



Full wwPDB EM Validation Report ⓘ

Aug 18, 2026 – 06:43 pm BST

PDB ID : 9SZ9 / pdb_00009sz9
EMDB ID : EMD-55362
Title : Capsid structure of Lactococcus phage Nocturne116
Authors : Rumnieks, J.; Tars, K.
Deposited on : 2025-10-14
Resolution : 2.63 Å(reported)
Based on initial model : .

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.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

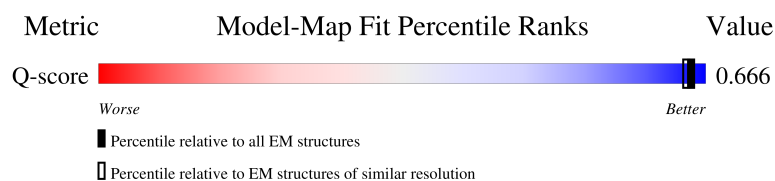
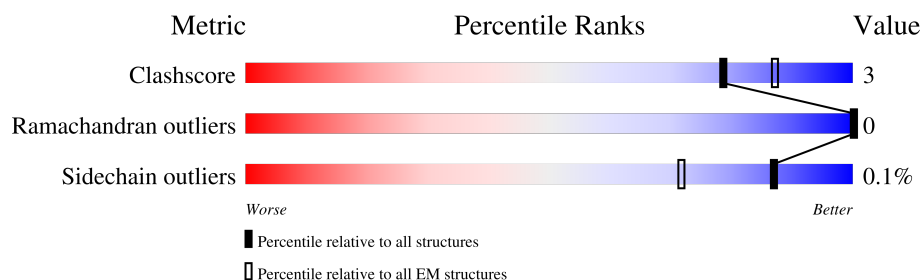
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.63 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.



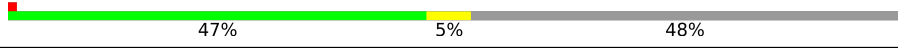
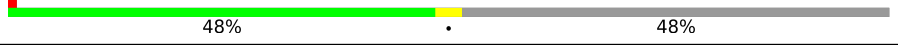
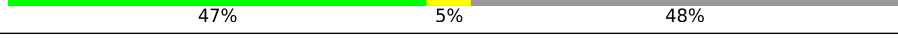
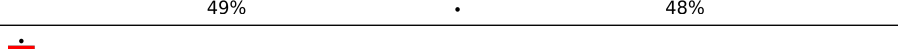
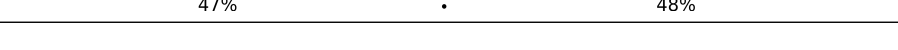
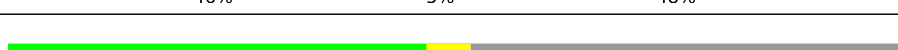
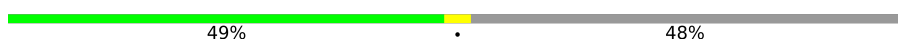
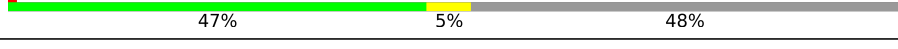
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8888 (2.13 - 3.13)

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	A0	516	
1	A1	516	
1	A2	516	
1	A3	516	

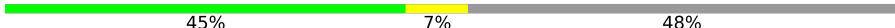
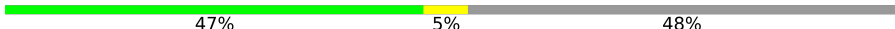
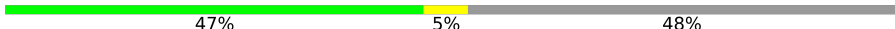
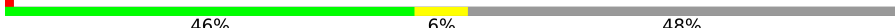
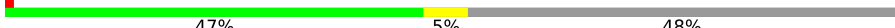
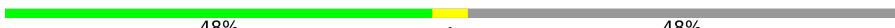
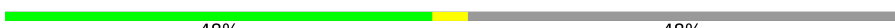
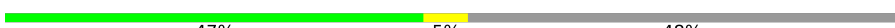
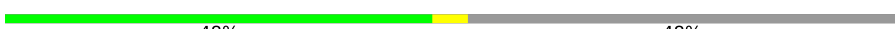
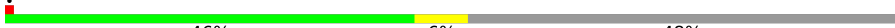
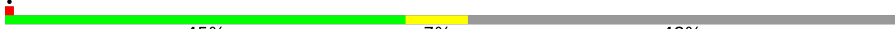
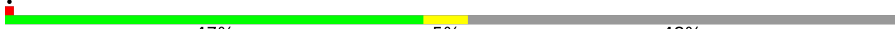
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Mol	Chain	Length	Quality of chain
1	A4	516	
1	A5	516	
1	A6	516	
1	A7	516	
1	AA	516	
1	AB	516	
1	AC	516	
1	AD	516	
1	AE	516	
1	AF	516	
1	AG	516	
1	AH	516	
1	AI	516	
1	AJ	516	
1	AK	516	
1	AL	516	
1	AM	516	
1	AN	516	
1	AO	516	
1	AP	516	
1	AQ	516	
1	AR	516	
1	AS	516	
1	AT	516	
1	AU	516	

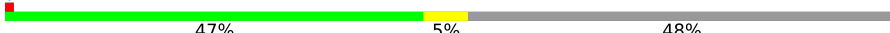
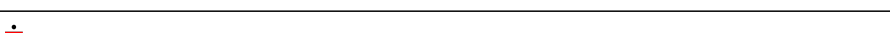
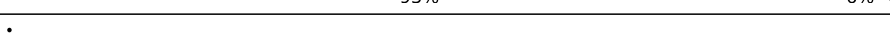
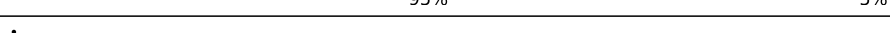
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Mol	Chain	Length	Quality of chain
1	AV	516	
1	AW	516	
1	AX	516	
1	AY	516	
1	AZ	516	
1	Aa	516	
1	Ab	516	
1	Ac	516	
1	Ad	516	
1	Ae	516	
1	Af	516	
1	Ag	516	
1	Ah	516	
1	Ai	516	
1	Aj	516	
1	Ak	516	
1	Al	516	
1	Am	516	
1	An	516	
1	Ao	516	
1	Ap	516	
1	Aq	516	
1	Ar	516	
1	As	516	
1	At	516	

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Mol	Chain	Length	Quality of chain
1	Au	516	
1	Av	516	
1	Aw	516	
1	Ax	516	
1	Ay	516	
1	Az	516	
2	FA	220	
2	FB	220	
2	FC	220	
2	FD	220	
2	FE	220	
2	FF	220	
2	FG	220	
2	FH	220	
2	FI	220	
2	FJ	220	
2	FK	220	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 142469 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 Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	267	Total	C	N	O	S	0	0
			2065	1311	347	401	6		
1	AB	267	Total	C	N	O	S	0	0
			2065	1311	347	401	6		
1	AC	267	Total	C	N	O	S	0	0
			2066	1311	348	401	6		
1	AD	267	Total	C	N	O	S	0	0
			2065	1311	347	401	6		
1	AE	267	Total	C	N	O	S	0	0
			2065	1311	347	401	6		
1	AF	267	Total	C	N	O	S	0	0
			2066	1311	348	401	6		
1	AG	267	Total	C	N	O	S	0	0
			2066	1311	348	401	6		
1	AH	267	Total	C	N	O	S	0	0
			2065	1311	347	401	6		
1	AI	267	Total	C	N	O	S	0	0
			2065	1311	347	401	6		
1	AJ	267	Total	C	N	O	S	0	0
			2065	1311	347	401	6		
1	AK	267	Total	C	N	O	S	0	0
			2065	1311	347	401	6		
1	AL	267	Total	C	N	O	S	0	0
			2066	1311	348	401	6		
1	AM	267	Total	C	N	O	S	0	0
			2065	1311	347	401	6		
1	AN	267	Total	C	N	O	S	0	0
			2065	1311	347	401	6		
1	AO	267	Total	C	N	O	S	0	0
			2065	1311	347	401	6		
1	AP	267	Total	C	N	O	S	0	0
			2065	1311	347	401	6		
1	AQ	267	Total	C	N	O	S	0	0
			2065	1311	347	401	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	AR	267	Total 2066	C 1311	N 348	O 401	S 6	0	0
1	AS	267	Total 2065	C 1311	N 347	O 401	S 6	0	0
1	AT	267	Total 2065	C 1311	N 347	O 401	S 6	0	0
1	AU	267	Total 2065	C 1311	N 347	O 401	S 6	0	0
1	AV	267	Total 2065	C 1311	N 347	O 401	S 6	0	0
1	AW	267	Total 2066	C 1311	N 348	O 401	S 6	0	0
1	AX	267	Total 2065	C 1311	N 347	O 401	S 6	0	0
1	AY	267	Total 2065	C 1311	N 347	O 401	S 6	0	0
1	AZ	267	Total 2065	C 1311	N 347	O 401	S 6	0	0
1	Aa	267	Total 2065	C 1311	N 347	O 401	S 6	0	0
1	Ab	267	Total 2065	C 1311	N 347	O 401	S 6	0	0
1	Ac	267	Total 2065	C 1311	N 347	O 401	S 6	0	0
1	Ad	267	Total 2065	C 1311	N 347	O 401	S 6	0	0
1	Ae	267	Total 2065	C 1311	N 347	O 401	S 6	0	0
1	Af	267	Total 2065	C 1311	N 347	O 401	S 6	0	0
1	Ag	267	Total 2066	C 1311	N 348	O 401	S 6	0	0
1	Ah	267	Total 2065	C 1311	N 347	O 401	S 6	0	0
1	Ai	267	Total 2065	C 1311	N 347	O 401	S 6	0	0
1	Aj	267	Total 2066	C 1311	N 348	O 401	S 6	0	0
1	Ak	267	Total 2066	C 1311	N 348	O 401	S 6	0	0
1	Al	267	Total 2065	C 1311	N 347	O 401	S 6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Am	267	Total 2065	C 1311	N 347	O 401	S 6	0	0
1	An	267	Total 2065	C 1311	N 347	O 401	S 6	0	0
1	Ao	267	Total 2065	C 1311	N 347	O 401	S 6	0	0
1	Ap	267	Total 2066	C 1311	N 348	O 401	S 6	0	0
1	Aq	267	Total 2065	C 1311	N 347	O 401	S 6	0	0
1	Ar	267	Total 2065	C 1311	N 347	O 401	S 6	0	0
1	As	267	Total 2065	C 1311	N 347	O 401	S 6	0	0
1	At	267	Total 2065	C 1311	N 347	O 401	S 6	0	0
1	Au	267	Total 2065	C 1311	N 347	O 401	S 6	0	0
1	Av	267	Total 2066	C 1311	N 348	O 401	S 6	0	0
1	Aw	267	Total 2065	C 1311	N 347	O 401	S 6	0	0
1	Ax	267	Total 2065	C 1311	N 347	O 401	S 6	0	0
1	Ay	267	Total 2065	C 1311	N 347	O 401	S 6	0	0
1	Az	267	Total 2065	C 1311	N 347	O 401	S 6	0	0
1	A0	267	Total 2066	C 1311	N 348	O 401	S 6	0	0
1	A1	267	Total 2065	C 1311	N 347	O 401	S 6	0	0
1	A2	267	Total 2065	C 1311	N 347	O 401	S 6	0	0
1	A3	267	Total 2065	C 1311	N 347	O 401	S 6	0	0
1	A4	267	Total 2065	C 1311	N 347	O 401	S 6	0	0
1	A5	267	Total 2065	C 1311	N 347	O 401	S 6	0	0
1	A6	267	Total 2065	C 1311	N 347	O 401	S 6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	A7	267	Total	C	N	O	S	0	0
			2065	1311	347	401	6		

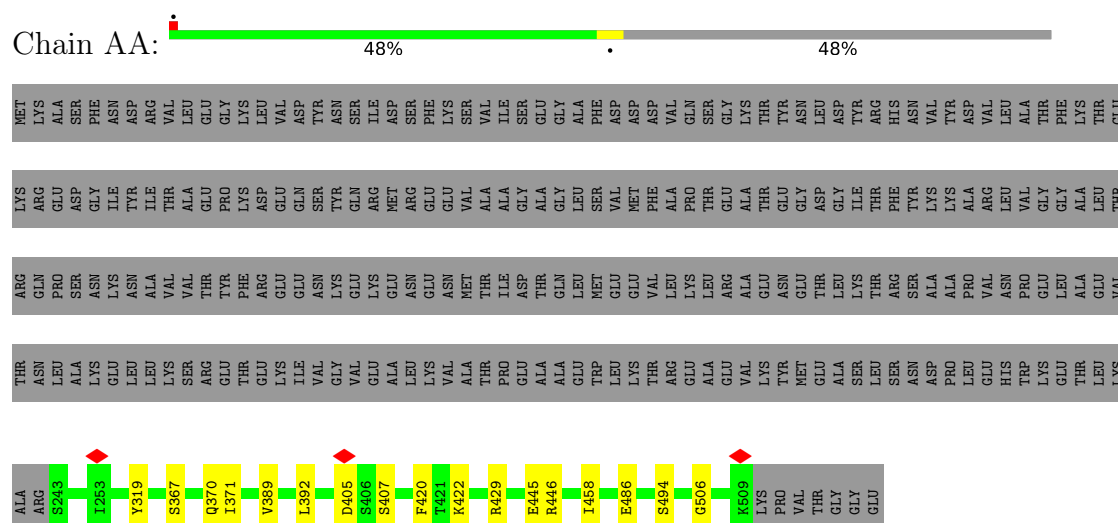
- Molecule 2 is a protein called Capsid vertex protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	FA	218	Total	C	N	O	S	0	0
			1687	1074	262	349	2		
2	FB	218	Total	C	N	O	S	0	0
			1687	1074	262	349	2		
2	FC	218	Total	C	N	O	S	0	0
			1687	1074	262	349	2		
2	FD	218	Total	C	N	O	S	0	0
			1687	1074	262	349	2		
2	FE	218	Total	C	N	O	S	0	0
			1687	1074	262	349	2		
2	FF	218	Total	C	N	O	S	0	0
			1687	1074	262	349	2		
2	FG	218	Total	C	N	O	S	0	0
			1687	1074	262	349	2		
2	FH	218	Total	C	N	O	S	0	0
			1687	1074	262	349	2		
2	FI	218	Total	C	N	O	S	0	0
			1687	1074	262	349	2		
2	FJ	218	Total	C	N	O	S	0	0
			1687	1074	262	349	2		
2	FK	218	Total	C	N	O	S	0	0
			1687	1074	262	349	2		

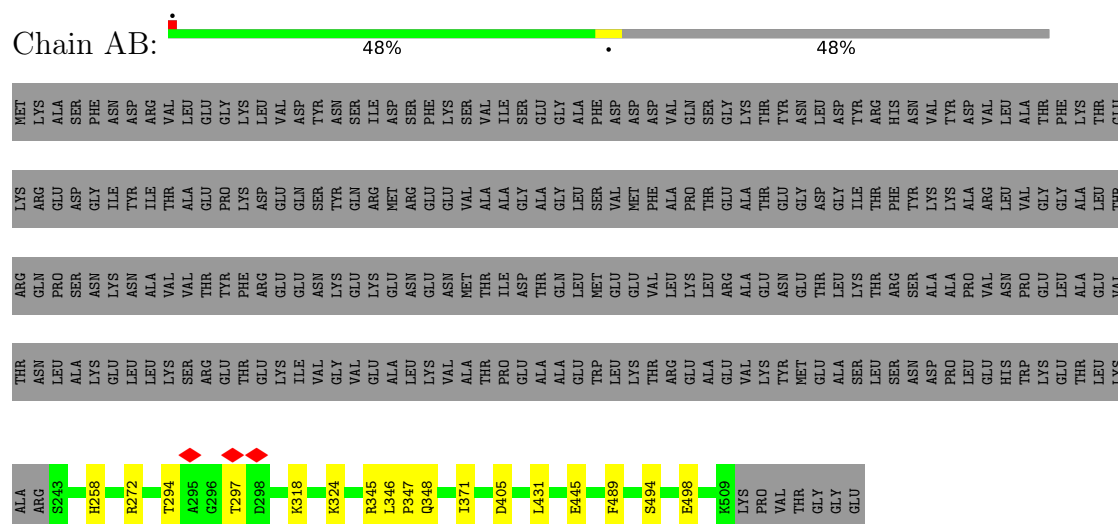
3 Residue-property plots

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

- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein

Response	Percentage
Yes, the U.S. is a democracy	47%
No, the U.S. is not a democracy	5%
Don't know	48%

- Molecule 1: Major capsid protein

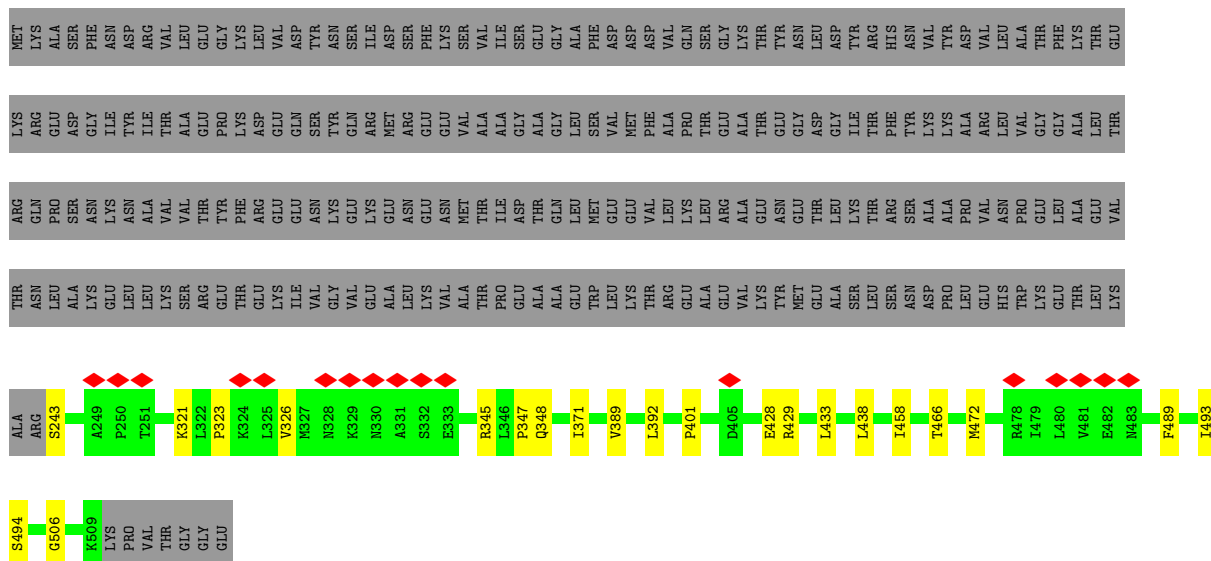
Response	Percentage
Yes, the U.S. is a democracy	48%
No, the U.S. is not a democracy	1%
Don't know	48%

- Molecule 1: Major capsid protein

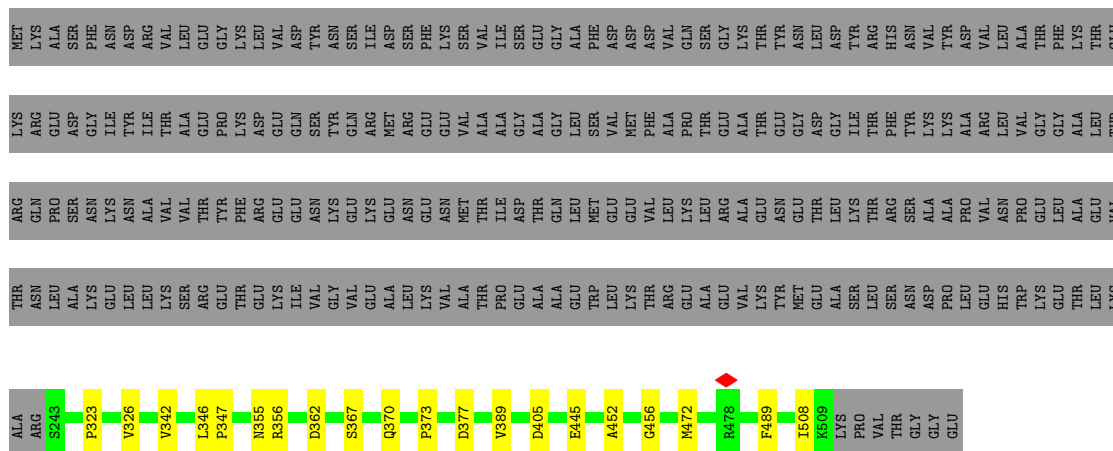
Response	Percentage
Yes, the U.S. is a democracy	49%
No, the U.S. is not a democracy	48%



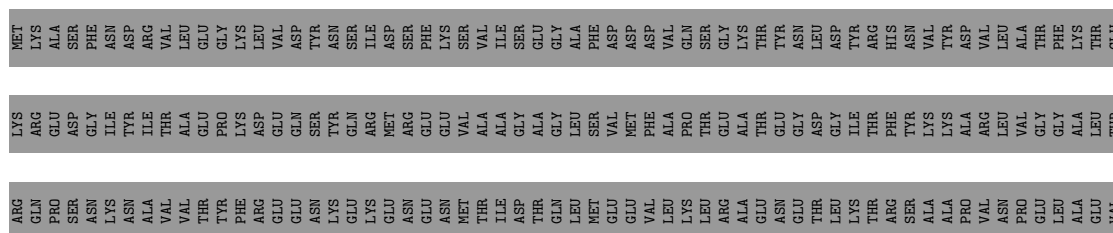
Chain AF: 47% 48%

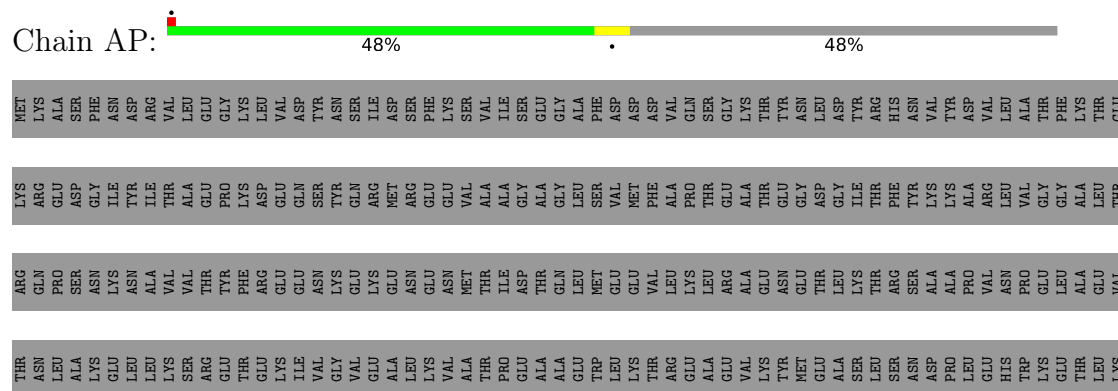


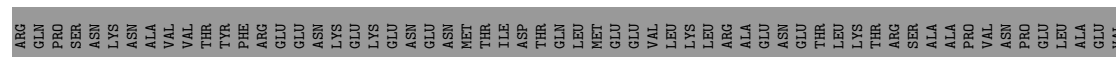
Chain AG:

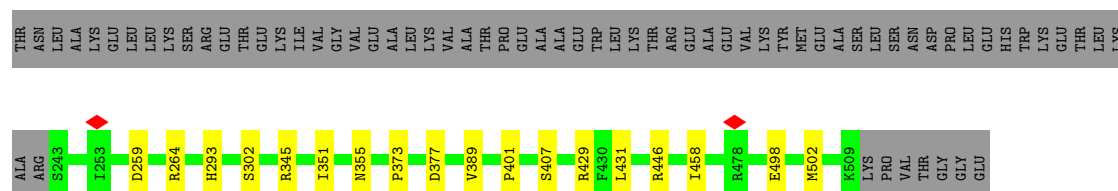


Chain AH:

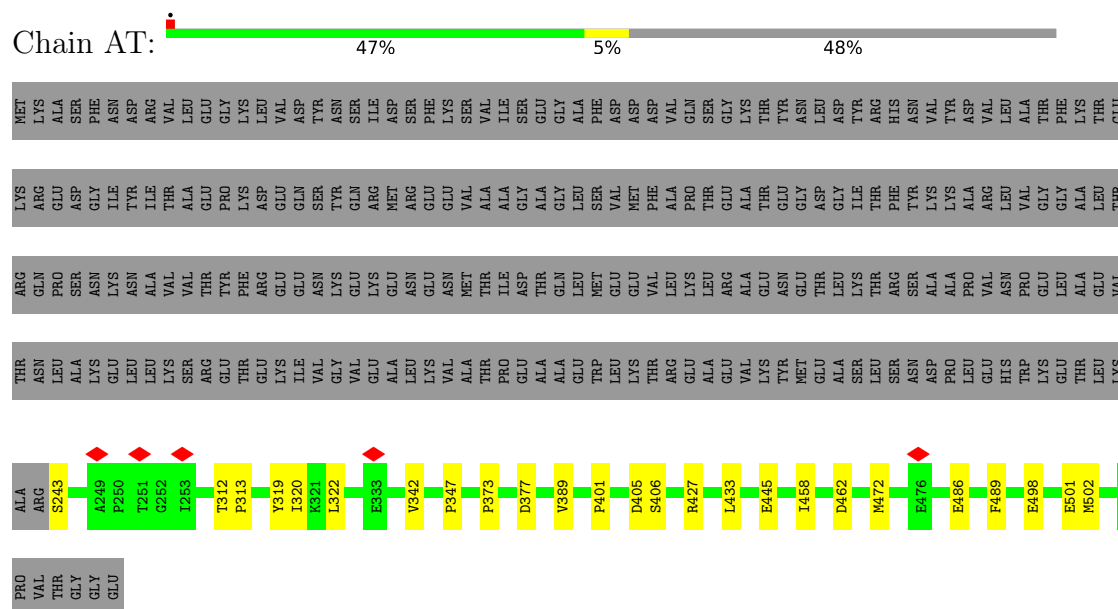




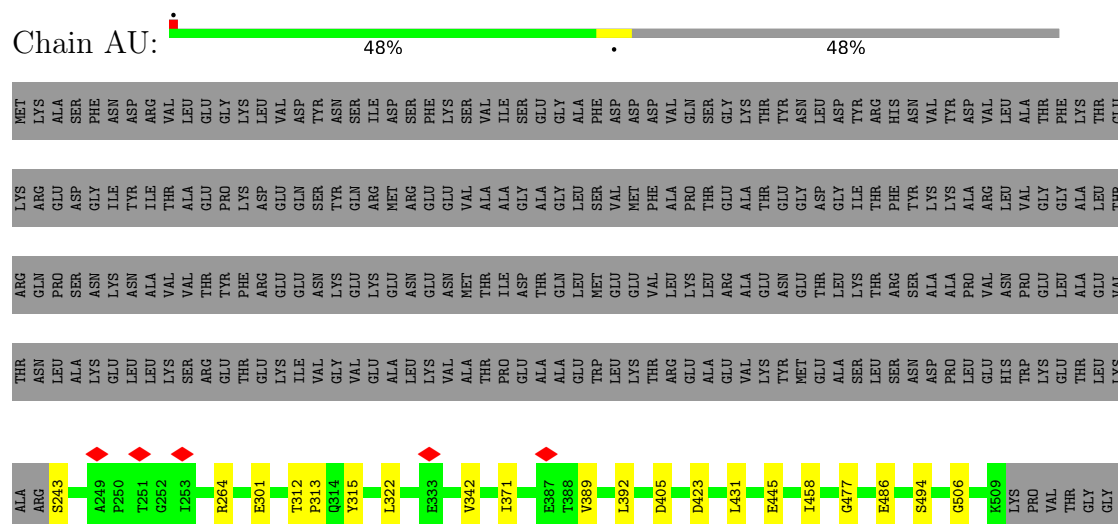




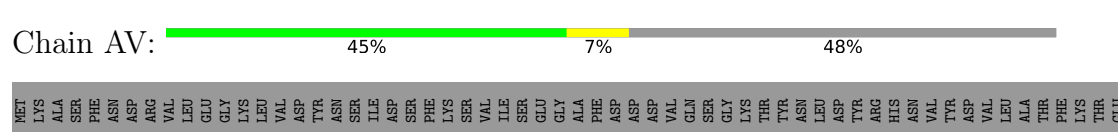
- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein

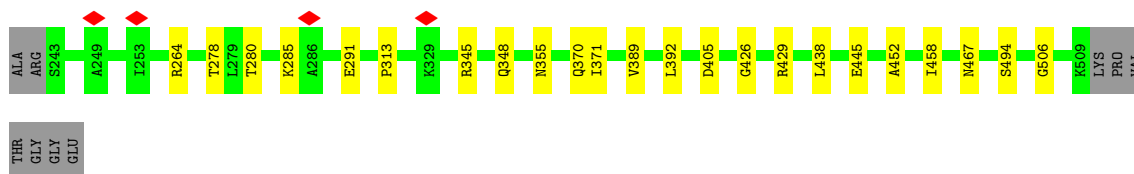


- Molecule 1: Major capsid protein

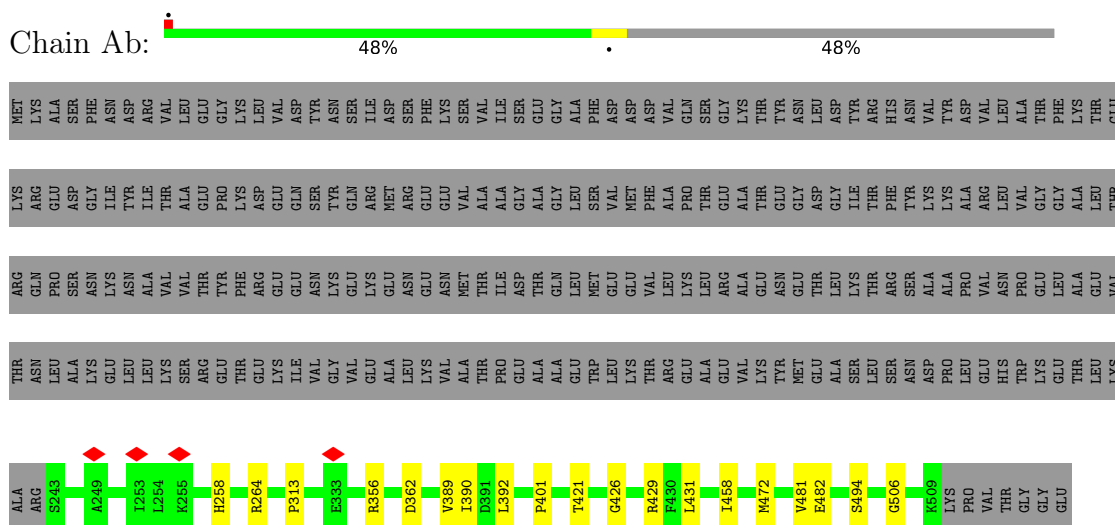




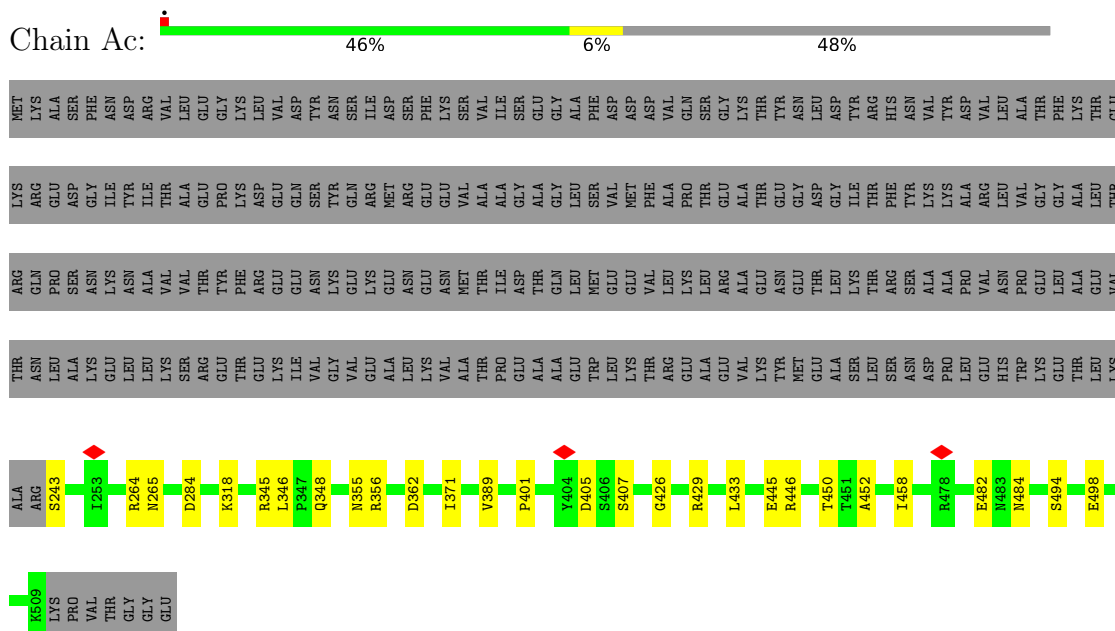
- [illegible]



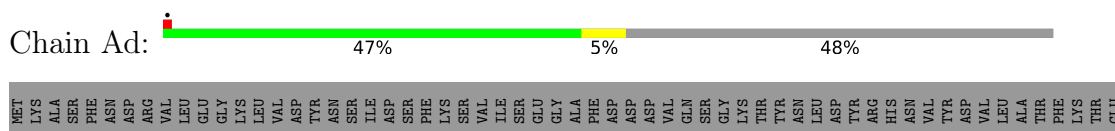
- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein



Response	Percentage
Yes, the U.S. is a democracy	48%
No, the U.S. is not a democracy	1%
Don't know	48%

Response	Percentage
Yes, the U.S. is a democracy	49%
No, the U.S. is not a democracy	48%

Response	Percentage
Yes, the U.S. is a democracy	47%
No, the U.S. is not a democracy	48%

49%

ALA	ARG	R264	T312	Y315	K321	E333	R345	Q348	S367	Q370	V389	P401	E428	R429	L433	I458	L480	K509	LVS	PRO	VAL	THR	GLY	GLY	GLU
-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----

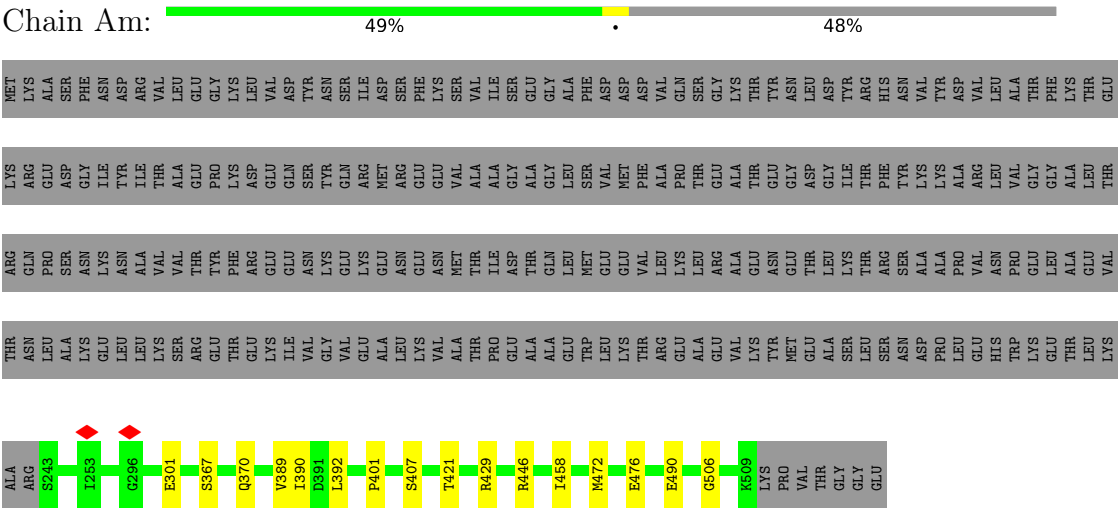
-
- | Response | Percentage |
|---|------------|
| Yes, the U.S. should take more action to reduce global warming | 48% |
| Not sure | 4% |
| No, the U.S. should not take more action to reduce global warming | 48% |

ALA	ARG	S243	R264	R272	V342	L346	P347	P373	D377	K386	V389	L392	P401	S407	R446	G456	M472	E475	F489	E498	E501	I508	K509	LYS	PRO	VAL	THR	GLY	GLY	GLU
-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----

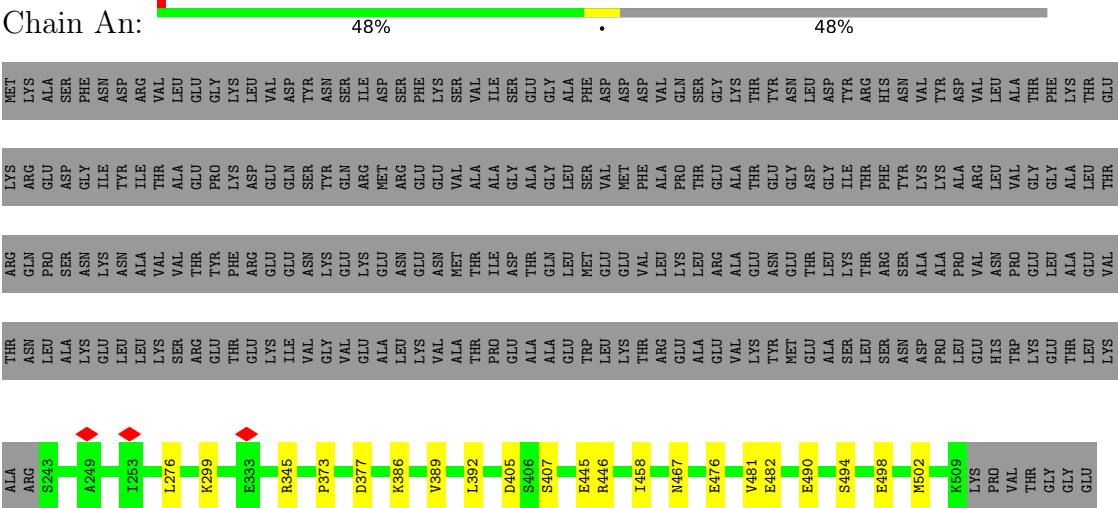
-
- | Response | Percentage |
|---------------------------------|------------|
| Yes, the U.S. is a democracy | 48% |
| No, the U.S. is not a democracy | 1% |
| Don't know | 48% |

ALA	ARG	S243	A249	R264	K324	R345	L346	P347	V354	N355	R356	D362	S367	Q370	P373	D377	P401	E428	A452	V453	D454	M472	F489	E490	M491	K509	LYS	PRO	VAL	THR	GLY	GLU
-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----

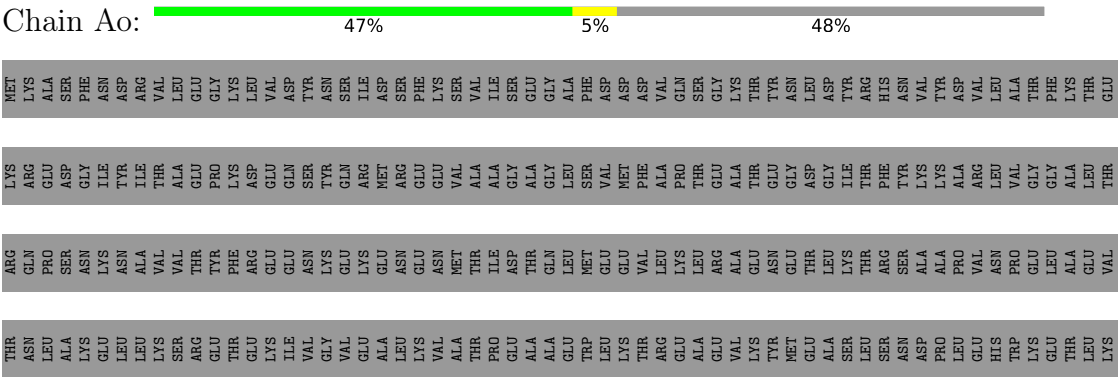
• Molecule 1: Major capsid protein



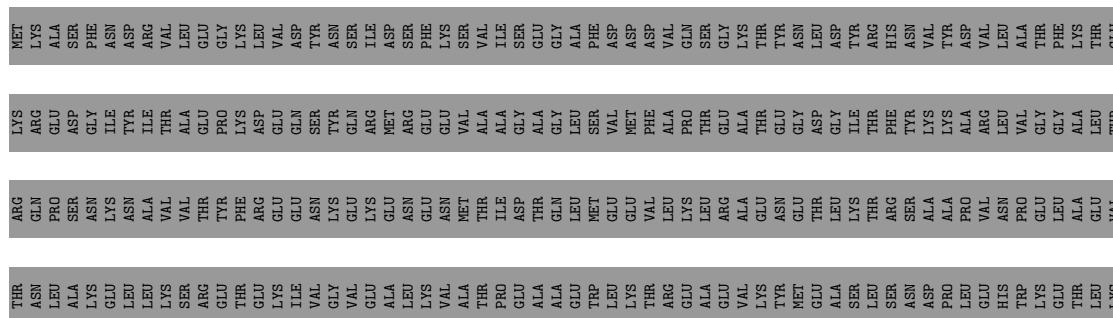
• Molecule 1: Major capsid protein



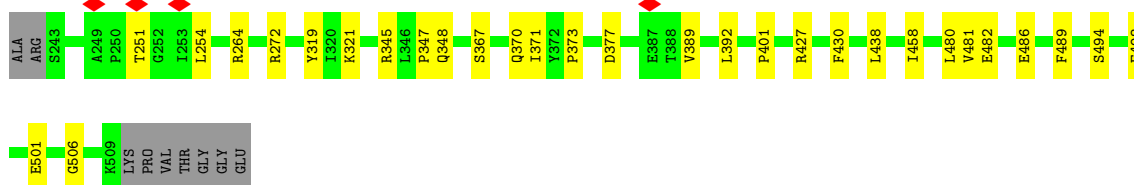
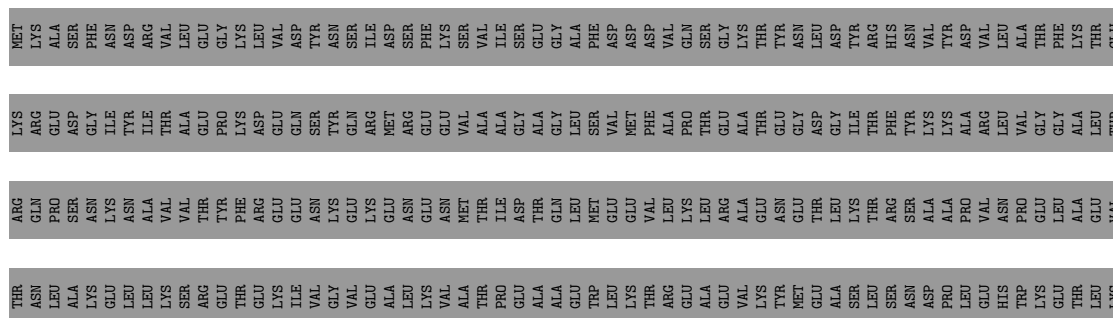
• Molecule 1: Major capsid protein



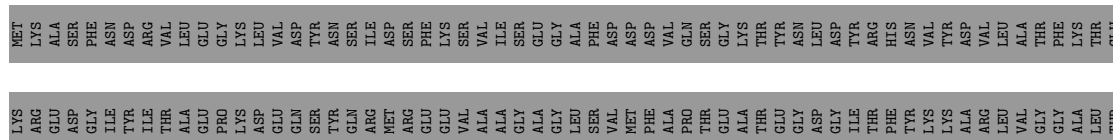
- Molecule 1: Major capsid protein



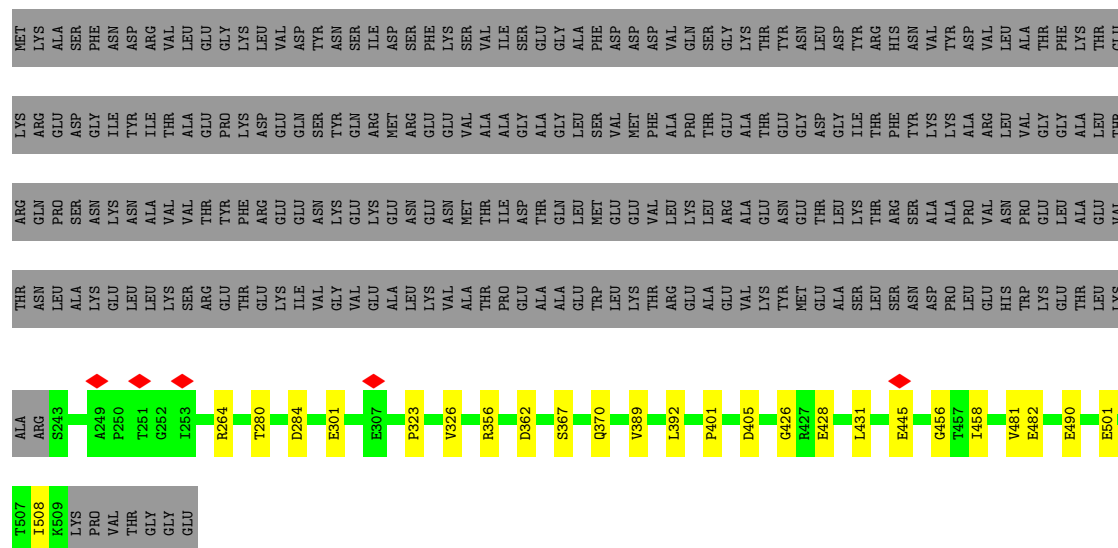
- Molecule 1: Major capsid protein



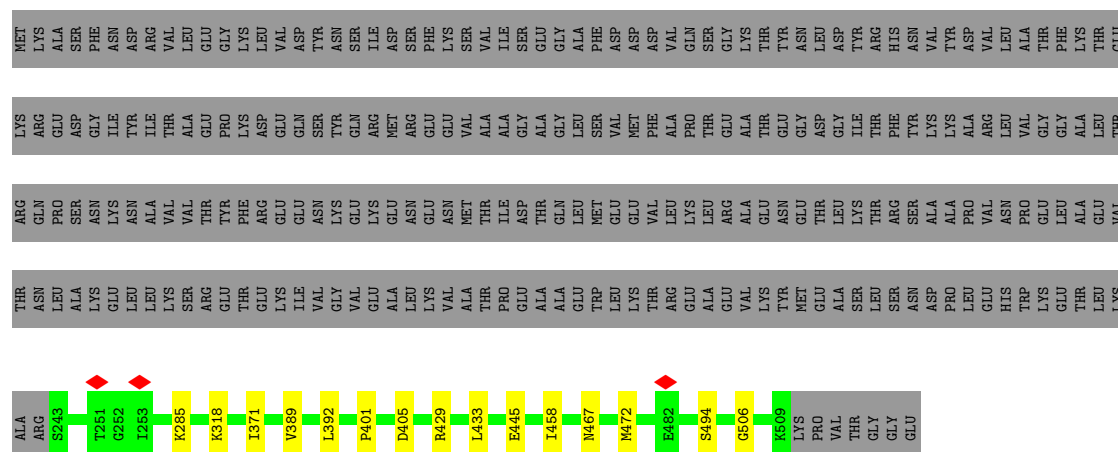
- Molecule 1: Major capsid protein



- Molecule 1: Major capsid protein

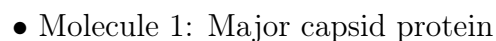


- Molecule 1: Major capsid protein

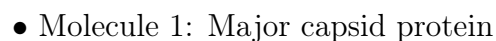


- Molecule 1: Major capsid protein

Satisfaction Level	Percentage
Very satisfied	48%
Satisfied	48%



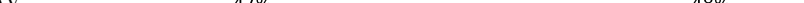
Frequency	Percentage
Every day	48%
Sometimes	48%
Never	4%

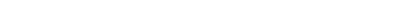


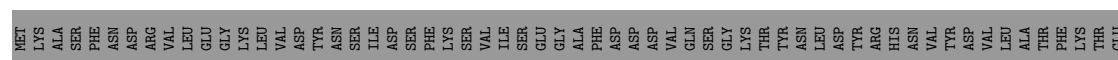
Satisfaction Level	Percentage
Very satisfied	48%
Satisfied	48%



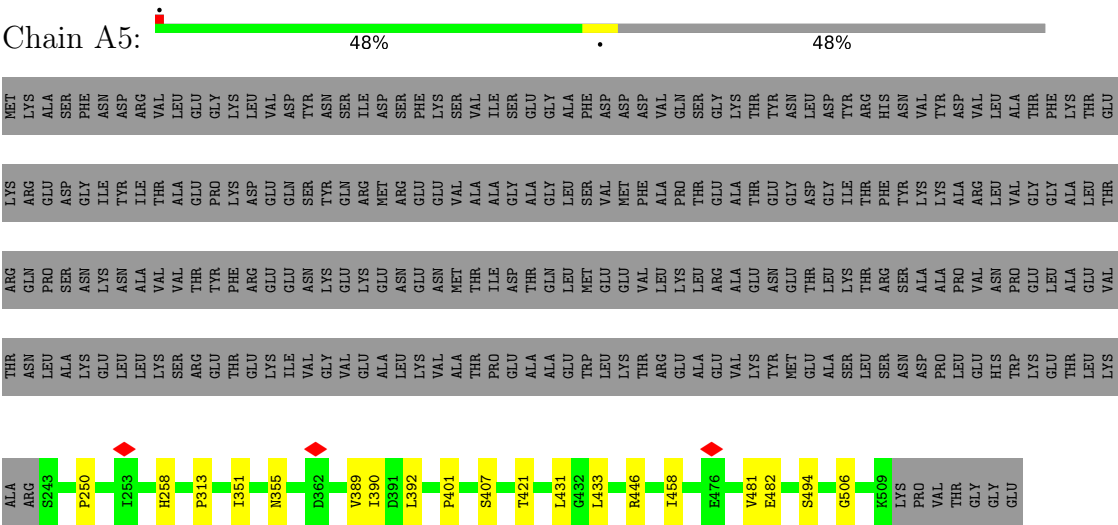
Chain Ax:

Chain A_y: 

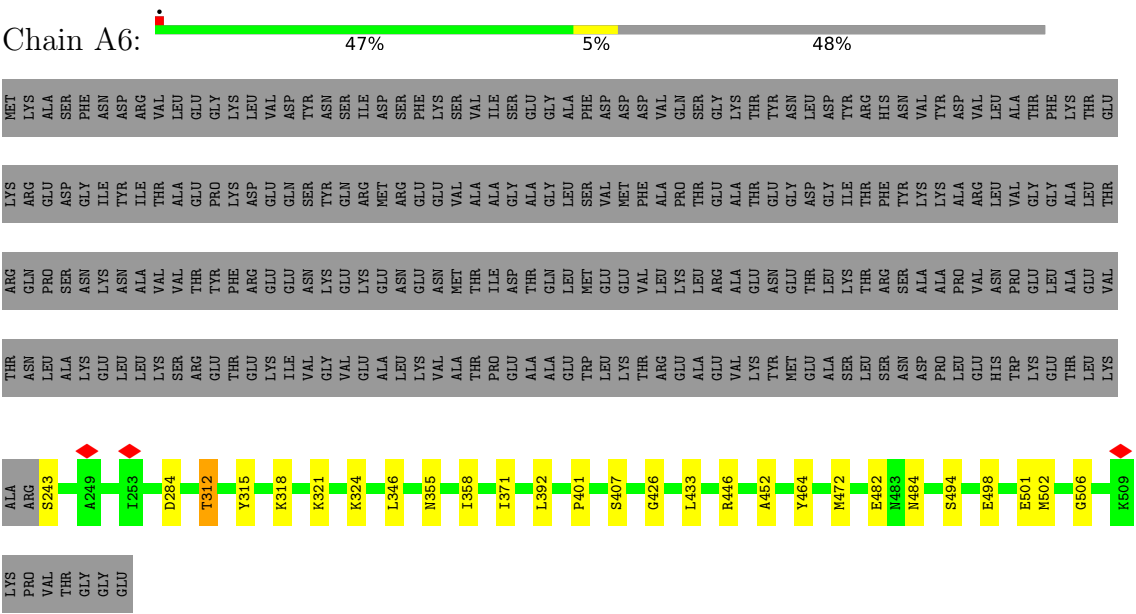
Chain Az: 



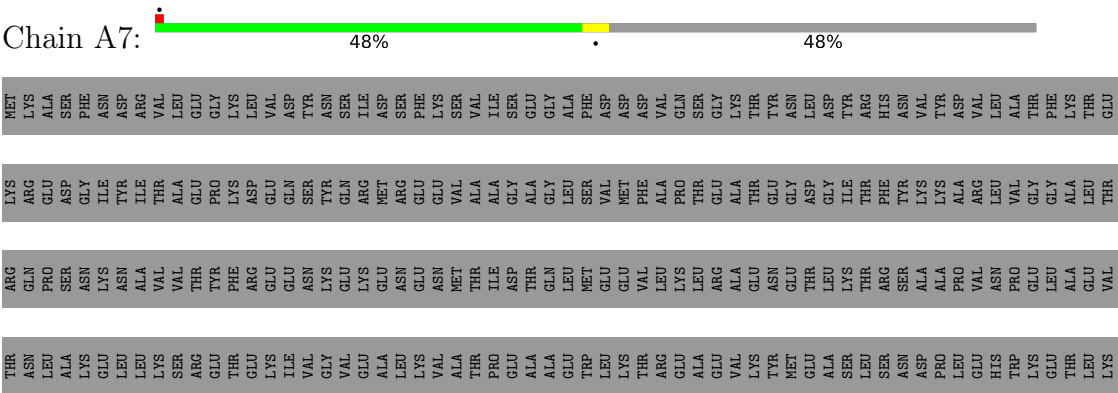
• Molecule 1: Major capsid protein



• Molecule 1: Major capsid protein



• Molecule 1: Major capsid protein





- Molecule 2: Capsid vertex protein

Chain FA: 92% 7%



- Molecule 2: Capsid vertex protein

Chain FB: 92% 7%



- Molecule 2: Capsid vertex protein

Chain FC: 91% 8%



- Molecule 2: Capsid vertex protein

Chain FD: 95% 5%



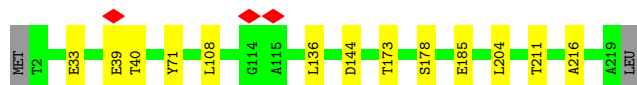
- Molecule 2: Capsid vertex protein

Chain FE: 93% 6%

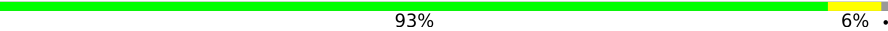


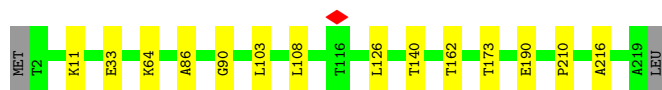
- Molecule 2: Capsid vertex protein

Chain FF: 93% 6%



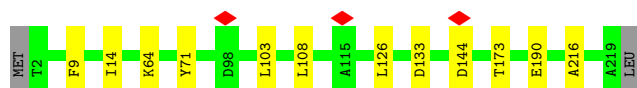
- Molecule 2: Capsid vertex protein

Chain FG:  93% 6%



- Molecule 2: Capsid vertex protein

Chain FH:  94% 5%



- Molecule 2: Capsid vertex protein

Chain FI:  93% 6%



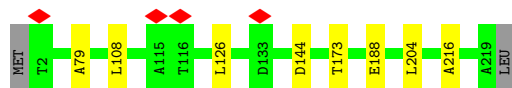
- Molecule 2: Capsid vertex protein

Chain FJ:  95% 5%



- Molecule 2: Capsid vertex protein

Chain FK:  95% 5%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	29793	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	165000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.043	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	801.792, 801.792, 801.792	wwPDB
Map dimensions	1024, 1024, 1024	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.783, 0.783, 0.783	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A0	0.10	0/2100	0.24	0/2846
1	A1	0.10	0/2099	0.23	0/2844
1	A2	0.09	0/2099	0.24	0/2844
1	A3	0.10	0/2099	0.24	0/2844
1	A4	0.11	0/2099	0.24	0/2844
1	A5	0.09	0/2099	0.24	0/2844
1	A6	0.09	0/2099	0.25	0/2844
1	A7	0.10	0/2099	0.24	0/2844
1	AA	0.10	0/2099	0.24	0/2844
1	AB	0.09	0/2099	0.24	0/2844
1	AC	0.10	0/2100	0.24	0/2846
1	AD	0.10	0/2099	0.23	0/2844
1	AE	0.10	0/2099	0.23	0/2844
1	AF	0.10	0/2100	0.22	0/2846
1	AG	0.10	0/2100	0.24	0/2846
1	AH	0.10	0/2099	0.23	0/2844
1	AI	0.10	0/2099	0.24	0/2844
1	AJ	0.09	0/2099	0.23	0/2844
1	AK	0.10	0/2099	0.23	0/2844
1	AL	0.10	0/2100	0.24	0/2846
1	AM	0.10	0/2099	0.23	0/2844
1	AN	0.09	0/2099	0.23	0/2844
1	AO	0.09	0/2099	0.23	0/2844
1	AP	0.09	0/2099	0.24	0/2844
1	AQ	0.09	0/2099	0.23	0/2844
1	AR	0.10	0/2100	0.25	0/2846
1	AS	0.10	0/2099	0.24	0/2844
1	AT	0.10	0/2099	0.24	0/2844
1	AU	0.11	0/2099	0.25	0/2844
1	AV	0.09	0/2099	0.24	0/2844
1	AW	0.09	0/2100	0.23	0/2846
1	AX	0.10	0/2099	0.24	0/2844
1	AY	0.09	0/2099	0.24	0/2844
1	AZ	0.09	0/2099	0.23	0/2844

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Aa	0.10	0/2099	0.24	0/2844
1	Ab	0.09	0/2099	0.24	0/2844
1	Ac	0.10	0/2099	0.25	0/2844
1	Ad	0.10	0/2099	0.23	0/2844
1	Ae	0.10	0/2099	0.25	0/2844
1	Af	0.10	0/2099	0.24	0/2844
1	Ag	0.10	0/2100	0.24	0/2846
1	Ah	0.10	0/2099	0.24	0/2844
1	Ai	0.10	0/2099	0.25	0/2844
1	Aj	0.10	0/2100	0.24	0/2846
1	Ak	0.10	0/2100	0.24	0/2846
1	Al	0.10	0/2099	0.24	0/2844
1	Am	0.10	0/2099	0.24	0/2844
1	An	0.10	0/2099	0.24	0/2844
1	Ao	0.10	0/2099	0.23	0/2844
1	Ap	0.10	0/2100	0.24	0/2846
1	Aq	0.10	0/2099	0.24	0/2844
1	Ar	0.09	0/2099	0.24	0/2844
1	As	0.09	0/2099	0.24	0/2844
1	At	0.09	0/2099	0.23	0/2844
1	Au	0.09	0/2099	0.23	0/2844
1	Av	0.10	0/2100	0.25	0/2846
1	Aw	0.10	0/2099	0.24	0/2844
1	Ax	0.10	0/2099	0.24	0/2844
1	Ay	0.10	0/2099	0.24	0/2844
1	Az	0.09	0/2099	0.24	0/2844
2	FA	0.11	0/1717	0.24	0/2337
2	FB	0.09	0/1717	0.23	0/2337
2	FC	0.10	0/1717	0.23	0/2337
2	FD	0.11	0/1717	0.24	0/2337
2	FE	0.10	0/1717	0.22	0/2337
2	FF	0.11	0/1717	0.25	0/2337
2	FG	0.09	0/1717	0.24	0/2337
2	FH	0.11	0/1717	0.24	0/2337
2	FI	0.11	0/1717	0.23	0/2337
2	FJ	0.11	0/1717	0.24	0/2337
2	FK	0.11	0/1717	0.25	0/2337
All	All	0.10	0/144839	0.24	0/196371

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	A0	2066	0	2093	15	0
1	A1	2065	0	2091	15	0
1	A2	2065	0	2091	16	0
1	A3	2065	0	2091	18	0
1	A4	2065	0	2091	14	0
1	A5	2065	0	2091	13	0
1	A6	2065	0	2093	18	0
1	A7	2065	0	2093	13	0
1	AA	2065	0	2093	10	0
1	AB	2065	0	2093	11	0
1	AC	2066	0	2095	16	0
1	AD	2065	0	2091	14	0
1	AE	2065	0	2091	12	0
1	AF	2066	0	2095	14	0
1	AG	2066	0	2095	12	0
1	AH	2065	0	2091	17	0
1	AI	2065	0	2091	16	0
1	AJ	2065	0	2091	10	0
1	AK	2065	0	2091	11	0
1	AL	2066	0	2095	12	0
1	AM	2065	0	2091	12	0
1	AN	2065	0	2091	13	0
1	AO	2065	0	2091	15	0
1	AP	2065	0	2091	16	0
1	AQ	2065	0	2093	11	0
1	AR	2066	0	2095	13	0
1	AS	2065	0	2091	13	0
1	AT	2065	0	2093	17	0
1	AU	2065	0	2093	14	0
1	AV	2065	0	2091	25	0
1	AW	2066	0	2093	17	0
1	AX	2065	0	2091	15	0
1	AY	2065	0	2091	18	0
1	AZ	2065	0	2091	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Aa	2065	0	2091	18	0
1	Ab	2065	0	2091	13	0
1	Ac	2065	0	2093	18	0
1	Ad	2065	0	2093	16	0
1	Ae	2065	0	2093	10	0
1	Af	2065	0	2093	12	0
1	Ag	2066	0	2095	14	0
1	Ah	2065	0	2091	10	0
1	Ai	2065	0	2091	14	0
1	Aj	2066	0	2095	12	0
1	Ak	2066	0	2095	12	0
1	Al	2065	0	2091	13	0
1	Am	2065	0	2091	11	0
1	An	2065	0	2091	14	0
1	Ao	2065	0	2091	16	0
1	Ap	2066	0	2095	13	0
1	Aq	2065	0	2091	18	0
1	Ar	2065	0	2090	25	0
1	As	2065	0	2091	19	0
1	At	2065	0	2091	12	0
1	Au	2065	0	2093	13	0
1	Av	2066	0	2095	11	0
1	Aw	2065	0	2091	12	0
1	Ax	2065	0	2093	16	0
1	Ay	2065	0	2093	16	0
1	Az	2065	0	2091	17	0
2	FA	1687	0	1666	11	0
2	FB	1687	0	1666	12	0
2	FC	1687	0	1666	13	0
2	FD	1687	0	1666	6	0
2	FE	1687	0	1666	11	0
2	FF	1687	0	1666	8	0
2	FG	1687	0	1666	9	0
2	FH	1687	0	1666	10	0
2	FI	1687	0	1666	10	0
2	FJ	1687	0	1666	8	0
2	FK	1687	0	1666	5	0
All	All	142469	0	143857	786	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 (786) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AD:356:ARG:NH2	1:AD:362:ASP:OD2	2.25	0.69
1:Ae:367:SER:HB3	1:Ae:370:GLN:HG3	1.76	0.68
1:Ai:428:GLU:OE2	1:Aj:429:ARG:NH2	2.26	0.66
1:A2:264:ARG:NH2	1:A3:401:PRO:O	2.30	0.65
1:Aj:480:LEU:HD11	2:FK:188:GLU:HG3	1.79	0.65
1:Ah:356:ARG:NH2	1:Ah:362:ASP:OD2	2.28	0.65
2:FC:74:ARG:NH2	2:FD:31:PRO:O	2.30	0.64
1:AB:318:LYS:HD2	1:AB:346:LEU:HD22	1.80	0.64
1:Au:498:GLU:HB2	1:Au:502:MET:HE1	1.80	0.64
1:Az:318:LYS:HD2	1:Az:346:LEU:HD22	1.78	0.64
1:AM:264:ARG:NH2	1:AN:401:PRO:O	2.30	0.64
1:Ar:264:ARG:NH2	1:As:401:PRO:O	2.31	0.64
1:Ad:356:ARG:NH2	1:Ad:362:ASP:OD2	2.32	0.63
1:AJ:276:LEU:O	1:AJ:467:ASN:ND2	2.32	0.63
1:AW:367:SER:HB3	1:AW:370:GLN:HG3	1.79	0.63
1:Ac:318:LYS:HD2	1:Ac:346:LEU:HD22	1.80	0.63
1:Ay:264:ARG:NH2	1:Az:401:PRO:O	2.32	0.63
1:AS:264:ARG:NH2	1:AT:401:PRO:O	2.31	0.62
1:Ak:389:VAL:HG22	1:Ak:508:ILE:HD13	1.81	0.62
1:Ar:478:ARG:HH11	1:Ar:480:LEU:HD21	1.64	0.62
1:A6:318:LYS:HD2	1:A6:346:LEU:HD22	1.81	0.62
1:Aq:264:ARG:NH2	1:Ar:401:PRO:O	2.32	0.62
1:Al:367:SER:HB3	1:Al:370:GLN:HG3	1.82	0.61
1:Ab:264:ARG:NH2	1:Ac:401:PRO:O	2.34	0.61
1:AC:243:SER:N	1:AC:321:LYS:O	2.34	0.61
2:FJ:119:GLN:HG2	2:FJ:152:ALA:HB2	1.83	0.61
1:Ag:356:ARG:NH2	1:Ag:362:ASP:OD2	2.29	0.60
1:Al:354:VAL:HG21	1:Al:491:MET:HE3	1.83	0.60
1:Ag:243:SER:N	1:Ag:321:LYS:O	2.34	0.60
1:A2:478:ARG:HH11	1:A2:480:LEU:HD21	1.65	0.60
1:As:301:GLU:OE2	1:A6:243:SER:N	2.34	0.60
1:Ar:243:SER:N	1:A6:321:LYS:O	2.34	0.60
1:Ay:431:LEU:HD21	1:Az:433:LEU:HD11	1.84	0.60
1:Ad:417:ALA:O	1:Ad:421:THR:OG1	2.20	0.59
1:Ao:423:ASP:OD2	1:Ap:427:ARG:NH1	2.34	0.59
1:AZ:321:LYS:O	1:Ax:243:SER:N	2.34	0.59
1:Aj:345:ARG:NH1	1:Aj:348:GLN:OE1	2.35	0.59
1:Ab:356:ARG:NH2	1:Ab:362:ASP:OD2	2.36	0.59
1:Az:371:ILE:HG12	1:Az:494:SER:HA	1.84	0.59
1:Aw:274:GLU:OE2	1:A1:255:LYS:NZ	2.32	0.59
1:Aw:431:LEU:HD21	1:Ax:433:LEU:HD11	1.84	0.59
1:Ao:356:ARG:NH2	1:Ao:362:ASP:OD2	2.29	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AX:345:ARG:NH1	1:AX:348:GLN:OE1	2.35	0.59
1:Ar:356:ARG:NH2	1:Ar:362:ASP:OD2	2.29	0.59
1:Au:345:ARG:NH1	1:Au:348:GLN:OE1	2.34	0.59
1:Aw:264:ARG:NH2	1:Ax:401:PRO:O	2.35	0.59
1:AF:243:SER:N	1:AF:321:LYS:O	2.36	0.59
1:AH:367:SER:HB3	1:AH:370:GLN:HG3	1.84	0.58
1:AX:367:SER:HB3	1:AX:370:GLN:HG3	1.84	0.58
1:A7:318:LYS:HD2	1:A7:346:LEU:HD22	1.85	0.58
1:Ap:272:ARG:NH2	1:Ap:498:GLU:OE2	2.36	0.58
1:Ar:272:ARG:NH2	1:Ar:498:GLU:OE2	2.36	0.58
1:AN:498:GLU:HB2	1:AN:502:MET:HE1	1.86	0.58
2:FB:11:LYS:HG2	2:FC:133:ASP:HA	1.85	0.58
1:Ad:405:ASP:HA	1:Ad:445:GLU:HG3	1.85	0.58
1:Aa:264:ARG:NH2	1:Ab:401:PRO:O	2.37	0.57
1:An:276:LEU:O	1:An:467:ASN:ND2	2.37	0.57
1:A1:367:SER:HB3	1:A1:370:GLN:HG3	1.86	0.57
1:A2:433:LEU:HD11	1:A7:431:LEU:HD21	1.84	0.57
1:Ao:345:ARG:NH1	1:Ao:348:GLN:OE1	2.38	0.57
1:AH:264:ARG:NH2	1:AI:401:PRO:O	2.38	0.57
1:AI:476:GLU:O	1:AQ:478:ARG:NH2	2.37	0.57
1:AC:264:ARG:NH2	1:AD:401:PRO:O	2.38	0.57
1:Am:367:SER:HB3	1:Am:370:GLN:HG3	1.86	0.57
1:As:264:ARG:NH2	1:At:401:PRO:O	2.38	0.57
1:Am:392:LEU:HD11	1:Am:506:GLY:HA3	1.86	0.57
1:A0:272:ARG:NH2	1:A0:498:GLU:OE2	2.36	0.57
1:AX:498:GLU:HB2	1:AX:502:MET:HE1	1.85	0.57
1:Ak:272:ARG:NH2	1:Ak:498:GLU:OE2	2.35	0.57
1:Ar:490:GLU:OE2	1:Az:324:LYS:NZ	2.33	0.57
1:Ay:389:VAL:HG23	1:Ay:458:ILE:HD11	1.87	0.56
1:Az:264:ARG:NH2	1:A0:401:PRO:O	2.38	0.56
1:Az:407:SER:HG	1:Az:446:ARG:HH11	1.53	0.56
1:A6:426:GLY:O	1:A7:429:ARG:NH1	2.37	0.56
1:AG:342:VAL:HG13	1:AG:346:LEU:HD12	1.88	0.56
1:Ar:498:GLU:HB2	1:Ar:502:MET:HE1	1.87	0.56
1:AQ:367:SER:HB3	1:AQ:370:GLN:HG3	1.86	0.56
1:Ag:301:GLU:OE2	1:Ao:243:SER:N	2.39	0.56
1:AN:264:ARG:NH2	1:AO:401:PRO:O	2.38	0.56
1:Aw:401:PRO:O	1:A1:264:ARG:NH2	2.38	0.56
1:Az:392:LEU:HD11	1:Az:506:GLY:HA3	1.87	0.56
1:AK:407:SER:OG	1:AK:446:ARG:NH1	2.39	0.56
1:AO:301:GLU:OE2	1:Ac:243:SER:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AS:431:LEU:HD21	1:AT:433:LEU:HD11	1.88	0.56
1:AC:318:LYS:HD2	1:AC:346:LEU:HD22	1.88	0.55
1:A1:405:ASP:HA	1:A1:445:GLU:HG3	1.87	0.55
1:A5:407:SER:OG	1:A5:446:ARG:NH1	2.35	0.55
2:FE:108:LEU:HD13	2:FE:216:ALA:HB2	1.88	0.55
1:Aq:367:SER:HB3	1:Aq:370:GLN:HG3	1.88	0.55
1:AG:389:VAL:HG22	1:AG:508:ILE:HD13	1.88	0.55
1:AL:301:GLU:OE2	1:AX:243:SER:N	2.40	0.55
1:A7:498:GLU:HB2	1:A7:502:MET:HE1	1.87	0.55
1:AO:389:VAL:HG22	1:AO:508:ILE:HD13	1.88	0.55
1:Am:407:SER:OG	1:Am:446:ARG:NH1	2.39	0.55
1:A2:244:ILE:HG13	1:A2:247:ILE:HD11	1.88	0.55
1:A2:498:GLU:HB2	1:A2:502:MET:HE1	1.88	0.55
1:Ay:251:THR:HB	1:A7:251:THR:HB	1.88	0.55
2:FE:119:GLN:HG2	2:FE:152:ALA:HB2	1.89	0.55
1:AS:498:GLU:HB2	1:AS:502:MET:HE1	1.89	0.55
1:Ac:407:SER:OG	1:Ac:446:ARG:NH1	2.35	0.55
1:AW:272:ARG:NH2	1:AW:498:GLU:OE2	2.39	0.55
1:Al:264:ARG:NH2	1:Am:401:PRO:O	2.39	0.55
1:AW:407:SER:OG	1:AW:446:ARG:NH1	2.39	0.54
1:A1:342:VAL:HG13	1:A1:346:LEU:HD12	1.89	0.54
1:Ac:426:GLY:O	1:Ad:429:ARG:NH1	2.41	0.54
2:FA:39:GLU:HG2	2:FA:40:THR:HG23	1.88	0.54
2:FJ:52:SER:HB3	2:FJ:201:ARG:HH11	1.72	0.54
2:FG:11:LYS:HG2	2:FH:133:ASP:HA	1.87	0.54
1:Ae:401:PRO:O	1:Aj:264:ARG:NH2	2.40	0.54
1:Au:264:ARG:NH2	1:Av:401:PRO:O	2.40	0.54
1:Av:388:THR:HG22	1:Av:390:ILE:H	1.72	0.54
1:AN:490:GLU:OE2	1:AV:324:LYS:NZ	2.37	0.54
1:AR:345:ARG:NH1	1:AR:348:GLN:OE1	2.40	0.54
1:AY:371:ILE:HG12	1:AY:494:SER:HA	1.88	0.54
1:Ar:321:LYS:O	1:A6:243:SER:N	2.41	0.54
1:AB:294:THR:HG23	1:AB:297:THR:HB	1.89	0.54
1:AB:324:LYS:NZ	1:AJ:490:GLU:OE2	2.38	0.54
1:AT:243:SER:N	1:A4:301:GLU:OE2	2.40	0.54
1:Af:478:ARG:NH2	1:An:476:GLU:O	2.40	0.54
1:Ak:401:PRO:HD2	1:Ak:501:GLU:HB3	1.89	0.54
2:FE:52:SER:HB3	2:FE:201:ARG:HH11	1.72	0.54
1:Af:272:ARG:NH2	1:Af:498:GLU:OE2	2.36	0.54
1:Aw:319:TYR:OH	1:Aw:486:GLU:OE2	2.25	0.54
1:A2:431:LEU:HD21	1:A3:433:LEU:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A4:431:LEU:HD21	1:A5:433:LEU:HD11	1.90	0.53
1:A5:431:LEU:HD21	1:A6:433:LEU:HD11	1.89	0.53
1:AH:354:VAL:HG21	1:AH:491:MET:HE3	1.91	0.53
1:Ah:467:ASN:OD1	1:Ah:494:SER:OG	2.24	0.53
1:Am:301:GLU:OE2	1:Au:243:SER:N	2.41	0.53
1:Ag:323:PRO:HB2	1:Ag:326:VAL:HG23	1.90	0.53
1:Aq:319:TYR:OH	1:Aq:486:GLU:OE2	2.26	0.53
1:A5:407:SER:HG	1:A5:446:ARG:HH11	1.53	0.53
1:AU:371:ILE:HG12	1:AU:494:SER:HA	1.89	0.53
1:Aa:313:PRO:HA	1:Aa:494:SER:HB3	1.89	0.53
1:Ao:407:SER:OG	1:Ao:446:ARG:NH1	2.39	0.53
1:Ac:356:ARG:NH2	1:Ac:362:ASP:OD2	2.37	0.53
1:AE:291:GLU:OE1	1:AE:300:ASN:ND2	2.41	0.53
1:AK:406:SER:HA	1:AK:462:ASP:HB2	1.89	0.53
1:Aw:429:ARG:NH2	1:A1:428:GLU:OE2	2.42	0.53
1:AV:371:ILE:HG12	1:AV:494:SER:HA	1.90	0.53
2:FF:71:TYR:OH	2:FG:33:GLU:OE2	2.22	0.53
1:AL:342:VAL:HG13	1:AL:346:LEU:HD12	1.91	0.53
1:Ac:498:GLU:HB2	1:Ac:502:MET:HE1	1.90	0.53
1:A6:482:GLU:OE1	1:A6:484:ASN:ND2	2.42	0.53
1:AI:367:SER:HB3	1:AI:370:GLN:HG3	1.90	0.52
1:AT:243:SER:N	1:A3:321:LYS:O	2.41	0.52
1:Al:428:GLU:OE2	1:Am:429:ARG:NH2	2.42	0.52
1:Ay:392:LEU:HD11	1:Ay:506:GLY:HA3	1.90	0.52
1:AA:392:LEU:HD11	1:AA:506:GLY:HA3	1.92	0.52
1:AZ:301:GLU:OE2	1:A2:243:SER:N	2.41	0.52
1:AI:458:ILE:HD11	1:AI:508:ILE:HD11	1.91	0.52
2:FA:71:TYR:OH	2:FB:33:GLU:OE2	2.21	0.52
1:AQ:498:GLU:HB2	1:AQ:502:MET:HE1	1.91	0.52
1:AY:392:LEU:HD11	1:AY:506:GLY:HA3	1.92	0.52
1:Ao:406:SER:HA	1:Ao:462:ASP:HB2	1.91	0.52
1:AP:371:ILE:HG12	1:AP:494:SER:HA	1.91	0.52
1:AU:243:SER:N	1:AY:301:GLU:OE2	2.42	0.52
1:An:498:GLU:HB2	1:An:502:MET:HE1	1.91	0.52
1:As:389:VAL:HG22	1:As:508:ILE:HD13	1.92	0.52
1:A0:407:SER:OG	1:A0:446:ARG:NH1	2.39	0.52
1:As:426:GLY:O	1:At:429:ARG:NH1	2.43	0.52
2:FF:39:GLU:HG2	2:FF:40:THR:HG23	1.92	0.52
1:Ae:467:ASN:OD1	1:Ae:494:SER:OG	2.22	0.52
1:Aw:433:LEU:HD11	1:A1:431:LEU:HD21	1.92	0.52
1:A2:356:ARG:NH2	1:A2:362:ASP:OD2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Av:345:ARG:NH1	1:Av:348:GLN:OE1	2.42	0.52
1:Aq:321:LYS:O	1:Az:243:SER:N	2.43	0.52
1:AE:430:PHE:HB3	1:AE:438:LEU:HD21	1.91	0.51
1:Ao:367:SER:HB3	1:Ao:370:GLN:HG3	1.92	0.51
1:A4:264:ARG:NH2	1:A5:401:PRO:O	2.43	0.51
1:A7:371:ILE:HG12	1:A7:494:SER:HA	1.92	0.51
1:AD:428:GLU:OE2	1:AE:429:ARG:NH2	2.43	0.51
1:AX:467:ASN:OD1	1:AX:494:SER:OG	2.20	0.51
2:FA:31:PRO:O	2:FE:74:ARG:NH1	2.43	0.51
2:FJ:108:LEU:HD13	2:FJ:216:ALA:HB2	1.93	0.51
1:AG:356:ARG:NH2	1:AG:362:ASP:OD2	2.38	0.51
1:AJ:299:LYS:HD3	1:AK:317:TYR:CD2	2.44	0.51
1:AM:367:SER:HB3	1:AM:370:GLN:HG3	1.93	0.51
1:Aq:480:LEU:HD12	1:A0:486:GLU:HB3	1.92	0.51
1:Aq:345:ARG:NH1	1:Aq:348:GLN:OE1	2.43	0.51
1:Au:367:SER:HB3	1:Au:370:GLN:HG3	1.91	0.51
1:A5:392:LEU:HD11	1:A5:506:GLY:HA3	1.92	0.51
1:AZ:498:GLU:HB2	1:AZ:502:MET:HE1	1.93	0.51
1:At:467:ASN:OD1	1:At:494:SER:OG	2.24	0.51
1:AM:371:ILE:HG12	1:AM:494:SER:HA	1.93	0.51
1:AS:389:VAL:HG23	1:AS:458:ILE:HD11	1.93	0.51
1:AY:478:ARG:NH2	1:A3:476:GLU:O	2.43	0.51
1:Af:324:LYS:NZ	1:An:490:GLU:OE2	2.42	0.51
1:AR:319:TYR:OH	1:AR:486:GLU:OE2	2.28	0.51
1:Av:323:PRO:HB2	1:Av:326:VAL:HG23	1.93	0.51
1:Aw:498:GLU:HB2	1:Aw:502:MET:HE1	1.92	0.51
1:AE:264:ARG:NH2	1:AF:401:PRO:O	2.43	0.51
1:AB:371:ILE:HG12	1:AB:494:SER:HA	1.91	0.51
1:AD:264:ARG:NH2	1:AE:401:PRO:O	2.44	0.51
1:Ak:407:SER:OG	1:Ak:446:ARG:NH1	2.43	0.51
1:As:456:GLY:HA2	1:As:508:ILE:HD12	1.93	0.51
1:Av:272:ARG:NH2	1:Av:498:GLU:OE2	2.42	0.51
1:AT:406:SER:HA	1:AT:462:ASP:HB2	1.93	0.50
1:AV:318:LYS:HD2	1:AV:346:LEU:HD22	1.92	0.50
1:Ac:482:GLU:OE1	1:Ac:484:ASN:ND2	2.45	0.50
1:Ap:243:SER:N	1:Ap:321:LYS:O	2.44	0.50
1:A1:401:PRO:HD2	1:A1:501:GLU:HB3	1.93	0.50
1:Ag:264:ARG:NH2	1:Ah:401:PRO:O	2.44	0.50
1:A4:392:LEU:HD11	1:A4:506:GLY:HA3	1.91	0.50
1:A5:389:VAL:HG23	1:A5:458:ILE:HD11	1.93	0.50
1:Ac:264:ARG:NH2	1:Ad:401:PRO:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A3:392:LEU:HD11	1:A3:506:GLY:HA3	1.93	0.50
1:AC:364:THR:HB	1:AD:291:GLU:HG2	1.94	0.50
1:AK:367:SER:HB3	1:AK:370:GLN:HG3	1.92	0.50
1:AM:407:SER:OG	1:AM:446:ARG:NH1	2.40	0.50
1:AX:342:VAL:HG13	1:AX:346:LEU:HD12	1.94	0.50
1:AP:356:ARG:NH2	1:AP:362:ASP:OD2	2.33	0.50
1:AY:243:SER:N	1:A3:301:GLU:OE2	2.44	0.50
2:FA:33:GLU:OE2	2:FE:71:TYR:OH	2.24	0.50
2:FI:17:LEU:HD13	2:FI:174:ILE:HG21	1.93	0.50
2:FE:52:SER:HB3	2:FE:201:ARG:NH1	2.27	0.50
1:AW:345:ARG:NH1	1:AW:348:GLN:OE1	2.44	0.50
1:As:405:ASP:HA	1:As:445:GLU:HG3	1.93	0.50
1:As:481:VAL:HG13	1:As:482:GLU:HG3	1.92	0.50
1:Au:389:VAL:HG23	1:Au:458:ILE:HD11	1.94	0.50
1:A2:317:TYR:CE2	1:A3:299:LYS:HB3	2.47	0.50
1:Ap:356:ARG:NH2	1:Ap:362:ASP:OD2	2.38	0.50
1:Ar:345:ARG:NH1	1:Ar:348:GLN:OE1	2.43	0.50
2:FD:71:TYR:OH	2:FE:33:GLU:OE2	2.26	0.50
1:AO:356:ARG:NH2	1:AO:362:ASP:OD2	2.40	0.49
1:AN:407:SER:OG	1:AN:446:ARG:NH1	2.44	0.49
1:AV:392:LEU:HD11	1:AV:506:GLY:HA3	1.94	0.49
1:Aq:272:ARG:NH2	1:Aq:498:GLU:OE2	2.37	0.49
1:A3:371:ILE:HG12	1:A3:494:SER:HA	1.93	0.49
2:FG:126:LEU:HD22	2:FG:173:THR:HG23	1.94	0.49
1:AF:371:ILE:HG12	1:AF:494:SER:HA	1.94	0.49
1:Ah:264:ARG:NH2	1:Ai:401:PRO:O	2.45	0.49
2:FH:108:LEU:HD13	2:FH:216:ALA:HB2	1.95	0.49
1:Ak:264:ARG:NH2	1:Al:401:PRO:O	2.46	0.49
1:AF:323:PRO:HB2	1:AF:326:VAL:HG23	1.93	0.49
1:AP:401:PRO:HD2	1:AP:501:GLU:HB3	1.94	0.49
1:Aa:405:ASP:HA	1:Aa:445:GLU:HG3	1.94	0.49
1:AI:389:VAL:HG23	1:AI:458:ILE:HD11	1.95	0.49
1:AT:401:PRO:HD2	1:AT:501:GLU:HB3	1.95	0.49
1:AZ:251:THR:HB	1:Ax:251:THR:HB	1.93	0.49
1:Ax:498:GLU:HB2	1:Ax:502:MET:HE1	1.95	0.49
1:AA:371:ILE:HG12	1:AA:494:SER:HA	1.94	0.49
1:AG:405:ASP:HA	1:AG:445:GLU:HG3	1.95	0.49
1:AV:254:LEU:HD13	1:AW:280:THR:HG22	1.94	0.49
1:AZ:324:LYS:NZ	1:Ay:490:GLU:OE2	2.32	0.49
1:AK:433:LEU:HD11	1:AL:431:LEU:HD21	1.95	0.49
1:AX:371:ILE:HG12	1:AX:494:SER:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:As:367:SER:HB3	1:As:370:GLN:HG3	1.95	0.49
1:A1:259:ASP:OD2	1:A1:345:ARG:NH2	2.46	0.49
2:FI:144:ASP:OD1	2:FI:144:ASP:N	2.46	0.49
1:AL:323:PRO:HB2	1:AL:326:VAL:HG23	1.94	0.49
1:AM:345:ARG:NH1	1:AM:348:GLN:OE1	2.46	0.49
1:Ab:389:VAL:HG23	1:Ab:458:ILE:HD11	1.94	0.49
1:A5:351:ILE:O	1:A5:355:ASN:ND2	2.46	0.49
1:AQ:264:ARG:NH2	1:AR:401:PRO:O	2.45	0.48
1:Av:392:LEU:HD11	1:Av:506:GLY:HA3	1.95	0.48
1:A4:389:VAL:HG23	1:A4:458:ILE:HD11	1.94	0.48
1:AP:467:ASN:OD1	1:AP:494:SER:OG	2.26	0.48
1:Am:476:GLU:O	1:Au:478:ARG:NH2	2.46	0.48
1:AJ:407:SER:OG	1:AJ:446:ARG:NH1	2.43	0.48
1:AM:481:VAL:HG13	1:AM:482:GLU:HG3	1.94	0.48
1:Aj:367:SER:HB3	1:Aj:370:GLN:HG3	1.95	0.48
1:AS:351:ILE:O	1:AS:355:ASN:ND2	2.38	0.48
1:AU:322:LEU:HD11	1:AU:342:VAL:HG21	1.95	0.48
1:AY:498:GLU:HB2	1:AY:502:MET:HE1	1.94	0.48
1:Ae:405:ASP:HA	1:Ae:445:GLU:HG3	1.95	0.48
1:AS:429:ARG:NH2	1:AX:428:GLU:OE2	2.46	0.48
1:Ay:407:SER:OG	1:Ay:446:ARG:NH1	2.45	0.48
1:Az:254:LEU:HD13	1:A0:280:THR:HG22	1.94	0.48
2:FI:178:SER:O	2:FI:211:THR:OG1	2.24	0.48
1:AF:345:ARG:NH1	1:AF:348:GLN:OE1	2.46	0.48
1:AH:356:ARG:NH2	1:AH:362:ASP:OD2	2.39	0.48
1:AK:389:VAL:HG13	1:AK:458:ILE:HD11	1.96	0.48
1:Ae:390:ILE:HG13	1:Ae:421:THR:HG21	1.96	0.48
1:Au:407:SER:HG	1:Au:446:ARG:HH11	1.59	0.48
2:FB:103:LEU:HD23	2:FB:210:PRO:HB3	1.95	0.48
1:Ad:498:GLU:HB2	1:Ad:502:MET:HE1	1.95	0.48
1:AU:392:LEU:HD11	1:AU:506:GLY:HA3	1.95	0.48
1:Ad:467:ASN:OD1	1:Ad:494:SER:OG	2.25	0.48
1:Ay:322:LEU:HD11	1:Ay:342:VAL:HG21	1.96	0.48
2:FJ:52:SER:HB3	2:FJ:201:ARG:NH1	2.28	0.48
1:AY:356:ARG:NH2	1:AY:362:ASP:OD2	2.47	0.48
1:Ay:321:LYS:O	1:A7:243:SER:N	2.47	0.48
1:AJ:481:VAL:HG13	1:AJ:482:GLU:HG3	1.95	0.48
1:AS:401:PRO:O	1:AX:264:ARG:NH2	2.47	0.48
1:AU:431:LEU:HD21	1:AV:433:LEU:HD11	1.95	0.48
1:AZ:392:LEU:HD11	1:AZ:506:GLY:HA3	1.96	0.48
1:AB:431:LEU:HD21	1:AC:433:LEU:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AS:407:SER:OG	1:AS:446:ARG:NH1	2.43	0.47
1:Ac:265:ASN:O	1:Ac:450:THR:OG1	2.32	0.47
1:AG:367:SER:HB3	1:AG:370:GLN:HG3	1.96	0.47
1:AK:345:ARG:NH1	1:AK:348:GLN:OE1	2.47	0.47
1:AO:264:ARG:NH2	1:AP:401:PRO:O	2.46	0.47
1:AY:251:THR:HB	1:A2:251:THR:HB	1.96	0.47
1:Ar:347:PRO:HG3	1:Ar:489:PHE:CE1	2.49	0.47
1:A2:392:LEU:HD11	1:A2:506:GLY:HA3	1.95	0.47
2:FA:174:ILE:HG13	2:FA:175:PRO:HD2	1.96	0.47
2:FD:144:ASP:OD1	2:FD:144:ASP:N	2.42	0.47
1:AI:392:LEU:HD11	1:AI:506:GLY:HA3	1.97	0.47
1:Aa:389:VAL:HG23	1:Aa:458:ILE:HD11	1.96	0.47
1:Ak:342:VAL:HG13	1:Ak:346:LEU:HD12	1.97	0.47
1:An:467:ASN:N	1:An:494:SER:O	2.35	0.47
1:Aq:251:THR:HB	1:Az:251:THR:OG1	2.15	0.47
1:A3:431:LEU:HD21	1:A4:433:LEU:HD11	1.96	0.47
1:An:299:LYS:HD3	1:Ao:317:TYR:CD2	2.49	0.47
1:A0:478:ARG:HH12	2:FH:190:GLU:HB2	1.78	0.47
2:FB:71:TYR:OH	2:FC:33:GLU:OE2	2.26	0.47
1:AO:291:GLU:OE1	1:AO:300:ASN:ND2	2.48	0.47
1:AO:481:VAL:HG13	1:AO:482:GLU:HG3	1.96	0.47
1:AZ:490:GLU:OE2	1:A2:324:LYS:NZ	2.44	0.47
1:A6:371:ILE:HG12	1:A6:494:SER:HA	1.95	0.47
1:A7:405:ASP:HA	1:A7:445:GLU:HG3	1.96	0.47
1:AH:401:PRO:HD2	1:AH:501:GLU:HB3	1.96	0.47
1:AV:312:THR:O	1:AV:370:GLN:NE2	2.44	0.47
1:Ab:426:GLY:O	1:Ac:429:ARG:NH1	2.47	0.47
1:Ad:371:ILE:HG12	1:Ad:494:SER:HA	1.96	0.47
1:AI:407:SER:OG	1:AI:446:ARG:NH1	2.45	0.47
1:Ao:371:ILE:HG12	1:Ao:494:SER:HA	1.96	0.47
1:Aq:347:PRO:HG3	1:Aq:489:PHE:CD2	2.50	0.47
1:A6:472:MET:HE2	1:A6:472:MET:HB2	1.82	0.47
1:Al:324:LYS:NZ	1:Av:490:GLU:OE2	2.39	0.47
1:Aq:389:VAL:HG23	1:Aq:458:ILE:HD11	1.97	0.47
1:Ax:264:ARG:NH2	1:Ay:401:PRO:O	2.48	0.47
1:Ax:373:PRO:O	1:Ax:377:ASP:HB2	2.14	0.47
1:A4:371:ILE:HG12	1:A4:494:SER:HA	1.95	0.47
1:AJ:327:MET:HE1	1:AJ:339:LEU:HB2	1.96	0.47
1:AS:259:ASP:OD2	1:AS:345:ARG:NH2	2.47	0.47
1:AY:345:ARG:NH1	1:AY:348:GLN:OE1	2.48	0.47
1:Aa:371:ILE:HG12	1:Aa:494:SER:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:As:490:GLU:OE2	1:A6:324:LYS:NZ	2.45	0.47
1:Aw:389:VAL:HG23	1:Aw:458:ILE:HD11	1.96	0.47
1:Aw:481:VAL:HG13	1:Aw:482:GLU:HG3	1.96	0.47
2:FC:144:ASP:OD1	2:FC:144:ASP:N	2.48	0.47
1:AD:467:ASN:OD1	1:AD:494:SER:OG	2.23	0.46
1:Ar:373:PRO:O	1:Ar:377:ASP:HB2	2.15	0.46
2:FB:58:PRO:HG2	2:FB:63:GLN:HG2	1.97	0.46
2:FH:9:PHE:CD1	2:FH:14:ILE:HD11	2.51	0.46
2:FH:126:LEU:HD22	2:FH:173:THR:HG23	1.97	0.46
1:AH:356:ARG:NH1	1:AH:454:ASP:OD1	2.46	0.46
1:Al:356:ARG:NH1	1:Al:454:ASP:OD1	2.47	0.46
1:Ar:254:LEU:HD13	1:As:280:THR:HG22	1.97	0.46
1:AL:313:PRO:HA	1:AL:494:SER:HB3	1.98	0.46
1:AZ:428:GLU:OE2	1:Aa:429:ARG:NH2	2.38	0.46
1:Ar:258:HIS:O	1:As:284:ASP:N	2.48	0.46
1:Ay:478:ARG:NH2	1:A2:476:GLU:O	2.48	0.46
1:A3:389:VAL:HG23	1:A3:458:ILE:HD11	1.97	0.46
2:FF:178:SER:O	2:FF:211:THR:OG1	2.28	0.46
1:AC:431:LEU:HD21	1:AD:433:LEU:HD11	1.97	0.46
1:AG:456:GLY:HA2	1:AG:508:ILE:HD12	1.97	0.46
1:AU:301:GLU:OE2	1:A3:243:SER:N	2.49	0.46
1:Aj:389:VAL:HG23	1:Aj:458:ILE:HD11	1.97	0.46
1:Aq:371:ILE:HG12	1:Aq:494:SER:HA	1.97	0.46
1:AN:392:LEU:HD11	1:AN:506:GLY:HA3	1.97	0.46
1:AR:323:PRO:HB2	1:AR:326:VAL:HG23	1.96	0.46
1:AV:301:GLU:OE2	1:Ad:243:SER:N	2.49	0.46
1:Ai:431:LEU:HD21	1:Aj:433:LEU:HD11	1.97	0.46
1:A0:386:LYS:HG3	1:A0:392:LEU:HA	1.98	0.46
1:AI:390:ILE:HG13	1:AI:421:THR:HG21	1.98	0.46
1:AL:480:LEU:HD13	2:FB:190:GLU:HB3	1.97	0.46
1:AR:392:LEU:HD11	1:AR:506:GLY:HA3	1.97	0.46
1:AW:405:ASP:HA	1:AW:445:GLU:HG3	1.95	0.46
1:AZ:389:VAL:HG23	1:AZ:458:ILE:HD11	1.98	0.46
1:Ac:371:ILE:HG12	1:Ac:494:SER:HA	1.97	0.46
1:AZ:364:THR:HB	1:Aa:291:GLU:HG2	1.97	0.46
1:Ac:405:ASP:HA	1:Ac:445:GLU:HG3	1.97	0.46
1:A0:472:MET:HB2	1:A0:472:MET:HE2	1.79	0.46
1:A3:364:THR:HB	1:A4:291:GLU:HG2	1.97	0.46
1:A6:407:SER:OG	1:A6:446:ARG:NH1	2.46	0.46
1:A6:498:GLU:HB2	1:A6:502:MET:HE1	1.98	0.46
1:AG:373:PRO:O	1:AG:377:ASP:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ai:392:LEU:HD11	1:Ai:506:GLY:HA3	1.98	0.46
1:Ak:472:MET:HE2	1:Ak:472:MET:HB2	1.83	0.46
2:FF:33:GLU:OE2	2:FJ:71:TYR:OH	2.24	0.46
1:AA:420:PHE:O	1:AA:422:LYS:NZ	2.49	0.46
1:AA:429:ARG:NH2	1:AF:428:GLU:OE2	2.47	0.46
1:AM:251:THR:HB	1:AV:251:THR:OG1	2.16	0.46
1:AR:407:SER:OG	1:AR:446:ARG:NH1	2.44	0.46
1:Ab:313:PRO:HA	1:Ab:494:SER:HB3	1.98	0.46
1:AU:405:ASP:HA	1:AU:445:GLU:HG3	1.98	0.45
1:AZ:483:ASN:HB2	1:Az:293:HIS:CE1	2.51	0.45
1:Af:373:PRO:O	1:Af:377:ASP:HB2	2.16	0.45
1:AC:323:PRO:HB2	1:AC:326:VAL:HG23	1.97	0.45
1:Ag:479:ILE:HD11	1:Ag:486:GLU:HG3	1.99	0.45
1:Az:390:ILE:HG21	1:Az:429:ARG:HH22	1.81	0.45
1:A2:279:LEU:HD23	1:A2:311:LEU:HD12	1.99	0.45
1:AB:345:ARG:NH1	1:AB:348:GLN:OE1	2.48	0.45
1:AT:427:ARG:NH1	1:AU:423:ASP:OD2	2.47	0.45
1:AW:323:PRO:HB2	1:AW:326:VAL:HG23	1.98	0.45
1:Aa:426:GLY:O	1:Ab:429:ARG:NH1	2.49	0.45
1:At:392:LEU:HD11	1:At:506:GLY:HA3	1.99	0.45
1:AI:401:PRO:HD2	1:AI:501:GLU:HB3	1.99	0.45
1:Af:392:LEU:HD11	1:Af:506:GLY:HA3	1.97	0.45
2:FF:185:GLU:HG2	2:FF:204:LEU:HD13	1.99	0.45
1:AN:373:PRO:O	1:AN:377:ASP:HB2	2.17	0.45
1:AQ:389:VAL:HG23	1:AQ:458:ILE:HD11	1.98	0.45
1:AV:405:ASP:HA	1:AV:445:GLU:HG3	1.98	0.45
1:AY:431:LEU:HD21	1:AZ:433:LEU:HD11	1.99	0.45
1:Am:390:ILE:HG13	1:Am:421:THR:HG21	1.98	0.45
1:AL:268:LEU:O	1:AL:470:ARG:NH1	2.50	0.45
1:Al:356:ARG:NH2	1:Al:362:ASP:OD2	2.32	0.45
1:A5:313:PRO:HA	1:A5:494:SER:HB3	1.99	0.45
1:AA:367:SER:HB3	1:AA:370:GLN:HG3	1.98	0.45
1:AE:431:LEU:HD21	1:AF:433:LEU:HD11	1.97	0.45
1:AY:280:THR:HG22	1:Ad:254:LEU:HD13	1.99	0.45
1:Az:407:SER:OG	1:Az:446:ARG:NH1	2.45	0.45
1:AC:427:ARG:NH1	1:AD:423:ASP:OD2	2.50	0.45
1:AM:480:LEU:HD12	1:AW:486:GLU:HB3	1.99	0.45
1:AT:472:MET:HE2	1:AT:472:MET:HB2	1.84	0.45
1:Ab:392:LEU:HD11	1:Ab:506:GLY:HA3	1.98	0.45
1:Ag:389:VAL:HG23	1:Ag:458:ILE:HD11	1.99	0.45
1:Am:472:MET:HE2	1:Am:472:MET:HB2	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ao:433:LEU:HD11	1:Ap:431:LEU:HD21	1.99	0.45
1:Ap:389:VAL:HG23	1:Ap:458:ILE:HD11	1.99	0.45
1:Aq:401:PRO:HD2	1:Aq:501:GLU:HB3	1.98	0.45
1:A4:405:ASP:HA	1:A4:445:GLU:HG3	1.97	0.45
1:AL:405:ASP:OD2	1:AL:446:ARG:NH2	2.50	0.45
1:AE:345:ARG:HD2	1:AE:345:ARG:HA	1.82	0.45
1:AE:401:PRO:HD2	1:AE:501:GLU:HB3	1.99	0.45
1:AK:347:PRO:HG3	1:AK:489:PHE:CD2	2.52	0.45
1:AW:386:LYS:HG3	1:AW:392:LEU:HA	1.99	0.45
1:Ai:345:ARG:HD2	1:Ai:345:ARG:HA	1.82	0.45
1:Ak:386:LYS:HG3	1:Ak:392:LEU:HA	1.99	0.45
1:Ao:389:VAL:HG13	1:Ao:458:ILE:HD11	1.99	0.45
1:Ay:371:ILE:HG12	1:Ay:494:SER:HA	1.99	0.45
2:FA:5:ILE:HD12	2:FA:76:VAL:HG13	1.99	0.45
2:FC:9:PHE:CD1	2:FC:14:ILE:HD11	2.51	0.45
2:FG:140:THR:OG1	2:FG:162:THR:OG1	2.34	0.45
2:FI:58:PRO:HD3	2:FJ:36:TYR:HB2	1.99	0.45
1:AB:405:ASP:HA	1:AB:445:GLU:HG3	2.00	0.44
1:Aa:278:THR:OG1	1:Ax:333:GLU:OE2	2.29	0.44
1:Ab:481:VAL:HG13	1:Ab:482:GLU:HG3	1.98	0.44
1:An:345:ARG:HD2	1:An:345:ARG:HA	1.83	0.44
2:FG:103:LEU:HD23	2:FG:210:PRO:HB3	1.98	0.44
1:AL:389:VAL:HG23	1:AL:458:ILE:HD11	1.99	0.44
1:AT:319:TYR:OH	1:AT:486:GLU:OE2	2.30	0.44
1:Ab:390:ILE:HG13	1:Ab:421:THR:HG21	1.99	0.44
1:Af:264:ARG:NH2	1:Ag:401:PRO:O	2.50	0.44
1:AU:264:ARG:NH2	1:AV:401:PRO:O	2.51	0.44
1:Ac:389:VAL:HG23	1:Ac:458:ILE:HD11	1.98	0.44
1:Al:355:ASN:HB3	1:Al:452:ALA:HB2	1.99	0.44
1:Aq:254:LEU:HD13	1:Ar:280:THR:HG22	1.99	0.44
1:AF:466:THR:HB	1:AF:493:ILE:HD11	1.99	0.44
1:AL:347:PRO:HG3	1:AL:489:PHE:CD2	2.52	0.44
1:AT:389:VAL:HG23	1:AT:458:ILE:HD11	2.00	0.44
1:AU:389:VAL:HG23	1:AU:458:ILE:HD11	2.00	0.44
1:Ai:264:ARG:NH2	1:Aj:401:PRO:O	2.50	0.44
1:Ap:371:ILE:HG12	1:Ap:494:SER:HA	1.99	0.44
1:As:356:ARG:NH2	1:As:362:ASP:OD2	2.44	0.44
1:AM:407:SER:HG	1:AM:446:ARG:HH11	1.63	0.44
1:Af:342:VAL:HG13	1:Af:346:LEU:HD22	1.99	0.44
1:Ag:401:PRO:HD2	1:Ag:501:GLU:HB3	1.99	0.44
1:AK:347:PRO:HG3	1:AK:489:PHE:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:An:481:VAL:HG13	1:An:482:GLU:HG3	2.00	0.44
2:FC:108:LEU:HD13	2:FC:216:ALA:HB2	1.98	0.44
2:FC:119:GLN:HG2	2:FC:152:ALA:HB2	1.99	0.44
1:AC:479:ILE:HD11	1:AC:486:GLU:HG3	1.98	0.44
1:AT:498:GLU:HB2	1:AT:502:MET:HE1	2.00	0.44
1:AV:392:LEU:HD23	1:AV:458:ILE:HD12	1.99	0.44
1:Ae:355:ASN:HB3	1:Ae:452:ALA:HB2	2.00	0.44
1:A1:438:LEU:HD23	1:A1:438:LEU:HA	1.78	0.44
1:A4:481:VAL:HG13	1:A4:482:GLU:HG3	1.99	0.44
1:A6:355:ASN:HB3	1:A6:452:ALA:HB2	1.99	0.44
1:AA:407:SER:HG	1:AA:446:ARG:HH11	1.61	0.44
1:AI:293:HIS:CE1	2:FD:196:ASN:HB2	2.53	0.44
1:AV:407:SER:OG	1:AV:446:ARG:NH1	2.49	0.44
1:AX:347:PRO:HG3	1:AX:489:PHE:CD2	2.52	0.44
1:Ah:386:LYS:HG3	1:Ah:392:LEU:HA	2.00	0.44
1:An:392:LEU:HD23	1:An:458:ILE:HD12	1.99	0.44
1:Az:314:GLN:NE2	1:Az:365:GLY:O	2.48	0.44
1:Az:389:VAL:HG23	1:Az:458:ILE:HD11	2.00	0.44
1:A0:347:PRO:HG3	1:A0:489:PHE:CD2	2.53	0.44
1:AB:345:ARG:HD2	1:AB:345:ARG:HA	1.85	0.44
1:AV:362:ASP:OD1	1:AV:362:ASP:N	2.51	0.44
1:Ab:258:HIS:O	1:Ac:284:ASP:N	2.48	0.44
1:Ao:498:GLU:HB3	1:Ap:258:HIS:CE1	2.53	0.44
1:Aw:371:ILE:HG12	1:Aw:494:SER:HA	2.00	0.44
1:AM:254:LEU:HD13	1:AN:280:THR:HG22	2.00	0.44
1:AN:347:PRO:HG3	1:AN:489:PHE:CE1	2.52	0.44
1:AP:431:LEU:HD21	1:AQ:433:LEU:HD11	1.99	0.44
1:AT:320:ILE:HA	1:AU:301:GLU:HG3	2.00	0.44
1:Ag:428:GLU:OE2	1:Ah:429:ARG:NH2	2.51	0.44
1:Ar:389:VAL:HG23	1:Ar:458:ILE:HD11	2.00	0.44
1:Az:362:ASP:OD1	1:Az:362:ASP:N	2.50	0.44
1:AA:407:SER:OG	1:AA:446:ARG:NH1	2.44	0.43
1:AC:371:ILE:HG12	1:AC:494:SER:HA	2.00	0.43
1:AE:392:LEU:HD11	1:AE:506:GLY:HA3	2.00	0.43
1:AL:351:ILE:O	1:AL:355:ASN:ND2	2.51	0.43
1:AV:285:LYS:HE2	1:AV:285:LYS:HB3	1.82	0.43
1:AY:313:PRO:HA	1:AY:494:SER:HB3	2.00	0.43
1:Ah:478:ARG:HH11	1:Ak:475:GLU:HG2	1.83	0.43
1:A4:397:SER:OG	1:A4:442:PHE:O	2.27	0.43
2:FH:144:ASP:N	2:FH:144:ASP:OD1	2.51	0.43
2:FI:71:TYR:OH	2:FJ:33:GLU:OE2	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AP:389:VAL:HG23	1:AP:458:ILE:HD11	1.99	0.43
1:Ad:481:VAL:HG13	1:Ad:482:GLU:HG3	1.99	0.43
1:Ae:345:ARG:HD2	1:Ae:345:ARG:HA	1.78	0.43
1:Ag:371:ILE:HG12	1:Ag:494:SER:HA	2.00	0.43
1:Aq:430:PHE:HB3	1:Aq:438:LEU:HD21	2.00	0.43
1:Aq:481:VAL:HG13	1:Aq:482:GLU:HG3	1.99	0.43
2:FK:144:ASP:OD1	2:FK:144:ASP:N	2.49	0.43
1:AN:258:HIS:O	1:AO:284:ASP:N	2.51	0.43
1:AY:423:ASP:HB2	1:Ad:425:ASN:O	2.18	0.43
1:A1:467:ASN:OD1	1:A1:494:SER:OG	2.24	0.43
1:A7:481:VAL:HG13	1:A7:482:GLU:HG3	1.99	0.43
1:AC:407:SER:OG	1:AC:446:ARG:NH1	2.49	0.43
1:AF:389:VAL:HG23	1:AF:458:ILE:HD11	1.99	0.43
1:AI:407:SER:OG	1:AI:446:ARG:NH1	2.47	0.43
1:AM:389:VAL:HG23	1:AM:458:ILE:HD11	2.01	0.43
1:Ad:386:LYS:HG3	1:Ad:392:LEU:HA	1.99	0.43
1:Ax:319:TYR:OH	1:Ax:486:GLU:OE2	2.34	0.43
1:A2:390:ILE:HG13	1:A2:421:THR:HG21	2.00	0.43
1:A6:401:PRO:HD2	1:A6:501:GLU:HB3	2.00	0.43
2:FG:108:LEU:HD13	2:FG:216:ALA:HB2	1.98	0.43
2:FH:71:TYR:HE1	2:FI:33:GLU:HG2	1.82	0.43
2:FK:126:LEU:HD22	2:FK:173:THR:HG23	2.00	0.43
1:AC:486:GLU:HB3	1:AK:480:LEU:HD12	2.01	0.43
1:AD:319:TYR:OH	1:AD:486:GLU:OE2	2.35	0.43
1:AH:389:VAL:HG23	1:AH:458:ILE:HD11	2.01	0.43
1:AQ:345:ARG:NH1	1:AQ:348:GLN:OE1	2.50	0.43
1:AW:386:LYS:HA	1:AW:386:LYS:HD3	1.86	0.43
1:Aa:467:ASN:OD1	1:Aa:494:SER:OG	2.35	0.43
1:Af:259:ASP:OD2	1:Af:345:ARG:NH2	2.50	0.43
1:Ar:319:TYR:OH	1:Ar:486:GLU:OE2	2.35	0.43
1:A3:428:GLU:OE2	1:A4:429:ARG:NH2	2.34	0.43
2:FB:174:ILE:HG13	2:FB:175:PRO:HD2	1.99	0.43
1:AT:312:THR:HA	1:AT:313:PRO:HD3	1.92	0.43
1:AT:347:PRO:HG3	1:AT:489:PHE:CE2	2.53	0.43
1:AY:433:LEU:HD11	1:Ad:431:LEU:HD21	1.99	0.43
1:AZ:323:PRO:HB2	1:AZ:326:VAL:HG23	2.00	0.43
1:AZ:405:ASP:HA	1:AZ:445:GLU:HG3	2.00	0.43
1:Ai:250:PRO:HG2	1:Aj:312:THR:HG21	2.00	0.43
1:A5:390:ILE:HG13	1:A5:421:THR:HG21	2.00	0.43
1:A7:285:LYS:HB3	1:A7:285:LYS:HE2	1.76	0.43
1:AH:319:TYR:OH	1:AH:486:GLU:OE2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AP:285:LYS:HE2	1:AP:285:LYS:HB3	1.86	0.43
1:AG:347:PRO:HG3	1:AG:489:PHE:CD2	2.54	0.43
1:AI:356:ARG:NH2	1:AI:362:ASP:OD2	2.44	0.43
1:AM:347:PRO:HG3	1:AM:489:PHE:CD2	2.54	0.43
1:Am:490:GLU:OE2	1:Au:324:LYS:NZ	2.38	0.43
1:Ax:329:LYS:HD3	1:Ax:335:ALA:HB3	2.00	0.43
1:A6:358:ILE:HG23	1:A6:464:TYR:CZ	2.54	0.43
2:FD:178:SER:O	2:FD:211:THR:OG1	2.22	0.43
2:FK:79:ALA:HB1	2:FK:204:LEU:HD22	2.01	0.43
1:AE:472:MET:HE2	1:AE:472:MET:HB2	1.78	0.43
1:AI:405:ASP:HA	1:AI:445:GLU:HG3	2.01	0.43
1:AL:405:ASP:HA	1:AL:445:GLU:HG3	1.99	0.43
1:Aa:355:ASN:HB3	1:Aa:452:ALA:HB2	2.00	0.43
1:Ab:431:LEU:HD21	1:Ac:433:LEU:HD11	2.00	0.43
1:Ai:356:ARG:NH2	1:Ai:454:ASP:OD1	2.40	0.43
1:Am:389:VAL:HG23	1:Am:458:ILE:HD11	2.00	0.43
1:As:431:LEU:HD21	1:At:433:LEU:HD11	2.01	0.43
2:FA:178:SER:O	2:FA:211:THR:OG1	2.32	0.43
1:AI:345:ARG:HD2	1:AI:345:ARG:HA	1.76	0.43
1:AV:356:ARG:NH2	1:AV:362:ASP:OD2	2.44	0.43
1:AW:332:SER:HB3	1:AW:335:ALA:HB2	2.00	0.43
1:AY:321:LYS:HG2	1:AZ:301:GLU:OE2	2.19	0.43
1:A0:347:PRO:HG3	1:A0:489:PHE:CE2	2.54	0.43
1:A2:438:LEU:HD23	1:A2:438:LEU:HA	1.91	0.43
1:AV:426:GLY:O	1:AW:429:ARG:NH1	2.52	0.42
1:At:285:LYS:HE2	1:At:285:LYS:HB3	1.84	0.42
1:Ax:427:ARG:NH1	1:Ay:423:ASP:OD2	2.46	0.42
1:Ay:243:SER:N	1:A7:321:LYS:O	2.53	0.42
1:AS:302:SER:OG	1:AX:318:LYS:NZ	2.40	0.42
1:Aa:345:ARG:HD2	1:Aa:345:ARG:HA	1.90	0.42
1:AI:345:ARG:HA	1:AI:345:ARG:HD2	1.83	0.42
1:Ar:342:VAL:O	1:Ar:346:LEU:HB2	2.20	0.42
2:FA:36:TYR:HB2	2:FE:58:PRO:HD3	2.00	0.42
2:FB:70:LEU:HD11	2:FC:31:PRO:HA	2.00	0.42
1:AS:373:PRO:O	1:AS:377:ASP:HB2	2.20	0.42
1:AW:467:ASN:OD1	1:AW:494:SER:OG	2.26	0.42
1:Ae:429:ARG:NH2	1:Aj:428:GLU:OE2	2.52	0.42
1:A0:345:ARG:NH1	1:A0:348:GLN:OE1	2.50	0.42
1:AA:405:ASP:HA	1:AA:445:GLU:HG3	2.01	0.42
1:AD:392:LEU:HD11	1:AD:506:GLY:HA3	2.01	0.42
1:AF:438:LEU:HD23	1:AF:438:LEU:HA	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Af:347:PRO:HG3	1:Af:489:PHE:CE2	2.55	0.42
1:Ak:373:PRO:O	1:Ak:377:ASP:HB2	2.20	0.42
1:Al:373:PRO:O	1:Al:377:ASP:HB2	2.20	0.42
1:Ap:472:MET:HE2	1:Ap:472:MET:HB2	1.76	0.42
1:Ar:472:MET:HE2	1:Ar:472:MET:HB2	1.86	0.42
1:A0:323:PRO:HB2	1:A0:326:VAL:HG23	2.02	0.42
1:AC:347:PRO:HG3	1:AC:489:PHE:CE2	2.55	0.42
1:Ai:481:VAL:HG13	1:Ai:482:GLU:HG3	2.01	0.42
1:An:373:PRO:O	1:An:377:ASP:HB2	2.20	0.42
1:An:405:ASP:HA	1:An:445:GLU:HG3	2.01	0.42
1:As:428:GLU:OE2	1:At:429:ARG:NH2	2.52	0.42
1:At:371:ILE:HG12	1:At:494:SER:HA	2.01	0.42
2:FG:64:LYS:HA	2:FG:64:LYS:HD3	1.90	0.42
1:AD:314:GLN:NE2	1:AD:365:GLY:O	2.52	0.42
1:AW:347:PRO:HG3	1:AW:489:PHE:CE2	2.54	0.42
1:Ar:401:PRO:HD2	1:Ar:501:GLU:HB3	2.02	0.42
1:Au:478:ARG:HE	1:Au:478:ARG:HB2	1.68	0.42
2:FF:108:LEU:HD13	2:FF:216:ALA:HB2	2.02	0.42
1:AN:291:GLU:OE1	1:AN:300:ASN:ND2	2.51	0.42
1:AO:317:TYR:CE2	1:AP:299:LYS:HB3	2.54	0.42
1:AP:318:LYS:HE3	1:AP:346:LEU:HD22	2.00	0.42
1:AY:428:GLU:OE2	1:AZ:429:ARG:NH2	2.45	0.42
1:Af:347:PRO:HG3	1:Af:489:PHE:CD2	2.54	0.42
1:Ah:438:LEU:HD23	1:Ah:438:LEU:HA	1.90	0.42
1:A1:389:VAL:HG23	1:A1:458:ILE:HD11	2.00	0.42
1:A3:326:VAL:O	1:A3:332:SER:OG	2.32	0.42
2:FC:126:LEU:HD22	2:FC:173:THR:HG23	2.02	0.42
1:AA:319:TYR:OH	1:AA:486:GLU:OE2	2.31	0.42
1:AA:389:VAL:HG23	1:AA:458:ILE:HD11	2.01	0.42
1:AF:347:PRO:HG3	1:AF:489:PHE:CD2	2.55	0.42
1:AW:472:MET:HE2	1:AW:472:MET:HB2	1.81	0.42
1:Ak:456:GLY:HA2	1:Ak:508:ILE:HD12	2.01	0.42
2:FC:103:LEU:HB3	2:FC:108:LEU:HG	2.02	0.42
1:AB:272:ARG:NH2	1:AB:498:GLU:OE2	2.41	0.42
1:AF:472:MET:HE2	1:AF:472:MET:HB2	1.79	0.42
1:AG:323:PRO:HB2	1:AG:326:VAL:HG23	2.01	0.42
1:AH:373:PRO:O	1:AH:377:ASP:HB2	2.20	0.42
1:AH:390:ILE:HG21	1:AH:429:ARG:NH2	2.34	0.42
1:AO:254:LEU:HD13	1:AP:280:THR:HG22	2.02	0.42
1:AO:474:PHE:HZ	1:AO:487:TYR:HD2	1.66	0.42
1:AP:264:ARG:NH2	1:AQ:401:PRO:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aa:345:ARG:NH1	1:Aa:348:GLN:OE1	2.51	0.42
1:Aa:392:LEU:HD11	1:Aa:506:GLY:HA3	2.01	0.42
1:Ag:345:ARG:HD2	1:Ag:345:ARG:HA	1.85	0.42
1:Au:356:ARG:NH2	1:Au:362:ASP:OD2	2.36	0.42
1:Aw:301:GLU:HG2	1:A1:320:ILE:HA	2.00	0.42
1:A0:255:LYS:HB3	1:A0:255:LYS:HE2	1.75	0.42
1:A0:386:LYS:HA	1:A0:386:LYS:HD3	1.86	0.42
2:FA:31:PRO:HA	2:FE:70:LEU:HD11	2.02	0.42
2:FA:70:LEU:HD11	2:FB:31:PRO:HA	2.01	0.42
2:FF:144:ASP:OD1	2:FF:144:ASP:N	2.51	0.42
2:FH:64:LYS:HE3	2:FI:43:PHE:CE2	2.54	0.42
1:Ab:472:MET:HE2	1:Ab:472:MET:HB2	1.96	0.42
1:A4:485:LYS:HE2	1:A4:485:LYS:HB3	1.85	0.42
2:FB:58:PRO:HD3	2:FC:36:TYR:HB2	2.01	0.42
2:FE:46:LEU:HD11	2:FE:209:MET:HB3	2.02	0.42
1:AC:355:ASN:HB3	1:AC:452:ALA:HB2	2.02	0.41
1:AB:258:HIS:O	1:AC:284:ASP:N	2.52	0.41
1:AD:389:VAL:HG23	1:AD:458:ILE:HD11	2.02	0.41
1:AE:428:GLU:OE2	1:AF:429:ARG:NH2	2.43	0.41
1:AJ:401:PRO:O	1:AK:264:ARG:NH2	2.53	0.41
1:AO:456:GLY:HA2	1:AO:508:ILE:HD12	2.02	0.41
1:AP:355:ASN:HB3	1:AP:452:ALA:HB2	2.02	0.41
1:An:389:VAL:HG23	1:An:458:ILE:HD11	2.02	0.41
1:An:407:SER:OG	1:An:446:ARG:NH1	2.47	0.41
1:Ar:386:LYS:HG3	1:Ar:392:LEU:HA	2.01	0.41
1:Au:426:GLY:O	1:Av:429:ARG:NH1	2.53	0.41
1:A0:405:ASP:HA	1:A0:445:GLU:HG3	2.03	0.41
1:A5:481:VAL:HG13	1:A5:482:GLU:HG3	2.02	0.41
1:AI:272:ARG:NH2	1:AI:498:GLU:OE2	2.46	0.41
1:AS:293:HIS:CE1	2:FB:196:ASN:HB2	2.55	0.41
1:AY:467:ASN:OD1	1:AY:494:SER:OG	2.35	0.41
1:As:392:LEU:HD11	1:As:506:GLY:HA3	2.03	0.41
1:Ay:319:TYR:OH	1:Ay:486:GLU:OE2	2.35	0.41
1:A3:356:ARG:NH2	1:A3:362:ASP:OD2	2.27	0.41
2:FB:108:LEU:HD13	2:FB:216:ALA:HB2	2.02	0.41
1:AG:347:PRO:HG3	1:AG:489:PHE:CE2	2.55	0.41
1:AG:355:ASN:HB3	1:AG:452:ALA:HB2	2.00	0.41
1:AR:264:ARG:HE	1:AR:264:ARG:HB2	1.67	0.41
1:AX:319:TYR:OH	1:AX:486:GLU:OE2	2.33	0.41
1:AX:371:ILE:HD11	1:AX:493:ILE:HG23	2.03	0.41
1:Ac:355:ASN:HB3	1:Ac:452:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ar:355:ASN:HB3	1:Ar:452:ALA:HB2	2.03	0.41
1:Au:345:ARG:HA	1:Au:345:ARG:HD2	1.89	0.41
1:Av:347:PRO:HG3	1:Av:489:PHE:CD1	2.55	0.41
1:Ax:389:VAL:HG23	1:Ax:458:ILE:HD11	2.02	0.41
1:A3:430:PHE:HB3	1:A3:438:LEU:HD21	2.02	0.41
1:A3:485:LYS:HE2	1:A3:485:LYS:HB3	1.95	0.41
1:A5:250:PRO:HG3	1:A6:312:THR:HG21	2.01	0.41
2:FF:136:LEU:HA	2:FF:173:THR:HG22	2.02	0.41
2:FI:64:LYS:HE3	2:FJ:43:PHE:CE2	2.56	0.41
1:AH:347:PRO:HG3	1:AH:489:PHE:CD2	2.55	0.41
1:AH:386:LYS:HG3	1:AH:392:LEU:HA	2.02	0.41
1:AV:264:ARG:NH2	1:AW:401:PRO:O	2.53	0.41
1:Ad:259:ASP:OD2	1:Ad:345:ARG:NH2	2.51	0.41
1:Ae:420:PHE:O	1:Ae:422:LYS:NZ	2.52	0.41
1:Ai:405:ASP:HA	1:Ai:445:GLU:HG3	2.02	0.41
1:An:386:LYS:HG3	1:An:392:LEU:HA	2.01	0.41
1:Ao:392:LEU:HD11	1:Ao:506:GLY:HA3	2.02	0.41
1:Ap:324:LYS:HE3	1:Ap:324:LYS:HB3	1.86	0.41
1:Ap:480:LEU:HD13	2:FG:190:GLU:HB3	2.02	0.41
1:As:323:PRO:HB2	1:As:326:VAL:HG23	2.03	0.41
2:FC:64:LYS:HA	2:FC:64:LYS:HD3	1.93	0.41
1:AH:345:ARG:HA	1:AH:345:ARG:HD2	1.84	0.41
1:AH:392:LEU:HD11	1:AH:506:GLY:HA3	2.03	0.41
1:AJ:498:GLU:HB2	1:AJ:502:MET:HE1	2.00	0.41
1:AT:322:LEU:HD11	1:AT:342:VAL:HG21	2.02	0.41
1:AT:405:ASP:HA	1:AT:445:GLU:HG3	2.02	0.41
1:AV:438:LEU:HD23	1:AV:438:LEU:HA	1.87	0.41
1:Aa:285:LYS:HB3	1:Aa:285:LYS:HE2	1.81	0.41
1:Aa:438:LEU:HD23	1:Aa:438:LEU:HA	1.91	0.41
1:Ah:371:ILE:HG12	1:Ah:494:SER:HA	2.03	0.41
1:Ap:355:ASN:HB3	1:Ap:452:ALA:HB2	2.02	0.41
1:Aq:373:PRO:O	1:Aq:377:ASP:HB2	2.21	0.41
1:Aq:392:LEU:HD11	1:Aq:506:GLY:HA3	2.02	0.41
1:As:401:PRO:HD2	1:As:501:GLU:HB3	2.02	0.41
1:Ax:371:ILE:HG12	1:Ax:494:SER:HA	2.02	0.41
2:FC:39:GLU:HG2	2:FC:40:THR:HG23	2.03	0.41
1:AF:392:LEU:HD11	1:AF:506:GLY:HA3	2.02	0.41
1:AJ:268:LEU:HG	1:AJ:355:ASN:HD21	1.84	0.41
1:AR:389:VAL:HG23	1:AR:458:ILE:HD11	2.03	0.41
1:AV:361:GLY:O	1:AV:368:LYS:HE2	2.20	0.41
1:AZ:319:TYR:OH	1:AZ:486:GLU:OE2	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:FG:86:ALA:HA	2:FG:90:GLY:HA2	2.02	0.41
1:AB:347:PRO:HG3	1:AB:489:PHE:CD2	2.56	0.41
1:AC:389:VAL:HG23	1:AC:458:ILE:HD11	2.02	0.41
1:AO:258:HIS:O	1:AP:284:ASP:N	2.53	0.41
1:AP:313:PRO:HA	1:AP:494:SER:HB3	2.02	0.41
1:AQ:345:ARG:HA	1:AQ:345:ARG:HD2	1.88	0.41
1:AR:318:LYS:HD2	1:AR:318:LYS:HA	1.93	0.41
1:AU:392:LEU:HD23	1:AU:458:ILE:HD12	2.03	0.41
1:AV:342:VAL:HG13	1:AV:346:LEU:HD12	2.02	0.41
1:AZ:254:LEU:HD13	1:Aa:280:THR:HG22	2.03	0.41
1:Ai:371:ILE:HG12	1:Ai:494:SER:HA	2.03	0.41
1:Ar:324:LYS:NZ	1:A7:490:GLU:OE2	2.48	0.41
1:A1:419:ARG:HE	1:A1:419:ARG:HB3	1.68	0.41
2:FI:142:THR:HG21	2:FI:170:TYR:CD1	2.56	0.41
1:AD:313:PRO:HA	1:AD:494:SER:HB3	2.02	0.41
1:AE:293:HIS:CE1	2:FE:196:ASN:HB2	2.56	0.41
1:AI:371:ILE:HG12	1:AI:494:SER:HA	2.02	0.41
1:AV:276:LEU:HD12	1:AV:279:LEU:HD13	2.01	0.41
1:AV:389:VAL:HG23	1:AV:458:ILE:HD11	2.03	0.41
1:AV:430:PHE:HB3	1:AV:438:LEU:HD21	2.02	0.41
1:AW:345:ARG:HA	1:AW:345:ARG:HD2	1.85	0.41
1:Ad:392:LEU:HD11	1:Ad:506:GLY:HA3	2.03	0.41
1:Ai:430:PHE:HB3	1:Ai:438:LEU:HD21	2.02	0.41
1:Aj:321:LYS:HB2	1:Aj:321:LYS:HE3	1.89	0.41
1:Aj:345:ARG:HD2	1:Aj:345:ARG:HA	1.86	0.41
1:Al:347:PRO:HG3	1:Al:489:PHE:CD2	2.56	0.41
1:Aq:427:ARG:HG2	1:Av:427:ARG:NH2	2.36	0.41
1:At:405:ASP:HA	1:At:445:GLU:HG3	2.03	0.41
1:At:472:MET:HE2	1:At:472:MET:HB2	1.91	0.41
1:Ax:406:SER:HA	1:Ax:462:ASP:HB2	2.03	0.41
2:FK:108:LEU:HD13	2:FK:216:ALA:HB2	2.03	0.41
1:AN:318:LYS:HD2	1:AN:318:LYS:HA	1.94	0.41
1:AO:345:ARG:HA	1:AO:345:ARG:HD2	1.83	0.41
1:AR:388:THR:HG23	1:AR:391:ASP:H	1.86	0.41
1:AU:477:GLY:O	1:AU:486:GLU:N	2.45	0.41
1:AY:345:ARG:HD2	1:AY:345:ARG:HA	1.88	0.41
1:Af:390:ILE:HG13	1:Af:421:THR:HG21	2.03	0.41
1:Ag:345:ARG:NH1	1:Ag:348:GLN:OE1	2.51	0.41
1:At:318:LYS:HD2	1:At:318:LYS:HA	1.88	0.41
1:Av:318:LYS:HD2	1:Av:318:LYS:HA	1.77	0.41
1:Ax:254:LEU:HD13	1:Ay:280:THR:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AH:467:ASN:OD1	1:AH:494:SER:OG	2.31	0.40
1:AN:253:ILE:HG23	1:AN:333:GLU:HB3	2.04	0.40
1:AR:347:PRO:HG3	1:AR:489:PHE:CD2	2.55	0.40
1:Ac:345:ARG:NH1	1:Ac:348:GLN:OE1	2.53	0.40
1:Ae:392:LEU:HD11	1:Ae:506:GLY:HA3	2.03	0.40
1:Ap:430:PHE:HB3	1:Ap:438:LEU:HD21	2.02	0.40
1:Ar:345:ARG:HA	1:Ar:345:ARG:HD2	1.92	0.40
1:A7:345:ARG:HA	1:A7:345:ARG:HD2	1.85	0.40
2:FA:136:LEU:HA	2:FA:173:THR:HG22	2.03	0.40
1:AH:392:LEU:HD23	1:AH:458:ILE:HD12	2.03	0.40
1:AK:356:ARG:NH2	1:AK:362:ASP:OD2	2.50	0.40
1:AP:318:LYS:HD3	1:AQ:290:GLY:HA2	2.04	0.40
1:Aa:370:GLN:O	1:Aa:494:SER:HB2	2.21	0.40
1:Ag:347:PRO:HG3	1:Ag:489:PHE:CD2	2.57	0.40
1:Ao:347:PRO:HG3	1:Ao:489:PHE:CD2	2.56	0.40
1:Ao:405:ASP:HA	1:Ao:445:GLU:HG3	2.03	0.40
1:As:389:VAL:HG13	1:As:458:ILE:HD11	2.04	0.40
2:FD:37:ASP:HB3	2:FD:40:THR:HG22	2.03	0.40
2:FH:71:TYR:CE1	2:FI:33:GLU:HG2	2.56	0.40
1:AI:347:PRO:HG3	1:AI:489:PHE:CD2	2.56	0.40
1:AS:345:ARG:HA	1:AS:345:ARG:HD2	1.88	0.40
1:At:389:VAL:HG23	1:At:458:ILE:HD11	2.02	0.40
1:AG:472:MET:HE2	1:AG:472:MET:HB2	1.85	0.40
1:AH:472:MET:HE2	1:AH:472:MET:HB2	1.96	0.40
1:AQ:258:HIS:O	1:AR:284:ASP:N	2.53	0.40
1:AT:373:PRO:O	1:AT:377:ASP:HB2	2.21	0.40
1:AU:312:THR:HA	1:AU:313:PRO:HD3	1.95	0.40
1:AV:358:ILE:HG23	1:AV:464:TYR:CZ	2.56	0.40
1:Af:389:VAL:HG23	1:Af:458:ILE:HD11	2.03	0.40
1:Ai:409:VAL:HB	1:Ai:459:VAL:HB	2.03	0.40
1:A1:361:GLY:O	1:A1:368:LYS:HE2	2.21	0.40
1:A3:401:PRO:HD2	1:A3:501:GLU:HB3	2.04	0.40
1:A5:258:HIS:O	1:A6:284:ASP:N	2.53	0.40
1:AD:409:VAL:HB	1:AD:459:VAL:HB	2.04	0.40
1:AJ:389:VAL:HG23	1:AJ:458:ILE:HD11	2.03	0.40
1:AO:417:ALA:O	1:AO:421:THR:OG1	2.36	0.40
1:AR:356:ARG:NH2	1:AR:362:ASP:OD2	2.40	0.40
1:AX:389:VAL:HG23	1:AX:458:ILE:HD11	2.03	0.40
1:AX:405:ASP:HA	1:AX:445:GLU:HG3	2.03	0.40
1:Ah:389:VAL:HG23	1:Ah:458:ILE:HD11	2.04	0.40
1:Al:472:MET:HE2	1:Al:472:MET:HB2	1.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ao:345:ARG:HA	1:Ao:345:ARG:HD2	1.89	0.40
1:Ar:405:ASP:HA	1:Ar:445:GLU:HG3	2.03	0.40
1:Ax:392:LEU:HD11	1:Ax:506:GLY:HA3	2.04	0.40
1:A4:345:ARG:HD2	1:A4:345:ARG:HA	1.93	0.40
1:A6:392:LEU:HD11	1:A6:506:GLY:HA3	2.04	0.40
2:FH:103:LEU:HB3	2:FH:108:LEU:HG	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A0	265/516 (51%)	259 (98%)	6 (2%)	0	100	100
1	A1	265/516 (51%)	262 (99%)	3 (1%)	0	100	100
1	A2	265/516 (51%)	263 (99%)	2 (1%)	0	100	100
1	A3	265/516 (51%)	262 (99%)	3 (1%)	0	100	100
1	A4	265/516 (51%)	261 (98%)	4 (2%)	0	100	100
1	A5	265/516 (51%)	261 (98%)	4 (2%)	0	100	100
1	A6	265/516 (51%)	258 (97%)	7 (3%)	0	100	100
1	A7	265/516 (51%)	261 (98%)	4 (2%)	0	100	100
1	AA	265/516 (51%)	263 (99%)	2 (1%)	0	100	100
1	AB	265/516 (51%)	261 (98%)	4 (2%)	0	100	100
1	AC	265/516 (51%)	261 (98%)	4 (2%)	0	100	100
1	AD	265/516 (51%)	262 (99%)	3 (1%)	0	100	100
1	AE	265/516 (51%)	262 (99%)	3 (1%)	0	100	100
1	AF	265/516 (51%)	263 (99%)	2 (1%)	0	100	100
1	AG	265/516 (51%)	261 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AH	265/516 (51%)	262 (99%)	3 (1%)	0	100	100
1	AI	265/516 (51%)	262 (99%)	3 (1%)	0	100	100
1	AJ	265/516 (51%)	261 (98%)	4 (2%)	0	100	100
1	AK	265/516 (51%)	260 (98%)	5 (2%)	0	100	100
1	AL	265/516 (51%)	260 (98%)	5 (2%)	0	100	100
1	AM	265/516 (51%)	260 (98%)	5 (2%)	0	100	100
1	AN	265/516 (51%)	261 (98%)	4 (2%)	0	100	100
1	AO	265/516 (51%)	258 (97%)	7 (3%)	0	100	100
1	AP	265/516 (51%)	259 (98%)	6 (2%)	0	100	100
1	AQ	265/516 (51%)	262 (99%)	3 (1%)	0	100	100
1	AR	265/516 (51%)	260 (98%)	5 (2%)	0	100	100
1	AS	265/516 (51%)	261 (98%)	4 (2%)	0	100	100
1	AT	265/516 (51%)	260 (98%)	5 (2%)	0	100	100
1	AU	265/516 (51%)	260 (98%)	5 (2%)	0	100	100
1	AV	265/516 (51%)	261 (98%)	4 (2%)	0	100	100
1	AW	265/516 (51%)	261 (98%)	4 (2%)	0	100	100
1	AX	265/516 (51%)	261 (98%)	4 (2%)	0	100	100
1	AY	265/516 (51%)	262 (99%)	3 (1%)	0	100	100
1	AZ	265/516 (51%)	261 (98%)	4 (2%)	0	100	100
1	Aa	265/516 (51%)	262 (99%)	3 (1%)	0	100	100
1	Ab	265/516 (51%)	259 (98%)	6 (2%)	0	100	100
1	Ac	265/516 (51%)	259 (98%)	6 (2%)	0	100	100
1	Ad	265/516 (51%)	261 (98%)	4 (2%)	0	100	100
1	Ae	265/516 (51%)	262 (99%)	3 (1%)	0	100	100
1	Af	265/516 (51%)	262 (99%)	3 (1%)	0	100	100
1	Ag	265/516 (51%)	259 (98%)	6 (2%)	0	100	100
1	Ah	265/516 (51%)	262 (99%)	3 (1%)	0	100	100
1	Ai	265/516 (51%)	262 (99%)	3 (1%)	0	100	100
1	Aj	265/516 (51%)	259 (98%)	6 (2%)	0	100	100
1	Ak	265/516 (51%)	262 (99%)	3 (1%)	0	100	100
1	Al	265/516 (51%)	262 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Am	265/516 (51%)	260 (98%)	5 (2%)	0	100	100
1	An	265/516 (51%)	261 (98%)	4 (2%)	0	100	100
1	Ao	265/516 (51%)	262 (99%)	3 (1%)	0	100	100
1	Ap	265/516 (51%)	261 (98%)	4 (2%)	0	100	100
1	Aq	265/516 (51%)	260 (98%)	5 (2%)	0	100	100
1	Ar	265/516 (51%)	260 (98%)	5 (2%)	0	100	100
1	As	265/516 (51%)	260 (98%)	5 (2%)	0	100	100
1	At	265/516 (51%)	261 (98%)	4 (2%)	0	100	100
1	Au	265/516 (51%)	262 (99%)	3 (1%)	0	100	100
1	Av	265/516 (51%)	260 (98%)	5 (2%)	0	100	100
1	Aw	265/516 (51%)	261 (98%)	4 (2%)	0	100	100
1	Ax	265/516 (51%)	261 (98%)	4 (2%)	0	100	100
1	Ay	265/516 (51%)	261 (98%)	4 (2%)	0	100	100
1	Az	265/516 (51%)	261 (98%)	4 (2%)	0	100	100
2	FA	216/220 (98%)	214 (99%)	2 (1%)	0	100	100
2	FB	216/220 (98%)	212 (98%)	4 (2%)	0	100	100
2	FC	216/220 (98%)	215 (100%)	1 (0%)	0	100	100
2	FD	216/220 (98%)	216 (100%)	0	0	100	100
2	FE	216/220 (98%)	213 (99%)	3 (1%)	0	100	100
2	FF	216/220 (98%)	214 (99%)	2 (1%)	0	100	100
2	FG	216/220 (98%)	213 (99%)	3 (1%)	0	100	100
2	FH	216/220 (98%)	215 (100%)	1 (0%)	0	100	100
2	FI	216/220 (98%)	214 (99%)	2 (1%)	0	100	100
2	FJ	216/220 (98%)	213 (99%)	3 (1%)	0	100	100
2	FK	216/220 (98%)	215 (100%)	1 (0%)	0	100	100
All	All	18276/33380 (55%)	18008 (98%)	268 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A0	226/438 (52%)	226 (100%)	0	100	100
1	A1	226/438 (52%)	226 (100%)	0	100	100
1	A2	226/438 (52%)	226 (100%)	0	100	100
1	A3	226/438 (52%)	225 (100%)	1 (0%)	84	91
1	A4	226/438 (52%)	226 (100%)	0	100	100
1	A5	226/438 (52%)	226 (100%)	0	100	100
1	A6	226/438 (52%)	224 (99%)	2 (1%)	70	82
1	A7	226/438 (52%)	226 (100%)	0	100	100
1	AA	226/438 (52%)	226 (100%)	0	100	100
1	AB	226/438 (52%)	226 (100%)	0	100	100
1	AC	226/438 (52%)	226 (100%)	0	100	100
1	AD	226/438 (52%)	226 (100%)	0	100	100
1	AE	226/438 (52%)	225 (100%)	1 (0%)	84	91
1	AF	226/438 (52%)	226 (100%)	0	100	100
1	AG	226/438 (52%)	226 (100%)	0	100	100
1	AH	226/438 (52%)	225 (100%)	1 (0%)	84	91
1	AI	226/438 (52%)	226 (100%)	0	100	100
1	AJ	226/438 (52%)	226 (100%)	0	100	100
1	AK	226/438 (52%)	226 (100%)	0	100	100
1	AL	226/438 (52%)	226 (100%)	0	100	100
1	AM	226/438 (52%)	226 (100%)	0	100	100
1	AN	226/438 (52%)	226 (100%)	0	100	100
1	AO	226/438 (52%)	225 (100%)	1 (0%)	84	91
1	AP	226/438 (52%)	226 (100%)	0	100	100
1	AQ	226/438 (52%)	226 (100%)	0	100	100
1	AR	226/438 (52%)	226 (100%)	0	100	100
1	AS	226/438 (52%)	226 (100%)	0	100	100
1	AT	226/438 (52%)	226 (100%)	0	100	100
1	AU	226/438 (52%)	225 (100%)	1 (0%)	84	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AV	226/438 (52%)	226 (100%)	0	100	100
1	AW	226/438 (52%)	226 (100%)	0	100	100
1	AX	226/438 (52%)	226 (100%)	0	100	100
1	AY	226/438 (52%)	226 (100%)	0	100	100
1	AZ	226/438 (52%)	226 (100%)	0	100	100
1	Aa	226/438 (52%)	226 (100%)	0	100	100
1	Ab	226/438 (52%)	226 (100%)	0	100	100
1	Ac	226/438 (52%)	226 (100%)	0	100	100
1	Ad	226/438 (52%)	226 (100%)	0	100	100
1	Ae	226/438 (52%)	226 (100%)	0	100	100
1	Af	226/438 (52%)	226 (100%)	0	100	100
1	Ag	226/438 (52%)	226 (100%)	0	100	100
1	Ah	226/438 (52%)	225 (100%)	1 (0%)	84	91
1	Ai	226/438 (52%)	226 (100%)	0	100	100
1	Aj	226/438 (52%)	225 (100%)	1 (0%)	84	91
1	Ak	226/438 (52%)	226 (100%)	0	100	100
1	Al	226/438 (52%)	226 (100%)	0	100	100
1	Am	226/438 (52%)	226 (100%)	0	100	100
1	An	226/438 (52%)	226 (100%)	0	100	100
1	Ao	226/438 (52%)	226 (100%)	0	100	100
1	Ap	226/438 (52%)	226 (100%)	0	100	100
1	Aq	226/438 (52%)	226 (100%)	0	100	100
1	Ar	226/438 (52%)	226 (100%)	0	100	100
1	As	226/438 (52%)	226 (100%)	0	100	100
1	At	226/438 (52%)	226 (100%)	0	100	100
1	Au	226/438 (52%)	226 (100%)	0	100	100
1	Av	226/438 (52%)	226 (100%)	0	100	100
1	Aw	226/438 (52%)	226 (100%)	0	100	100
1	Ax	226/438 (52%)	226 (100%)	0	100	100
1	Ay	226/438 (52%)	226 (100%)	0	100	100
1	Az	226/438 (52%)	226 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	FA	187/189 (99%)	187 (100%)	0	100	100
2	FB	187/189 (99%)	187 (100%)	0	100	100
2	FC	187/189 (99%)	187 (100%)	0	100	100
2	FD	187/189 (99%)	187 (100%)	0	100	100
2	FE	187/189 (99%)	187 (100%)	0	100	100
2	FF	187/189 (99%)	187 (100%)	0	100	100
2	FG	187/189 (99%)	187 (100%)	0	100	100
2	FH	187/189 (99%)	187 (100%)	0	100	100
2	FI	187/189 (99%)	186 (100%)	1 (0%)	81	89
2	FJ	187/189 (99%)	187 (100%)	0	100	100
2	FK	187/189 (99%)	187 (100%)	0	100	100
All	All	15617/28359 (55%)	15607 (100%)	10 (0%)	87	95

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AE	251	THR
1	AH	346	LEU
1	AO	315	TYR
1	AU	315	TYR
1	Ah	294	THR
1	Aj	315	TYR
1	A3	320	ILE
1	A6	312	THR
1	A6	315	TYR
2	FI	136	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (106) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	265	ASN
1	AB	265	ASN
1	AB	293	HIS
1	AC	293	HIS
1	AC	355	ASN
1	AC	441	HIS
1	AE	258	HIS

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Mol	Chain	Res	Type
1	AE	262	ASN
1	AE	370	GLN
1	AE	484	ASN
1	AF	293	HIS
1	AF	441	HIS
1	AI	265	ASN
1	AI	441	HIS
1	AJ	265	ASN
1	AK	265	ASN
1	AK	275	ASN
1	AL	258	HIS
1	AM	262	ASN
1	AM	265	ASN
1	AP	265	ASN
1	AP	370	GLN
1	AQ	265	ASN
1	AQ	275	ASN
1	AR	293	HIS
1	AS	441	HIS
1	AT	275	ASN
1	AT	441	HIS
1	AU	265	ASN
1	AU	275	ASN
1	AU	441	HIS
1	AV	265	ASN
1	AW	293	HIS
1	AW	300	ASN
1	AX	275	ASN
1	AX	441	HIS
1	AY	265	ASN
1	AY	275	ASN
1	AZ	355	ASN
1	Aa	275	ASN
1	Aa	305	GLN
1	Ab	275	ASN
1	Ac	275	ASN
1	Ac	425	ASN
1	Af	258	HIS
1	Af	265	ASN
1	Af	275	ASN
1	Af	441	HIS
1	Ag	258	HIS

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Mol	Chain	Res	Type
1	Ag	293	HIS
1	Ag	355	ASN
1	Ai	258	HIS
1	Aj	293	HIS
1	Aj	441	HIS
1	Ak	355	ASN
1	Al	265	ASN
1	Al	275	ASN
1	Al	293	HIS
1	Am	265	ASN
1	Am	441	HIS
1	An	265	ASN
1	An	275	ASN
1	Ao	293	HIS
1	Ao	441	HIS
1	Ap	258	HIS
1	Aq	262	ASN
1	Aq	265	ASN
1	Aq	441	HIS
1	As	275	ASN
1	At	265	ASN
1	At	293	HIS
1	Au	275	ASN
1	Au	441	HIS
1	Aw	258	HIS
1	Aw	425	ASN
1	Aw	441	HIS
1	Ax	293	HIS
1	Ax	441	HIS
1	Ay	258	HIS
1	Ay	275	ASN
1	Ay	441	HIS
1	Ay	484	ASN
1	Az	293	HIS
1	A1	275	ASN
1	A2	265	ASN
1	A2	275	ASN
1	A2	293	HIS
1	A2	484	ASN
1	A3	293	HIS
1	A3	370	GLN
1	A4	275	ASN

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Mol	Chain	Res	Type
1	A5	441	HIS
1	A6	258	HIS
1	A6	262	ASN
1	A6	355	ASN
1	A7	265	ASN
1	A7	441	HIS
2	FA	32	ASN
2	FE	50	GLN
2	FF	32	ASN
2	FF	195	ASN
2	FH	184	ASN
2	FH	195	ASN
2	FI	50	GLN
2	FI	73	ASN
2	FK	16	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

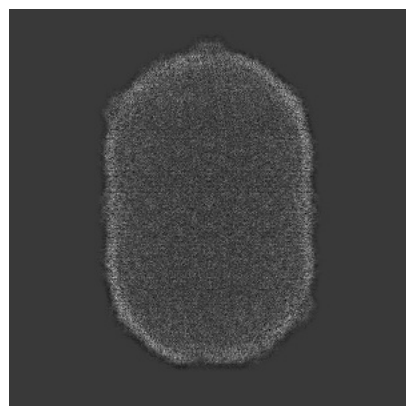
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55362. These allow visual inspection of the internal detail of the map and identification of artifacts.

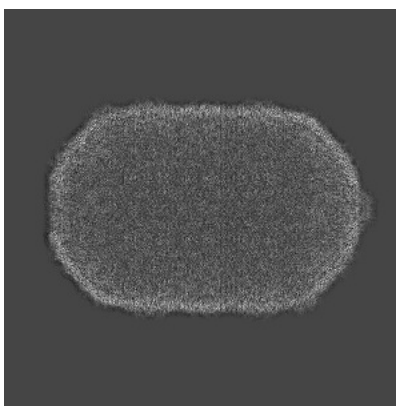
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

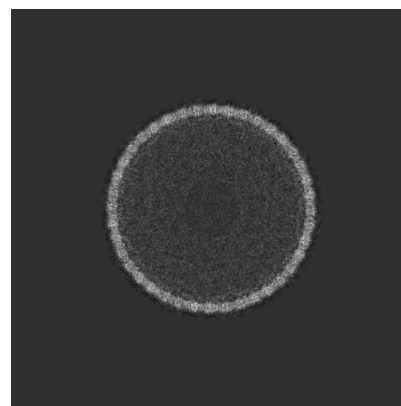
6.1.1 Primary map



X

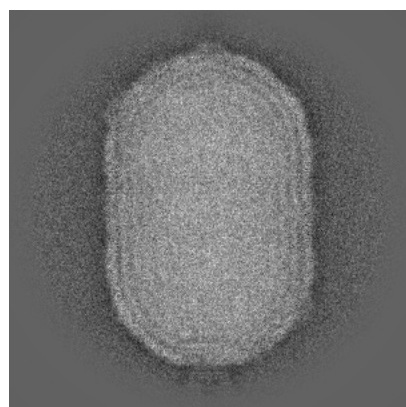


Y

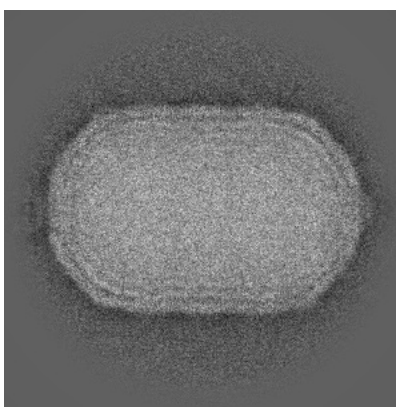


Z

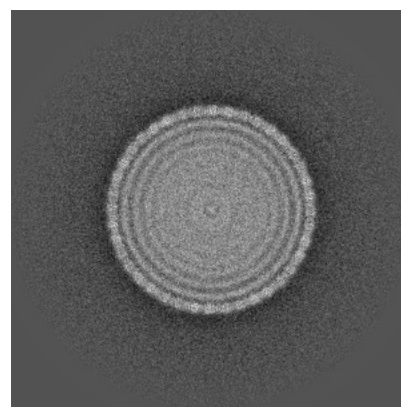
6.1.2 Raw map



X



Y

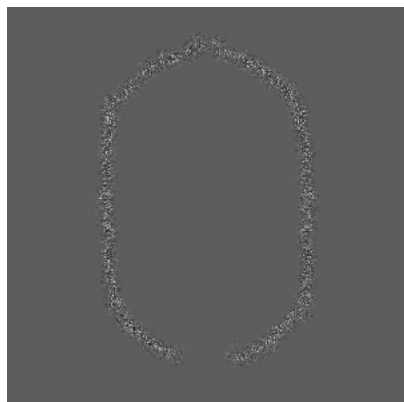


Z

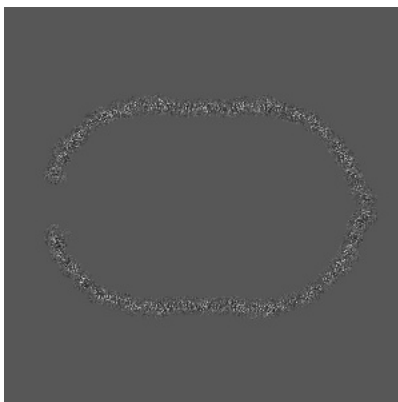
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 512

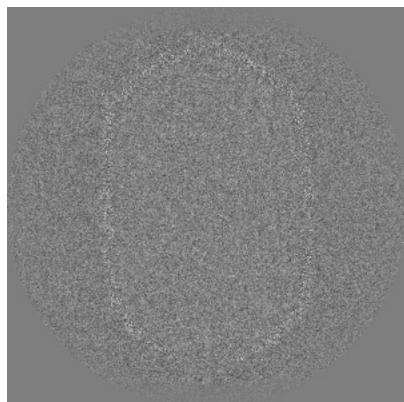


Y Index: 512

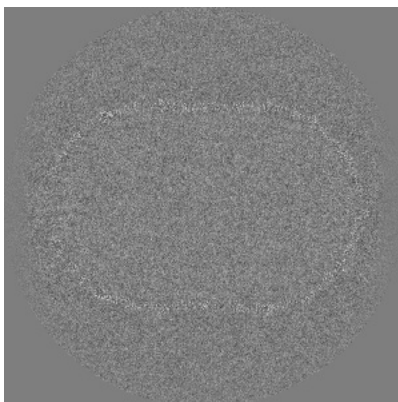


Z Index: 512

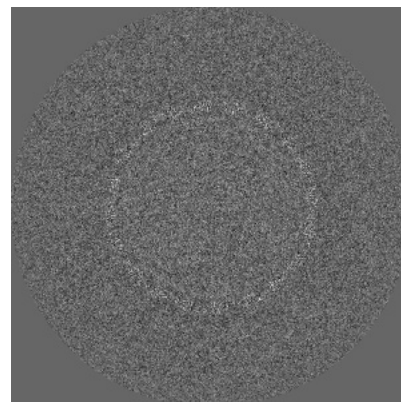
6.2.2 Raw map



X Index: 512



Y Index: 512

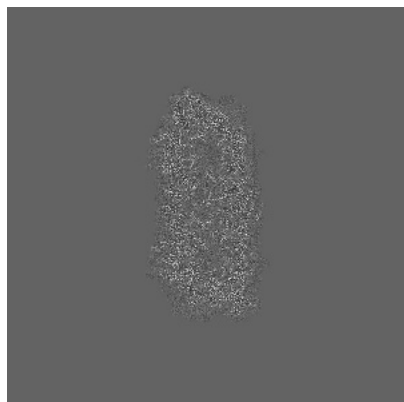


Z Index: 512

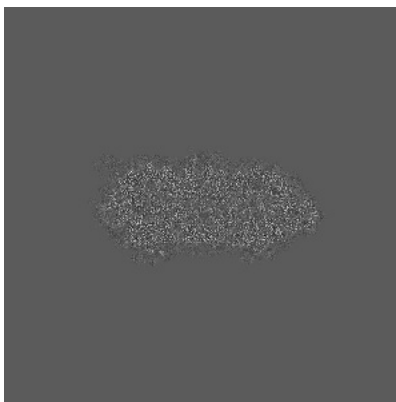
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

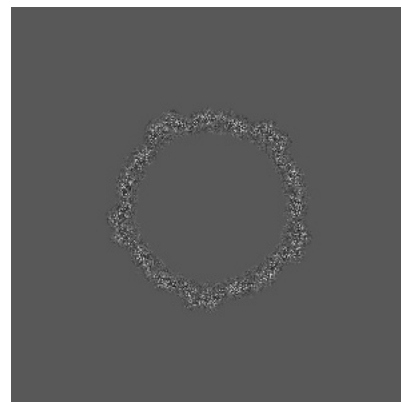
6.3.1 Primary map



X Index: 270

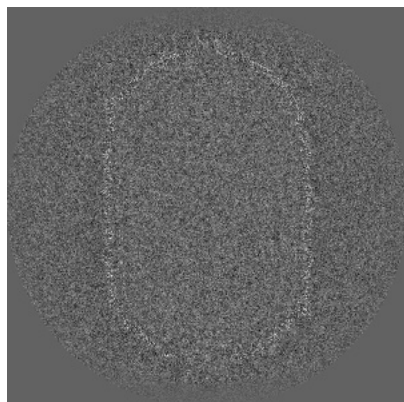


Y Index: 265

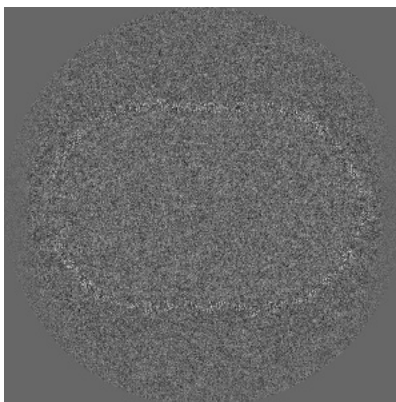


Z Index: 786

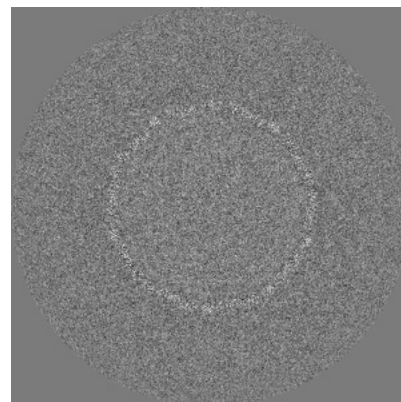
6.3.2 Raw map



X Index: 510



Y Index: 505

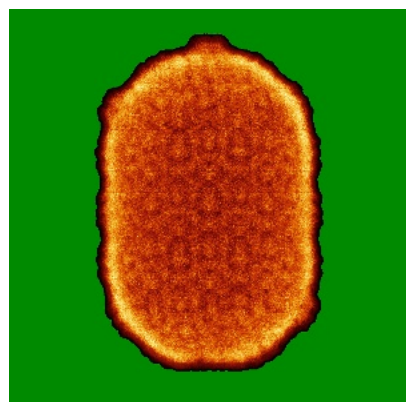


Z Index: 474

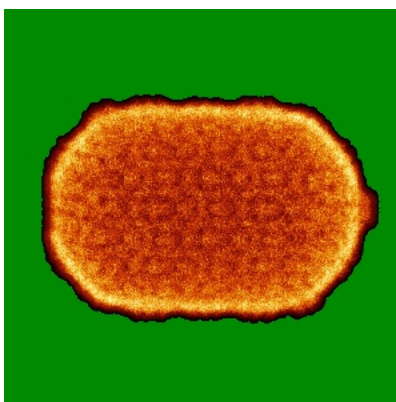
The images above show the largest variance slices of the map in three orthogonal directions.

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

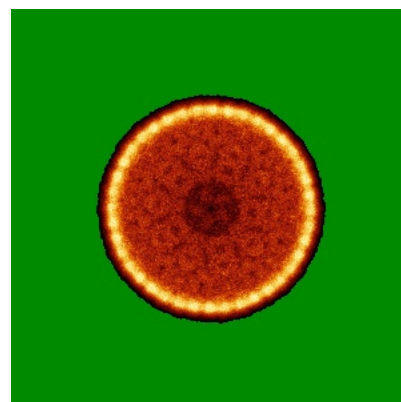
6.4.1 Primary map



X

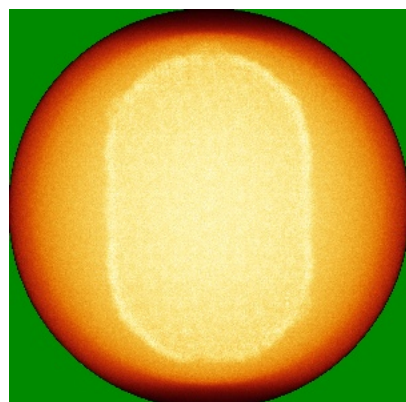


Y

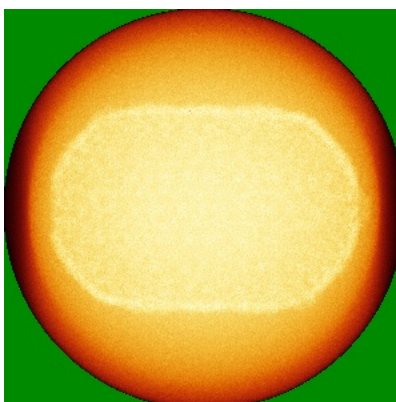


Z

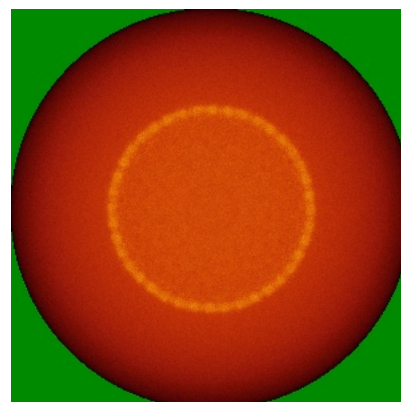
6.4.2 Raw map



X



Y

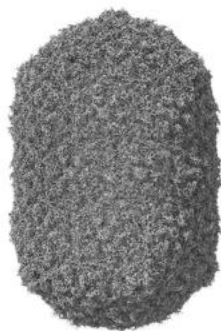


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



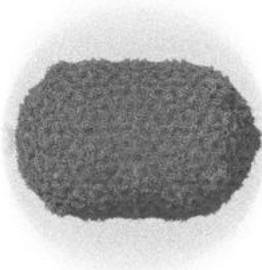
Z

The images above show the 3D surface view of the map at the recommended contour level 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

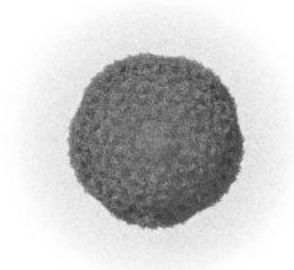
6.5.2 Raw map



X



Y



Z

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.

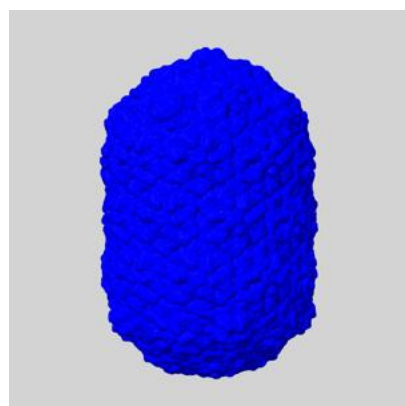
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

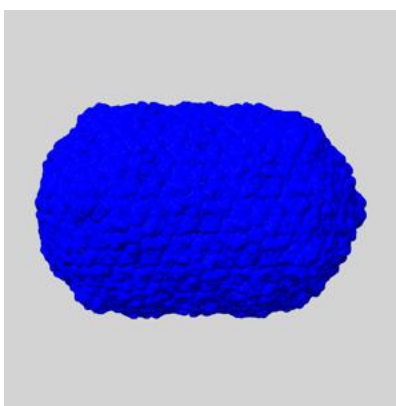
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

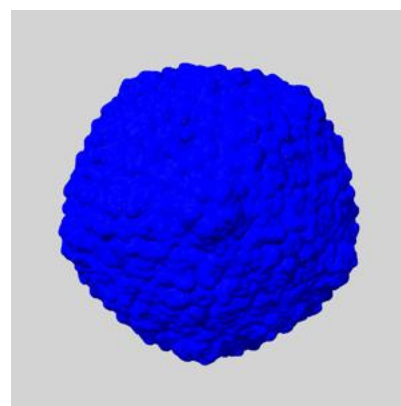
6.6.1 emd_55362_msk_1.map [i](#)



X



Y

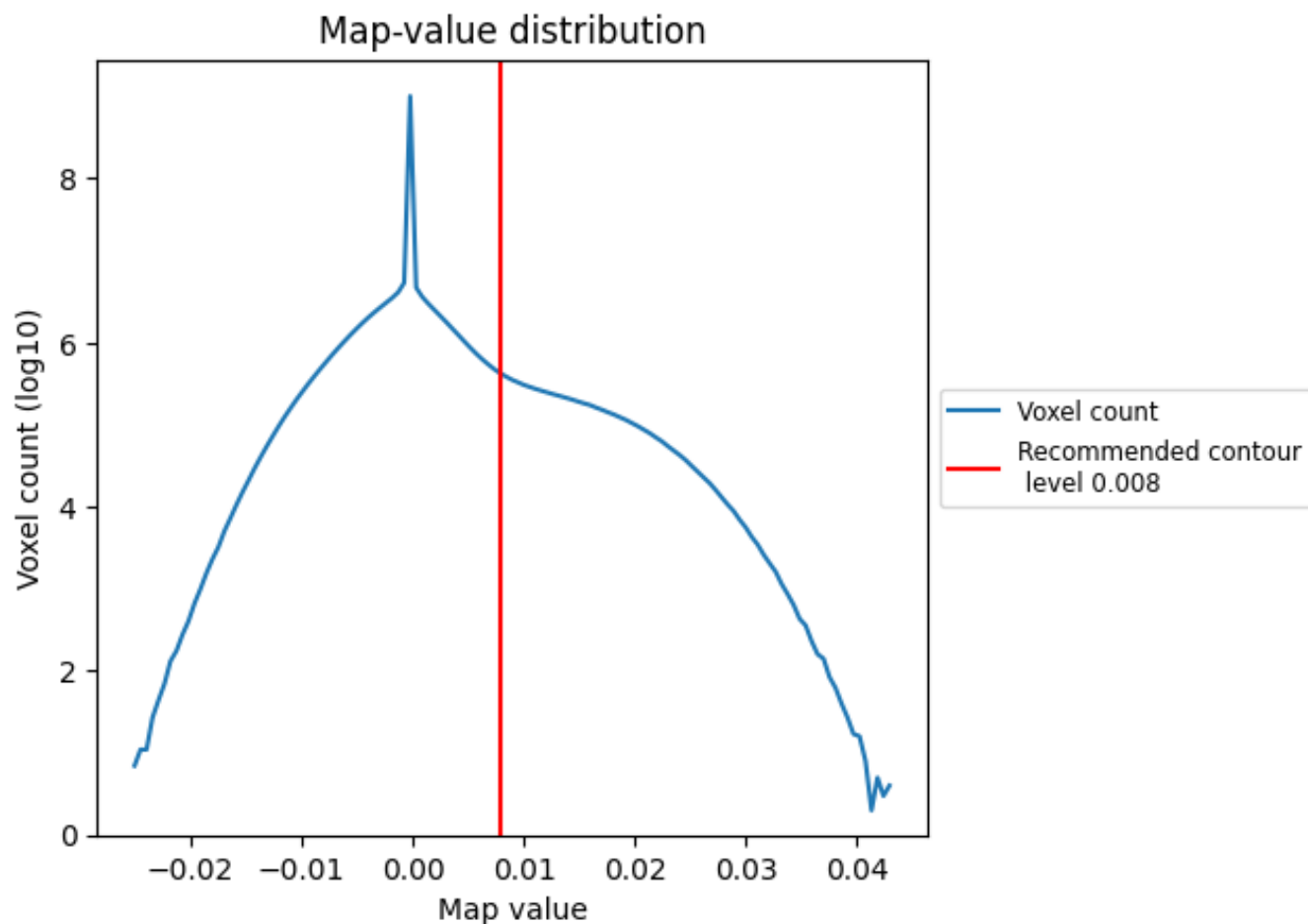


Z

7 Map analysis [i](#)

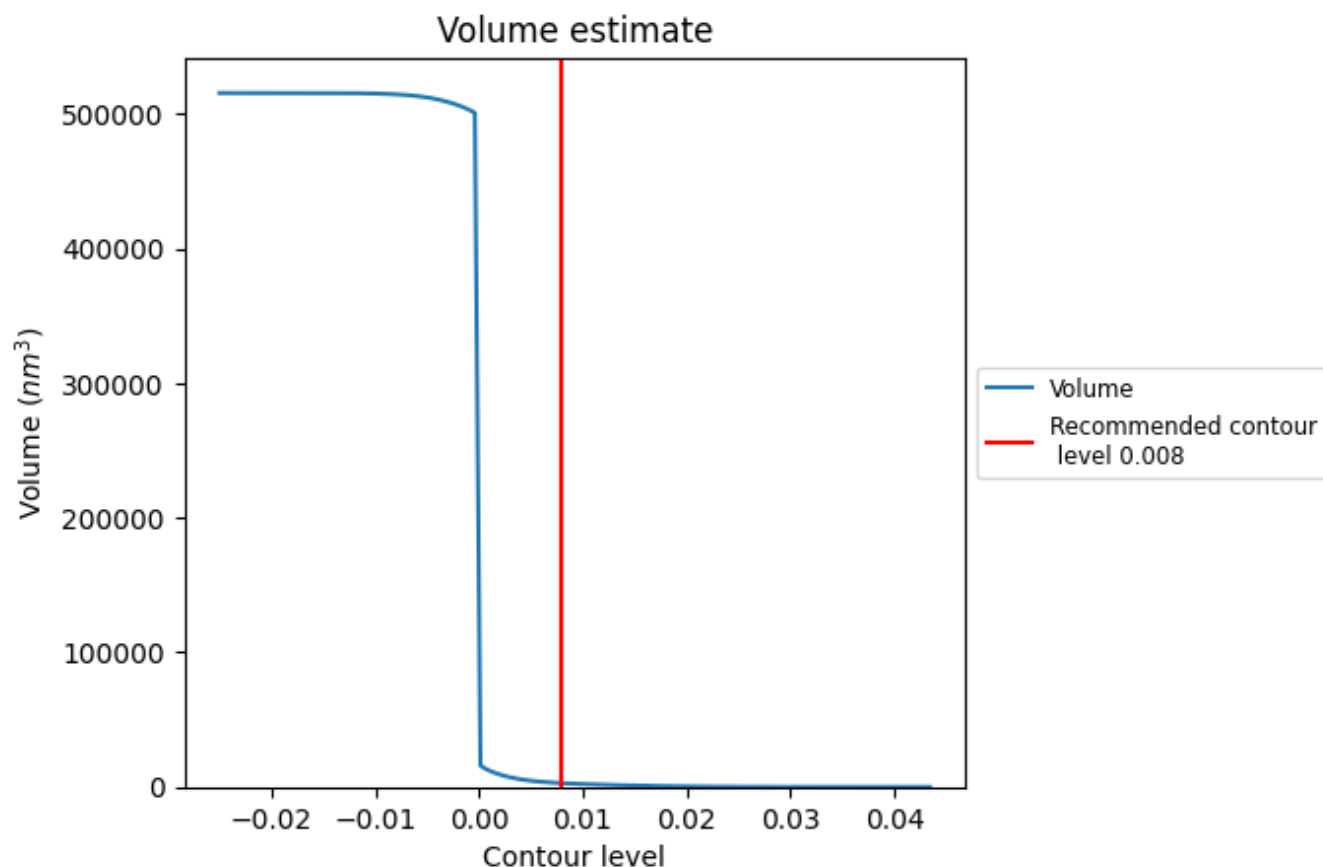
This section contains the results of statistical analysis of the map.

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.

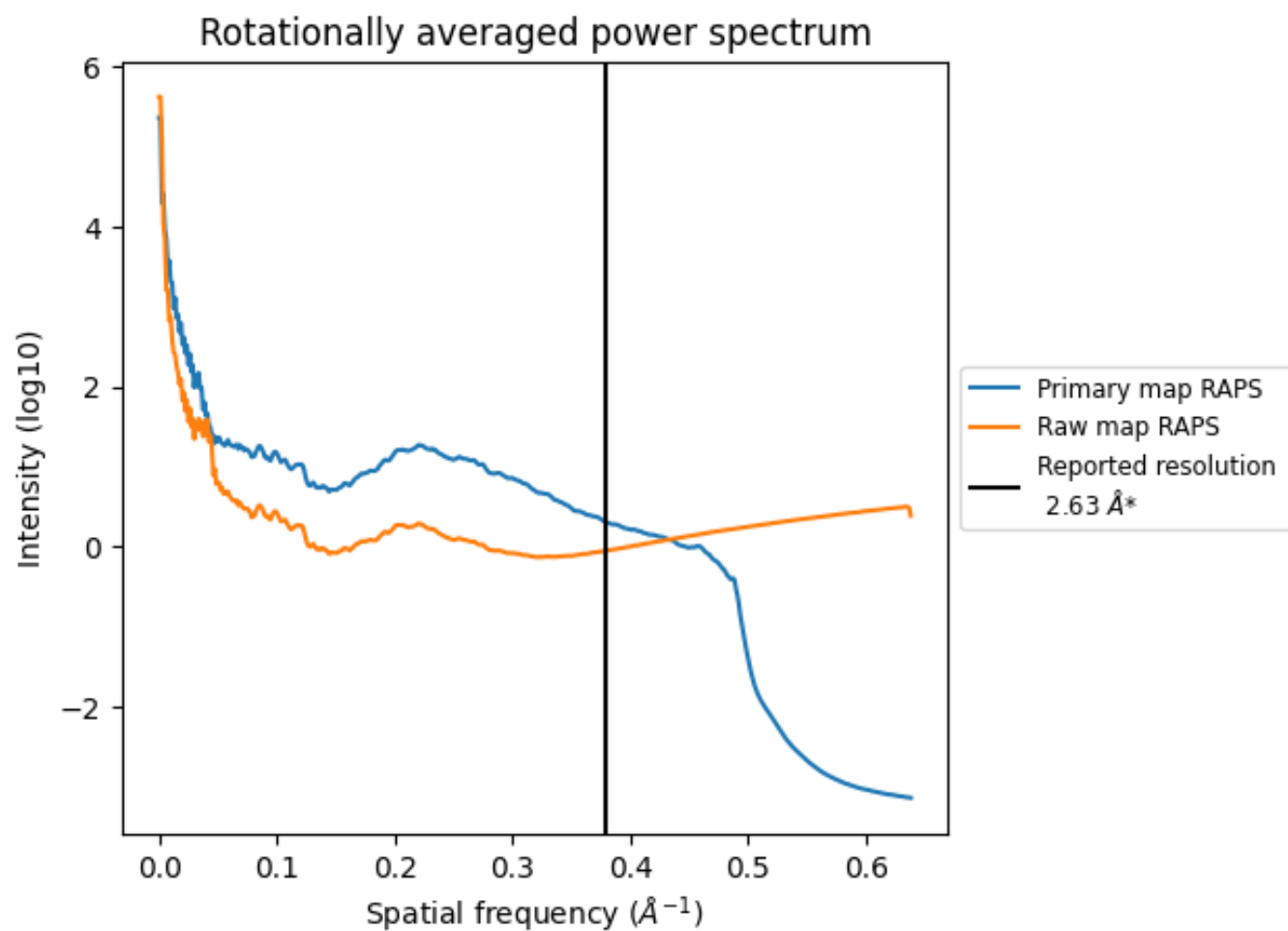
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2826 nm³; this corresponds to an approximate mass of 2553 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 ⓘ

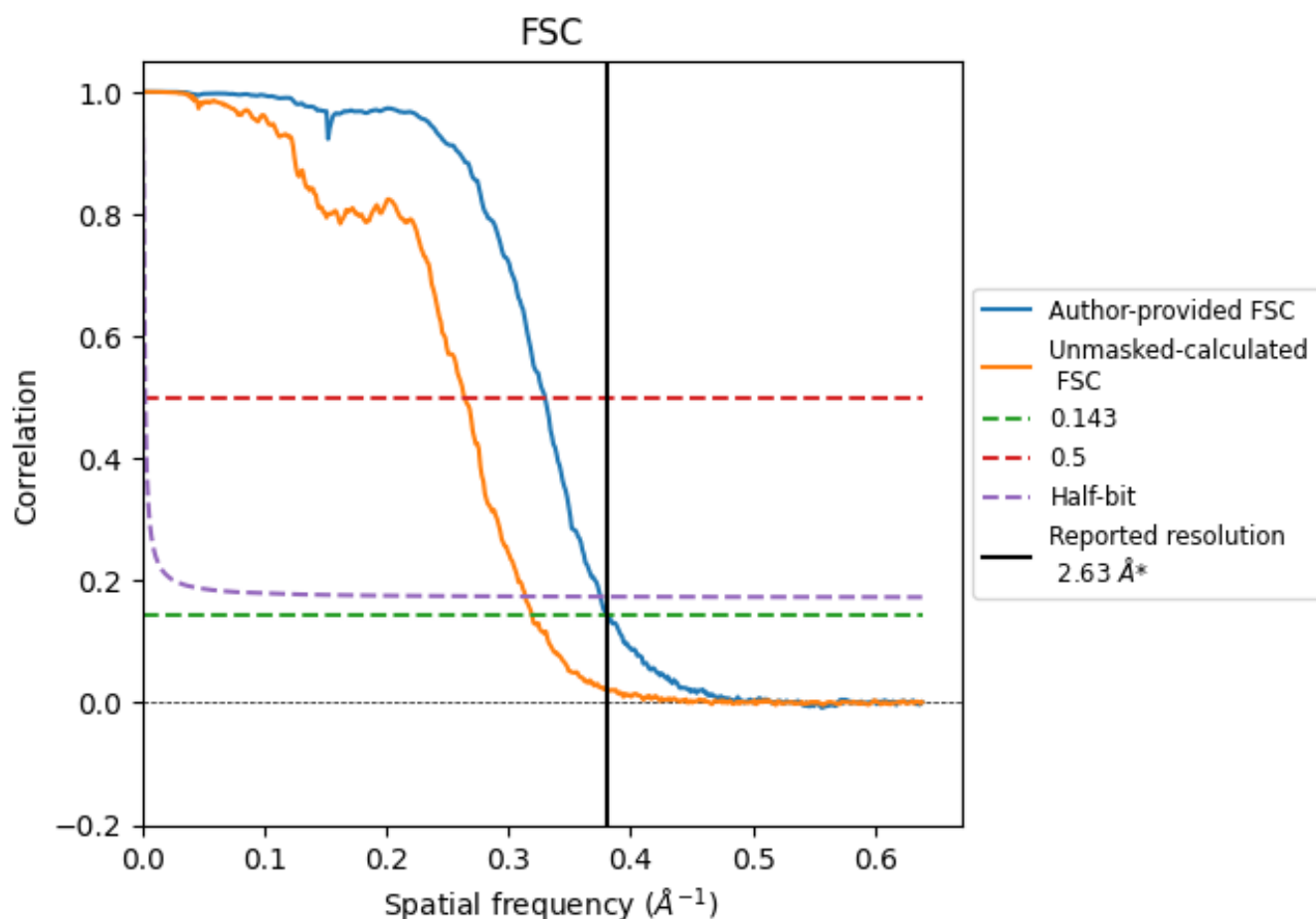


*Reported resolution corresponds to spatial frequency of 0.380 $\text{\AA}^{-1}$

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 0.380 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.63	-	-
Author-provided FSC curve	2.63	3.03	2.67
Unmasked-calculated*	3.13	3.79	3.19

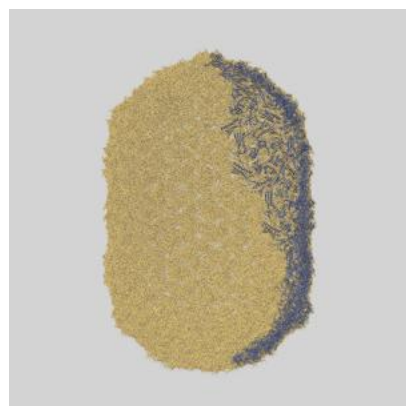
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.13 differs from the reported value 2.63 by more than 10 %

9 Map-model fit [i](#)

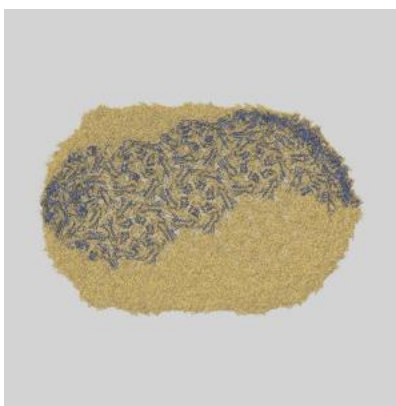
This section contains information regarding the fit between EMDB map EMD-55362 and PDB model 9SZ9. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlays

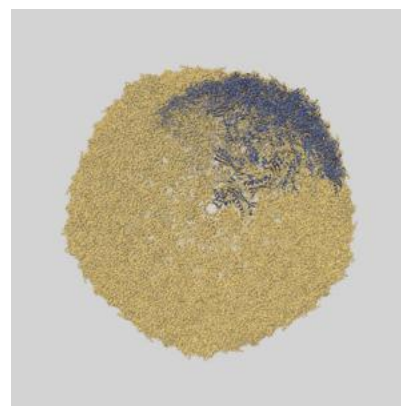
9.1.1 Map-model overlay [i](#)



X

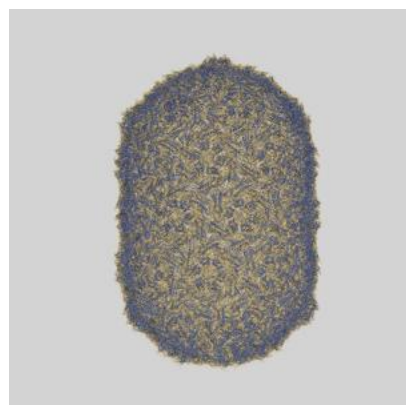


Y

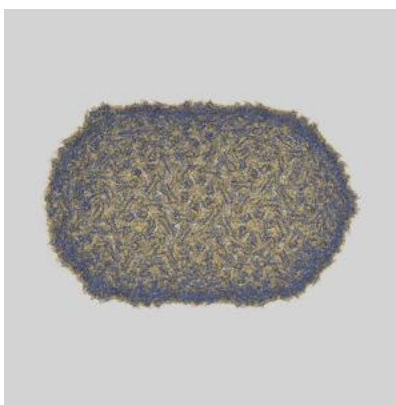


Z

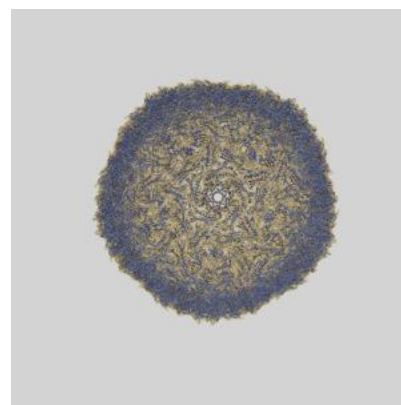
9.1.2 Map-model assembly overlay [i](#)



X



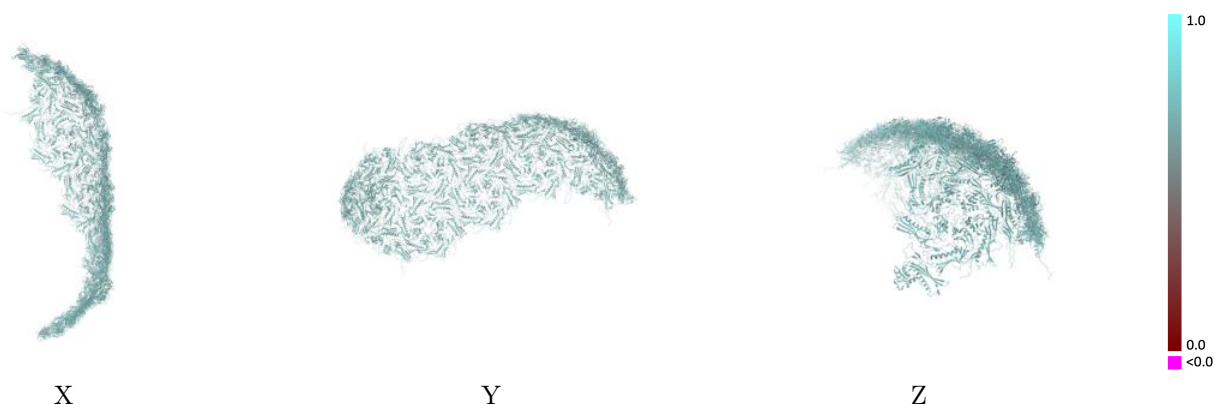
Y



Z

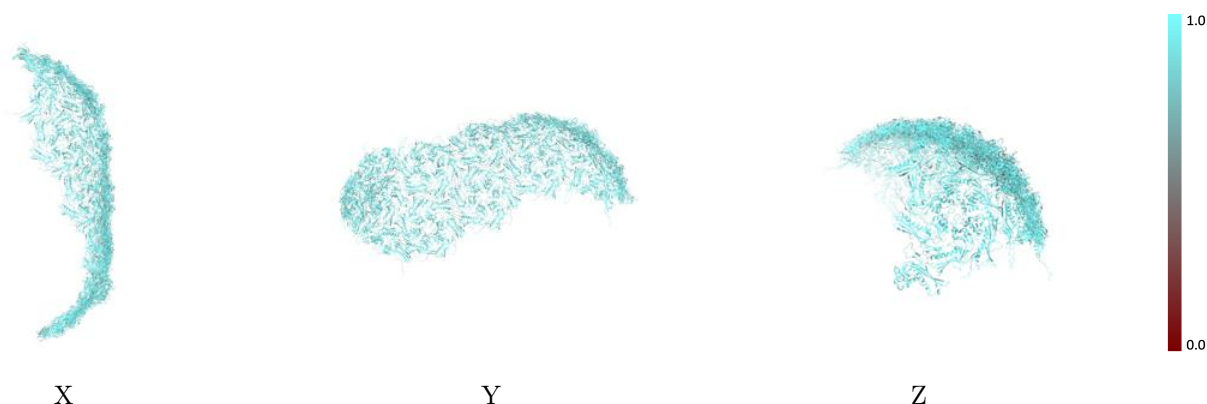
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



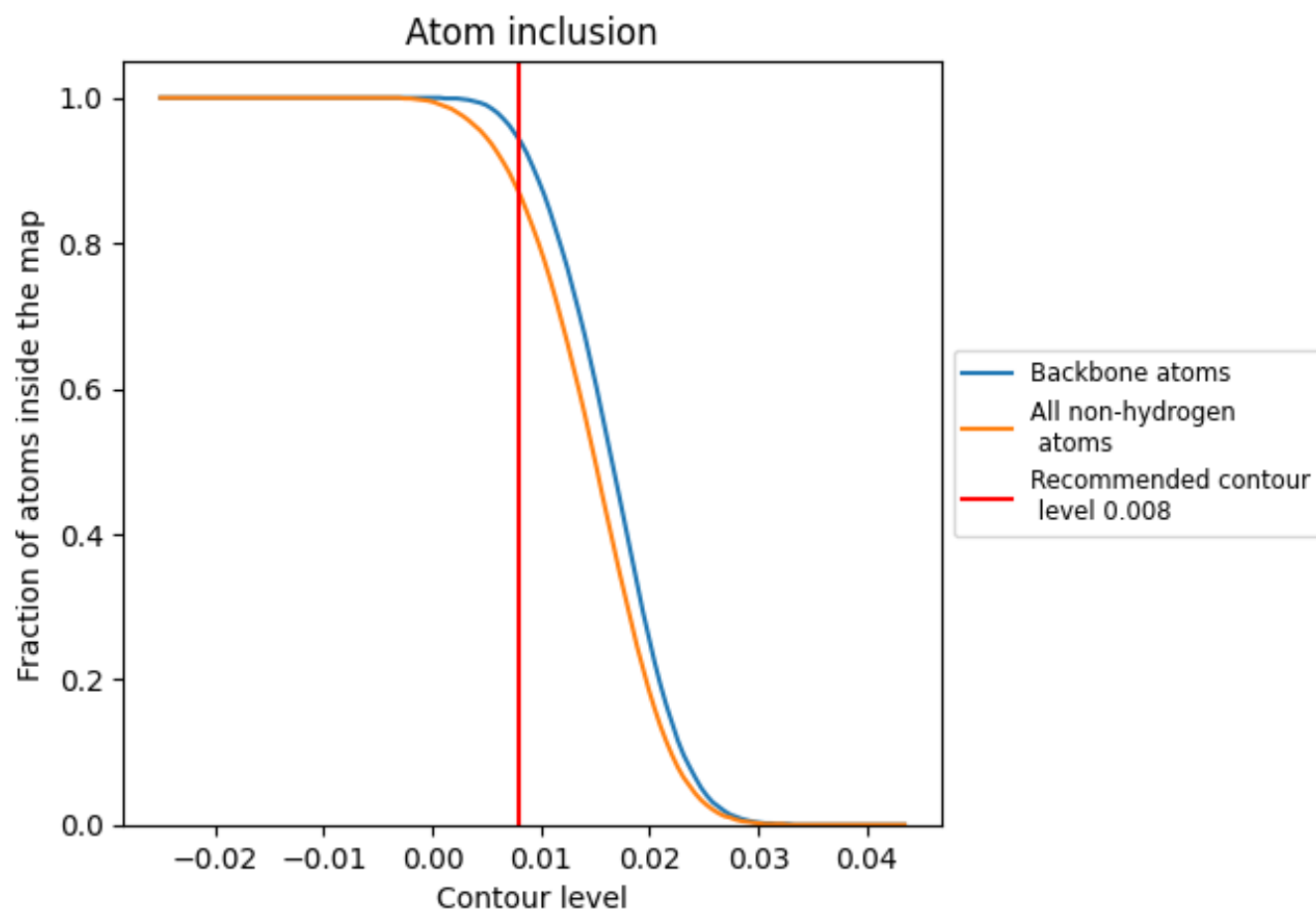
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.008).

9.4 Atom inclusion ⓘ



At the recommended contour level, 94% of all backbone atoms, 87% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8690	 0.6660
A0	 0.8720	 0.6670
A1	 0.8860	 0.6650
A2	 0.8380	 0.6520
A3	 0.8490	 0.6530
A4	 0.8520	 0.6580
A5	 0.8450	 0.6590
A6	 0.8340	 0.6590
A7	 0.8490	 0.6530
AA	 0.8570	 0.6550
AB	 0.8830	 0.6670
AC	 0.8900	 0.6770
AD	 0.8850	 0.6730
AE	 0.8850	 0.6690
AF	 0.8280	 0.6510
AG	 0.8930	 0.6770
AH	 0.8940	 0.6820
AI	 0.8940	 0.6780
AJ	 0.8930	 0.6770
AK	 0.8880	 0.6740
AL	 0.8850	 0.6780
AM	 0.8930	 0.6750
AN	 0.8690	 0.6720
AO	 0.8600	 0.6690
AP	 0.8750	 0.6710
AQ	 0.8890	 0.6780
AR	 0.8870	 0.6790
AS	 0.8860	 0.6770
AT	 0.8690	 0.6770
AU	 0.8550	 0.6680
AV	 0.8740	 0.6700
AW	 0.8790	 0.6740
AX	 0.8840	 0.6780
AY	 0.8550	 0.6670
AZ	 0.8590	 0.6670



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Chain	Atom inclusion	Q-score
Aa	 0.8540	 0.6600
Ab	 0.8590	 0.6670
Ac	 0.8540	 0.6600
Ad	 0.8570	 0.6660
Ae	 0.8800	 0.6590
Af	 0.8840	 0.6640
Ag	 0.8910	 0.6700
Ah	 0.8850	 0.6630
Ai	 0.8880	 0.6710
Aj	 0.8770	 0.6640
Ak	 0.8920	 0.6710
Al	 0.8830	 0.6660
Am	 0.8850	 0.6720
An	 0.8860	 0.6680
Ao	 0.8870	 0.6690
Ap	 0.8830	 0.6670
Aq	 0.8740	 0.6670
Ar	 0.8620	 0.6600
As	 0.8460	 0.6530
At	 0.8570	 0.6610
Au	 0.8710	 0.6660
Av	 0.8720	 0.6680
Aw	 0.8730	 0.6680
Ax	 0.8660	 0.6590
Ay	 0.8510	 0.6590
Az	 0.8650	 0.6600
FA	 0.8610	 0.6690
FB	 0.8630	 0.6710
FC	 0.8640	 0.6700
FD	 0.8570	 0.6680
FE	 0.8660	 0.6690
FF	 0.8520	 0.6530
FG	 0.8490	 0.6580
FH	 0.8470	 0.6550
FI	 0.8430	 0.6540
FJ	 0.8540	 0.6520
FK	 0.8170	 0.6370