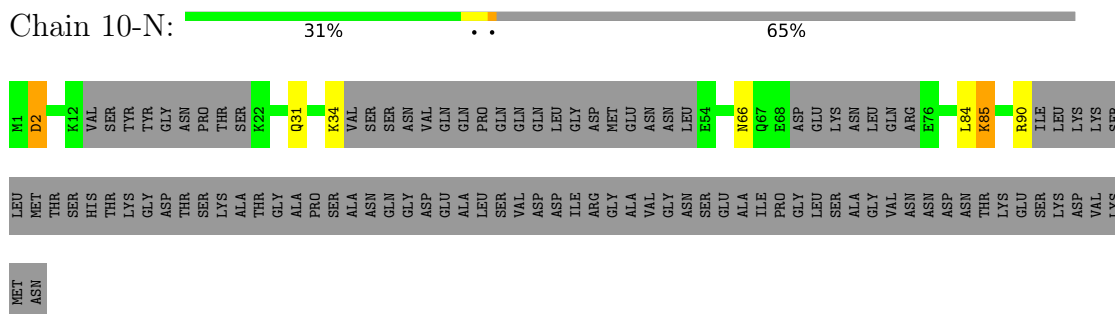
- Molecule 4: Regulator of Ty1 transposition protein 102



- Molecule 4: Regulator of Ty1 transposition protein 102



- Molecule 4: Regulator of Ty1 transposition protein 102



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	415957	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	36000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.043	Depositor
Minimum map value	-0.014	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	278.4, 278.4, 278.4	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ATP

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	1-L	0.71	0/3220	0.75	22/4355 (0.5%)
1	2-L	0.71	0/3220	0.75	22/4355 (0.5%)
1	3-L	0.71	0/3220	0.75	22/4355 (0.5%)
1	4-L	0.71	0/3220	0.75	22/4355 (0.5%)
1	5-L	0.71	0/3220	0.75	22/4355 (0.5%)
1	6-L	0.71	0/3220	0.75	22/4355 (0.5%)
1	7-L	0.71	0/3220	0.75	22/4355 (0.5%)
1	8-L	0.71	0/3220	0.75	22/4355 (0.5%)
1	9-L	0.71	0/3220	0.75	22/4355 (0.5%)
1	10-L	0.71	0/3220	0.75	22/4355 (0.5%)
2	1-M	0.68	0/3259	0.72	22/4417 (0.5%)
2	2-M	0.68	0/3259	0.72	22/4417 (0.5%)
2	3-M	0.68	0/3259	0.72	22/4417 (0.5%)
2	4-M	0.68	0/3259	0.72	22/4417 (0.5%)
2	5-M	0.68	0/3259	0.72	22/4417 (0.5%)
2	6-M	0.68	0/3259	0.72	22/4417 (0.5%)
2	7-M	0.68	0/3259	0.72	22/4417 (0.5%)
2	8-M	0.68	0/3259	0.72	22/4417 (0.5%)
2	9-M	0.68	0/3259	0.72	22/4417 (0.5%)
2	10-M	0.68	0/3259	0.72	22/4417 (0.5%)
3	1-K	0.64	0/543	0.38	0/716
3	2-K	0.64	0/543	0.38	0/716
3	3-K	0.64	0/543	0.38	0/716
3	4-K	0.64	0/543	0.38	0/716
3	5-K	0.64	0/543	0.38	0/716
3	6-K	0.64	0/543	0.38	0/716
3	7-K	0.64	0/543	0.38	0/716
3	8-K	0.64	0/543	0.38	0/716
3	9-K	0.64	0/543	0.38	0/716
3	10-K	0.64	0/543	0.38	0/716
4	1-N	0.64	0/505	0.77	4/674 (0.6%)
4	2-N	0.64	0/505	0.77	4/674 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	3-N	0.64	0/505	0.77	4/674 (0.6%)
4	4-N	0.64	0/505	0.77	4/674 (0.6%)
4	5-N	0.64	0/505	0.77	4/674 (0.6%)
4	6-N	0.64	0/505	0.77	4/674 (0.6%)
4	7-N	0.64	0/505	0.77	4/674 (0.6%)
4	8-N	0.64	0/505	0.77	4/674 (0.6%)
4	9-N	0.64	0/505	0.77	4/674 (0.6%)
4	10-N	0.64	0/505	0.77	4/674 (0.6%)
All	All	0.69	0/75270	0.72	480/101620 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	2-L	0	1
1	3-L	0	2
1	6-L	0	2
1	8-L	0	2
1	10-L	0	2
2	1-M	0	2
2	2-M	0	2
2	3-M	0	2
2	4-M	0	2
2	5-M	0	4
2	6-M	0	2
2	7-M	0	4
2	9-M	0	2
2	10-M	0	2
All	All	0	31

There are no bond length outliers.

All (480) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-L	416	PHE	CA-C-N	8.25	127.89	119.56
1	1-L	416	PHE	C-N-CA	8.25	127.89	119.56
1	2-L	416	PHE	CA-C-N	8.25	127.89	119.56
1	2-L	416	PHE	C-N-CA	8.25	127.89	119.56
1	3-L	416	PHE	CA-C-N	8.25	127.89	119.56
1	3-L	416	PHE	C-N-CA	8.25	127.89	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4-L	416	PHE	CA-C-N	8.25	127.89	119.56
1	4-L	416	PHE	C-N-CA	8.25	127.89	119.56
1	5-L	416	PHE	CA-C-N	8.25	127.89	119.56
1	5-L	416	PHE	C-N-CA	8.25	127.89	119.56
1	6-L	416	PHE	CA-C-N	8.25	127.89	119.56
1	6-L	416	PHE	C-N-CA	8.25	127.89	119.56
1	7-L	416	PHE	CA-C-N	8.25	127.89	119.56
1	7-L	416	PHE	C-N-CA	8.25	127.89	119.56
1	8-L	416	PHE	CA-C-N	8.25	127.89	119.56
1	8-L	416	PHE	C-N-CA	8.25	127.89	119.56
1	9-L	416	PHE	CA-C-N	8.25	127.89	119.56
1	9-L	416	PHE	C-N-CA	8.25	127.89	119.56
1	10-L	416	PHE	CA-C-N	8.25	127.89	119.56
1	10-L	416	PHE	C-N-CA	8.25	127.89	119.56
2	1-M	202	LEU	CA-C-N	8.07	127.80	119.56
2	1-M	202	LEU	C-N-CA	8.07	127.80	119.56
2	2-M	202	LEU	CA-C-N	8.07	127.80	119.56
2	2-M	202	LEU	C-N-CA	8.07	127.80	119.56
2	3-M	202	LEU	CA-C-N	8.07	127.80	119.56
2	3-M	202	LEU	C-N-CA	8.07	127.80	119.56
2	4-M	202	LEU	CA-C-N	8.07	127.80	119.56
2	4-M	202	LEU	C-N-CA	8.07	127.80	119.56
2	5-M	202	LEU	CA-C-N	8.07	127.80	119.56
2	5-M	202	LEU	C-N-CA	8.07	127.80	119.56
2	6-M	202	LEU	CA-C-N	8.07	127.80	119.56
2	6-M	202	LEU	C-N-CA	8.07	127.80	119.56
2	7-M	202	LEU	CA-C-N	8.07	127.80	119.56
2	7-M	202	LEU	C-N-CA	8.07	127.80	119.56
2	8-M	202	LEU	CA-C-N	8.07	127.80	119.56
2	8-M	202	LEU	C-N-CA	8.07	127.80	119.56
2	9-M	202	LEU	CA-C-N	8.07	127.80	119.56
2	9-M	202	LEU	C-N-CA	8.07	127.80	119.56
2	10-M	202	LEU	CA-C-N	8.07	127.80	119.56
2	10-M	202	LEU	C-N-CA	8.07	127.80	119.56
1	1-L	102	LEU	CA-C-N	7.70	127.62	119.85
1	1-L	102	LEU	C-N-CA	7.70	127.62	119.85
1	2-L	102	LEU	CA-C-N	7.70	127.62	119.85
1	2-L	102	LEU	C-N-CA	7.70	127.62	119.85
1	3-L	102	LEU	CA-C-N	7.70	127.62	119.85
1	3-L	102	LEU	C-N-CA	7.70	127.62	119.85
1	4-L	102	LEU	CA-C-N	7.70	127.62	119.85
1	4-L	102	LEU	C-N-CA	7.70	127.62	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5-L	102	LEU	CA-C-N	7.70	127.62	119.85
1	5-L	102	LEU	C-N-CA	7.70	127.62	119.85
1	6-L	102	LEU	CA-C-N	7.70	127.62	119.85
1	6-L	102	LEU	C-N-CA	7.70	127.62	119.85
1	7-L	102	LEU	CA-C-N	7.70	127.62	119.85
1	7-L	102	LEU	C-N-CA	7.70	127.62	119.85
1	8-L	102	LEU	CA-C-N	7.70	127.62	119.85
1	8-L	102	LEU	C-N-CA	7.70	127.62	119.85
1	9-L	102	LEU	CA-C-N	7.70	127.62	119.85
1	9-L	102	LEU	C-N-CA	7.70	127.62	119.85
1	10-L	102	LEU	CA-C-N	7.70	127.62	119.85
1	10-L	102	LEU	C-N-CA	7.70	127.62	119.85
4	1-N	31	GLN	CA-C-N	6.83	126.80	119.76
4	1-N	31	GLN	C-N-CA	6.83	126.80	119.76
4	2-N	31	GLN	CA-C-N	6.83	126.80	119.76
4	2-N	31	GLN	C-N-CA	6.83	126.80	119.76
4	3-N	31	GLN	CA-C-N	6.83	126.80	119.76
4	3-N	31	GLN	C-N-CA	6.83	126.80	119.76
4	4-N	31	GLN	CA-C-N	6.83	126.80	119.76
4	4-N	31	GLN	C-N-CA	6.83	126.80	119.76
4	5-N	31	GLN	CA-C-N	6.83	126.80	119.76
4	5-N	31	GLN	C-N-CA	6.83	126.80	119.76
4	6-N	31	GLN	CA-C-N	6.83	126.80	119.76
4	6-N	31	GLN	C-N-CA	6.83	126.80	119.76
4	7-N	31	GLN	CA-C-N	6.83	126.80	119.76
4	7-N	31	GLN	C-N-CA	6.83	126.80	119.76
4	8-N	31	GLN	CA-C-N	6.83	126.80	119.76
4	8-N	31	GLN	C-N-CA	6.83	126.80	119.76
4	9-N	31	GLN	CA-C-N	6.83	126.80	119.76
4	9-N	31	GLN	C-N-CA	6.83	126.80	119.76
4	10-N	31	GLN	CA-C-N	6.83	126.80	119.76
4	10-N	31	GLN	C-N-CA	6.83	126.80	119.76
1	1-L	108	MET	CA-C-N	6.75	126.71	120.03
1	1-L	108	MET	C-N-CA	6.75	126.71	120.03
1	2-L	108	MET	CA-C-N	6.75	126.71	120.03
1	2-L	108	MET	C-N-CA	6.75	126.71	120.03
1	3-L	108	MET	CA-C-N	6.75	126.71	120.03
1	3-L	108	MET	C-N-CA	6.75	126.71	120.03
1	4-L	108	MET	CA-C-N	6.75	126.71	120.03
1	4-L	108	MET	C-N-CA	6.75	126.71	120.03
1	5-L	108	MET	CA-C-N	6.75	126.71	120.03
1	5-L	108	MET	C-N-CA	6.75	126.71	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6-L	108	MET	CA-C-N	6.75	126.71	120.03
1	6-L	108	MET	C-N-CA	6.75	126.71	120.03
1	7-L	108	MET	CA-C-N	6.75	126.71	120.03
1	7-L	108	MET	C-N-CA	6.75	126.71	120.03
1	8-L	108	MET	CA-C-N	6.75	126.71	120.03
1	8-L	108	MET	C-N-CA	6.75	126.71	120.03
1	9-L	108	MET	CA-C-N	6.75	126.71	120.03
1	9-L	108	MET	C-N-CA	6.75	126.71	120.03
1	10-L	108	MET	CA-C-N	6.75	126.71	120.03
1	10-L	108	MET	C-N-CA	6.75	126.71	120.03
2	1-M	216	SER	CA-C-N	6.66	128.16	119.84
2	1-M	216	SER	C-N-CA	6.66	128.16	119.84
2	2-M	216	SER	CA-C-N	6.66	128.16	119.84
2	2-M	216	SER	C-N-CA	6.66	128.16	119.84
2	3-M	216	SER	CA-C-N	6.66	128.16	119.84
2	3-M	216	SER	C-N-CA	6.66	128.16	119.84
2	4-M	216	SER	CA-C-N	6.66	128.16	119.84
2	4-M	216	SER	C-N-CA	6.66	128.16	119.84
2	5-M	216	SER	CA-C-N	6.66	128.16	119.84
2	5-M	216	SER	C-N-CA	6.66	128.16	119.84
2	6-M	216	SER	CA-C-N	6.66	128.16	119.84
2	6-M	216	SER	C-N-CA	6.66	128.16	119.84
2	7-M	216	SER	CA-C-N	6.66	128.16	119.84
2	7-M	216	SER	C-N-CA	6.66	128.16	119.84
2	8-M	216	SER	CA-C-N	6.66	128.16	119.84
2	8-M	216	SER	C-N-CA	6.66	128.16	119.84
2	9-M	216	SER	CA-C-N	6.66	128.16	119.84
2	9-M	216	SER	C-N-CA	6.66	128.16	119.84
2	10-M	216	SER	CA-C-N	6.66	128.16	119.84
2	10-M	216	SER	C-N-CA	6.66	128.16	119.84
2	1-M	442	HIS	CA-C-N	6.52	126.14	119.56
2	1-M	442	HIS	C-N-CA	6.52	126.14	119.56
2	2-M	442	HIS	CA-C-N	6.52	126.14	119.56
2	2-M	442	HIS	C-N-CA	6.52	126.14	119.56
2	3-M	442	HIS	CA-C-N	6.52	126.14	119.56
2	3-M	442	HIS	C-N-CA	6.52	126.14	119.56
2	4-M	442	HIS	CA-C-N	6.52	126.14	119.56
2	4-M	442	HIS	C-N-CA	6.52	126.14	119.56
2	5-M	442	HIS	CA-C-N	6.52	126.14	119.56
2	5-M	442	HIS	C-N-CA	6.52	126.14	119.56
2	6-M	442	HIS	CA-C-N	6.52	126.14	119.56
2	6-M	442	HIS	C-N-CA	6.52	126.14	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7-M	442	HIS	CA-C-N	6.52	126.14	119.56
2	7-M	442	HIS	C-N-CA	6.52	126.14	119.56
2	8-M	442	HIS	CA-C-N	6.52	126.14	119.56
2	8-M	442	HIS	C-N-CA	6.52	126.14	119.56
2	9-M	442	HIS	CA-C-N	6.52	126.14	119.56
2	9-M	442	HIS	C-N-CA	6.52	126.14	119.56
2	10-M	442	HIS	CA-C-N	6.52	126.14	119.56
2	10-M	442	HIS	C-N-CA	6.52	126.14	119.56
2	1-M	66	LYS	CA-C-N	6.48	127.94	119.84
2	1-M	66	LYS	C-N-CA	6.48	127.94	119.84
2	2-M	66	LYS	CA-C-N	6.48	127.94	119.84
2	2-M	66	LYS	C-N-CA	6.48	127.94	119.84
2	3-M	66	LYS	CA-C-N	6.48	127.94	119.84
2	3-M	66	LYS	C-N-CA	6.48	127.94	119.84
2	4-M	66	LYS	CA-C-N	6.48	127.94	119.84
2	4-M	66	LYS	C-N-CA	6.48	127.94	119.84
2	5-M	66	LYS	CA-C-N	6.48	127.94	119.84
2	5-M	66	LYS	C-N-CA	6.48	127.94	119.84
2	6-M	66	LYS	CA-C-N	6.48	127.94	119.84
2	6-M	66	LYS	C-N-CA	6.48	127.94	119.84
2	7-M	66	LYS	CA-C-N	6.48	127.94	119.84
2	7-M	66	LYS	C-N-CA	6.48	127.94	119.84
2	8-M	66	LYS	CA-C-N	6.48	127.94	119.84
2	8-M	66	LYS	C-N-CA	6.48	127.94	119.84
2	9-M	66	LYS	CA-C-N	6.48	127.94	119.84
2	9-M	66	LYS	C-N-CA	6.48	127.94	119.84
2	10-M	66	LYS	CA-C-N	6.48	127.94	119.84
2	10-M	66	LYS	C-N-CA	6.48	127.94	119.84
4	1-N	2	ASP	CA-C-N	6.47	126.39	119.28
4	1-N	2	ASP	C-N-CA	6.47	126.39	119.28
4	2-N	2	ASP	CA-C-N	6.47	126.39	119.28
4	2-N	2	ASP	C-N-CA	6.47	126.39	119.28
4	3-N	2	ASP	CA-C-N	6.47	126.39	119.28
4	3-N	2	ASP	C-N-CA	6.47	126.39	119.28
4	4-N	2	ASP	CA-C-N	6.47	126.39	119.28
4	4-N	2	ASP	C-N-CA	6.47	126.39	119.28
4	5-N	2	ASP	CA-C-N	6.47	126.39	119.28
4	5-N	2	ASP	C-N-CA	6.47	126.39	119.28
4	6-N	2	ASP	CA-C-N	6.47	126.39	119.28
4	6-N	2	ASP	C-N-CA	6.47	126.39	119.28
4	7-N	2	ASP	CA-C-N	6.47	126.39	119.28
4	7-N	2	ASP	C-N-CA	6.47	126.39	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	8-N	2	ASP	CA-C-N	6.47	126.39	119.28
4	8-N	2	ASP	C-N-CA	6.47	126.39	119.28
4	9-N	2	ASP	CA-C-N	6.47	126.39	119.28
4	9-N	2	ASP	C-N-CA	6.47	126.39	119.28
4	10-N	2	ASP	CA-C-N	6.47	126.39	119.28
4	10-N	2	ASP	C-N-CA	6.47	126.39	119.28
2	1-M	416	PHE	CA-C-N	6.43	127.88	119.84
2	1-M	416	PHE	C-N-CA	6.43	127.88	119.84
2	2-M	416	PHE	CA-C-N	6.43	127.88	119.84
2	2-M	416	PHE	C-N-CA	6.43	127.88	119.84
2	3-M	416	PHE	CA-C-N	6.43	127.88	119.84
2	3-M	416	PHE	C-N-CA	6.43	127.88	119.84
2	4-M	416	PHE	CA-C-N	6.43	127.88	119.84
2	4-M	416	PHE	C-N-CA	6.43	127.88	119.84
2	5-M	416	PHE	CA-C-N	6.43	127.88	119.84
2	5-M	416	PHE	C-N-CA	6.43	127.88	119.84
2	6-M	416	PHE	CA-C-N	6.43	127.88	119.84
2	6-M	416	PHE	C-N-CA	6.43	127.88	119.84
2	7-M	416	PHE	CA-C-N	6.43	127.88	119.84
2	7-M	416	PHE	C-N-CA	6.43	127.88	119.84
2	8-M	416	PHE	CA-C-N	6.43	127.88	119.84
2	8-M	416	PHE	C-N-CA	6.43	127.88	119.84
2	9-M	416	PHE	CA-C-N	6.43	127.88	119.84
2	9-M	416	PHE	C-N-CA	6.43	127.88	119.84
2	10-M	416	PHE	CA-C-N	6.43	127.88	119.84
2	10-M	416	PHE	C-N-CA	6.43	127.88	119.84
2	1-M	37	ILE	CA-C-N	6.38	126.72	119.83
2	1-M	37	ILE	C-N-CA	6.38	126.72	119.83
2	2-M	37	ILE	CA-C-N	6.38	126.72	119.83
2	2-M	37	ILE	C-N-CA	6.38	126.72	119.83
2	3-M	37	ILE	CA-C-N	6.38	126.72	119.83
2	3-M	37	ILE	C-N-CA	6.38	126.72	119.83
2	4-M	37	ILE	CA-C-N	6.38	126.72	119.83
2	4-M	37	ILE	C-N-CA	6.38	126.72	119.83
2	5-M	37	ILE	CA-C-N	6.38	126.72	119.83
2	5-M	37	ILE	C-N-CA	6.38	126.72	119.83
2	6-M	37	ILE	CA-C-N	6.38	126.72	119.83
2	6-M	37	ILE	C-N-CA	6.38	126.72	119.83
2	7-M	37	ILE	CA-C-N	6.38	126.72	119.83
2	7-M	37	ILE	C-N-CA	6.38	126.72	119.83
2	8-M	37	ILE	CA-C-N	6.38	126.72	119.83
2	8-M	37	ILE	C-N-CA	6.38	126.72	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	9-M	37	ILE	CA-C-N	6.38	126.72	119.83
2	9-M	37	ILE	C-N-CA	6.38	126.72	119.83
2	10-M	37	ILE	CA-C-N	6.38	126.72	119.83
2	10-M	37	ILE	C-N-CA	6.38	126.72	119.83
2	1-M	458	GLY	CA-C-N	6.25	125.94	119.56
2	1-M	458	GLY	C-N-CA	6.25	125.94	119.56
2	2-M	458	GLY	CA-C-N	6.25	125.94	119.56
2	2-M	458	GLY	C-N-CA	6.25	125.94	119.56
2	3-M	458	GLY	CA-C-N	6.25	125.94	119.56
2	3-M	458	GLY	C-N-CA	6.25	125.94	119.56
2	4-M	458	GLY	CA-C-N	6.25	125.94	119.56
2	4-M	458	GLY	C-N-CA	6.25	125.94	119.56
2	5-M	458	GLY	CA-C-N	6.25	125.94	119.56
2	5-M	458	GLY	C-N-CA	6.25	125.94	119.56
2	6-M	458	GLY	CA-C-N	6.25	125.94	119.56
2	6-M	458	GLY	C-N-CA	6.25	125.94	119.56
2	7-M	458	GLY	CA-C-N	6.25	125.94	119.56
2	7-M	458	GLY	C-N-CA	6.25	125.94	119.56
2	8-M	458	GLY	CA-C-N	6.25	125.94	119.56
2	8-M	458	GLY	C-N-CA	6.25	125.94	119.56
2	9-M	458	GLY	CA-C-N	6.25	125.94	119.56
2	9-M	458	GLY	C-N-CA	6.25	125.94	119.56
2	10-M	458	GLY	CA-C-N	6.25	125.94	119.56
2	10-M	458	GLY	C-N-CA	6.25	125.94	119.56
1	1-L	282	ASN	CA-C-N	6.16	125.84	119.56
1	1-L	282	ASN	C-N-CA	6.16	125.84	119.56
1	2-L	282	ASN	CA-C-N	6.16	125.84	119.56
1	2-L	282	ASN	C-N-CA	6.16	125.84	119.56
1	3-L	282	ASN	CA-C-N	6.16	125.84	119.56
1	3-L	282	ASN	C-N-CA	6.16	125.84	119.56
1	4-L	282	ASN	CA-C-N	6.16	125.84	119.56
1	4-L	282	ASN	C-N-CA	6.16	125.84	119.56
1	5-L	282	ASN	CA-C-N	6.16	125.84	119.56
1	5-L	282	ASN	C-N-CA	6.16	125.84	119.56
1	6-L	282	ASN	CA-C-N	6.16	125.84	119.56
1	6-L	282	ASN	C-N-CA	6.16	125.84	119.56
1	7-L	282	ASN	CA-C-N	6.16	125.84	119.56
1	7-L	282	ASN	C-N-CA	6.16	125.84	119.56
1	8-L	282	ASN	CA-C-N	6.16	125.84	119.56
1	8-L	282	ASN	C-N-CA	6.16	125.84	119.56
1	9-L	282	ASN	CA-C-N	6.16	125.84	119.56
1	9-L	282	ASN	C-N-CA	6.16	125.84	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	10-L	282	ASN	CA-C-N	6.16	125.84	119.56
1	10-L	282	ASN	C-N-CA	6.16	125.84	119.56
1	1-L	76	LEU	CA-C-N	6.14	126.09	119.76
1	1-L	76	LEU	C-N-CA	6.14	126.09	119.76
1	2-L	76	LEU	CA-C-N	6.14	126.09	119.76
1	2-L	76	LEU	C-N-CA	6.14	126.09	119.76
1	3-L	76	LEU	CA-C-N	6.14	126.09	119.76
1	3-L	76	LEU	C-N-CA	6.14	126.09	119.76
1	4-L	76	LEU	CA-C-N	6.14	126.09	119.76
1	4-L	76	LEU	C-N-CA	6.14	126.09	119.76
1	5-L	76	LEU	CA-C-N	6.14	126.09	119.76
1	5-L	76	LEU	C-N-CA	6.14	126.09	119.76
1	6-L	76	LEU	CA-C-N	6.14	126.09	119.76
1	6-L	76	LEU	C-N-CA	6.14	126.09	119.76
1	7-L	76	LEU	CA-C-N	6.14	126.09	119.76
1	7-L	76	LEU	C-N-CA	6.14	126.09	119.76
1	8-L	76	LEU	CA-C-N	6.14	126.09	119.76
1	8-L	76	LEU	C-N-CA	6.14	126.09	119.76
1	9-L	76	LEU	CA-C-N	6.14	126.09	119.76
1	9-L	76	LEU	C-N-CA	6.14	126.09	119.76
1	10-L	76	LEU	CA-C-N	6.14	126.09	119.76
1	10-L	76	LEU	C-N-CA	6.14	126.09	119.76
2	1-M	32	VAL	CA-C-N	6.10	126.01	119.85
2	1-M	32	VAL	C-N-CA	6.10	126.01	119.85
2	2-M	32	VAL	CA-C-N	6.10	126.01	119.85
2	2-M	32	VAL	C-N-CA	6.10	126.01	119.85
2	3-M	32	VAL	CA-C-N	6.10	126.01	119.85
2	3-M	32	VAL	C-N-CA	6.10	126.01	119.85
2	4-M	32	VAL	CA-C-N	6.10	126.01	119.85
2	4-M	32	VAL	C-N-CA	6.10	126.01	119.85
2	5-M	32	VAL	CA-C-N	6.10	126.01	119.85
2	5-M	32	VAL	C-N-CA	6.10	126.01	119.85
2	6-M	32	VAL	CA-C-N	6.10	126.01	119.85
2	6-M	32	VAL	C-N-CA	6.10	126.01	119.85
2	7-M	32	VAL	CA-C-N	6.10	126.01	119.85
2	7-M	32	VAL	C-N-CA	6.10	126.01	119.85
2	8-M	32	VAL	CA-C-N	6.10	126.01	119.85
2	8-M	32	VAL	C-N-CA	6.10	126.01	119.85
2	9-M	32	VAL	CA-C-N	6.10	126.01	119.85
2	9-M	32	VAL	C-N-CA	6.10	126.01	119.85
2	10-M	32	VAL	CA-C-N	6.10	126.01	119.85
2	10-M	32	VAL	C-N-CA	6.10	126.01	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1-M	423	GLY	N-CA-C	-6.06	105.00	112.33
2	2-M	423	GLY	N-CA-C	-6.06	105.00	112.33
2	3-M	423	GLY	N-CA-C	-6.06	105.00	112.33
2	4-M	423	GLY	N-CA-C	-6.06	105.00	112.33
2	5-M	423	GLY	N-CA-C	-6.06	105.00	112.33
2	6-M	423	GLY	N-CA-C	-6.06	105.00	112.33
2	7-M	423	GLY	N-CA-C	-6.06	105.00	112.33
2	8-M	423	GLY	N-CA-C	-6.06	105.00	112.33
2	9-M	423	GLY	N-CA-C	-6.06	105.00	112.33
2	10-M	423	GLY	N-CA-C	-6.06	105.00	112.33
1	1-L	26	LEU	CA-C-N	6.05	125.97	119.85
1	1-L	26	LEU	C-N-CA	6.05	125.97	119.85
1	2-L	26	LEU	CA-C-N	6.05	125.97	119.85
1	2-L	26	LEU	C-N-CA	6.05	125.97	119.85
1	3-L	26	LEU	CA-C-N	6.05	125.97	119.85
1	3-L	26	LEU	C-N-CA	6.05	125.97	119.85
1	4-L	26	LEU	CA-C-N	6.05	125.97	119.85
1	4-L	26	LEU	C-N-CA	6.05	125.97	119.85
1	5-L	26	LEU	CA-C-N	6.05	125.97	119.85
1	5-L	26	LEU	C-N-CA	6.05	125.97	119.85
1	6-L	26	LEU	CA-C-N	6.05	125.97	119.85
1	6-L	26	LEU	C-N-CA	6.05	125.97	119.85
1	7-L	26	LEU	CA-C-N	6.05	125.97	119.85
1	7-L	26	LEU	C-N-CA	6.05	125.97	119.85
1	8-L	26	LEU	CA-C-N	6.05	125.97	119.85
1	8-L	26	LEU	C-N-CA	6.05	125.97	119.85
1	9-L	26	LEU	CA-C-N	6.05	125.97	119.85
1	9-L	26	LEU	C-N-CA	6.05	125.97	119.85
1	10-L	26	LEU	CA-C-N	6.05	125.97	119.85
1	10-L	26	LEU	C-N-CA	6.05	125.97	119.85
1	1-L	324	SER	CA-C-N	5.95	125.82	119.28
1	1-L	324	SER	C-N-CA	5.95	125.82	119.28
1	2-L	324	SER	CA-C-N	5.95	125.82	119.28
1	2-L	324	SER	C-N-CA	5.95	125.82	119.28
1	3-L	324	SER	CA-C-N	5.95	125.82	119.28
1	3-L	324	SER	C-N-CA	5.95	125.82	119.28
1	4-L	324	SER	CA-C-N	5.95	125.82	119.28
1	4-L	324	SER	C-N-CA	5.95	125.82	119.28
1	5-L	324	SER	CA-C-N	5.95	125.82	119.28
1	5-L	324	SER	C-N-CA	5.95	125.82	119.28
1	6-L	324	SER	CA-C-N	5.95	125.82	119.28
1	6-L	324	SER	C-N-CA	5.95	125.82	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	7-L	324	SER	CA-C-N	5.95	125.82	119.28
1	7-L	324	SER	C-N-CA	5.95	125.82	119.28
1	8-L	324	SER	CA-C-N	5.95	125.82	119.28
1	8-L	324	SER	C-N-CA	5.95	125.82	119.28
1	9-L	324	SER	CA-C-N	5.95	125.82	119.28
1	9-L	324	SER	C-N-CA	5.95	125.82	119.28
1	10-L	324	SER	CA-C-N	5.95	125.82	119.28
1	10-L	324	SER	C-N-CA	5.95	125.82	119.28
1	1-L	330	GLY	CA-C-N	5.92	125.46	119.19
1	1-L	330	GLY	C-N-CA	5.92	125.46	119.19
1	2-L	330	GLY	CA-C-N	5.92	125.46	119.19
1	2-L	330	GLY	C-N-CA	5.92	125.46	119.19
1	3-L	330	GLY	CA-C-N	5.92	125.46	119.19
1	3-L	330	GLY	C-N-CA	5.92	125.46	119.19
1	4-L	330	GLY	CA-C-N	5.92	125.46	119.19
1	4-L	330	GLY	C-N-CA	5.92	125.46	119.19
1	5-L	330	GLY	CA-C-N	5.92	125.46	119.19
1	5-L	330	GLY	C-N-CA	5.92	125.46	119.19
1	6-L	330	GLY	CA-C-N	5.92	125.46	119.19
1	6-L	330	GLY	C-N-CA	5.92	125.46	119.19
1	7-L	330	GLY	CA-C-N	5.92	125.46	119.19
1	7-L	330	GLY	C-N-CA	5.92	125.46	119.19
1	8-L	330	GLY	CA-C-N	5.92	125.46	119.19
1	8-L	330	GLY	C-N-CA	5.92	125.46	119.19
1	9-L	330	GLY	CA-C-N	5.92	125.46	119.19
1	9-L	330	GLY	C-N-CA	5.92	125.46	119.19
1	10-L	330	GLY	CA-C-N	5.92	125.46	119.19
1	10-L	330	GLY	C-N-CA	5.92	125.46	119.19
2	1-M	361	GLU	CA-C-N	5.71	126.98	119.84
2	1-M	361	GLU	C-N-CA	5.71	126.98	119.84
2	2-M	361	GLU	CA-C-N	5.71	126.98	119.84
2	2-M	361	GLU	C-N-CA	5.71	126.98	119.84
2	3-M	361	GLU	CA-C-N	5.71	126.98	119.84
2	3-M	361	GLU	C-N-CA	5.71	126.98	119.84
2	4-M	361	GLU	CA-C-N	5.71	126.98	119.84
2	4-M	361	GLU	C-N-CA	5.71	126.98	119.84
2	5-M	361	GLU	CA-C-N	5.71	126.98	119.84
2	5-M	361	GLU	C-N-CA	5.71	126.98	119.84
2	6-M	361	GLU	CA-C-N	5.71	126.98	119.84
2	6-M	361	GLU	C-N-CA	5.71	126.98	119.84
2	7-M	361	GLU	CA-C-N	5.71	126.98	119.84
2	7-M	361	GLU	C-N-CA	5.71	126.98	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	8-M	361	GLU	CA-C-N	5.71	126.98	119.84
2	8-M	361	GLU	C-N-CA	5.71	126.98	119.84
2	9-M	361	GLU	CA-C-N	5.71	126.98	119.84
2	9-M	361	GLU	C-N-CA	5.71	126.98	119.84
2	10-M	361	GLU	CA-C-N	5.71	126.98	119.84
2	10-M	361	GLU	C-N-CA	5.71	126.98	119.84
2	1-M	412	TYR	CA-C-N	5.59	126.83	119.84
2	1-M	412	TYR	C-N-CA	5.59	126.83	119.84
2	2-M	412	TYR	CA-C-N	5.59	126.83	119.84
2	2-M	412	TYR	C-N-CA	5.59	126.83	119.84
2	3-M	412	TYR	CA-C-N	5.59	126.83	119.84
2	3-M	412	TYR	C-N-CA	5.59	126.83	119.84
2	4-M	412	TYR	CA-C-N	5.59	126.83	119.84
2	4-M	412	TYR	C-N-CA	5.59	126.83	119.84
2	5-M	412	TYR	CA-C-N	5.59	126.83	119.84
2	5-M	412	TYR	C-N-CA	5.59	126.83	119.84
2	6-M	412	TYR	CA-C-N	5.59	126.83	119.84
2	6-M	412	TYR	C-N-CA	5.59	126.83	119.84
2	7-M	412	TYR	CA-C-N	5.59	126.83	119.84
2	7-M	412	TYR	C-N-CA	5.59	126.83	119.84
2	8-M	412	TYR	CA-C-N	5.59	126.83	119.84
2	8-M	412	TYR	C-N-CA	5.59	126.83	119.84
2	9-M	412	TYR	CA-C-N	5.59	126.83	119.84
2	9-M	412	TYR	C-N-CA	5.59	126.83	119.84
2	10-M	412	TYR	CA-C-N	5.59	126.83	119.84
2	10-M	412	TYR	C-N-CA	5.59	126.83	119.84
1	1-L	98	SER	CA-C-N	5.55	126.78	119.84
1	1-L	98	SER	C-N-CA	5.55	126.78	119.84
1	2-L	98	SER	CA-C-N	5.55	126.78	119.84
1	2-L	98	SER	C-N-CA	5.55	126.78	119.84
1	3-L	98	SER	CA-C-N	5.55	126.78	119.84
1	3-L	98	SER	C-N-CA	5.55	126.78	119.84
1	4-L	98	SER	CA-C-N	5.55	126.78	119.84
1	4-L	98	SER	C-N-CA	5.55	126.78	119.84
1	5-L	98	SER	CA-C-N	5.55	126.78	119.84
1	5-L	98	SER	C-N-CA	5.55	126.78	119.84
1	6-L	98	SER	CA-C-N	5.55	126.78	119.84
1	6-L	98	SER	C-N-CA	5.55	126.78	119.84
1	7-L	98	SER	CA-C-N	5.55	126.78	119.84
1	7-L	98	SER	C-N-CA	5.55	126.78	119.84
1	8-L	98	SER	CA-C-N	5.55	126.78	119.84
1	8-L	98	SER	C-N-CA	5.55	126.78	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9-L	98	SER	CA-C-N	5.55	126.78	119.84
1	9-L	98	SER	C-N-CA	5.55	126.78	119.84
1	10-L	98	SER	CA-C-N	5.55	126.78	119.84
1	10-L	98	SER	C-N-CA	5.55	126.78	119.84
1	1-L	198	ALA	CA-C-N	5.36	125.42	119.32
1	1-L	198	ALA	C-N-CA	5.36	125.42	119.32
1	2-L	198	ALA	CA-C-N	5.36	125.42	119.32
1	2-L	198	ALA	C-N-CA	5.36	125.42	119.32
1	3-L	198	ALA	CA-C-N	5.36	125.42	119.32
1	3-L	198	ALA	C-N-CA	5.36	125.42	119.32
1	4-L	198	ALA	CA-C-N	5.36	125.42	119.32
1	4-L	198	ALA	C-N-CA	5.36	125.42	119.32
1	5-L	198	ALA	CA-C-N	5.36	125.42	119.32
1	5-L	198	ALA	C-N-CA	5.36	125.42	119.32
1	6-L	198	ALA	CA-C-N	5.36	125.42	119.32
1	6-L	198	ALA	C-N-CA	5.36	125.42	119.32
1	7-L	198	ALA	CA-C-N	5.36	125.42	119.32
1	7-L	198	ALA	C-N-CA	5.36	125.42	119.32
1	8-L	198	ALA	CA-C-N	5.36	125.42	119.32
1	8-L	198	ALA	C-N-CA	5.36	125.42	119.32
1	9-L	198	ALA	CA-C-N	5.36	125.42	119.32
1	9-L	198	ALA	C-N-CA	5.36	125.42	119.32
1	10-L	198	ALA	CA-C-N	5.36	125.42	119.32
1	10-L	198	ALA	C-N-CA	5.36	125.42	119.32
2	1-M	168	HIS	CA-CB-CG	-5.15	108.65	113.80
2	2-M	168	HIS	CA-CB-CG	-5.15	108.65	113.80
2	3-M	168	HIS	CA-CB-CG	-5.15	108.65	113.80
2	4-M	168	HIS	CA-CB-CG	-5.15	108.65	113.80
2	5-M	168	HIS	CA-CB-CG	-5.15	108.65	113.80
2	6-M	168	HIS	CA-CB-CG	-5.15	108.65	113.80
2	7-M	168	HIS	CA-CB-CG	-5.15	108.65	113.80
2	8-M	168	HIS	CA-CB-CG	-5.15	108.65	113.80
2	9-M	168	HIS	CA-CB-CG	-5.15	108.65	113.80
2	10-M	168	HIS	CA-CB-CG	-5.15	108.65	113.80
1	1-L	31	ILE	CA-C-N	5.09	126.20	119.84
1	1-L	31	ILE	C-N-CA	5.09	126.20	119.84
1	2-L	31	ILE	CA-C-N	5.09	126.20	119.84
1	2-L	31	ILE	C-N-CA	5.09	126.20	119.84
1	3-L	31	ILE	CA-C-N	5.09	126.20	119.84
1	3-L	31	ILE	C-N-CA	5.09	126.20	119.84
1	4-L	31	ILE	CA-C-N	5.09	126.20	119.84
1	4-L	31	ILE	C-N-CA	5.09	126.20	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5-L	31	ILE	CA-C-N	5.09	126.20	119.84
1	5-L	31	ILE	C-N-CA	5.09	126.20	119.84
1	6-L	31	ILE	CA-C-N	5.09	126.20	119.84
1	6-L	31	ILE	C-N-CA	5.09	126.20	119.84
1	7-L	31	ILE	CA-C-N	5.09	126.20	119.84
1	7-L	31	ILE	C-N-CA	5.09	126.20	119.84
1	8-L	31	ILE	CA-C-N	5.09	126.20	119.84
1	8-L	31	ILE	C-N-CA	5.09	126.20	119.84
1	9-L	31	ILE	CA-C-N	5.09	126.20	119.84
1	9-L	31	ILE	C-N-CA	5.09	126.20	119.84
1	10-L	31	ILE	CA-C-N	5.09	126.20	119.84
1	10-L	31	ILE	C-N-CA	5.09	126.20	119.84

There are no chirality outliers.

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1-M	3	PRO	Mainchain,Peptide
1	10-L	343	SER	Mainchain,Peptide
2	10-M	3	PRO	Mainchain,Peptide
1	2-L	49	PHE	Mainchain
2	2-M	3	PRO	Mainchain,Peptide
1	3-L	343	SER	Mainchain,Peptide
2	3-M	3	PRO	Mainchain,Peptide
2	4-M	3	PRO	Mainchain,Peptide
2	5-M	3	PRO	Mainchain,Peptide
2	5-M	466	GLN	Mainchain,Peptide
1	6-L	343	SER	Mainchain,Peptide
2	6-M	3	PRO	Mainchain,Peptide
2	7-M	3	PRO	Mainchain,Peptide
2	7-M	466	GLN	Mainchain,Peptide
1	8-L	343	SER	Mainchain,Peptide
2	9-M	3	PRO	Mainchain,Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-L	3154	0	3173	12	0
1	2-L	3154	0	3173	12	0
1	3-L	3154	0	3173	25	0
1	4-L	3154	0	3173	18	0
1	5-L	3154	0	3173	22	0
1	6-L	3154	0	3173	17	0
1	7-L	3154	0	3173	22	0
1	8-L	3154	0	3173	25	0
1	9-L	3154	0	3173	20	0
1	10-L	3154	0	3173	20	0
2	1-M	3192	0	3180	10	0
2	2-M	3192	0	3180	14	0
2	3-M	3192	0	3180	17	0
2	4-M	3192	0	3180	18	0
2	5-M	3192	0	3180	17	0
2	6-M	3192	0	3180	17	0
2	7-M	3192	0	3180	18	0
2	8-M	3192	0	3180	13	0
2	9-M	3192	0	3180	16	0
2	10-M	3192	0	3180	18	0
3	1-K	537	0	546	2	0
3	2-K	537	0	546	0	0
3	3-K	537	0	546	1	0
3	4-K	537	0	546	1	0
3	5-K	537	0	546	4	0
3	6-K	537	0	546	1	0
3	7-K	537	0	546	2	0
3	8-K	537	0	546	1	0
3	9-K	537	0	546	2	0
3	10-K	537	0	546	5	0
4	1-N	494	0	473	6	0
4	2-N	494	0	473	6	0
4	3-N	494	0	473	4	0
4	4-N	494	0	473	6	0
4	5-N	494	0	473	6	0
4	6-N	494	0	473	4	0
4	7-N	494	0	473	4	0
4	8-N	494	0	473	7	0
4	9-N	494	0	473	5	0
4	10-N	494	0	473	8	0
5	1-L	31	0	12	1	0
5	2-L	31	0	12	2	0
5	3-L	31	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	4-L	31	0	12	0	0
5	5-L	31	0	12	2	0
5	6-L	31	0	12	1	0
5	7-L	31	0	12	1	0
5	8-L	31	0	12	1	0
5	9-L	31	0	12	1	0
5	10-L	31	0	12	2	0
All	All	74080	0	73840	432	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 3.

All (432) 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)
2:M:154:ILE:HG22	2:M:154:ILE:O	1.74	0.86
2:M:154:ILE:HG22	2:M:154:ILE:O	1.76	0.84
1:L:256:ILE:O	1:L:256:ILE:HG23	1.77	0.83
1:L:465:ARG:O	1:L:465:ARG:NH1	2.15	0.76
3:K:346:GLU:N	3:K:346:GLU:OE1	2.19	0.75
2:M:154:ILE:HG22	2:M:154:ILE:O	1.85	0.75
2:M:438:GLN:O	2:M:438:GLN:HG3	1.88	0.74
2:M:154:ILE:HG22	2:M:154:ILE:O	1.87	0.72
2:M:6:GLN:N	2:M:6:GLN:OE1	2.22	0.72
5:L:501:ATP:O1G	5:L:501:ATP:O1B	2.05	0.70
2:M:154:ILE:HG22	2:M:154:ILE:O	1.90	0.70
3:K:346:GLU:N	3:K:346:GLU:OE1	2.26	0.69
5:L:501:ATP:O1G	5:L:501:ATP:O1B	2.08	0.68
5:L:501:ATP:O2B	5:L:501:ATP:O2G	2.12	0.68
2:M:418:GLU:OE1	2:M:418:GLU:N	2.26	0.67
2:M:154:ILE:HG22	2:M:154:ILE:O	1.93	0.67
2:M:363:GLU:CD	2:M:363:GLU:H	2.03	0.66
1:L:227:TRP:C	1:L:227:TRP:CD1	2.75	0.64
1:L:302:ASP:C	1:L:302:ASP:OD1	2.40	0.64
2:M:363:GLU:OE1	2:M:363:GLU:N	2.27	0.64
1:L:302:ASP:C	1:L:302:ASP:OD1	2.40	0.64
1:L:302:ASP:C	1:L:302:ASP:OD1	2.42	0.63
2:M:154:ILE:HG22	2:M:154:ILE:O	1.97	0.63
1:L:256:ILE:HG22	1:L:256:ILE:O	1.97	0.63
2:M:6:GLN:N	2:M:6:GLN:OE1	2.29	0.62
2:M:363:GLU:OE1	2:M:363:GLU:N	2.26	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:302:ASP:C	1:L:302:ASP:OD1	2.42	0.62
2:M:418:GLU:OE1	2:M:418:GLU:N	2.25	0.62
1:L:256:ILE:O	1:L:256:ILE:HG23	1.99	0.62
2:M:363:GLU:OE1	2:M:363:GLU:N	2.29	0.61
3:K:345:GLN:OE1	3:K:345:GLN:N	2.26	0.61
1:L:87:TRP:HA	1:L:87:TRP:CE3	2.35	0.61
2:M:462:LEU:HD12	2:M:462:LEU:O	1.99	0.61
1:L:240:GLU:H	1:L:240:GLU:CD	2.09	0.61
2:M:418:GLU:OE1	2:M:418:GLU:N	2.26	0.61
4:N:34:LYS:O	4:N:34:LYS:HG2	2.00	0.61
2:M:363:GLU:CD	2:M:363:GLU:H	2.04	0.60
1:L:344:ILE:O	1:L:344:ILE:HG22	2.01	0.60
2:M:363:GLU:OE1	2:M:363:GLU:N	2.26	0.60
2:M:6:GLN:OE1	2:M:6:GLN:N	2.27	0.60
2:M:418:GLU:OE1	2:M:418:GLU:N	2.27	0.60
1:L:136:PHE:C	1:L:136:PHE:CD2	2.80	0.59
4:N:34:LYS:O	4:N:34:LYS:HG2	2.03	0.59
2:M:6:GLN:OE1	2:M:6:GLN:N	2.31	0.59
2:M:206:ASP:OD1	2:M:206:ASP:C	2.44	0.59
2:M:154:ILE:O	2:M:154:ILE:CG2	2.47	0.59
4:N:34:LYS:O	4:N:34:LYS:HG2	2.01	0.59
4:N:34:LYS:O	4:N:34:LYS:HG2	2.03	0.59
1:L:87:TRP:HA	1:L:87:TRP:HE3	1.68	0.59
4:N:34:LYS:O	4:N:34:LYS:HG2	2.01	0.58
5:L:501:ATP:O2B	5:L:501:ATP:O2G	2.22	0.58
4:N:34:LYS:O	4:N:34:LYS:HG2	2.03	0.58
4:N:34:LYS:O	4:N:34:LYS:HG2	2.02	0.57
2:M:363:GLU:OE1	2:M:363:GLU:N	2.33	0.57
2:M:445:ASP:OD1	2:M:445:ASP:C	2.46	0.56
1:L:427:GLN:OE1	1:L:427:GLN:N	2.32	0.56
4:N:34:LYS:O	4:N:34:LYS:HG2	2.04	0.56
1:L:427:GLN:OE1	1:L:427:GLN:N	2.31	0.56
1:L:302:ASP:C	1:L:302:ASP:OD1	2.43	0.56
2:M:363:GLU:OE1	2:M:363:GLU:N	2.32	0.56
2:M:206:ASP:OD1	2:M:206:ASP:C	2.46	0.56
5:L:501:ATP:O2B	5:L:501:ATP:O1A	2.21	0.56
2:M:418:GLU:OE1	2:M:418:GLU:N	2.31	0.56
1:L:79:ASN:OD1	1:L:79:ASN:C	2.48	0.56
2:M:276:ASN:OD1	2:M:276:ASN:N	2.38	0.56
1:L:240:GLU:OE1	1:L:240:GLU:N	2.33	0.55
1:L:326:GLU:OE1	1:L:326:GLU:N	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:276:ASN:OD1	2:M:276:ASN:N	2.39	0.55
1:L:427:GLN:OE1	1:L:427:GLN:N	2.31	0.55
1:L:458:GLU:OE1	1:L:458:GLU:N	2.35	0.55
1:L:427:GLN:OE1	1:L:427:GLN:N	2.34	0.55
1:L:427:GLN:OE1	1:L:427:GLN:N	2.33	0.55
2:M:276:ASN:OD1	2:M:276:ASN:N	2.39	0.54
4:N:85:LYS:NZ	4:N:85:LYS:HB2	2.23	0.54
2:M:349:LEU:C	2:M:349:LEU:HD23	2.32	0.54
1:L:427:GLN:OE1	1:L:427:GLN:N	2.33	0.54
1:L:427:GLN:OE1	1:L:427:GLN:N	2.32	0.54
2:M:276:ASN:OD1	2:M:276:ASN:N	2.40	0.54
2:M:363:GLU:OE1	2:M:363:GLU:N	2.34	0.54
4:N:90:ARG:O	4:N:90:ARG:HG3	2.07	0.54
1:L:72:ASP:C	1:L:72:ASP:OD1	2.51	0.53
3:K:343:SER:OG	3:K:344:ARG:N	2.39	0.53
2:M:418:GLU:OE1	2:M:418:GLU:N	2.33	0.53
2:M:13:TYR:CD1	2:M:13:TYR:C	2.84	0.53
1:L:72:ASP:C	1:L:72:ASP:OD1	2.51	0.53
2:M:141:ILE:HG23	2:M:141:ILE:O	2.08	0.53
2:M:363:GLU:OE1	2:M:363:GLU:N	2.32	0.53
2:M:462:LEU:C	2:M:462:LEU:HD12	2.33	0.53
1:L:463:LEU:C	1:L:463:LEU:HD23	2.34	0.53
1:L:72:ASP:C	1:L:72:ASP:OD1	2.52	0.53
2:M:462:LEU:C	2:M:462:LEU:HD12	2.34	0.53
1:L:136:PHE:C	1:L:136:PHE:CD2	2.86	0.53
1:L:72:ASP:C	1:L:72:ASP:OD1	2.51	0.53
2:M:13:TYR:C	2:M:13:TYR:CD2	2.86	0.53
1:L:463:LEU:C	1:L:463:LEU:HD23	2.34	0.52
2:M:112:LEU:C	2:M:112:LEU:HD23	2.34	0.52
1:L:79:ASN:OD1	1:L:79:ASN:C	2.52	0.52
1:L:79:ASN:OD1	1:L:79:ASN:C	2.52	0.52
4:N:66:ASN:OD1	4:N:66:ASN:C	2.51	0.52
5:L:501:ATP:O2B	5:L:501:ATP:O1A	2.27	0.52
1:L:79:ASN:OD1	1:L:79:ASN:C	2.52	0.52
2:M:438:GLN:O	2:M:438:GLN:CG	2.56	0.52
1:L:240:GLU:OE1	1:L:240:GLU:N	2.30	0.52
1:L:79:ASN:OD1	1:L:79:ASN:C	2.50	0.52
2:M:445:ASP:OD1	2:M:445:ASP:C	2.53	0.52
2:M:112:LEU:C	2:M:112:LEU:HD23	2.34	0.52
1:L:458:GLU:OE1	1:L:458:GLU:N	2.37	0.52
4:N:85:LYS:NZ	4:N:85:LYS:HB2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:154:ILE:HG22	2:M:154:ILE:O	2.09	0.52
5:L:501:ATP:O2B	5:L:501:ATP:O1A	2.23	0.52
2:M:119:TRP:CD1	2:M:119:TRP:N	2.75	0.52
2:M:361:GLU:OE1	2:M:361:GLU:N	2.41	0.52
1:L:72:ASP:C	1:L:72:ASP:OD1	2.51	0.52
2:M:112:LEU:C	2:M:112:LEU:HD23	2.35	0.52
2:M:445:ASP:OD1	2:M:445:ASP:C	2.53	0.52
1:L:326:GLU:OE1	1:L:326:GLU:N	2.38	0.52
2:M:363:GLU:OE1	2:M:363:GLU:N	2.36	0.52
2:M:112:LEU:C	2:M:112:LEU:HD23	2.35	0.52
2:M:462:LEU:C	2:M:462:LEU:HD12	2.36	0.51
3:K:341:GLN:O	3:K:342:TRP:C	2.52	0.51
1:L:79:ASN:OD1	1:L:79:ASN:C	2.50	0.51
2:M:418:GLU:OE1	2:M:418:GLU:N	2.34	0.51
1:L:122:ARG:NE	1:L:122:ARG:HA	2.25	0.51
2:M:154:ILE:O	2:M:154:ILE:CG2	2.49	0.51
1:L:72:ASP:C	1:L:72:ASP:OD1	2.52	0.51
2:M:462:LEU:HD12	2:M:462:LEU:C	2.36	0.51
3:K:341:GLN:O	3:K:342:TRP:C	2.53	0.51
2:M:107:SER:OG	2:M:108:ASN:N	2.41	0.51
1:L:72:ASP:C	1:L:72:ASP:OD1	2.50	0.51
2:M:107:SER:OG	2:M:108:ASN:N	2.41	0.51
3:K:342:TRP:O	3:K:342:TRP:CG	2.64	0.51
1:L:326:GLU:OE1	1:L:326:GLU:N	2.38	0.51
1:L:79:ASN:OD1	1:L:79:ASN:C	2.51	0.51
2:M:119:TRP:CD1	2:M:119:TRP:N	2.77	0.51
1:L:136:PHE:C	1:L:136:PHE:CD2	2.89	0.51
4:N:85:LYS:NZ	4:N:85:LYS:HB2	2.25	0.50
2:M:119:TRP:CD1	2:M:119:TRP:N	2.79	0.50
4:N:85:LYS:NZ	4:N:85:LYS:HB2	2.26	0.50
1:L:326:GLU:OE1	1:L:326:GLU:N	2.38	0.50
1:L:79:ASN:OD1	1:L:79:ASN:C	2.52	0.50
2:M:119:TRP:CD1	2:M:119:TRP:N	2.77	0.50
1:L:463:LEU:C	1:L:463:LEU:HD23	2.37	0.50
1:L:463:LEU:C	1:L:463:LEU:HD23	2.37	0.50
1:L:256:ILE:O	1:L:256:ILE:CG2	2.49	0.50
1:L:458:GLU:OE1	1:L:458:GLU:N	2.39	0.50
1:L:449:TRP:C	1:L:449:TRP:CD1	2.89	0.50
2:M:119:TRP:CD1	2:M:119:TRP:N	2.78	0.50
2:M:445:ASP:OD1	2:M:445:ASP:C	2.55	0.50
2:M:119:TRP:CD1	2:M:119:TRP:N	2.78	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:119:TRP:CD1	2:M:119:TRP:N	2.78	0.50
1:L:72:ASP:C	1:L:72:ASP:OD1	2.51	0.50
4:N:85:LYS:NZ	4:N:85:LYS:HB2	2.26	0.49
2:M:119:TRP:CD1	2:M:119:TRP:N	2.78	0.49
1:L:72:ASP:C	1:L:72:ASP:OD1	2.51	0.49
4:N:85:LYS:NZ	4:N:85:LYS:HB2	2.27	0.49
1:L:11:HIS:C	1:L:11:HIS:ND1	2.70	0.49
1:L:326:GLU:OE1	1:L:326:GLU:N	2.39	0.49
1:L:79:ASN:OD1	1:L:79:ASN:C	2.54	0.49
1:L:201:ILE:O	1:L:202:LYS:CB	2.60	0.49
2:M:119:TRP:CD1	2:M:119:TRP:N	2.79	0.49
1:L:79:ASN:OD1	1:L:79:ASN:C	2.55	0.49
1:L:215:LYS:O	1:L:218:THR:OG1	2.27	0.49
1:L:463:LEU:C	1:L:463:LEU:HD23	2.38	0.48
5:L:501:ATP:O2B	5:L:501:ATP:O1A	2.30	0.48
1:L:463:LEU:C	1:L:463:LEU:HD23	2.37	0.48
2:M:354:LEU:C	2:M:354:LEU:HD23	2.38	0.48
2:M:322:ASP:OD1	2:M:322:ASP:C	2.56	0.48
1:L:72:ASP:C	1:L:72:ASP:OD1	2.52	0.48
2:M:418:GLU:OE1	2:M:418:GLU:N	2.31	0.48
1:L:329:LEU:C	1:L:329:LEU:HD23	2.39	0.48
2:M:286:ASP:OD1	2:M:286:ASP:C	2.55	0.48
2:M:119:TRP:CD1	2:M:119:TRP:N	2.80	0.48
2:M:139:ASN:OD1	2:M:139:ASN:C	2.56	0.48
1:L:428:VAL:HG12	1:L:428:VAL:O	2.13	0.48
1:L:281:ASN:OD1	1:L:281:ASN:C	2.56	0.48
1:L:311:GLU:HA	1:L:311:GLU:OE1	2.14	0.48
1:L:343:SER:OG	1:L:344:ILE:HA	2.14	0.48
1:L:428:VAL:O	1:L:430:MET:N	2.47	0.48
1:L:155:PHE:CE1	1:L:388:LEU:HB3	2.49	0.48
5:L:501:ATP:O2A	5:L:501:ATP:O2B	2.31	0.48
1:L:7:CYS:SG	1:L:22:SER:HB3	2.54	0.48
1:L:87:TRP:CE3	1:L:87:TRP:CA	2.96	0.48
1:L:343:SER:CB	1:L:344:ILE:HA	2.44	0.48
1:L:7:CYS:SG	1:L:22:SER:HB3	2.54	0.47
1:L:4:ASN:OD1	1:L:4:ASN:C	2.57	0.47
1:L:281:ASN:OD1	1:L:281:ASN:C	2.57	0.47
5:L:501:ATP:O2B	5:L:501:ATP:O1A	2.27	0.47
1:L:141:GLU:HB2	1:L:142:PRO:CD	2.45	0.47
1:L:343:SER:CB	1:L:344:ILE:HA	2.45	0.47
1:L:281:ASN:OD1	1:L:281:ASN:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:341:GLN:O	3:K:342:TRP:C	2.58	0.47
4:N:85:LYS:HB2	4:N:85:LYS:HZ2	1.80	0.47
2:M:154:ILE:O	2:M:154:ILE:CG2	2.58	0.47
1:L:343:SER:OG	1:L:344:ILE:HA	2.15	0.47
2:M:418:GLU:H	2:M:418:GLU:CD	2.14	0.47
4:N:66:ASN:OD1	4:N:66:ASN:C	2.55	0.47
1:L:122:ARG:NE	1:L:122:ARG:HA	2.29	0.47
2:M:322:ASP:OD1	2:M:322:ASP:C	2.58	0.47
4:N:85:LYS:NZ	4:N:85:LYS:HB2	2.30	0.47
5:L:501:ATP:O2A	5:L:501:ATP:O2B	2.33	0.47
2:M:286:ASP:OD1	2:M:286:ASP:C	2.57	0.46
2:M:154:ILE:O	2:M:155:SER:C	2.58	0.46
2:M:354:LEU:C	2:M:354:LEU:HD23	2.40	0.46
3:K:342:TRP:O	3:K:342:TRP:CD1	2.69	0.46
2:M:75:ASP:C	2:M:75:ASP:OD1	2.57	0.46
3:K:376:GLN:O	3:K:377:ARG:HB2	2.15	0.46
2:M:322:ASP:OD1	2:M:322:ASP:C	2.58	0.46
3:K:320:ARG:NE	3:K:320:ARG:HA	2.31	0.46
4:N:66:ASN:OD1	4:N:66:ASN:C	2.58	0.46
3:K:341:GLN:O	3:K:343:SER:N	2.49	0.46
2:M:213:LEU:HD23	2:M:213:LEU:C	2.41	0.46
1:L:382:GLU:H	1:L:382:GLU:CD	2.23	0.46
3:K:347:ARG:H	3:K:347:ARG:HD2	1.81	0.46
2:M:322:ASP:OD1	2:M:322:ASP:C	2.58	0.46
4:N:66:ASN:OD1	4:N:66:ASN:C	2.58	0.46
2:M:57:ASN:OD1	2:M:57:ASN:C	2.56	0.46
3:K:376:GLN:O	3:K:377:ARG:HB2	2.16	0.46
2:M:75:ASP:C	2:M:75:ASP:OD1	2.57	0.46
4:N:85:LYS:NZ	4:N:85:LYS:HB2	2.31	0.46
2:M:98:ASN:O	2:M:99:GLN:HB2	2.16	0.46
4:N:85:LYS:NZ	4:N:85:LYS:HB2	2.31	0.46
2:M:322:ASP:OD1	2:M:322:ASP:C	2.58	0.46
2:M:75:ASP:C	2:M:75:ASP:OD1	2.58	0.45
4:N:66:ASN:OD1	4:N:66:ASN:C	2.57	0.45
2:M:418:GLU:OE1	2:M:418:GLU:N	2.37	0.45
1:L:198:ALA:HB3	1:L:199:PRO:HD3	1.98	0.45
2:M:139:ASN:OD1	2:M:139:ASN:C	2.59	0.45
1:L:293:LYS:HB3	1:L:294:PRO:HD3	1.98	0.45
4:N:85:LYS:NZ	4:N:85:LYS:HB2	2.32	0.45
1:L:122:ARG:NE	1:L:122:ARG:HA	2.31	0.45
1:L:198:ALA:HB3	1:L:199:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:465:ARG:HA	1:L:465:ARG:NE	2.32	0.45
1:L:256:ILE:HG22	1:L:256:ILE:O	2.16	0.45
3:K:376:GLN:O	3:K:377:ARG:HB2	2.16	0.45
1:L:302:ASP:OD1	1:L:302:ASP:O	2.35	0.45
2:M:57:ASN:OD1	2:M:57:ASN:C	2.58	0.45
2:M:146:SER:OG	2:M:147:LEU:N	2.50	0.45
1:L:198:ALA:HB3	1:L:199:PRO:HD3	1.98	0.45
3:K:376:GLN:O	3:K:377:ARG:HB2	2.16	0.45
2:M:154:ILE:O	2:M:155:SER:C	2.60	0.45
2:M:146:SER:OG	2:M:147:LEU:N	2.50	0.45
1:L:158:ASP:OD1	1:L:158:ASP:C	2.59	0.45
2:M:369:ARG:HA	2:M:369:ARG:NE	2.32	0.44
4:N:80:ASP:OD1	4:N:80:ASP:C	2.60	0.44
1:L:343:SER:HB3	1:L:344:ILE:HA	1.99	0.44
4:N:80:ASP:OD1	4:N:80:ASP:C	2.57	0.44
1:L:240:GLU:CD	1:L:240:GLU:N	2.75	0.44
2:M:154:ILE:O	2:M:155:SER:C	2.60	0.44
1:L:198:ALA:HB3	1:L:199:PRO:HD3	1.99	0.44
1:L:343:SER:HB3	1:L:344:ILE:HA	1.99	0.44
2:M:57:ASN:OD1	2:M:57:ASN:C	2.60	0.44
1:L:201:ILE:O	1:L:202:LYS:HB3	2.17	0.44
1:L:158:ASP:OD1	1:L:158:ASP:C	2.60	0.44
1:L:429:MET:SD	2:M:322:ASP:HA	2.58	0.44
2:M:57:ASN:OD1	2:M:57:ASN:C	2.60	0.44
2:M:286:ASP:OD1	2:M:286:ASP:C	2.59	0.44
2:M:57:ASN:OD1	2:M:57:ASN:C	2.60	0.44
2:M:418:GLU:H	2:M:418:GLU:CD	2.19	0.44
2:M:144:PRO:O	2:M:145:ALA:C	2.61	0.44
2:M:98:ASN:O	2:M:99:GLN:HB3	2.18	0.44
2:M:141:ILE:HG23	2:M:141:ILE:O	2.16	0.44
2:M:13:TYR:HD2	2:M:13:TYR:O	2.01	0.44
1:L:38:ARG:HB2	1:L:46:GLU:HB3	2.00	0.44
2:M:462:LEU:C	2:M:462:LEU:HD12	2.42	0.44
4:N:80:ASP:OD1	4:N:80:ASP:C	2.59	0.44
1:L:136:PHE:O	1:L:136:PHE:HD2	2.01	0.44
4:N:2:ASP:OD1	4:N:2:ASP:C	2.61	0.44
1:L:87:TRP:CD1	1:L:87:TRP:N	2.83	0.44
1:L:320:SER:OG	1:L:321:ASP:N	2.51	0.43
4:N:2:ASP:OD1	4:N:2:ASP:C	2.61	0.43
1:L:4:ASN:OD1	1:L:4:ASN:C	2.61	0.43
2:M:322:ASP:OD1	2:M:322:ASP:C	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:320:SER:OG	1:L:321:ASP:N	2.51	0.43
1:L:198:ALA:HB3	1:L:199:PRO:HD3	1.99	0.43
4:N:80:ASP:OD1	4:N:80:ASP:C	2.59	0.43
2:M:98:ASN:O	2:M:99:GLN:HB3	2.19	0.43
2:M:146:SER:OG	2:M:147:LEU:N	2.51	0.43
1:L:320:SER:OG	1:L:321:ASP:N	2.51	0.43
2:M:146:SER:OG	2:M:147:LEU:N	2.50	0.43
1:L:256:ILE:O	1:L:256:ILE:CG2	2.64	0.43
1:L:320:SER:OG	1:L:321:ASP:N	2.51	0.43
1:L:141:GLU:CB	1:L:142:PRO:CD	2.97	0.43
1:L:112:ASN:OD1	1:L:112:ASN:C	2.62	0.43
1:L:141:GLU:HB2	1:L:142:PRO:CD	2.49	0.43
4:N:2:ASP:OD1	4:N:2:ASP:C	2.61	0.43
2:M:286:ASP:OD1	2:M:286:ASP:C	2.60	0.43
1:L:320:SER:OG	1:L:321:ASP:N	2.51	0.43
1:L:215:LYS:O	1:L:218:THR:OG1	2.30	0.43
1:L:382:GLU:H	1:L:382:GLU:CD	2.26	0.43
1:L:465:ARG:HA	1:L:465:ARG:NE	2.34	0.43
2:M:75:ASP:C	2:M:75:ASP:OD1	2.60	0.43
2:M:121:GLN:HG3	2:M:463:TRP:CZ2	2.54	0.43
1:L:7:CYS:SG	1:L:22:SER:HB3	2.58	0.43
1:L:198:ALA:HB3	1:L:199:PRO:HD3	2.00	0.43
1:L:4:ASN:OD1	1:L:4:ASN:C	2.62	0.43
1:L:4:ASN:OD1	1:L:4:ASN:C	2.60	0.43
1:L:38:ARG:HB2	1:L:46:GLU:HB3	2.01	0.43
4:N:34:LYS:O	4:N:34:LYS:CG	2.67	0.43
1:L:293:LYS:HB3	1:L:294:PRO:HD3	2.00	0.43
2:M:57:ASN:OD1	2:M:57:ASN:C	2.61	0.43
1:L:38:ARG:HB2	1:L:46:GLU:HB3	2.01	0.43
2:M:368:LYS:HA	2:M:368:LYS:HD3	1.87	0.43
1:L:4:ASN:OD1	1:L:4:ASN:C	2.62	0.43
1:L:159:ILE:HG22	1:L:398:THR:HB	2.01	0.43
1:L:112:ASN:OD1	1:L:112:ASN:C	2.62	0.43
4:N:84:LEU:O	4:N:85:LYS:HB2	2.19	0.43
1:L:241:LYS:O	1:L:242:ASP:C	2.62	0.43
1:L:133:VAL:O	1:L:134:PRO:C	2.61	0.43
1:L:4:ASN:OD1	1:L:4:ASN:O	2.36	0.43
1:L:429:MET:SD	2:M:322:ASP:HA	2.59	0.43
2:M:75:ASP:C	2:M:75:ASP:OD1	2.60	0.42
1:L:112:ASN:OD1	1:L:112:ASN:C	2.62	0.42
1:L:293:LYS:HB3	1:L:294:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:98:ASN:O	2:M:99:GLN:HB3	2.18	0.42
2:M:94:ARG:HA	2:M:94:ARG:HD3	1.78	0.42
2:M:57:ASN:OD1	2:M:57:ASN:C	2.59	0.42
1:L:7:CYS:SG	1:L:22:SER:HB3	2.59	0.42
1:L:4:ASN:OD1	1:L:4:ASN:C	2.60	0.42
2:M:27:GLU:O	2:M:28:GLU:C	2.62	0.42
1:L:114:LYS:HB3	1:L:115:PRO:HD3	2.01	0.42
4:N:84:LEU:O	4:N:85:LYS:HB2	2.19	0.42
1:L:117:MET:C	1:L:117:MET:SD	3.02	0.42
1:L:158:ASP:OD1	1:L:158:ASP:C	2.60	0.42
1:L:382:GLU:H	1:L:382:GLU:CD	2.27	0.42
2:M:322:ASP:OD1	2:M:322:ASP:C	2.60	0.42
1:L:434:ILE:O	1:L:435:GLN:C	2.63	0.42
2:M:454:TYR:O	2:M:458:GLY:N	2.53	0.42
4:N:34:LYS:O	4:N:34:LYS:CG	2.67	0.42
4:N:34:LYS:O	4:N:34:LYS:CG	2.67	0.42
1:L:429:MET:SD	2:M:322:ASP:HA	2.60	0.42
1:L:465:ARG:O	1:L:466:ASP:CB	2.67	0.42
1:L:141:GLU:HB2	1:L:142:PRO:CD	2.50	0.42
2:M:418:GLU:H	2:M:418:GLU:CD	2.16	0.42
4:N:85:LYS:HB2	4:N:85:LYS:HZ2	1.85	0.42
1:L:7:CYS:SG	1:L:22:SER:HB3	2.60	0.42
2:M:75:ASP:C	2:M:75:ASP:OD1	2.61	0.42
2:M:7:ASP:HA	2:M:24:GLY:HA2	2.01	0.42
4:N:84:LEU:O	4:N:85:LYS:HB2	2.19	0.42
1:L:15:HIS:CD2	1:L:16:ARG:HG3	2.55	0.42
1:L:198:ALA:HB3	1:L:199:PRO:HD3	2.01	0.42
2:M:3:PRO:HA	2:M:4:PHE:HA	1.90	0.42
3:K:345:GLN:HA	3:K:348:CYS:SG	2.59	0.42
2:M:88:VAL:O	2:M:88:VAL:HG22	2.19	0.42
4:N:84:LEU:O	4:N:85:LYS:HB2	2.20	0.42
1:L:198:ALA:HB3	1:L:199:PRO:HD3	2.02	0.42
4:N:84:LEU:O	4:N:85:LYS:HB2	2.19	0.42
1:L:227:TRP:CD1	1:L:227:TRP:O	2.73	0.42
5:L:501:ATP:O1A	5:L:501:ATP:O2B	2.38	0.42
4:N:84:LEU:O	4:N:85:LYS:HB2	2.20	0.42
4:N:84:LEU:O	4:N:85:LYS:HB2	2.20	0.42
1:L:256:ILE:O	1:L:256:ILE:HG22	2.19	0.42
2:M:369:ARG:HA	2:M:369:ARG:NE	2.35	0.42
4:N:34:LYS:O	4:N:34:LYS:CG	2.68	0.42
4:N:34:LYS:O	4:N:34:LYS:CG	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:429:MET:SD	2:M:322:ASP:HA	2.60	0.41
1:L:11:HIS:ND1	1:L:11:HIS:C	2.78	0.41
4:N:84:LEU:O	4:N:85:LYS:HB2	2.20	0.41
1:L:215:LYS:O	1:L:218:THR:OG1	2.29	0.41
1:L:302:ASP:OD1	1:L:302:ASP:O	2.38	0.41
2:M:322:ASP:OD1	2:M:322:ASP:C	2.62	0.41
2:M:75:ASP:OD1	2:M:75:ASP:C	2.62	0.41
4:N:80:ASP:C	4:N:80:ASP:OD1	2.63	0.41
1:L:38:ARG:HB2	1:L:46:GLU:HB3	2.02	0.41
1:L:464:LYS:HD3	1:L:464:LYS:HA	1.84	0.41
2:M:75:ASP:C	2:M:75:ASP:OD1	2.61	0.41
2:M:13:TYR:C	2:M:13:TYR:HD2	2.28	0.41
2:M:46:ARG:NH2	2:M:50:SER:OG	2.49	0.41
2:M:13:TYR:C	2:M:13:TYR:CD2	2.98	0.41
2:M:139:ASN:OD1	2:M:139:ASN:C	2.63	0.41
4:N:80:ASP:OD1	4:N:80:ASP:C	2.60	0.41
1:L:158:ASP:C	1:L:158:ASP:OD1	2.60	0.41
1:L:158:ASP:C	1:L:158:ASP:OD1	2.61	0.41
1:L:316:PRO:HA	1:L:319:ILE:HD12	2.02	0.41
2:M:104:ALA:O	2:M:106:LEU:N	2.52	0.41
1:L:155:PHE:CE1	1:L:388:LEU:HB3	2.55	0.41
1:L:255:ASP:O	1:L:256:ILE:C	2.63	0.41
1:L:112:ASN:OD1	1:L:112:ASN:C	2.62	0.41
1:L:112:ASN:OD1	1:L:112:ASN:C	2.63	0.41
1:L:7:CYS:SG	1:L:22:SER:HB3	2.60	0.41
2:M:98:ASN:OD1	2:M:98:ASN:C	2.63	0.41
1:L:136:PHE:CD1	1:L:136:PHE:C	2.98	0.41
1:L:293:LYS:HB3	1:L:294:PRO:HD3	2.01	0.41
2:M:98:ASN:OD1	2:M:98:ASN:C	2.61	0.41
3:K:376:GLN:O	3:K:377:ARG:HB2	2.20	0.41
1:L:293:LYS:HB3	1:L:294:PRO:HD3	2.02	0.41
1:L:392:VAL:HB	1:L:423:THR:HG22	2.03	0.41
1:L:107:THR:OG1	1:L:108:MET:N	2.53	0.41
1:L:7:CYS:SG	1:L:22:SER:HB3	2.61	0.41
1:L:282:ASN:OD1	1:L:282:ASN:C	2.63	0.41
2:M:3:PRO:HB2	2:M:4:PHE:HA	2.03	0.41
1:L:155:PHE:CE1	1:L:388:LEU:HB3	2.56	0.41
1:L:133:VAL:HA	1:L:134:PRO:HD3	1.98	0.41
1:L:282:ASN:OD1	1:L:282:ASN:C	2.62	0.41
2:M:141:ILE:O	2:M:141:ILE:HG23	2.21	0.41
4:N:84:LEU:O	4:N:85:LYS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:418:GLU:H	2:M:418:GLU:CD	2.17	0.41
1:L:15:HIS:CD2	1:L:16:ARG:HG3	2.56	0.41
2:M:139:ASN:OD1	2:M:139:ASN:C	2.63	0.41
4:N:34:LYS:O	4:N:34:LYS:CG	2.68	0.41
2:M:143:LEU:HA	2:M:144:PRO:HD2	1.94	0.41
1:L:282:ASN:OD1	1:L:282:ASN:C	2.63	0.41
2:M:415:TYR:CZ	3:K:363:GLU:HG2	2.56	0.41
2:M:57:ASN:C	2:M:57:ASN:OD1	2.61	0.41
2:M:163:ASP:C	2:M:163:ASP:OD1	2.62	0.41
1:L:100:GLU:H	1:L:100:GLU:CD	2.27	0.41
1:L:100:GLU:H	1:L:100:GLU:CD	2.27	0.41
1:L:429:MET:SD	2:M:322:ASP:HA	2.61	0.41
2:M:368:LYS:HD3	2:M:368:LYS:HA	1.91	0.41
4:N:56:TYR:O	4:N:58:PHE:N	2.54	0.40
4:N:34:LYS:O	4:N:34:LYS:CG	2.69	0.40
1:L:239:SER:O	1:L:407:ARG:HD2	2.21	0.40
1:L:158:ASP:OD1	1:L:158:ASP:C	2.61	0.40
4:N:2:ASP:OD1	4:N:2:ASP:C	2.64	0.40
4:N:84:LEU:O	4:N:85:LYS:HB2	2.20	0.40
1:L:342:ALA:O	1:L:343:SER:C	2.63	0.40
1:L:282:ASN:OD1	1:L:282:ASN:C	2.63	0.40
1:L:4:ASN:OD1	1:L:4:ASN:C	2.65	0.40
1:L:282:ASN:OD1	1:L:282:ASN:C	2.63	0.40
2:M:322:ASP:OD1	2:M:322:ASP:C	2.62	0.40
1:L:201:ILE:O	1:L:203:GLU:N	2.54	0.40
1:L:158:ASP:OD1	1:L:158:ASP:C	2.62	0.40
1:L:11:HIS:ND1	1:L:11:HIS:C	2.78	0.40
1:L:293:LYS:HB3	1:L:294:PRO:HD3	2.02	0.40
1:L:7:CYS:SG	1:L:22:SER:HB3	2.62	0.40
4:N:34:LYS:O	4:N:34:LYS:CG	2.69	0.40
2:M:361:GLU:OE1	2:M:361:GLU:N	2.44	0.40
1:L:426:ASN:OD1	1:L:426:ASN:C	2.65	0.40
1:L:7:CYS:SG	1:L:22:SER:HB3	2.62	0.40
1:L:112:ASN:OD1	1:L:112:ASN:C	2.64	0.40
2:M:13:TYR:CD2	2:M:13:TYR:C	3.00	0.40
4:N:84:LEU:O	4:N:85:LYS:CB	2.70	0.40
2:M:29:THR:OG1	2:M:30:PHE:N	2.54	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	1-L	383/477 (80%)	370 (97%)	12 (3%)	1 (0%)	36	71
1	2-L	383/477 (80%)	368 (96%)	10 (3%)	5 (1%)	9	41
1	3-L	383/477 (80%)	366 (96%)	15 (4%)	2 (0%)	24	62
1	4-L	383/477 (80%)	366 (96%)	13 (3%)	4 (1%)	12	47
1	5-L	383/477 (80%)	368 (96%)	12 (3%)	3 (1%)	16	52
1	6-L	383/477 (80%)	362 (94%)	17 (4%)	4 (1%)	12	47
1	7-L	383/477 (80%)	371 (97%)	11 (3%)	1 (0%)	36	71
1	8-L	383/477 (80%)	367 (96%)	12 (3%)	4 (1%)	12	47
1	9-L	383/477 (80%)	369 (96%)	12 (3%)	2 (0%)	24	62
1	10-L	383/477 (80%)	369 (96%)	13 (3%)	1 (0%)	36	71
2	1-M	390/467 (84%)	371 (95%)	13 (3%)	6 (2%)	8	38
2	2-M	390/467 (84%)	373 (96%)	14 (4%)	3 (1%)	16	52
2	3-M	390/467 (84%)	374 (96%)	10 (3%)	6 (2%)	8	38
2	4-M	390/467 (84%)	367 (94%)	20 (5%)	3 (1%)	16	52
2	5-M	390/467 (84%)	373 (96%)	14 (4%)	3 (1%)	16	52
2	6-M	390/467 (84%)	369 (95%)	18 (5%)	3 (1%)	16	52
2	7-M	390/467 (84%)	368 (94%)	20 (5%)	2 (0%)	24	62
2	8-M	390/467 (84%)	369 (95%)	15 (4%)	6 (2%)	8	38
2	9-M	390/467 (84%)	365 (94%)	21 (5%)	4 (1%)	12	47
2	10-M	390/467 (84%)	370 (95%)	18 (5%)	2 (0%)	24	62
3	1-K	60/813 (7%)	59 (98%)	1 (2%)	0	100	100
3	2-K	60/813 (7%)	59 (98%)	0	1 (2%)	7	35
3	3-K	60/813 (7%)	59 (98%)	1 (2%)	0	100	100
3	4-K	60/813 (7%)	57 (95%)	2 (3%)	1 (2%)	7	35
3	5-K	60/813 (7%)	57 (95%)	0	3 (5%)	1	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	6-K	60/813 (7%)	60 (100%)	0	0	100	100
3	7-K	60/813 (7%)	59 (98%)	1 (2%)	0	100	100
3	8-K	60/813 (7%)	59 (98%)	0	1 (2%)	7	35
3	9-K	60/813 (7%)	60 (100%)	0	0	100	100
3	10-K	60/813 (7%)	57 (95%)	1 (2%)	2 (3%)	3	21
4	1-N	47/157 (30%)	44 (94%)	2 (4%)	1 (2%)	5	30
4	2-N	47/157 (30%)	45 (96%)	1 (2%)	1 (2%)	5	30
4	3-N	47/157 (30%)	44 (94%)	1 (2%)	2 (4%)	2	18
4	4-N	47/157 (30%)	43 (92%)	3 (6%)	1 (2%)	5	30
4	5-N	47/157 (30%)	43 (92%)	3 (6%)	1 (2%)	5	30
4	6-N	47/157 (30%)	44 (94%)	2 (4%)	1 (2%)	5	30
4	7-N	47/157 (30%)	44 (94%)	2 (4%)	1 (2%)	5	30
4	8-N	47/157 (30%)	45 (96%)	1 (2%)	1 (2%)	5	30
4	9-N	47/157 (30%)	44 (94%)	2 (4%)	1 (2%)	5	30
4	10-N	47/157 (30%)	45 (96%)	1 (2%)	1 (2%)	5	30
All	All	8800/19140 (46%)	8402 (96%)	314 (4%)	84 (1%)	15	47

All (84) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-L	202	LYS
2	1-M	155	SER
2	1-M	363	GLU
1	2-L	51	THR
2	3-M	58	LYS
4	3-N	57	PRO
1	4-L	429	MET
3	5-K	341	GLN
1	6-L	175	VAL
2	6-M	104	ALA
1	8-L	435	GLN
2	8-M	27	GLU
2	9-M	402	GLN
3	10-K	342	TRP
4	1-N	85	LYS
1	2-L	45	ALA
1	2-L	429	MET

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Mol	Chain	Res	Type
2	2-M	155	SER
3	2-K	341	GLN
4	2-N	85	LYS
1	3-L	202	LYS
2	3-M	27	GLU
2	3-M	146	SER
2	3-M	155	SER
4	3-N	85	LYS
1	4-L	45	ALA
4	4-N	85	LYS
2	5-M	27	GLU
2	5-M	155	SER
4	5-N	85	LYS
2	6-M	155	SER
4	6-N	85	LYS
1	7-L	134	PRO
2	7-M	155	SER
4	7-N	85	LYS
1	8-L	45	ALA
2	8-M	155	SER
4	8-N	85	LYS
2	9-M	155	SER
4	9-N	85	LYS
2	10-M	27	GLU
2	10-M	105	GLU
4	10-N	85	LYS
2	1-M	104	ALA
2	1-M	107	SER
2	1-M	362	PRO
1	2-L	77	PRO
1	3-L	115	PRO
1	4-L	115	PRO
2	4-M	28	GLU
1	5-L	115	PRO
2	5-M	104	ALA
1	6-L	464	LYS
2	7-M	146	SER
1	8-L	115	PRO
2	8-M	104	ALA
2	8-M	398	ILE
3	8-K	342	TRP
1	9-L	115	PRO

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Mol	Chain	Res	Type
2	9-M	107	SER
1	10-L	115	PRO
2	1-M	173	PRO
2	2-M	173	PRO
2	3-M	173	PRO
1	5-L	168	PRO
3	5-K	345	GLN
1	6-L	115	PRO
1	6-L	449	TRP
2	8-M	173	PRO
2	2-M	154	ILE
2	3-M	154	ILE
3	4-K	342	TRP
1	8-L	141	GLU
2	4-M	27	GLU
3	5-K	344	ARG
1	9-L	134	PRO
3	10-K	341	GLN
2	4-M	154	ILE
2	6-M	154	ILE
2	8-M	154	ILE
2	9-M	154	ILE
1	2-L	135	VAL
1	4-L	325	PRO
1	5-L	325	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-L	349/420 (83%)	349 (100%)	0	100	100
1	2-L	349/420 (83%)	349 (100%)	0	100	100
1	3-L	349/420 (83%)	349 (100%)	0	100	100
1	4-L	349/420 (83%)	349 (100%)	0	100	100
1	5-L	349/420 (83%)	349 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	6-L	349/420 (83%)	349 (100%)	0	100	100
1	7-L	349/420 (83%)	349 (100%)	0	100	100
1	8-L	349/420 (83%)	349 (100%)	0	100	100
1	9-L	349/420 (83%)	349 (100%)	0	100	100
1	10-L	349/420 (83%)	349 (100%)	0	100	100
2	1-M	362/423 (86%)	362 (100%)	0	100	100
2	2-M	362/423 (86%)	362 (100%)	0	100	100
2	3-M	362/423 (86%)	362 (100%)	0	100	100
2	4-M	362/423 (86%)	362 (100%)	0	100	100
2	5-M	362/423 (86%)	362 (100%)	0	100	100
2	6-M	362/423 (86%)	362 (100%)	0	100	100
2	7-M	362/423 (86%)	362 (100%)	0	100	100
2	8-M	362/423 (86%)	362 (100%)	0	100	100
2	9-M	362/423 (86%)	362 (100%)	0	100	100
2	10-M	362/423 (86%)	362 (100%)	0	100	100
3	1-K	58/735 (8%)	58 (100%)	0	100	100
3	2-K	58/735 (8%)	58 (100%)	0	100	100
3	3-K	58/735 (8%)	58 (100%)	0	100	100
3	4-K	58/735 (8%)	58 (100%)	0	100	100
3	5-K	58/735 (8%)	58 (100%)	0	100	100
3	6-K	58/735 (8%)	58 (100%)	0	100	100
3	7-K	58/735 (8%)	58 (100%)	0	100	100
3	8-K	58/735 (8%)	58 (100%)	0	100	100
3	9-K	58/735 (8%)	58 (100%)	0	100	100
3	10-K	58/735 (8%)	58 (100%)	0	100	100
4	1-N	54/140 (39%)	54 (100%)	0	100	100
4	2-N	54/140 (39%)	54 (100%)	0	100	100
4	3-N	54/140 (39%)	54 (100%)	0	100	100
4	4-N	54/140 (39%)	54 (100%)	0	100	100
4	5-N	54/140 (39%)	54 (100%)	0	100	100
4	6-N	54/140 (39%)	54 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	7-N	54/140 (39%)	54 (100%)	0	100	100
4	8-N	54/140 (39%)	54 (100%)	0	100	100
4	9-N	54/140 (39%)	54 (100%)	0	100	100
4	10-N	54/140 (39%)	54 (100%)	0	100	100
All	All	8230/17180 (48%)	8230 (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 (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-L	74	GLN
1	1-L	194	HIS
1	1-L	214	GLN
2	1-M	6	GLN
2	1-M	17	GLN
1	2-L	74	GLN
1	2-L	194	HIS
1	2-L	214	GLN
1	2-L	253	GLN
1	2-L	391	ASN
2	2-M	17	GLN
3	2-K	323	HIS
1	3-L	74	GLN
1	3-L	214	GLN
1	3-L	391	ASN
2	3-M	17	GLN
2	3-M	179	GLN
3	3-K	323	HIS
1	4-L	214	GLN
1	4-L	391	ASN
3	4-K	323	HIS
3	4-K	341	GLN
1	5-L	194	HIS
1	5-L	214	GLN
2	5-M	17	GLN
2	5-M	438	GLN
1	6-L	194	HIS
1	6-L	308	GLN
1	6-L	391	ASN

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Mol	Chain	Res	Type
2	6-M	17	GLN
1	7-L	74	GLN
1	7-L	194	HIS
1	7-L	214	GLN
2	7-M	17	GLN
1	8-L	214	GLN
1	8-L	391	ASN
2	8-M	81	GLN
3	8-K	323	HIS
1	9-L	74	GLN
1	9-L	194	HIS
1	9-L	214	GLN
2	9-M	6	GLN
2	9-M	352	GLN
1	10-L	12	ASN
1	10-L	15	HIS
1	10-L	194	HIS
1	10-L	214	GLN
2	10-M	17	GLN
3	10-K	323	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ATP	5-L	501	-	32,33,33	1.45	6 (18%)	48,52,52	1.83	11 (22%)
5	ATP	7-L	501	-	32,33,33	1.51	8 (25%)	48,52,52	1.85	11 (22%)
5	ATP	3-L	501	-	32,33,33	1.48	6 (18%)	48,52,52	1.86	11 (22%)
5	ATP	9-L	501	-	32,33,33	1.49	7 (21%)	48,52,52	1.86	11 (22%)
5	ATP	2-L	501	-	32,33,33	1.46	7 (21%)	48,52,52	1.80	9 (18%)
5	ATP	4-L	501	-	32,33,33	1.45	6 (18%)	48,52,52	1.83	9 (18%)
5	ATP	8-L	501	-	32,33,33	1.42	6 (18%)	48,52,52	1.84	11 (22%)
5	ATP	1-L	501	-	32,33,33	1.49	8 (25%)	48,52,52	1.85	10 (20%)
5	ATP	6-L	501	-	32,33,33	1.47	7 (21%)	48,52,52	1.87	11 (22%)
5	ATP	10-L	501	-	32,33,33	1.48	7 (21%)	48,52,52	1.82	10 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ATP	5-L	501	-	-	6/22/38/38	0/3/3/3
5	ATP	7-L	501	-	-	7/22/38/38	0/3/3/3
5	ATP	3-L	501	-	-	6/22/38/38	0/3/3/3
5	ATP	9-L	501	-	-	7/22/38/38	0/3/3/3
5	ATP	2-L	501	-	-	7/22/38/38	0/3/3/3
5	ATP	4-L	501	-	-	6/22/38/38	0/3/3/3
5	ATP	8-L	501	-	-	4/22/38/38	0/3/3/3
5	ATP	1-L	501	-	-	2/22/38/38	0/3/3/3
5	ATP	6-L	501	-	-	4/22/38/38	0/3/3/3
5	ATP	10-L	501	-	-	6/22/38/38	0/3/3/3

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	7-L	501	ATP	C5-C4	4.01	1.46	1.39
5	5-L	501	ATP	C5-C4	4.00	1.46	1.39
5	3-L	501	ATP	C5-C4	3.98	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1-L	501	ATP	C5-C4	3.98	1.46	1.39
5	6-L	501	ATP	C5-C4	3.97	1.46	1.39
5	9-L	501	ATP	C5-C4	3.97	1.46	1.39
5	8-L	501	ATP	C5-C4	3.94	1.46	1.39
5	10-L	501	ATP	C5-C4	3.90	1.46	1.39
5	2-L	501	ATP	C5-C4	3.88	1.46	1.39
5	4-L	501	ATP	C5-C4	3.85	1.46	1.39
5	3-L	501	ATP	C5-N7	-2.99	1.33	1.39
5	1-L	501	ATP	C5-N7	-2.96	1.33	1.39
5	10-L	501	ATP	C5-N7	-2.94	1.33	1.39
5	6-L	501	ATP	C5-N7	-2.94	1.33	1.39
5	9-L	501	ATP	C5-N7	-2.94	1.33	1.39
5	4-L	501	ATP	C5-N7	-2.92	1.33	1.39
5	5-L	501	ATP	C5-N7	-2.91	1.33	1.39
5	7-L	501	ATP	C5-N7	-2.90	1.33	1.39
5	2-L	501	ATP	C5-N7	-2.86	1.33	1.39
5	8-L	501	ATP	C5-N7	-2.77	1.34	1.39
5	1-L	501	ATP	PB-O3B	-2.72	1.56	1.59
5	3-L	501	ATP	PB-O3B	-2.63	1.56	1.59
5	7-L	501	ATP	PB-O3B	-2.62	1.56	1.59
5	6-L	501	ATP	PB-O3B	-2.61	1.56	1.59
5	9-L	501	ATP	PB-O3B	-2.49	1.56	1.59
5	3-L	501	ATP	C8-N9	-2.44	1.33	1.37
5	5-L	501	ATP	PB-O3B	-2.44	1.56	1.59
5	10-L	501	ATP	C4-N9	-2.43	1.32	1.37
5	2-L	501	ATP	C4-N9	-2.43	1.32	1.37
5	4-L	501	ATP	C8-N9	-2.42	1.33	1.37
5	2-L	501	ATP	C8-N9	-2.42	1.33	1.37
5	9-L	501	ATP	C8-N9	-2.41	1.33	1.37
5	1-L	501	ATP	C8-N9	-2.40	1.33	1.37
5	8-L	501	ATP	PB-O3B	-2.39	1.56	1.59
5	9-L	501	ATP	C4-N9	-2.39	1.32	1.37
5	10-L	501	ATP	PB-O3B	-2.38	1.56	1.59
5	4-L	501	ATP	PB-O3B	-2.37	1.56	1.59
5	3-L	501	ATP	C4-N9	-2.37	1.32	1.37
5	8-L	501	ATP	C8-N9	-2.36	1.33	1.37
5	7-L	501	ATP	C4-N9	-2.36	1.32	1.37
5	5-L	501	ATP	C8-N9	-2.35	1.33	1.37
5	10-L	501	ATP	C8-N9	-2.35	1.33	1.37
5	8-L	501	ATP	C4-N9	-2.34	1.32	1.37
5	7-L	501	ATP	C8-N9	-2.32	1.33	1.37
5	5-L	501	ATP	C4-N9	-2.31	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1-L	501	ATP	C4-N9	-2.28	1.33	1.37
5	4-L	501	ATP	C4-N9	-2.27	1.33	1.37
5	7-L	501	ATP	PB-O3A	-2.26	1.57	1.59
5	2-L	501	ATP	PB-O3B	-2.25	1.57	1.59
5	6-L	501	ATP	C8-N9	-2.25	1.33	1.37
5	6-L	501	ATP	PB-O3A	-2.19	1.57	1.59
5	6-L	501	ATP	C4-N9	-2.18	1.33	1.37
5	5-L	501	ATP	C5-C6	2.13	1.46	1.41
5	6-L	501	ATP	C5-C6	2.12	1.46	1.41
5	7-L	501	ATP	PA-O3A	-2.11	1.57	1.59
5	10-L	501	ATP	PB-O3A	-2.11	1.57	1.59
5	7-L	501	ATP	C5-C6	2.10	1.46	1.41
5	1-L	501	ATP	C5-C6	2.08	1.46	1.41
5	10-L	501	ATP	C5-C6	2.08	1.46	1.41
5	9-L	501	ATP	PB-O3A	-2.07	1.57	1.59
5	2-L	501	ATP	C5-C6	2.07	1.46	1.41
5	9-L	501	ATP	C5-C6	2.07	1.46	1.41
5	4-L	501	ATP	C5-C6	2.07	1.46	1.41
5	2-L	501	ATP	PB-O3A	-2.05	1.57	1.59
5	1-L	501	ATP	PB-O3A	-2.05	1.57	1.59
5	8-L	501	ATP	C5-C6	2.04	1.46	1.41
5	3-L	501	ATP	C5-C6	2.03	1.46	1.41
5	1-L	501	ATP	PA-O3A	-2.02	1.57	1.59

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	6-L	501	ATP	C5-C4-N3	-6.54	117.72	126.72
5	4-L	501	ATP	C5-C4-N3	-6.40	117.90	126.72
5	3-L	501	ATP	C5-C4-N3	-6.36	117.96	126.72
5	5-L	501	ATP	C5-C4-N3	-6.32	118.02	126.72
5	9-L	501	ATP	C5-C4-N3	-6.31	118.03	126.72
5	1-L	501	ATP	C5-C4-N3	-6.28	118.07	126.72
5	7-L	501	ATP	C5-C4-N3	-6.26	118.10	126.72
5	8-L	501	ATP	C5-C4-N3	-6.25	118.11	126.72
5	2-L	501	ATP	C5-C4-N3	-6.16	118.23	126.72
5	10-L	501	ATP	C5-C4-N3	-6.13	118.28	126.72
5	3-L	501	ATP	N3-C4-N9	5.13	135.89	127.17
5	9-L	501	ATP	N3-C4-N9	5.13	135.89	127.17
5	4-L	501	ATP	N3-C4-N9	5.08	135.81	127.17
5	6-L	501	ATP	N3-C4-N9	5.07	135.79	127.17
5	5-L	501	ATP	N3-C4-N9	5.06	135.78	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1-L	501	ATP	N3-C4-N9	5.04	135.73	127.17
5	8-L	501	ATP	N3-C4-N9	5.01	135.69	127.17
5	7-L	501	ATP	N3-C4-N9	4.99	135.66	127.17
5	2-L	501	ATP	N3-C4-N9	4.95	135.59	127.17
5	10-L	501	ATP	N3-C4-N9	4.95	135.59	127.17
5	6-L	501	ATP	C2-N3-C4	3.90	121.36	111.83
5	4-L	501	ATP	C2-N3-C4	3.82	121.16	111.83
5	1-L	501	ATP	C2-N3-C4	3.80	121.12	111.83
5	2-L	501	ATP	C2-N3-C4	3.79	121.08	111.83
5	9-L	501	ATP	C2-N3-C4	3.78	121.07	111.83
5	5-L	501	ATP	C2-N3-C4	3.77	121.04	111.83
5	10-L	501	ATP	C2-N3-C4	3.74	120.97	111.83
5	7-L	501	ATP	C2-N3-C4	3.73	120.95	111.83
5	8-L	501	ATP	C2-N3-C4	3.73	120.94	111.83
5	3-L	501	ATP	C2-N3-C4	3.72	120.92	111.83
5	6-L	501	ATP	C4-C5-N7	-3.30	106.81	110.58
5	4-L	501	ATP	C4-C5-N7	-3.25	106.87	110.58
5	1-L	501	ATP	C4-C5-N7	-3.22	106.90	110.58
5	3-L	501	ATP	C4-C5-N7	-3.19	106.94	110.58
5	5-L	501	ATP	C4-C5-N7	-3.19	106.94	110.58
5	7-L	501	ATP	C4-C5-N7	-3.18	106.95	110.58
5	8-L	501	ATP	C4-C5-N7	-3.15	106.98	110.58
5	9-L	501	ATP	C4-C5-N7	-3.14	106.99	110.58
5	2-L	501	ATP	C4-C5-N7	-3.14	106.99	110.58
5	2-L	501	ATP	N3-C2-N1	-3.14	123.83	128.58
5	1-L	501	ATP	N3-C2-N1	-3.10	123.89	128.58
5	10-L	501	ATP	C4-C5-N7	-3.08	107.06	110.58
5	10-L	501	ATP	N3-C2-N1	-3.07	123.93	128.58
5	9-L	501	ATP	N3-C2-N1	-3.06	123.94	128.58
5	6-L	501	ATP	N3-C2-N1	-3.04	123.97	128.58
5	4-L	501	ATP	N3-C2-N1	-3.04	123.99	128.58
5	5-L	501	ATP	N3-C2-N1	-3.04	123.99	128.58
5	8-L	501	ATP	N3-C2-N1	-2.99	124.06	128.58
5	7-L	501	ATP	N3-C2-N1	-2.96	124.10	128.58
5	3-L	501	ATP	N3-C2-N1	-2.92	124.16	128.58
5	7-L	501	ATP	O3G-PG-O2G	2.79	118.27	107.80
5	3-L	501	ATP	O3G-PG-O2G	2.76	118.16	107.80
5	4-L	501	ATP	O3G-PG-O2G	2.74	118.08	107.80
5	2-L	501	ATP	O3G-PG-O2G	2.67	117.81	107.80
5	9-L	501	ATP	O3G-PG-O2G	2.66	117.77	107.80
5	10-L	501	ATP	O3G-PG-O2G	2.65	117.73	107.80
5	6-L	501	ATP	O3G-PG-O2G	2.61	117.60	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	2-L	501	ATP	C4-N9-C8	2.60	108.47	105.74
5	1-L	501	ATP	O3G-PG-O2G	2.60	117.56	107.80
5	9-L	501	ATP	C4-N9-C8	2.59	108.45	105.74
5	10-L	501	ATP	C4-N9-C8	2.57	108.43	105.74
5	3-L	501	ATP	C4-N9-C8	2.49	108.36	105.74
5	10-L	501	ATP	C2'-C1'-N9	-2.49	107.12	113.30
5	5-L	501	ATP	C4-N9-C8	2.47	108.33	105.74
5	6-L	501	ATP	C2'-C1'-N9	-2.46	107.19	113.30
5	1-L	501	ATP	C3'-C2'-C1'	2.46	106.11	101.46
5	1-L	501	ATP	C4-N9-C8	2.45	108.31	105.74
5	8-L	501	ATP	C4-N9-C8	2.44	108.30	105.74
5	4-L	501	ATP	C4-N9-C8	2.42	108.27	105.74
5	7-L	501	ATP	C2'-C1'-N9	-2.39	107.37	113.30
5	7-L	501	ATP	C4-N9-C8	2.38	108.24	105.74
5	5-L	501	ATP	C2'-C1'-N9	-2.38	107.39	113.30
5	8-L	501	ATP	C2'-C1'-N9	-2.36	107.44	113.30
5	8-L	501	ATP	O3G-PG-O2G	2.35	116.62	107.80
5	5-L	501	ATP	O3G-PG-O2G	2.34	116.59	107.80
5	6-L	501	ATP	C5-N7-C8	2.28	107.04	103.45
5	3-L	501	ATP	C2'-C1'-N9	-2.27	107.66	113.30
5	6-L	501	ATP	C3'-C2'-C1'	2.26	105.74	101.46
5	4-L	501	ATP	C5-N7-C8	2.26	107.00	103.45
5	1-L	501	ATP	C5-N7-C8	2.26	107.00	103.45
5	7-L	501	ATP	C3'-C2'-C1'	2.22	105.66	101.46
5	9-L	501	ATP	C3'-C2'-C1'	2.22	105.65	101.46
5	5-L	501	ATP	C5-N7-C8	2.21	106.92	103.45
5	3-L	501	ATP	C5-N7-C8	2.21	106.92	103.45
5	9-L	501	ATP	O2B-PB-O1B	2.21	122.71	112.44
5	9-L	501	ATP	C5-N7-C8	2.19	106.90	103.45
5	9-L	501	ATP	C2'-C1'-N9	-2.19	107.86	113.30
5	6-L	501	ATP	C4-N9-C8	2.17	108.01	105.74
5	7-L	501	ATP	C5-N7-C8	2.15	106.84	103.45
5	7-L	501	ATP	O2B-PB-O1B	2.15	122.45	112.44
5	4-L	501	ATP	O2B-PB-O1B	2.15	122.44	112.44
5	10-L	501	ATP	C5-N7-C8	2.15	106.82	103.45
5	2-L	501	ATP	C5-N7-C8	2.14	106.82	103.45
5	5-L	501	ATP	O2B-PB-O1B	2.14	122.39	112.44
5	3-L	501	ATP	O2B-PB-O1B	2.11	122.24	112.44
5	2-L	501	ATP	O2B-PB-O1B	2.10	122.22	112.44
5	8-L	501	ATP	C5-N7-C8	2.10	106.75	103.45
5	6-L	501	ATP	O2B-PB-O1B	2.09	122.16	112.44
5	8-L	501	ATP	C3'-C2'-C1'	2.08	105.41	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	3-L	501	ATP	C3'-C2'-C1'	2.07	105.38	101.46
5	5-L	501	ATP	C3'-C2'-C1'	2.06	105.36	101.46
5	1-L	501	ATP	O2B-PB-O1B	2.04	121.94	112.44
5	10-L	501	ATP	O2B-PB-O1B	2.04	121.92	112.44
5	8-L	501	ATP	O2B-PB-O1B	2.01	121.78	112.44

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	3-L	501	ATP	PB-O3B-PG-O3G
5	4-L	501	ATP	PB-O3B-PG-O3G
5	6-L	501	ATP	O4'-C4'-C5'-O5'
5	6-L	501	ATP	C3'-C4'-C5'-O5'
5	7-L	501	ATP	C5'-O5'-PA-O1A
5	9-L	501	ATP	PB-O3B-PG-O3G
5	9-L	501	ATP	C5'-O5'-PA-O1A
5	9-L	501	ATP	C5'-O5'-PA-O3A
5	4-L	501	ATP	O4'-C4'-C5'-O5'
5	5-L	501	ATP	O4'-C4'-C5'-O5'
5	7-L	501	ATP	C3'-C4'-C5'-O5'
5	3-L	501	ATP	O4'-C4'-C5'-O5'
5	3-L	501	ATP	C3'-C4'-C5'-O5'
5	4-L	501	ATP	C3'-C4'-C5'-O5'
5	5-L	501	ATP	C3'-C4'-C5'-O5'
5	7-L	501	ATP	O4'-C4'-C5'-O5'
5	9-L	501	ATP	O4'-C4'-C5'-O5'
5	9-L	501	ATP	C3'-C4'-C5'-O5'
5	8-L	501	ATP	C3'-C4'-C5'-O5'
5	2-L	501	ATP	PA-O3A-PB-O1B
5	10-L	501	ATP	PA-O3A-PB-O1B
5	8-L	501	ATP	O4'-C4'-C5'-O5'
5	1-L	501	ATP	C2'-C1'-N9-C8
5	2-L	501	ATP	C3'-C4'-C5'-O5'
5	7-L	501	ATP	PB-O3B-PG-O3G
5	10-L	501	ATP	C3'-C4'-C5'-O5'
5	2-L	501	ATP	C5'-O5'-PA-O1A
5	4-L	501	ATP	C5'-O5'-PA-O1A
5	5-L	501	ATP	C5'-O5'-PA-O1A
5	6-L	501	ATP	C5'-O5'-PA-O1A
5	7-L	501	ATP	C5'-O5'-PA-O3A
5	8-L	501	ATP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
5	2-L	501	ATP	PA-O3A-PB-O2B
5	3-L	501	ATP	PA-O3A-PB-O2B
5	5-L	501	ATP	PA-O3A-PB-O2B
5	9-L	501	ATP	PA-O3A-PB-O2B
5	10-L	501	ATP	PA-O3A-PB-O2B
5	2-L	501	ATP	O4'-C4'-C5'-O5'
5	10-L	501	ATP	O4'-C4'-C5'-O5'
5	10-L	501	ATP	PB-O3B-PG-O1G
5	2-L	501	ATP	PB-O3B-PG-O3G
5	10-L	501	ATP	PB-O3B-PG-O3G
5	3-L	501	ATP	C2'-C1'-N9-C8
5	8-L	501	ATP	C2'-C1'-N9-C8
5	1-L	501	ATP	PA-O3A-PB-O1B
5	3-L	501	ATP	PA-O3A-PB-O1B
5	4-L	501	ATP	PA-O3A-PB-O2B
5	5-L	501	ATP	PA-O3A-PB-O1B
5	7-L	501	ATP	PA-O3A-PB-O2B
5	9-L	501	ATP	PA-O3A-PB-O1B
5	5-L	501	ATP	C2'-C1'-N9-C8
5	7-L	501	ATP	C2'-C1'-N9-C8
5	2-L	501	ATP	PB-O3B-PG-O1G
5	4-L	501	ATP	C2'-C1'-N9-C8
5	6-L	501	ATP	PA-O3A-PB-O1B

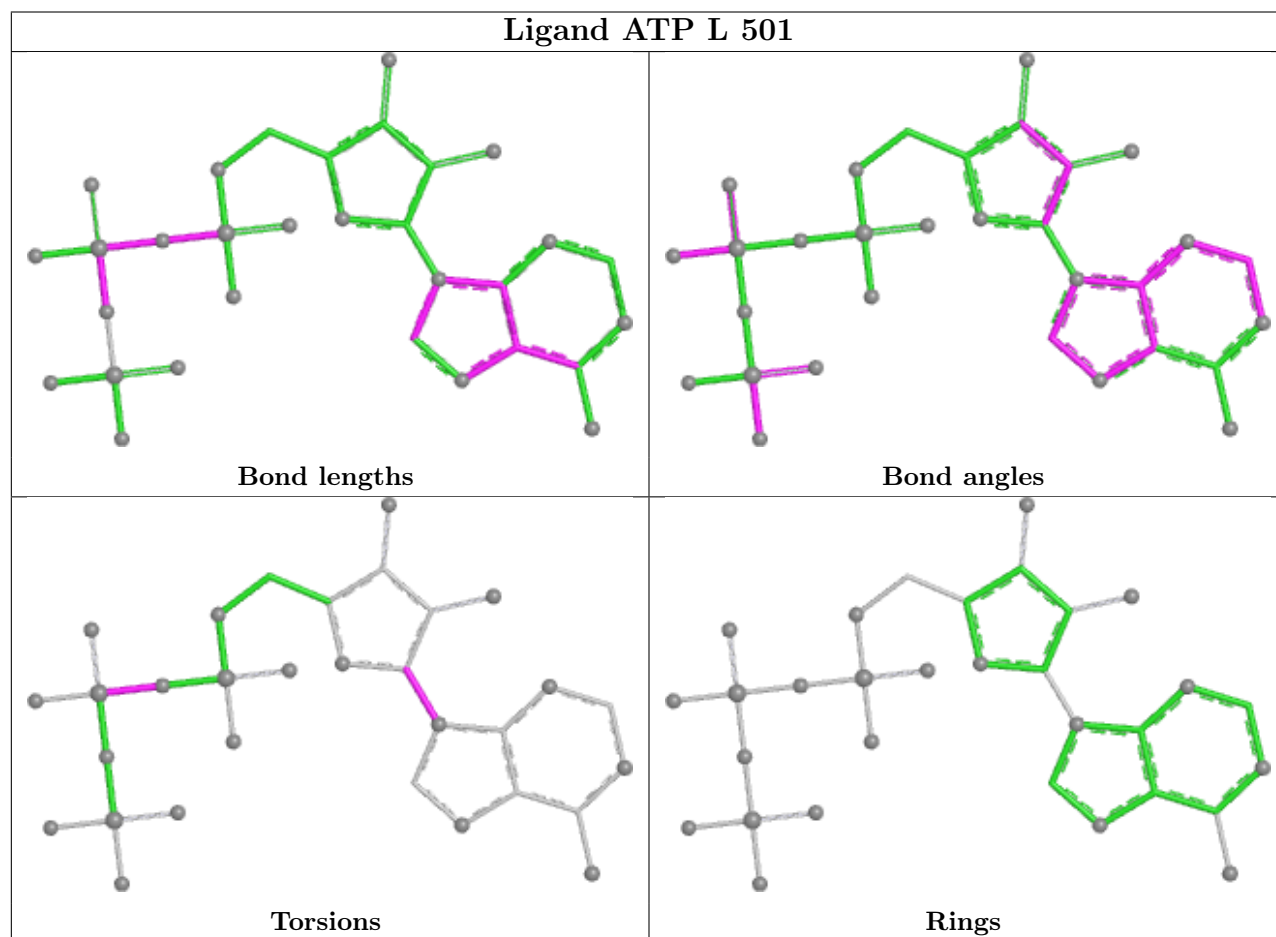
There are no ring outliers.

9 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	5-L	501	ATP	2	0
5	7-L	501	ATP	1	0
5	3-L	501	ATP	1	0
5	9-L	501	ATP	1	0
5	2-L	501	ATP	2	0
5	8-L	501	ATP	1	0
5	1-L	501	ATP	1	0
5	6-L	501	ATP	1	0
5	10-L	501	ATP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

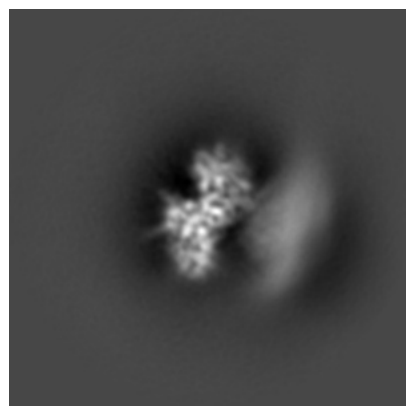
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21489. These allow visual inspection of the internal detail of the map and identification of artifacts.

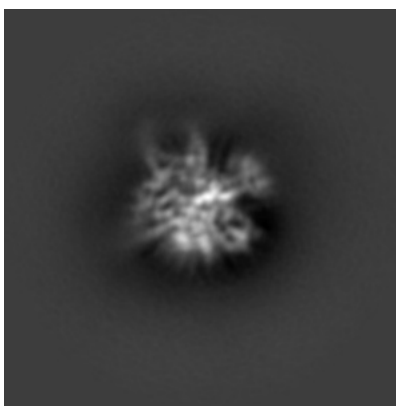
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

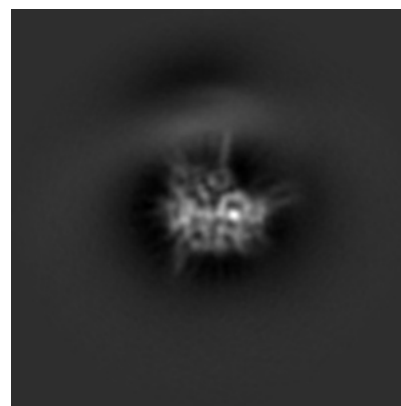
6.1.1 Primary map



X

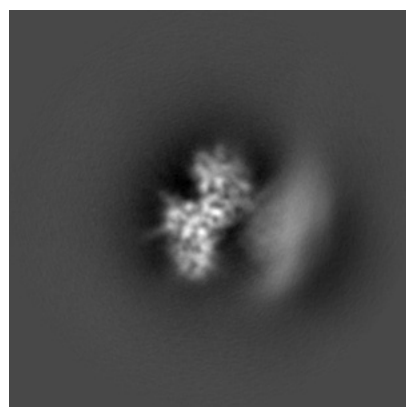


Y

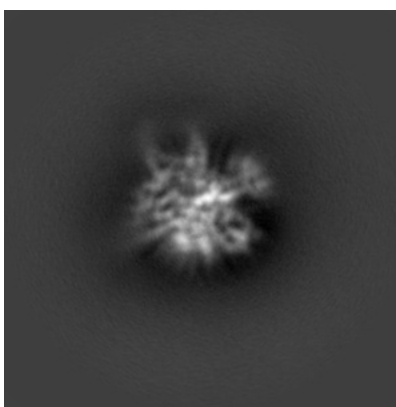


Z

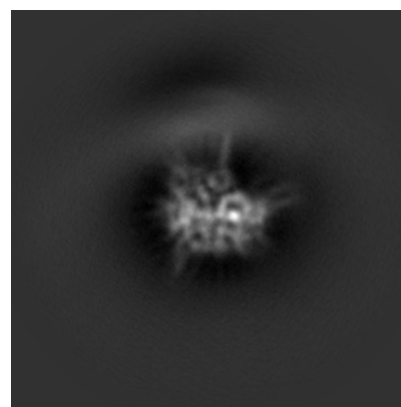
6.1.2 Raw map



X



Y

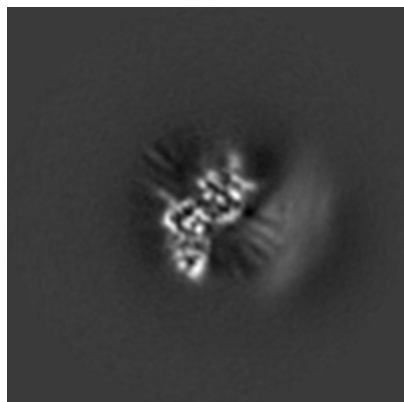


Z

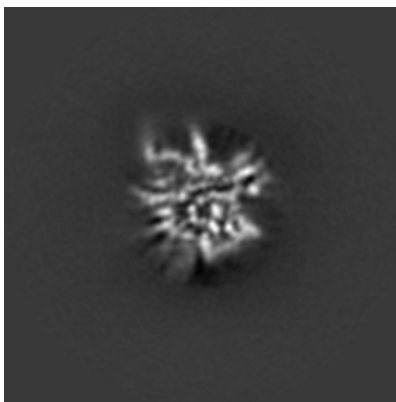
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

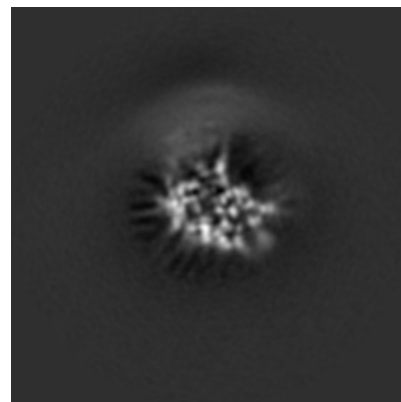
6.2.1 Primary map



X Index: 120

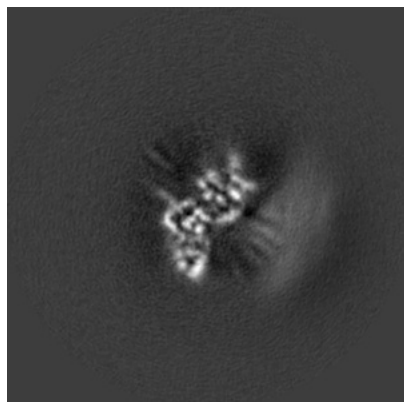


Y Index: 120

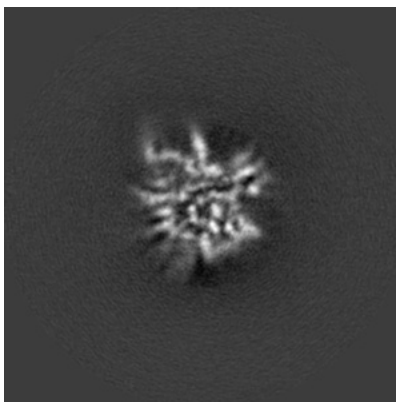


Z Index: 120

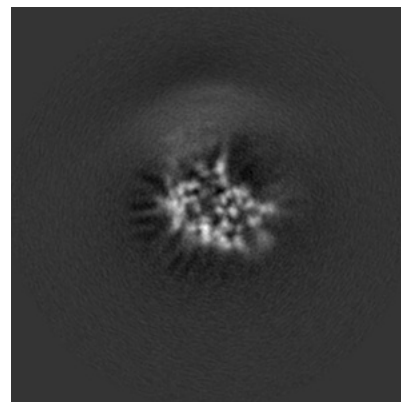
6.2.2 Raw map



X Index: 120



Y Index: 120

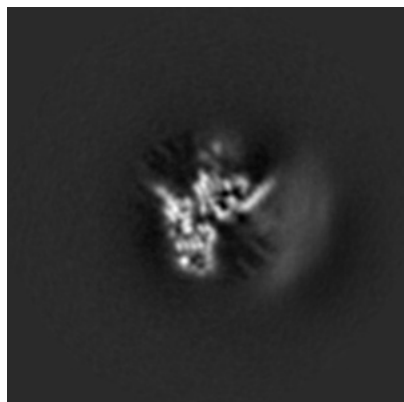


Z Index: 120

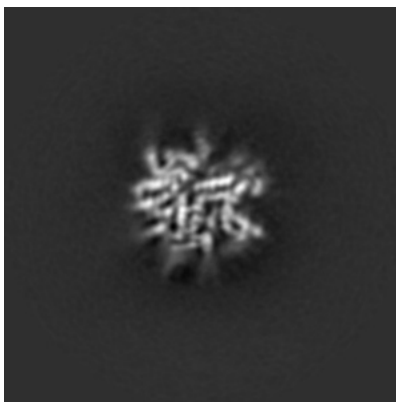
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

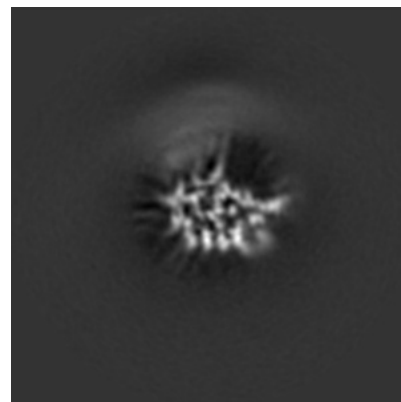
6.3.1 Primary map



X Index: 126

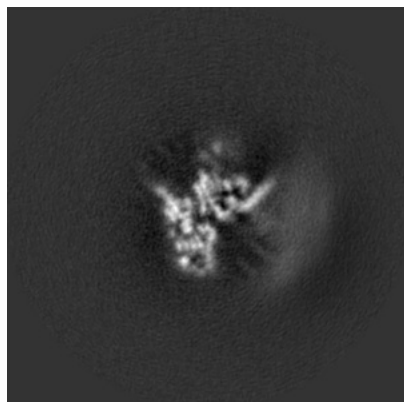


Y Index: 116

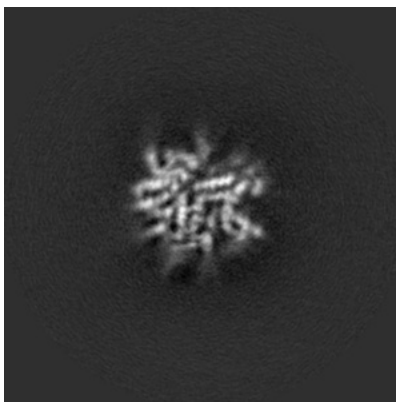


Z Index: 117

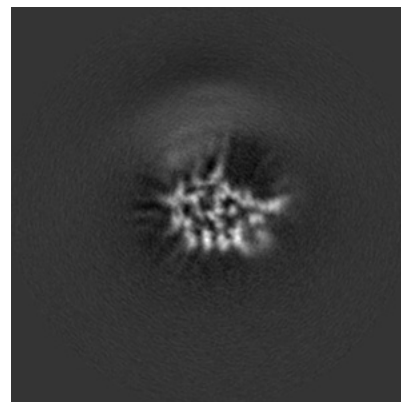
6.3.2 Raw map



X Index: 126



Y Index: 116

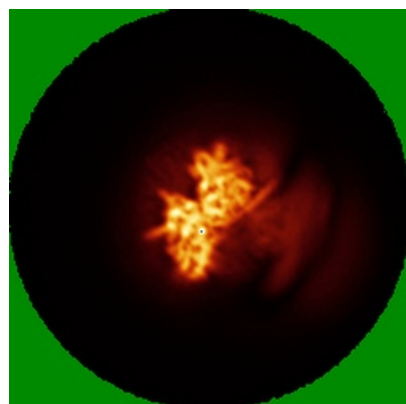


Z Index: 117

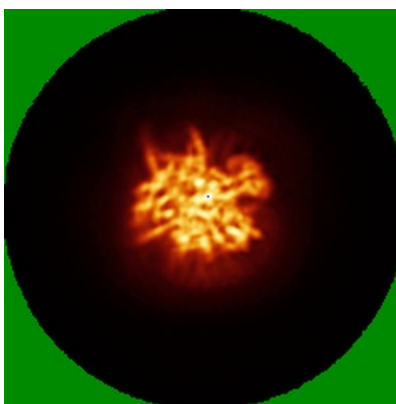
The images above show the largest variance slices of the map in three orthogonal directions.

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

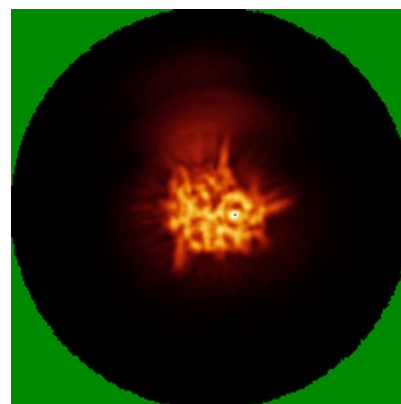
6.4.1 Primary map



X

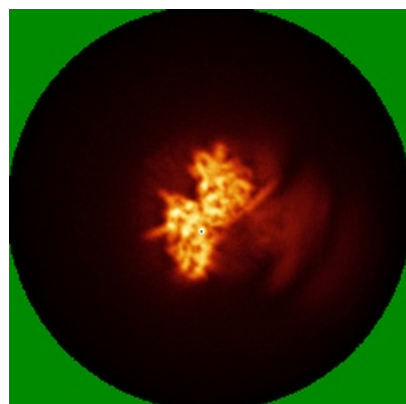


Y

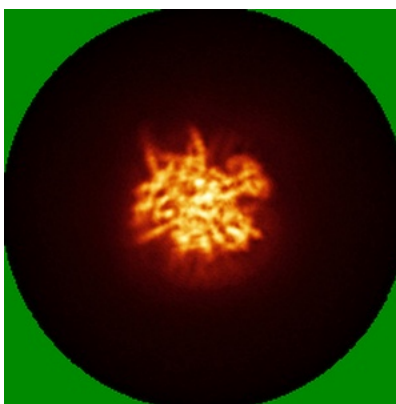


Z

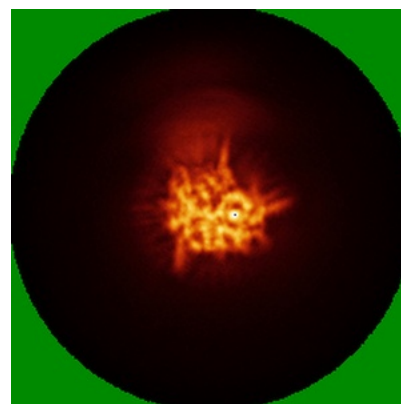
6.4.2 Raw map



X



Y



Z

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

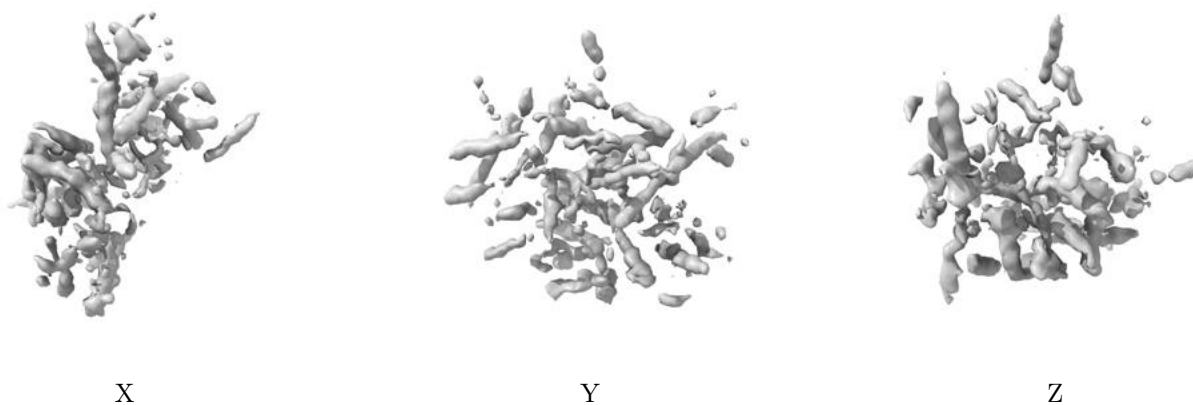
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

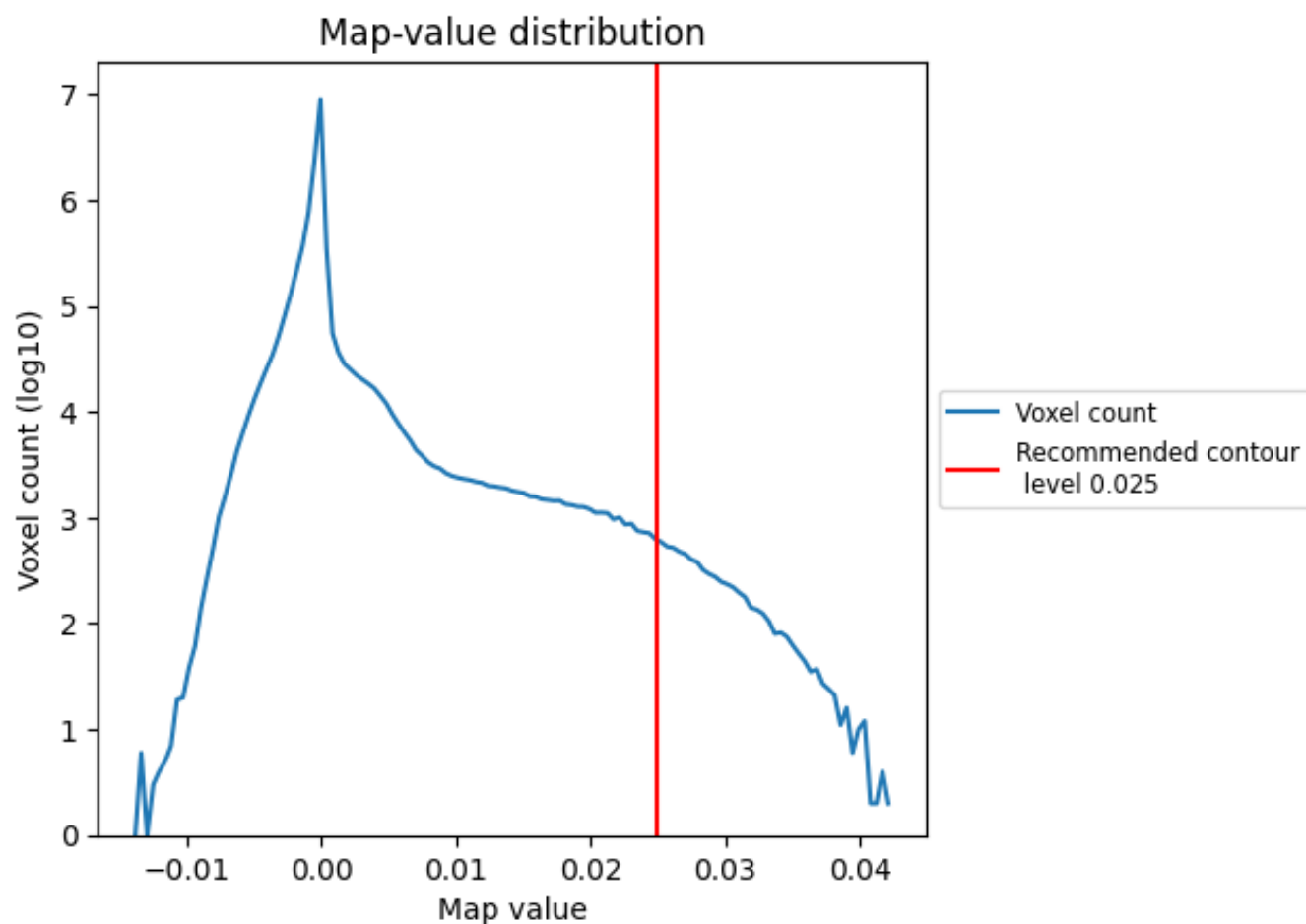
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

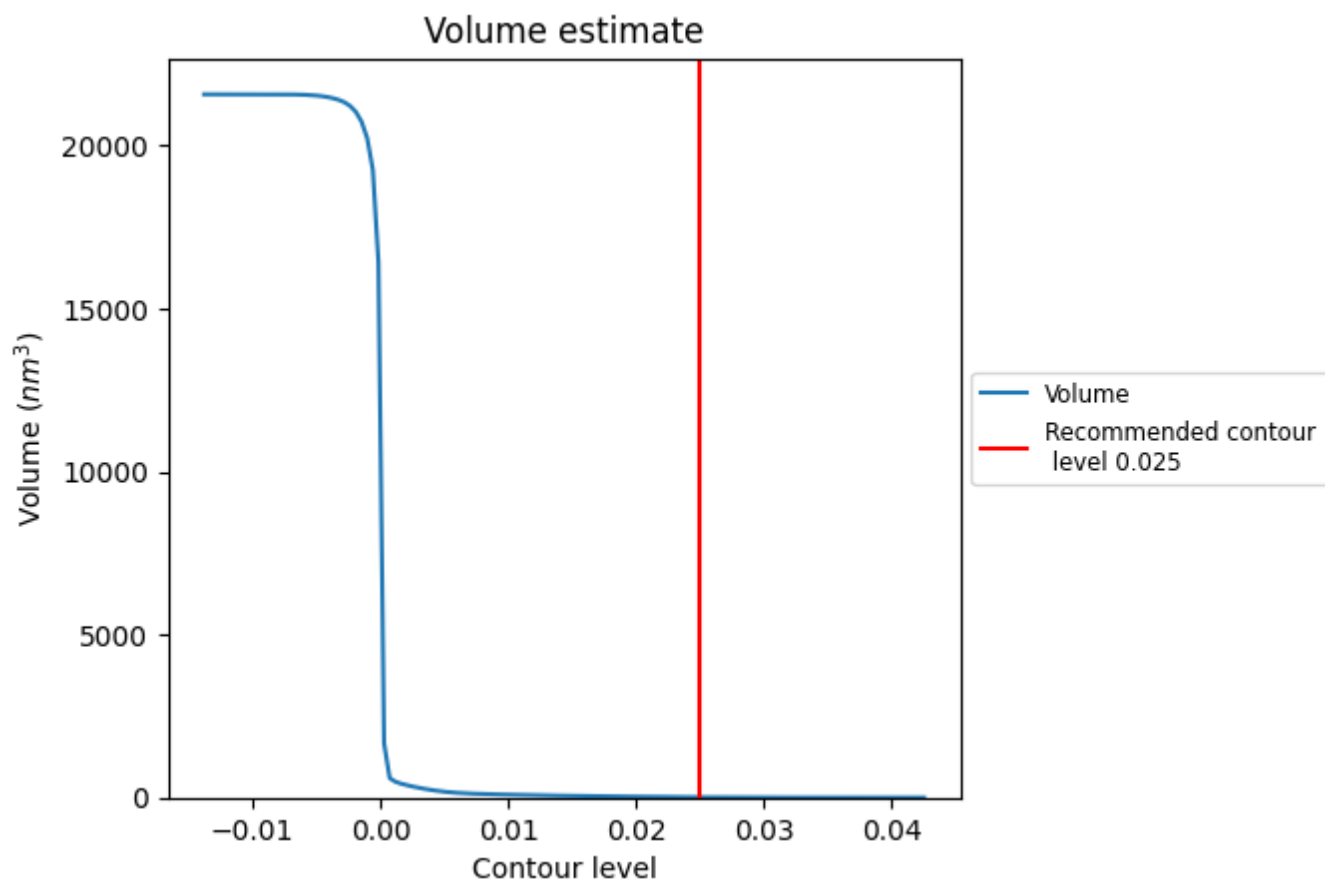
This section contains the results of statistical analysis of the map.

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.

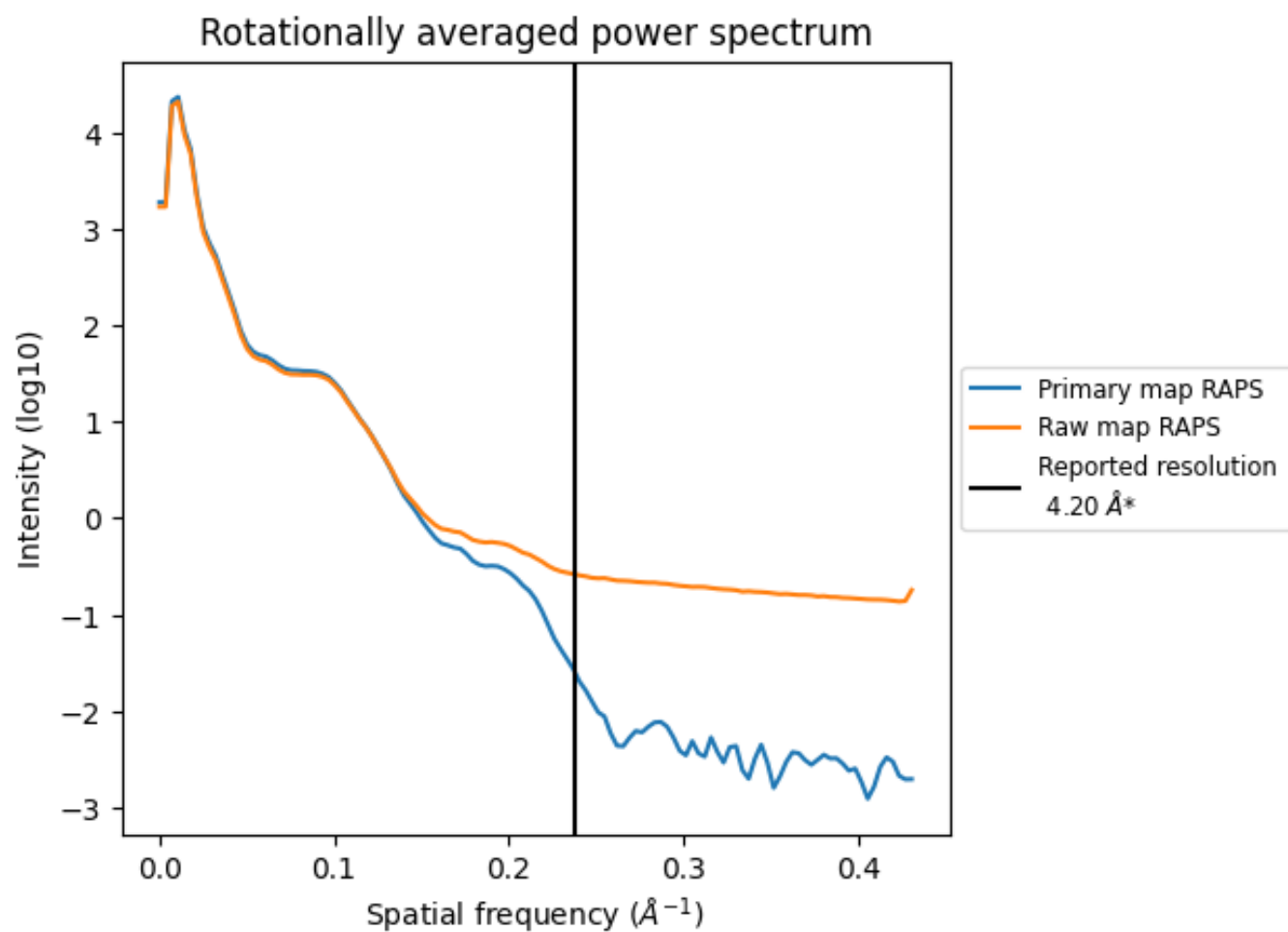
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 11 nm³; this corresponds to an approximate mass of 10 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 ⓘ

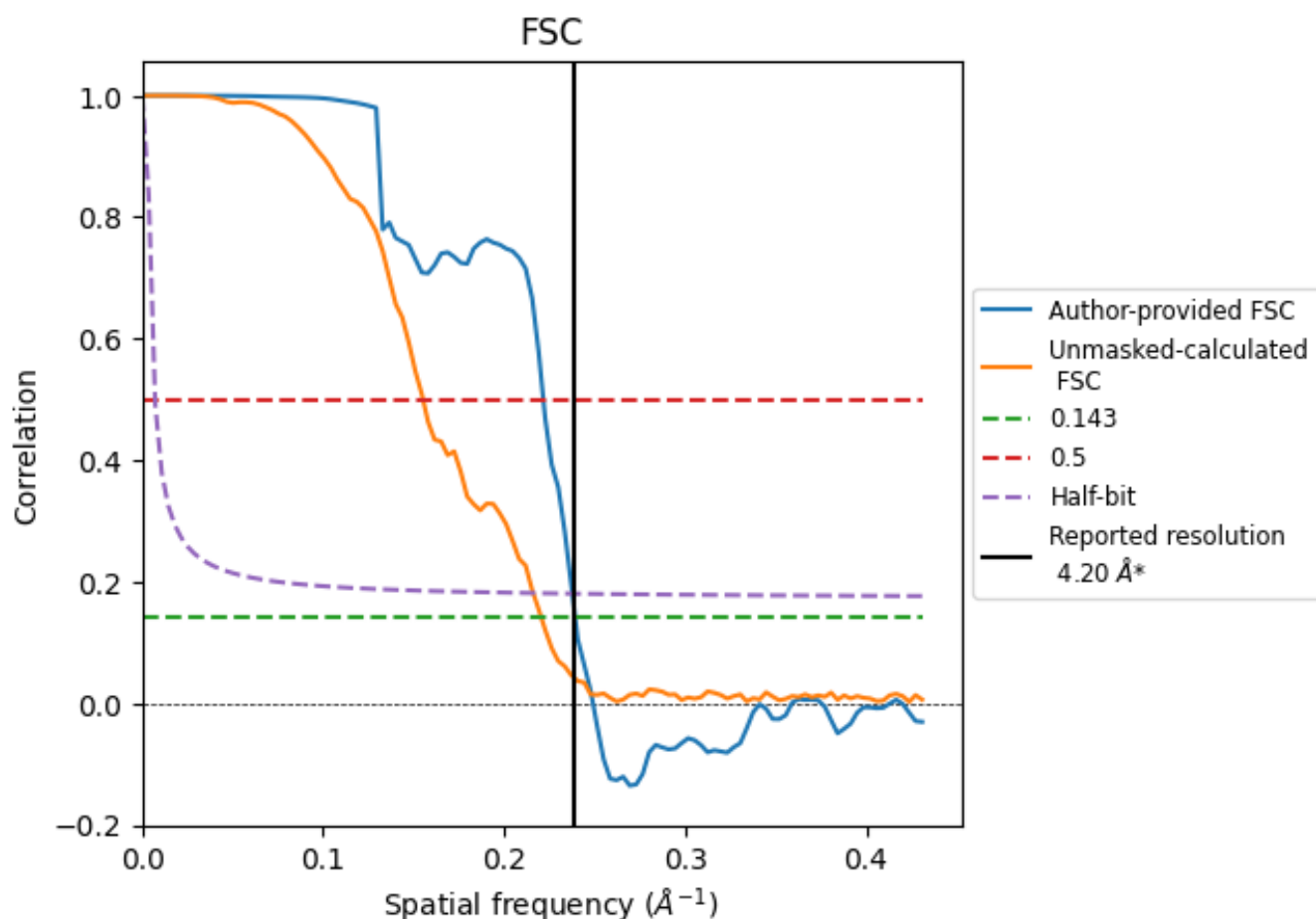


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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 0.238 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

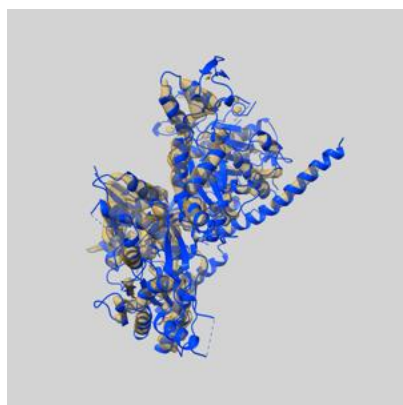
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.18	4.51	4.21
Unmasked-calculated*	4.54	6.45	4.63

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

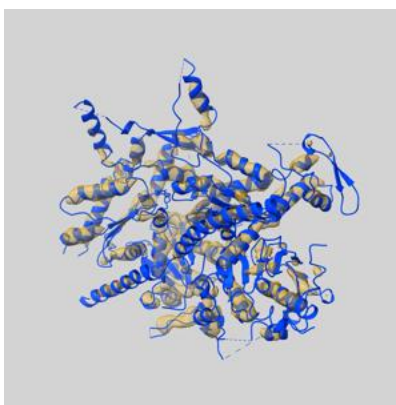
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21489 and PDB model 6VZG. Per-residue inclusion information can be found in section 3 on page 9.

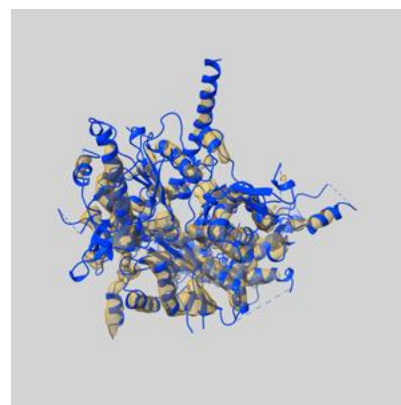
9.1 Map-model overlay [i](#)



X



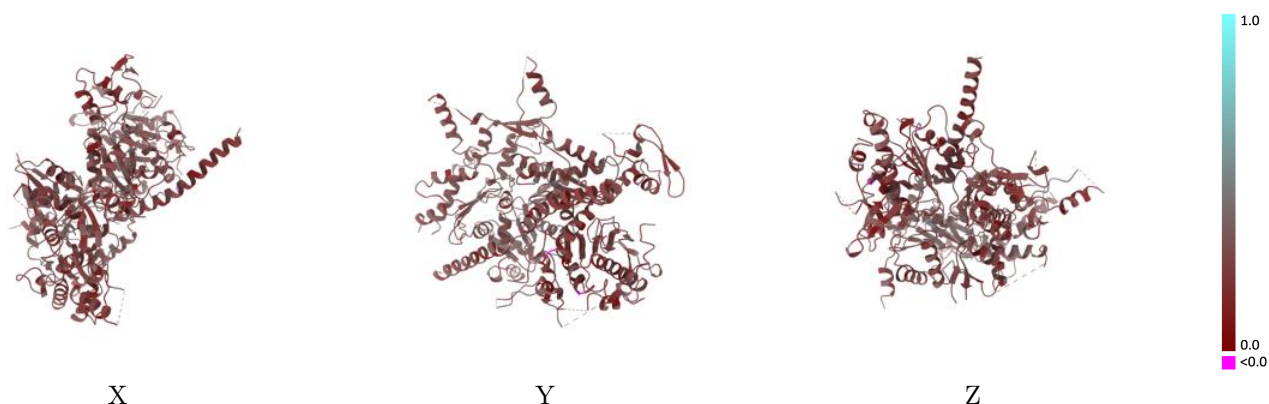
Y



Z

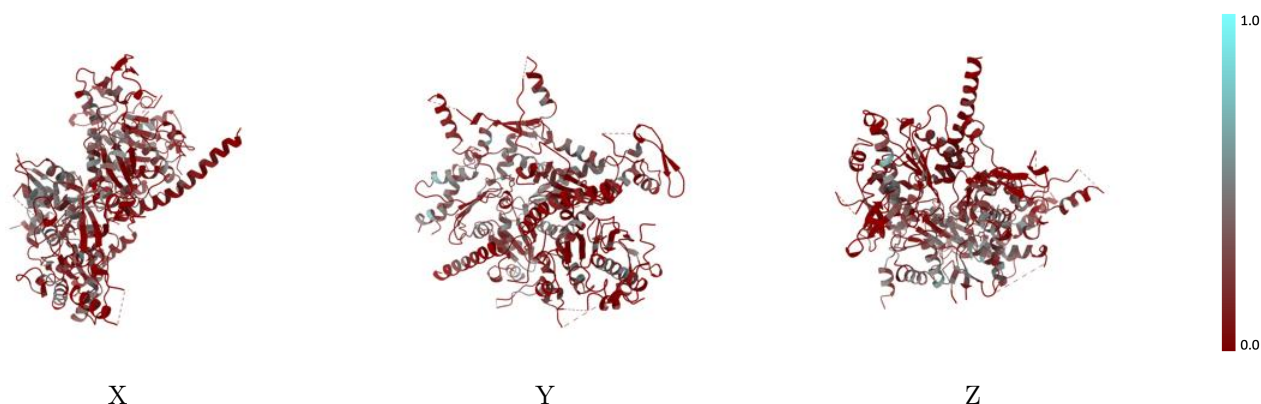
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



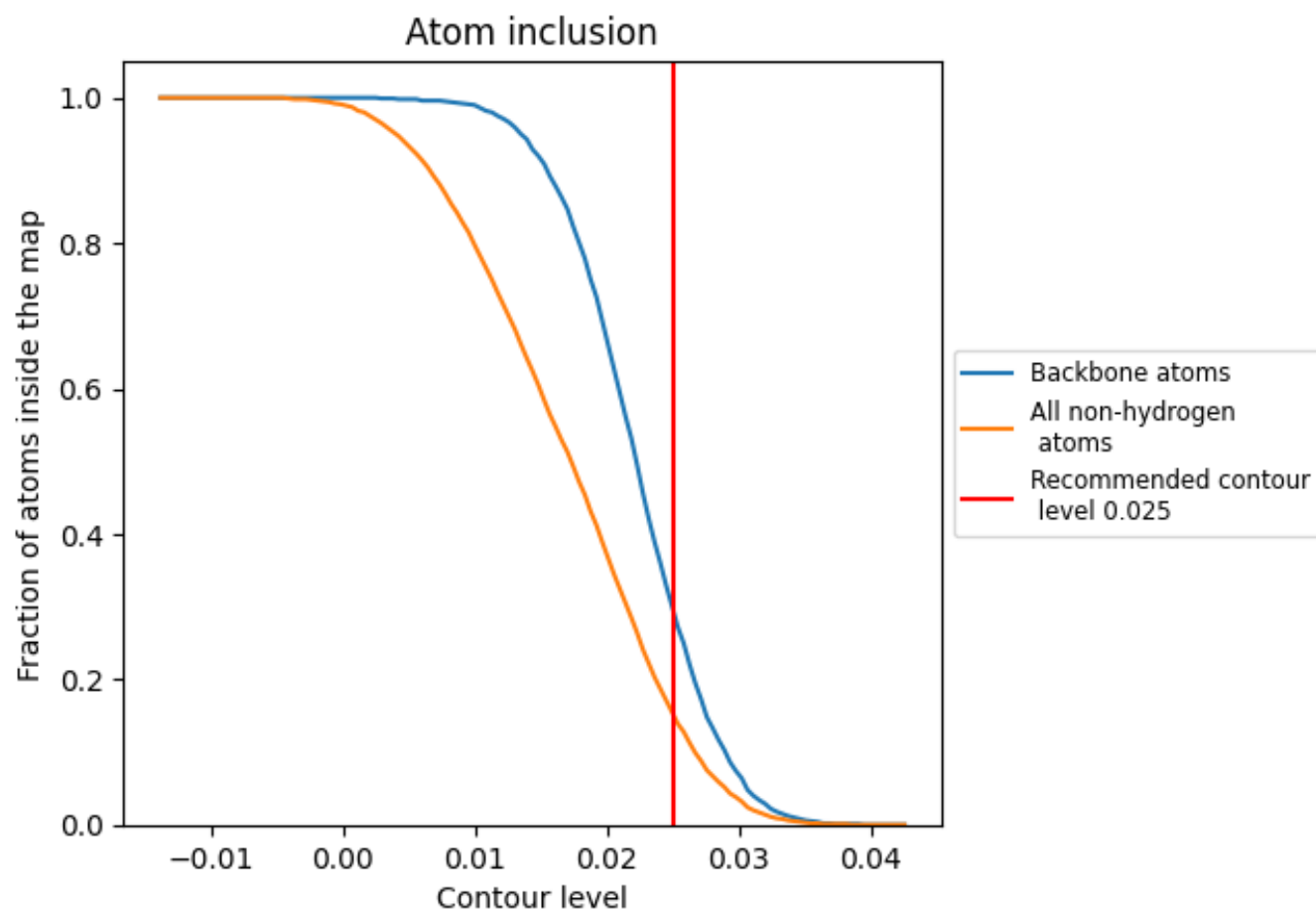
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 30% of all backbone atoms, 15% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.1530	0.2610
K	0.0540	0.2350
L	0.2000	0.2660
M	0.1310	0.2620
N	0.0960	0.2560

