



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:50 PM UTC

PDB ID : 7LVV / pdb_00007lvv
EMDB ID : EMD-23543
Title : cryoEM structure DrdV-DNA complex
Authors : Shen, B.W.; Stoddard, B.L.
Deposited on : 2021-02-26
Resolution : 3.25 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
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

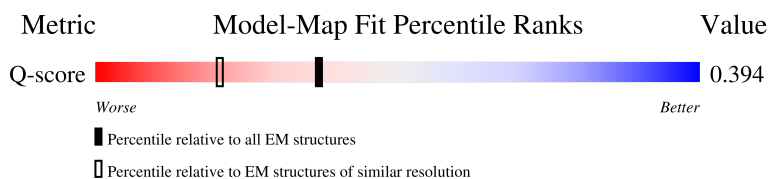
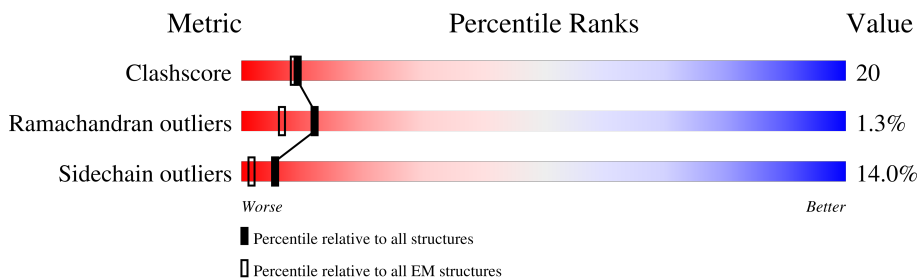
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.25 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	14599 (2.75 - 3.75)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1029	8% 59% 32% 7% .
1	B	1029	. 60% 32% 6% .
1	C	1029	8% 5% 86%
1	D	1029	9% 9% . . 86%

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Mol	Chain	Length	Quality of chain
2	E	29	66%31%•
2	G	29	69%28%•
3	F	29	83%10%7%
3	H	29	76%14%•7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21020 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 Site-specific DNA-methyltransferase (adenine-specific).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1011	Total	C	N	O	S	0	0
			8216	5222	1439	1536	19		
1	B	1012	Total	C	N	O	S	0	0
			8219	5223	1440	1537	19		
1	C	143	Total	C	N	O	S	0	0
			1126	704	197	223	2		
1	D	146	Total	C	N	O	S	0	0
			1149	719	201	227	2		

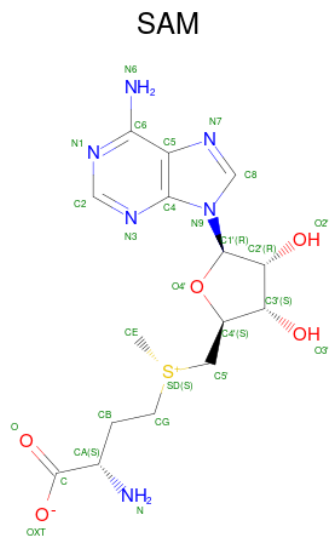
- Molecule 2 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	28	Total	C	N	O	P	0	0
			561	265	107	161	28		
2	G	28	Total	C	N	O	P	0	0
			561	265	107	161	28		

- Molecule 3 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	27	Total	C	N	O	P	0	0
			565	266	103	169	27		
3	H	27	Total	C	N	O	P	0	0
			565	266	103	169	27		

- Molecule 4 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: C₁₅H₂₂N₆O₅S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 27	C 15	N 6	O 5	S 1	0
4	B	1	Total 27	C 15	N 6	O 5	S 1	0

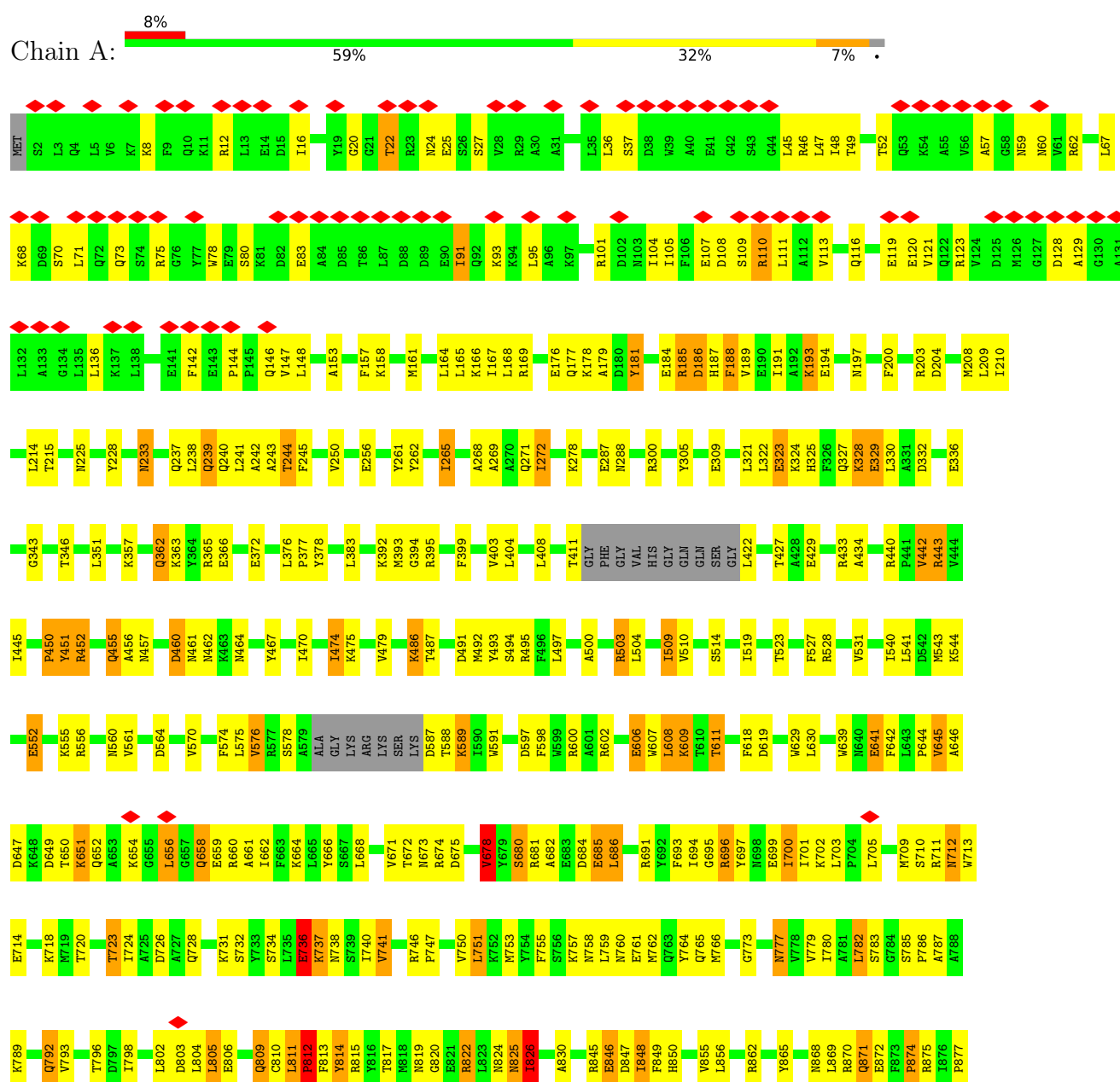
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

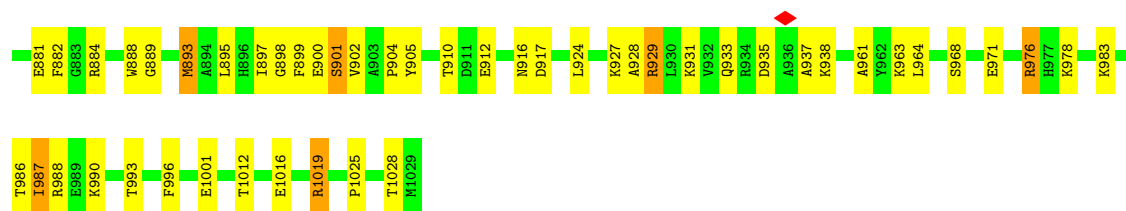
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total 1	Ca 1	0
5	B	1	Total 1	Ca 1	0
5	C	1	Total 1	Ca 1	0
5	D	1	Total 1	Ca 1	0

3 Residue-property plots

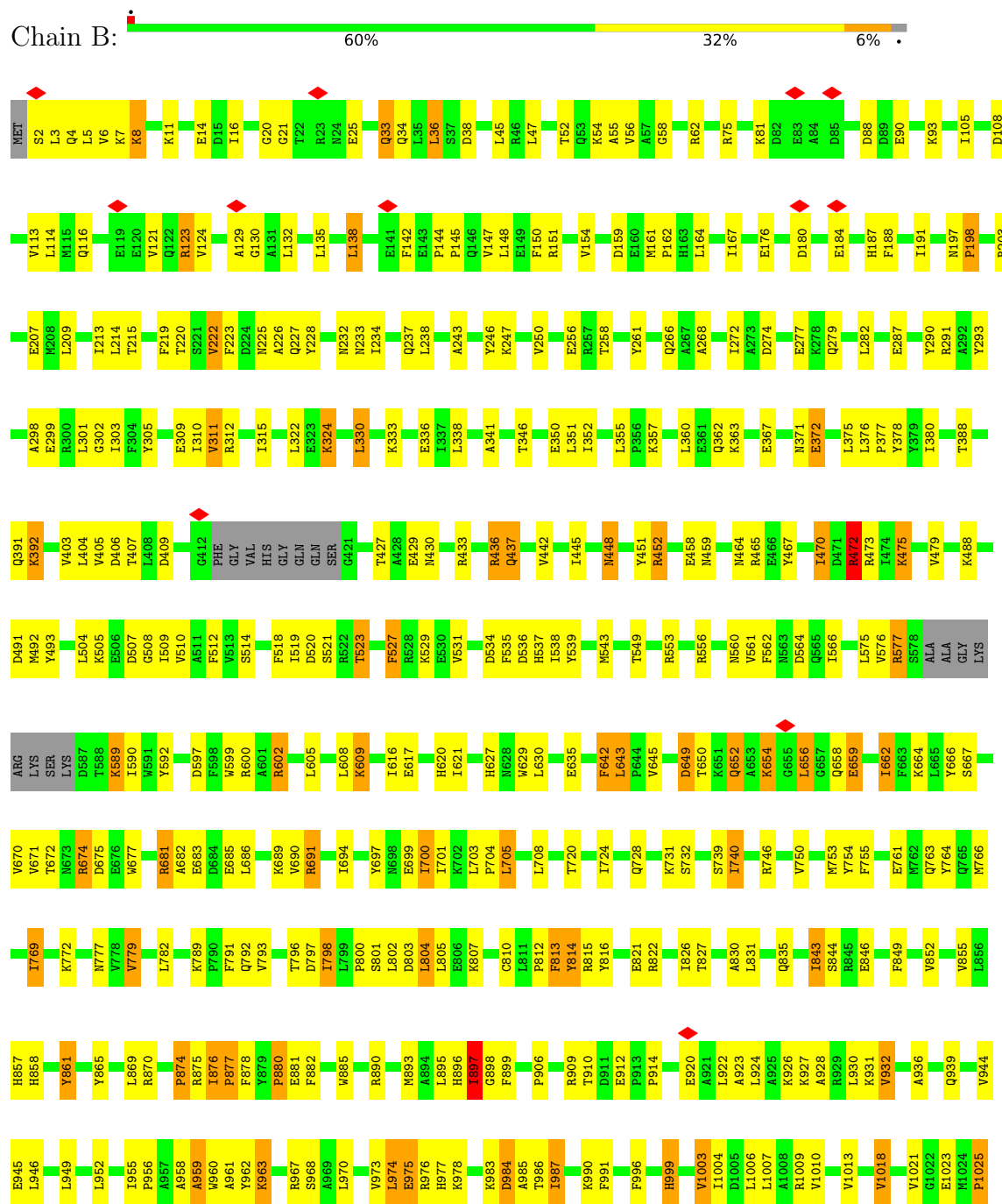
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Site-specific DNA-methyltransferase (adenine-specific)





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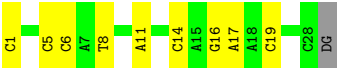
Chain C: 86%

GLY	ILE	PRO	ALA	ALA	ALA	TRP	GLU	VAL	GLY	GLU	GLY	LYS	VAL	PHE	GLY	VAL	ASP	GLY	ILE	GLY	PHE	GLY	VAL	GLY	ASN	PRO	ILE	ALA	S109	
THR	PRO	HIS	LEU	THR	GLY	GLY	ASP	GLY	LEU	GLY	ASP	GLN	HIS	VAL	SER	VAL	PRO	GLY	ILE	GLY	THR	GLY	GLN	GLY	GLY	ALA	GLN	ALA	R110	
ALA	ALA	ILE	ILE	HIS	ILE	VAL	ASN	ASN	ILE	GLY	ASP	GLN	THR	TYR	GLY	GLY	HIS	LYS	GLN	GLY	GLY	GLY	GLY	GLY	ALA	GLY	GLY	ALA	L111	
ALA	ALA	GLY	PHE	VAL	GLY	VAL	VAL	VAL	GLY	GLY	TRP	GLY	TYR	TYR	GLY	GLN	ILE	LYS	GLN	VAL	GLY	GLY	GLY	GLY	ALA	GLY	GLY	ALA	A112	
TRP	TRP	PHE	GLU	ASP	THR	ILE	ILE	ILE	ARG	THR	ARG	ARG	ALA	VAL	GLN	SER	ILE	LYS	GLN	GLY	GLY	GLY	GLY	GLY	ALA	GLY	GLY	ALA	V113	
ALA	ALA	GLU	GLU	ASP	THR	ILE	ARG	ALA	LEU	ALA	ILE	ILE	ALA	ALA	GLY	GLY	LEU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	GLY	GLY	ALA	L114	
TRP	TRP	VAL	VAL	THR	ALA	ALA	ALA	ALA	ALA	ALA	ARG	ALA	ALA	ALA	GLY	SER	LEU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	GLY	GLY	ALA	M115	
ALA	ALA	SER	GLU	SER	ALA	ALA	ALA	ALA	ILE	ARG	GLY	GLY	ALA	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	GLY	GLY	ALA	Q116	
TRP	TRP	ALA	ALA	THR	ALA	ALA	ALA	ALA	PHE	THR	ILE	LYS	ALA	ALA	PHE	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	GLY	GLY	ALA	N117	
ALA	ALA	PRO	GLY	SER	LYS	ILE	LYS	LYS	LEU	GLY	LYS	GLY	GLN	GLY	TYR	SER	ARG	TYR	THR	GLY	THR	THR	THR	GLY	GLY	GLY	GLY	ALA	G118	
ALA	ALA	TYR	GLY	ARG	ALA	ALA	ASP	GLY	ALA	GLY	LEU	GLY	GLN	SER	GLY	SER	ARG	TYR	PHE	THR	THR	THR	THR	GLY	GLY	GLY	GLY	ALA	E119	
ALA	ALA	PRO	ASP	GLY	PRO	GLY	PRO	GLY	TYR	GLY	GLY	GLY	LYS	GLY	GLY	GLY	ARG	TYR	PHE	THR	THR	THR	THR	GLY	GLY	GLY	GLY	ALA	E120	
ALA	ALA	LEU	ASP	THR	ASP	ALA	ALA	ALA	SER	TRP	TRP	TRP	THR	GLY	GLY	GLY	GLY	VAL	ASP	GLY	THR	THR	THR	ASP	ASP	ASP	ASP	ALA	V121	
ALA	ALA	LYS	LYS	ILE	LEU	GLN	LEU	LEU	LEU	LEU	LEU	LEU	LYS	ALA	ALA	GLY	GLY	GLY	HIS	LYS	LYS	LYS	LYS	HIS	HIS	HIS	HIS	ALA	Q122	
ALA	ALA	ARG	THR	PHE	GLY	LYS	LYS	LYS	GLY	GLY	LYS	GLY	LEU	LYS	GLY	GLY	LEU	GLY	PHE	VAL	GLY	PRO	VAL	VAL	VAL	VAL	VAL	ALA	R123	
ALA	ALA	THR	GLY	THR	GLY	VAL	VAL	VAL	VAL	THR	THR	THR	VAL	THR	SER	ASN	CYS	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	V124	
ALA	ALA	ASP	GLY	THR	GLY	LYS	LYS	LYS	GLY	GLY	GLY	GLY	ASP	MET	GLY	LEU	ASN	GLY	ILE	VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	ALA	A31	
ALA	ALA	GLY	THR	VAL	GLY	SER	THR	THR	THR	THR	THR	THR	ASP	ILE	GLY	GLY	ASN	GLY	LYS	ILE	ILE	ILE	ILE	ILE	ILE	ALA	ALA	ALA	M126	
ALA	ALA	PRO	VAL	VAL	VAL	VAL	PHE	PHE	ASN	TYR	PHE	GLY	ARG	MET	GLY	GLY	GLY	GLY	ARG	ARG	ARG	ARG	ARG	ARG	ALA	ALA	ALA	ALA	D127	
ALA	ALA	PRO	VAL	VAL	VAL	VAL	VAL	VAL	ASP	GLY	GLY	ASP	ARG	SER	ARG	ALA	ALA	ALA	ILE	ILE	ILE	ILE	ILE	ILE	ALA	ALA	ALA	ALA	D128	
ALA	ALA	ASN	GLY	THR	GLY	GLY	ILE	PHE	ILE	GLY	GLY	GLY	GLN	PHE	GLY	GLY	LEU	LEU	GLY	GLY	GLY	GLY	GLY	GLY	ASN	ASN	ASN	ASN	L132	
ALA	ALA	THR	THR	PRO	ILE	VAL	ASP	ASP	THR	THR	ASP	THR	TRP	ARG	ASN	ASN	PRO	PRO	THR	THR	THR	THR	THR	THR	PRO	PRO	PRO	PRO	G134	
ALA	ALA	PRO	GLY	ALA	GLY	GLY	HIS	ASP	ILE	ILE	ILE	ILE	ALA	TRP	GLY	GLY	LEU	LEU	GLY	GLY	GLY	GLY	GLY	GLY	PRO	PRO	PRO	PRO	L135	
ALA	ALA	ALA	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	ALA	ALA	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ASP	ASP	ASP	ASP	L136	
ALA	ALA	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	K137	
ALA	ALA	PRO	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	L138	
ALA	ALA	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	GLY	GLY	GLY	GLY	E143	
ALA	ALA	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	P144	
ALA	ALA	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	N60	
ALA	ALA	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	PRO	
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	GLN	T66
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	GLY	L67
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	LEU	K68
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	LEU	D69
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	PHE	S70
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ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	VAL	D82
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ASP	E83
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	THR	L87
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	LYS	Q92
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	GLY	K93
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	THR	K94
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	HIS	L95
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	LEU	A96
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	LEU	K97
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ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	HIS	K94
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	GLY	L95
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	LEU	A96
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	LEU	K97
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	LYS	Q92
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ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	HIS	K94
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	GLY	L95
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ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	LYS	Q92
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	THR	R93
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	GLY	K94
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	HIS	L95
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	LEU	A96
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA													



GLU	TRP	VAL	LEU	GLU	ARG	HIS	LYS	GLU	THR	THR	PRO	LYS	ASP	ALA	THR	ILE	ARG	GLU	LYS	PHE	ASN	THR	TYR	ARG	PHE	ALA	ASP	HIS	LYS	GLU	ARG	VAL	ILE	ASP	LEU	LEU	ALA	ARG	VAL	THR	THR	VAL	SER	VAL	GLU	THR	THR	VAL	ARG	ILE	VAL	GLY	GLU	MET	PRO	ALA	GLU	THR	MET
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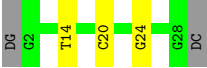
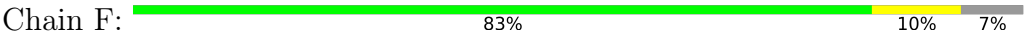
• Molecule 2: DNA (28-MER)



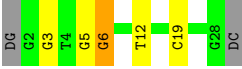
• Molecule 2: DNA (28-MER)



• Molecule 3: DNA (27-MER)



• Molecule 3: DNA (27-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	34554	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	37000	Depositor
Image detector	FEI CETA (4k x 4k)	Depositor
Maximum map value	2.203	Depositor
Minimum map value	-0.745	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.375	Depositor
Map size ($\text{\AA}$)	464.0, 464.0, 464.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.16, 1.16, 1.16	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.97	3/8396 (0.0%)	1.38	59/11348 (0.5%)
1	B	0.97	3/8399 (0.0%)	1.34	39/11351 (0.3%)
1	C	0.98	0/1141	1.36	1/1534 (0.1%)
1	D	0.93	0/1165	1.35	2/1568 (0.1%)
2	E	0.47	0/628	0.85	3/962 (0.3%)
2	G	0.46	0/628	0.81	2/962 (0.2%)
3	F	0.46	0/633	0.86	2/979 (0.2%)
3	H	0.43	0/633	0.82	3/979 (0.3%)
All	All	0.92	6/21623 (0.0%)	1.31	111/29683 (0.4%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	712	ASN	C-N	-6.07	1.25	1.33
1	B	844	SER	C-N	-5.76	1.26	1.33
1	A	741	VAL	C-N	5.50	1.40	1.33
1	A	702	LYS	C-N	5.33	1.41	1.33
1	B	144	PRO	C-O	-5.18	1.18	1.24
1	B	814	TYR	C-N	5.10	1.40	1.33

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	987	ILE	N-CA-C	-8.82	104.56	113.47
1	B	299	GLU	N-CA-C	-8.82	103.10	114.04
1	B	728	GLN	N-CA-C	-8.60	102.92	112.72
1	A	929	ARG	N-CA-C	-8.39	104.08	112.97
1	A	486	LYS	CA-C-N	-8.31	110.94	123.07
1	A	486	LYS	C-N-CA	-8.31	110.94	123.07
1	A	244	THR	N-CA-C	-8.06	103.65	113.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	503	ARG	N-CA-C	-7.63	102.09	111.40
1	A	268	ALA	N-CA-C	-7.58	104.94	114.56
1	A	239	GLN	N-CA-C	-7.45	102.84	112.23
1	A	91	ILE	N-CA-C	-7.35	103.36	110.42
1	B	1023	GLU	CA-C-N	-7.34	109.37	120.60
1	B	1023	GLU	C-N-CA	-7.34	109.37	120.60
2	G	23	DC	C2'-C3'-O3'	-7.29	100.57	111.50
1	B	650	THR	CA-CB-OG1	-7.26	98.70	109.60
2	E	14	DC	C2'-C3'-O3'	-7.25	100.63	111.50
1	B	33	GLN	N-CA-C	-7.24	103.33	111.07
1	B	897	ILE	N-CA-C	-7.24	103.57	112.76
1	B	861	TYR	N-CA-C	-7.22	103.13	112.23
2	E	19	DC	C4'-C3'-O3'	7.11	120.66	110.00
1	B	674	ARG	CB-CA-C	-6.91	102.49	111.40
1	A	606	GLU	N-CA-C	-6.83	104.94	113.55
3	F	20	DC	C2'-C3'-O3'	-6.75	101.38	111.50
1	A	904	PRO	CB-CA-C	-6.72	101.06	111.40
1	A	181	TYR	CB-CA-C	-6.67	100.69	110.96
1	B	763	GLN	N-CA-C	-6.65	103.64	113.61
1	A	904	PRO	N-CA-C	6.56	120.71	111.33
1	B	33	GLN	CB-CA-C	-6.56	100.59	110.88
1	B	391	GLN	N-CA-C	-6.40	106.01	113.88
1	B	388	THR	N-CA-C	-6.32	105.70	113.41
2	E	1	DC	C2'-C3'-O3'	-6.27	102.10	111.50
1	A	179	ALA	N-CA-C	-6.23	105.62	113.72
1	A	187	HIS	N-CA-C	-6.21	105.83	113.41
1	B	769	ILE	N-CA-C	-6.16	106.26	111.56
1	A	809	GLN	CB-CA-C	-6.08	101.43	110.62
1	A	243	ALA	N-CA-C	-6.07	104.95	113.20
1	A	443	ARG	CA-C-N	-6.06	115.28	123.10
1	A	443	ARG	C-N-CA	-6.06	115.28	123.10
3	F	14	DT	C2'-C3'-O3'	-6.04	102.44	111.50
1	A	736	GLU	CA-C-N	6.03	133.06	121.54
1	A	736	GLU	C-N-CA	6.03	133.06	121.54
1	A	450	PRO	CA-C-N	-6.00	113.07	122.73
1	A	450	PRO	C-N-CA	-6.00	113.07	122.73
1	A	193	LYS	N-CA-C	-5.99	105.29	112.59
1	B	923	ALA	O-C-N	5.97	129.62	122.27
1	A	399	PHE	CB-CA-C	-5.97	101.31	110.26
1	A	764	TYR	CB-CA-C	-5.94	103.43	112.11
1	B	813	PHE	N-CA-C	-5.94	106.64	114.31
1	A	897	ILE	N-CA-C	-5.91	105.95	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	810	CYS	CB-CA-C	-5.87	100.43	110.22
1	A	460	ASP	CA-C-O	-5.86	113.73	120.24
1	B	877	PRO	CB-CA-C	-5.86	101.23	110.96
1	B	755	PHE	CB-CA-C	-5.86	101.75	111.41
1	B	508	GLY	CA-C-O	-5.84	116.21	122.05
1	C	97	LYS	N-CA-C	-5.83	106.20	113.38
1	B	577	ARG	CB-CA-C	-5.82	100.49	110.16
1	B	1003	VAL	N-CA-C	-5.81	104.85	110.72
1	A	188	PHE	N-CA-C	-5.75	104.92	111.07
1	B	880	PRO	N-CA-C	5.72	124.24	112.47
1	B	388	THR	CB-CA-C	5.67	119.16	109.24
1	B	303	ILE	CB-CA-C	5.65	117.51	111.35
1	A	177	GLN	N-CA-C	-5.63	106.41	113.28
2	G	1	DC	C2'-C3'-O3'	-5.63	103.06	111.50
1	A	825	ASN	CA-C-O	-5.60	113.31	120.31
1	B	472	ARG	N-CA-C	-5.60	105.32	111.82
1	B	148	LEU	N-CA-C	-5.59	105.27	111.36
1	A	269	ALA	N-CA-C	-5.56	106.50	113.28
1	A	71	LEU	N-CA-C	-5.56	104.92	112.26
1	A	848	ILE	O-C-N	5.54	127.34	121.91
1	A	36	LEU	N-CA-C	-5.47	105.31	111.28
1	A	777	ASN	CB-CA-C	5.46	118.84	109.51
1	A	761	GLU	CA-C-N	-5.44	115.32	122.99
1	A	761	GLU	C-N-CA	-5.44	115.32	122.99
1	B	683	GLU	N-CA-C	-5.43	106.49	113.01
1	B	691	ARG	N-CA-C	-5.43	105.52	111.82
1	A	144	PRO	CB-CA-C	-5.42	106.30	111.39
1	A	814	TYR	CB-CA-C	-5.41	103.14	111.74
3	H	3	DG	C2'-C3'-O3'	5.38	119.56	111.50
1	B	56	VAL	CA-C-O	-5.35	116.23	121.58
1	B	539	TYR	CA-C-O	-5.34	114.45	120.32
1	A	455	GLN	CB-CG-CD	-5.33	103.55	112.60
1	A	777	ASN	CA-CB-CG	5.32	117.92	112.60
1	B	642	PHE	CA-C-O	-5.32	112.90	120.51
1	D	8	LYS	N-CA-C	-5.31	107.46	114.31
1	B	123	ARG	CB-CA-C	-5.31	103.30	111.74
1	A	812	PRO	CB-CA-C	-5.30	102.81	111.56
1	B	924	LEU	N-CA-C	-5.28	107.02	112.93
1	B	798	ILE	CA-C-O	-5.28	115.16	121.28
1	B	699	GLU	N-CA-C	-5.27	105.59	112.23
1	A	332	ASP	CA-C-N	-5.25	115.40	122.86
1	A	332	ASP	C-N-CA	-5.25	115.40	122.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	819	ASN	CB-CA-C	-5.24	104.09	111.95
3	H	12	DT	C2'-C3'-O3'	-5.22	103.67	111.50
1	A	609	LYS	N-CA-C	-5.21	106.01	112.93
1	B	527	PHE	N-CA-C	-5.20	105.61	111.28
1	A	757	LYS	N-CA-C	-5.19	106.45	112.89
1	A	697	TYR	N-CA-C	-5.16	105.65	111.28
1	A	186	ASP	N-CA-C	-5.16	107.01	113.72
1	A	758	ASN	CB-CA-C	-5.14	103.04	110.96
1	D	9	PHE	N-CA-C	-5.14	105.67	111.28
1	B	108	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	901	SER	N-CA-C	-5.13	107.67	114.04
1	A	321	LEU	N-CA-C	-5.13	106.99	114.12
3	H	6	DG	C2'-C3'-O3'	-5.12	103.81	111.50
1	A	265	ILE	O-C-N	5.11	127.03	121.87
1	A	609	LYS	CB-CA-C	-5.11	102.05	110.08
1	A	658	GLN	N-CA-C	-5.07	106.93	113.01
1	B	789	LYS	CA-C-O	-5.03	115.69	120.97
1	A	731	LYS	O-C-N	5.03	128.77	122.63
1	A	574	PHE	CA-CB-CG	5.02	118.82	113.80
1	B	372	GLU	CA-C-O	-5.01	115.87	121.23

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	A	8216	0	8108	361	0
1	B	8219	0	8109	391	0
1	C	1126	0	1115	47	0
1	D	1149	0	1139	40	0
2	E	561	0	310	10	0
2	G	561	0	310	18	0
3	F	565	0	306	3	0
3	H	565	0	306	3	0
4	A	27	0	22	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	27	0	22	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	1	0
All	All	21020	0	19747	828	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 20.

All (828) 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:B:509:ILE:CG2	1:B:576:VAL:HG22	1.32	1.58
1:B:543:MET:HE2	1:B:561:VAL:CG1	1.42	1.50
1:B:782:LEU:CD2	1:B:793:VAL:HG12	1.39	1.50
1:B:543:MET:CE	1:B:561:VAL:HG11	1.40	1.46
1:A:209:LEU:HD21	1:A:245:PHE:CZ	1.51	1.44
1:B:543:MET:CE	1:B:608:LEU:HD11	1.50	1.41
1:B:930:LEU:HD23	1:B:946:LEU:CD2	1.54	1.37
1:B:973:VAL:HG21	1:B:1006:LEU:CD2	1.53	1.37
1:B:529:LYS:HD2	1:B:627:HIS:CE1	1.62	1.34
1:B:509:ILE:HG22	1:B:576:VAL:CG2	1.59	1.31
1:B:973:VAL:CG2	1:B:1006:LEU:HD23	1.61	1.29
1:B:543:MET:SD	1:B:608:LEU:HD11	1.83	1.19
1:B:807:LYS:HE3	2:G:8:DT:C6	1.77	1.19
1:B:45:LEU:CD2	1:B:75:ARG:HD3	1.73	1.18
1:A:189:VAL:CG1	1:A:193:LYS:HE3	1.73	1.18
1:B:930:LEU:CD2	1:B:946:LEU:HD22	1.74	1.16
1:A:120:GLU:OE1	1:A:123:ARG:HG3	1.47	1.15
1:B:543:MET:CE	1:B:608:LEU:CD1	2.26	1.14
1:A:45:LEU:HD11	1:A:75:ARG:HD3	1.31	1.13
1:A:309:GLU:HG2	1:A:609:LYS:CE	1.79	1.12
1:B:3:LEU:O	1:B:7:LYS:HG2	1.48	1.12
1:B:930:LEU:CD2	1:B:946:LEU:CD2	2.27	1.12
1:B:782:LEU:HD23	1:B:793:VAL:HG12	1.17	1.12
1:B:560:ASN:ND2	1:B:566:ILE:HG12	1.64	1.12
1:B:114:LEU:HB2	1:B:135:LEU:HD11	1.20	1.11
1:B:3:LEU:HD21	1:B:130:GLY:HA2	1.29	1.11
1:B:234:ILE:HD13	1:B:404:LEU:CD2	1.81	1.10
1:B:543:MET:HE3	1:B:608:LEU:HD11	1.22	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:VAL:HG13	1:A:193:LYS:HE3	1.16	1.09
1:B:782:LEU:CD2	1:B:793:VAL:CG1	2.32	1.08
1:A:309:GLU:CG	1:A:609:LYS:CE	2.30	1.08
1:A:924:LEU:HD23	1:A:927:LYS:HE3	1.35	1.08
1:B:403:VAL:HG12	1:B:405:VAL:HG23	1.28	1.08
1:B:643:LEU:HD21	1:B:875:ARG:HD2	1.24	1.07
1:B:45:LEU:HD21	1:B:75:ARG:HD3	1.22	1.07
1:B:519:ILE:HG21	1:B:630:LEU:CD1	1.84	1.07
1:A:157:PHE:O	1:A:161:MET:HG3	1.56	1.06
1:C:13:LEU:HD13	1:C:28:VAL:HG13	1.33	1.06
1:A:649:ASP:OD2	1:A:661:ALA:HB3	1.53	1.06
1:A:924:LEU:HD23	1:A:927:LYS:CE	1.85	1.06
1:A:153:ALA:HB1	1:A:265:ILE:HD13	1.36	1.05
1:B:930:LEU:HD23	1:B:946:LEU:HD23	1.08	1.05
1:A:209:LEU:CD2	1:A:245:PHE:CZ	2.40	1.05
1:A:45:LEU:CD1	1:A:75:ARG:HD3	1.84	1.05
1:A:48:ILE:HD13	1:D:20:GLY:HA3	1.35	1.05
1:B:510:VAL:HG22	1:B:575:LEU:HB2	1.37	1.05
1:A:309:GLU:HG2	1:A:609:LYS:HE3	1.38	1.04
1:B:510:VAL:CG2	1:B:575:LEU:HB2	1.88	1.04
1:A:491:ASP:CG	1:A:493:TYR:CE2	2.36	1.03
1:B:234:ILE:HD13	1:B:404:LEU:HD23	1.05	1.03
1:A:762:MET:HE1	2:E:5:DC:C6	1.94	1.03
1:B:330:LEU:CD1	1:B:355:LEU:HD21	1.87	1.03
1:B:234:ILE:CD1	1:B:404:LEU:HD23	1.87	1.03
1:A:200:PHE:HZ	1:A:208:MET:SD	1.82	1.02
1:A:120:GLU:HG3	1:A:123:ARG:HE	1.23	1.02
1:B:782:LEU:HD21	1:B:793:VAL:HG12	1.34	1.01
1:B:922:LEU:HD11	1:B:926:LYS:HE3	1.43	1.01
1:A:209:LEU:HD21	1:A:245:PHE:HZ	1.22	1.00
1:B:643:LEU:HD23	1:B:875:ARG:HG2	1.37	1.00
1:A:309:GLU:CG	1:A:609:LYS:HE2	1.89	0.99
1:B:519:ILE:CG2	1:B:630:LEU:HD12	1.93	0.99
1:A:895:LEU:HD21	1:A:1016:GLU:HB2	1.42	0.99
1:B:807:LYS:CE	2:G:8:DT:C6	2.44	0.99
1:B:543:MET:SD	1:B:608:LEU:CD1	2.51	0.99
1:B:930:LEU:HD21	1:B:946:LEU:HD22	1.43	0.98
1:A:895:LEU:HD12	1:A:902:VAL:HG21	1.44	0.98
1:B:509:ILE:CG2	1:B:576:VAL:CG2	2.29	0.97
1:B:54:LYS:HE2	1:B:58:GLY:HA2	1.44	0.97
1:B:45:LEU:HD21	1:B:75:ARG:CD	1.94	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:VAL:CG1	1:B:405:VAL:HG23	1.94	0.96
1:B:556:ARG:HG2	1:B:597:ASP:OD1	1.65	0.96
1:B:643:LEU:HD21	1:B:875:ARG:CD	1.96	0.96
1:B:643:LEU:CD2	1:B:875:ARG:CD	2.43	0.96
1:A:309:GLU:CG	1:A:609:LYS:HE3	1.95	0.96
1:B:519:ILE:HG21	1:B:630:LEU:HD12	1.48	0.96
1:B:1006:LEU:CD1	1:B:1010:VAL:HG23	1.96	0.95
1:B:509:ILE:HG21	1:B:576:VAL:HG22	1.46	0.95
1:C:69:ASP:CG	1:C:70:SER:H	1.75	0.95
1:B:560:ASN:ND2	1:B:566:ILE:CG1	2.29	0.95
1:B:529:LYS:CD	1:B:627:HIS:CE1	2.49	0.94
1:A:924:LEU:CD2	1:A:927:LYS:NZ	2.29	0.94
1:B:1006:LEU:HD11	1:B:1010:VAL:CG2	1.96	0.94
1:B:643:LEU:HD23	1:B:875:ARG:CG	1.97	0.94
1:A:153:ALA:O	1:A:265:ILE:HD11	1.66	0.93
1:B:560:ASN:HD22	1:B:566:ILE:HG12	1.32	0.93
1:B:3:LEU:CD2	1:B:130:GLY:HA2	1.98	0.93
1:B:643:LEU:HG	1:B:875:ARG:CZ	1.99	0.92
1:A:924:LEU:HD23	1:A:927:LYS:NZ	1.83	0.92
1:B:330:LEU:HD13	1:B:330:LEU:O	1.70	0.92
1:A:83:GLU:HB3	1:A:110:ARG:NE	1.84	0.92
1:A:48:ILE:CD1	1:D:20:GLY:CA	2.48	0.91
1:A:48:ILE:HD13	1:D:20:GLY:CA	2.00	0.91
1:C:13:LEU:CD1	1:C:28:VAL:HG13	2.00	0.91
1:B:643:LEU:CD2	1:B:875:ARG:HD2	2.01	0.91
1:D:54:LYS:HG3	1:D:55:ALA:H	1.36	0.90
1:B:150:PHE:HB2	1:B:272:ILE:HD11	1.51	0.90
1:A:309:GLU:HG3	1:A:609:LYS:HE2	1.53	0.90
1:B:164:LEU:HD13	1:B:261:TYR:CD2	2.06	0.90
1:B:807:LYS:HE2	2:G:8:DT:C2'	2.01	0.90
1:B:333:LYS:HE3	1:B:362:GLN:NE2	1.87	0.90
1:D:52:THR:HB	1:D:60:ASN:HD21	1.36	0.90
1:B:234:ILE:CD1	1:B:404:LEU:CD2	2.49	0.90
1:A:681:ARG:HH11	1:A:751:LEU:HD21	1.32	0.90
1:B:543:MET:HE3	1:B:608:LEU:CD1	1.98	0.90
1:A:209:LEU:HD21	1:A:245:PHE:CE2	2.06	0.90
1:A:272:ILE:HD11	1:A:278:LYS:CG	2.01	0.90
1:A:45:LEU:HD11	1:A:75:ARG:CD	2.03	0.89
1:A:895:LEU:CD2	1:A:1016:GLU:HB2	2.03	0.89
1:A:309:GLU:OE2	1:A:609:LYS:HE3	1.72	0.88
1:B:371:ASN:HD22	1:B:407:THR:HG22	1.37	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:592:TYR:CE1	1:B:630:LEU:HD11	2.08	0.88
1:B:330:LEU:HD12	1:B:355:LEU:CD2	2.04	0.87
1:B:114:LEU:HB2	1:B:135:LEU:CD1	2.05	0.87
1:B:519:ILE:CG2	1:B:630:LEU:CD1	2.52	0.87
1:B:807:LYS:CE	2:G:8:DT:H6	1.86	0.87
1:D:69:ASP:OD1	1:D:70:SER:N	2.07	0.87
1:A:209:LEU:HD11	1:A:245:PHE:CZ	2.10	0.86
1:B:114:LEU:HD21	1:B:138:LEU:HD12	1.53	0.86
1:B:215:THR:HG23	1:B:219:PHE:CE1	2.10	0.86
1:A:673:ASN:HB3	1:A:720:THR:HG21	1.57	0.86
1:D:54:LYS:HG3	1:D:55:ALA:N	1.92	0.85
1:A:372:GLU:OE2	1:A:377:PRO:HB2	1.75	0.85
1:A:491:ASP:OD2	1:A:493:TYR:HE2	1.59	0.85
1:B:556:ARG:CG	1:B:597:ASP:OD1	2.24	0.85
1:A:649:ASP:OD2	1:A:661:ALA:CB	2.24	0.85
1:A:48:ILE:CD1	1:D:20:GLY:N	2.41	0.84
1:D:118:GLY:O	1:D:119:GLU:HG3	1.77	0.83
1:B:779:VAL:HG22	1:B:796:THR:CG2	2.08	0.82
1:A:200:PHE:CZ	1:A:208:MET:SD	2.71	0.82
1:A:209:LEU:CD2	1:A:245:PHE:HZ	1.84	0.81
1:A:487:THR:HG21	3:F:24:DG:H5'	1.60	0.81
1:B:974:LEU:O	1:B:978:LYS:HG3	1.78	0.81
1:B:1006:LEU:CD1	1:B:1010:VAL:CG2	2.57	0.81
1:A:602:ARG:O	1:A:606:GLU:HG2	1.80	0.81
1:B:779:VAL:HG22	1:B:796:THR:HG22	1.62	0.81
1:A:895:LEU:HD12	1:A:902:VAL:CG2	2.10	0.81
1:B:54:LYS:CE	1:B:58:GLY:HA2	2.11	0.81
1:A:491:ASP:OD2	1:A:493:TYR:CE2	2.33	0.80
1:B:138:LEU:HD13	1:B:138:LEU:C	2.06	0.80
1:B:1006:LEU:HD12	1:B:1010:VAL:HG23	1.62	0.80
1:B:910:THR:HG22	1:B:912:GLU:OE1	1.82	0.80
1:B:330:LEU:HD11	1:B:355:LEU:HD21	1.62	0.80
1:B:510:VAL:HG22	1:B:575:LEU:CB	2.11	0.80
1:B:330:LEU:CD1	1:B:355:LEU:CD2	2.58	0.80
1:A:895:LEU:CD2	1:A:1016:GLU:CB	2.59	0.80
1:A:519:ILE:CG2	1:A:630:LEU:HD11	2.12	0.79
1:A:895:LEU:CD1	1:A:902:VAL:HG21	2.12	0.79
1:A:120:GLU:CD	1:A:123:ARG:HG3	2.06	0.79
1:D:76:GLY:HA2	1:D:103:ASN:HB3	1.64	0.79
1:A:188:PHE:HZ	1:A:208:MET:CE	1.96	0.79
1:A:309:GLU:CD	1:A:609:LYS:HE3	2.08	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:LEU:CD2	1:B:138:LEU:HD12	2.13	0.79
1:B:330:LEU:HD13	1:B:330:LEU:C	2.08	0.79
1:A:309:GLU:HG2	1:A:609:LYS:CG	2.12	0.79
1:B:592:TYR:CZ	1:B:630:LEU:HD11	2.18	0.79
1:B:518:PHE:CE1	1:B:519:ILE:HD11	2.17	0.78
1:A:272:ILE:HD11	1:A:278:LYS:HG2	1.64	0.78
1:A:272:ILE:HD11	1:A:278:LYS:HG3	1.65	0.78
1:B:529:LYS:HD2	1:B:627:HIS:NE2	1.98	0.78
1:B:807:LYS:HE2	2:G:8:DT:H2''	1.64	0.78
1:B:782:LEU:HD21	1:B:793:VAL:CG1	2.05	0.77
1:B:807:LYS:HG2	2:G:8:DT:H72	1.65	0.77
1:B:45:LEU:HD23	1:B:75:ARG:HD3	1.63	0.77
1:B:643:LEU:HD23	1:B:875:ARG:CD	2.15	0.77
1:A:588:THR:HG22	1:A:589:LYS:N	1.99	0.77
1:C:66:THR:HG22	1:C:66:THR:O	1.84	0.76
1:B:20:GLY:HA3	1:C:48:ILE:CD1	2.15	0.76
1:A:519:ILE:HG21	1:A:630:LEU:HD11	1.66	0.76
1:B:973:VAL:CG2	1:B:1006:LEU:CD2	2.40	0.75
1:A:762:MET:CE	2:E:5:DC:C6	2.70	0.75
1:B:371:ASN:ND2	1:B:407:THR:HG22	2.02	0.75
1:B:519:ILE:HG21	1:B:630:LEU:HD11	1.69	0.74
1:B:643:LEU:CD2	1:B:875:ARG:HG2	2.15	0.74
1:B:150:PHE:CD1	1:B:272:ILE:HD12	2.23	0.74
1:B:782:LEU:HD23	1:B:793:VAL:CG1	2.10	0.74
1:B:592:TYR:CE2	1:B:630:LEU:HD21	2.22	0.74
1:A:48:ILE:CD1	1:D:20:GLY:HA3	2.11	0.74
1:A:153:ALA:O	1:A:265:ILE:CD1	2.34	0.74
1:B:330:LEU:HD12	1:B:355:LEU:HD23	1.69	0.74
1:A:924:LEU:CD2	1:A:927:LYS:HZ1	2.01	0.74
1:B:519:ILE:HG22	1:B:630:LEU:HD12	1.69	0.74
1:A:322:LEU:HD13	1:A:509:ILE:HD11	1.70	0.74
1:D:54:LYS:CG	1:D:55:ALA:H	2.01	0.74
1:A:209:LEU:CG	1:A:245:PHE:HZ	2.01	0.74
1:A:188:PHE:HZ	1:A:208:MET:HE1	1.52	0.73
1:A:272:ILE:CD1	1:A:278:LYS:HG3	2.18	0.73
1:A:492:MET:SD	1:A:495:ARG:NH1	2.61	0.73
1:A:895:LEU:HD21	1:A:1016:GLU:CB	2.17	0.73
1:A:287:GLU:OE2	1:A:305:TYR:HD1	1.72	0.72
1:A:491:ASP:OD1	1:A:493:TYR:CD2	2.42	0.72
1:B:589:LYS:HA	1:B:620:HIS:CE1	2.24	0.72
1:B:3:LEU:HB3	1:B:7:LYS:HE2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:LEU:HD11	1:A:245:PHE:HZ	1.52	0.71
1:A:710:SER:OG	1:A:712:ASN:ND2	2.23	0.71
1:B:895:LEU:HD22	1:B:1013:VAL:HA	1.69	0.71
1:B:88:ASP:CG	1:B:123:ARG:HH12	1.98	0.71
1:B:509:ILE:HG22	1:B:576:VAL:HG22	0.72	0.71
1:B:197:ASN:OD1	1:B:197:ASN:O	2.08	0.71
1:B:488:LYS:HB2	1:B:523:THR:HG21	1.71	0.71
1:A:491:ASP:CG	1:A:493:TYR:CD2	2.68	0.71
1:B:592:TYR:CD2	1:B:630:LEU:HD21	2.24	0.71
1:B:861:TYR:HA	1:B:1028:THR:HG21	1.72	0.71
1:B:549:THR:HG21	1:B:553:ARG:HG2	1.74	0.70
1:A:184:GLU:OE1	1:A:244:THR:HG21	1.90	0.70
1:A:116:GLN:NE2	1:A:142:PHE:CD1	2.60	0.70
1:A:588:THR:HG22	1:A:589:LYS:H	1.55	0.70
1:C:83:GLU:HB3	1:C:109:SER:HB2	1.73	0.70
1:B:643:LEU:CD2	1:B:875:ARG:CG	2.70	0.70
1:A:309:GLU:CD	1:A:609:LYS:CE	2.64	0.70
1:A:645:VAL:HG11	1:A:666:TYR:HB3	1.73	0.70
1:A:929:ARG:O	1:A:931:LYS:HG3	1.91	0.70
1:B:114:LEU:CB	1:B:135:LEU:HD11	2.13	0.69
1:B:164:LEU:CD1	1:B:258:THR:HG22	2.22	0.69
1:C:4:GLN:HG2	1:C:5:LEU:N	2.08	0.69
1:B:560:ASN:HD21	1:B:566:ILE:CD1	2.05	0.69
1:B:807:LYS:HE2	2:G:8:DT:H2'	1.72	0.69
1:B:138:LEU:HD13	1:B:138:LEU:O	1.92	0.69
1:B:543:MET:CE	1:B:561:VAL:CG1	2.26	0.69
1:B:215:THR:CG2	1:B:219:PHE:CE1	2.76	0.69
1:B:543:MET:HE1	1:B:608:LEU:CD1	2.23	0.69
1:B:560:ASN:HD21	1:B:566:ILE:HD11	1.58	0.69
1:B:560:ASN:ND2	1:B:562:PHE:HB2	2.08	0.69
1:A:905:TYR:HB2	1:A:1012:THR:HG23	1.75	0.69
1:B:207:GLU:HG2	1:B:293:TYR:CE2	2.28	0.69
1:A:672:THR:HG21	1:A:678:VAL:HG11	1.76	0.68
1:B:4:GLN:HG2	1:B:8:LYS:NZ	2.08	0.68
1:B:333:LYS:HG3	1:B:362:GLN:NE2	2.09	0.68
1:A:91:ILE:O	1:A:95:LEU:HG	1.94	0.68
1:A:209:LEU:CD1	1:A:245:PHE:HZ	2.06	0.68
1:B:518:PHE:CZ	1:B:519:ILE:HD11	2.28	0.68
1:A:120:GLU:CD	1:A:123:ARG:CG	2.67	0.68
1:A:924:LEU:CD2	1:A:927:LYS:HZ2	2.04	0.68
1:B:782:LEU:HD22	1:B:791:PHE:CZ	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:SER:C	1:D:71:LEU:HD12	2.19	0.68
1:B:973:VAL:HG22	1:B:977:HIS:CD2	2.28	0.68
1:A:225:ASN:ND2	1:A:228:TYR:HB2	2.08	0.67
1:A:83:GLU:HG2	1:A:109:SER:HB3	1.77	0.67
1:B:643:LEU:HG	1:B:875:ARG:NE	2.09	0.67
1:A:161:MET:SD	1:A:288:ASN:HB3	2.34	0.67
1:A:1016:GLU:OE1	1:A:1019:ARG:NH2	2.27	0.67
1:B:642:PHE:HZ	1:B:830:ALA:HA	1.59	0.67
1:B:671:VAL:HG23	1:B:764:TYR:HE2	1.60	0.67
1:A:467:TYR:CE2	1:A:492:MET:HE1	2.30	0.67
1:D:25:GLU:OE2	5:D:1101:CA:CA	1.70	0.67
1:A:750:VAL:HG23	1:A:899:PHE:HZ	1.60	0.66
1:A:862:ARG:HG2	1:A:869:LEU:HD13	1.76	0.66
1:B:807:LYS:HE2	2:G:8:DT:H6	1.58	0.66
1:A:762:MET:HE2	2:E:6:DC:H5	1.58	0.66
1:B:975:GLU:HA	1:B:978:LYS:HD2	1.77	0.66
1:B:150:PHE:CB	1:B:272:ILE:HD11	2.22	0.66
1:D:33:GLN:NE2	1:D:49:THR:HG21	2.09	0.66
1:D:71:LEU:HD12	1:D:71:LEU:N	2.11	0.66
1:B:518:PHE:CE1	1:B:519:ILE:CD1	2.78	0.66
1:A:242:ALA:C	1:A:244:THR:H	2.04	0.66
1:B:643:LEU:CD2	1:B:875:ARG:NE	2.59	0.66
1:A:422:LEU:HG	1:A:422:LEU:O	1.95	0.66
1:A:895:LEU:HG	1:A:895:LEU:O	1.96	0.65
1:B:164:LEU:HD12	1:B:258:THR:HG22	1.76	0.65
1:B:970:LEU:HD21	1:B:1007:LEU:HA	1.77	0.65
1:A:189:VAL:CG1	1:A:193:LYS:CE	2.64	0.65
1:B:333:LYS:HE3	1:B:362:GLN:HE21	1.58	0.65
1:B:592:TYR:CE2	1:B:630:LEU:CD2	2.80	0.65
1:A:850:HIS:HE1	1:A:893:MET:SD	2.19	0.65
1:B:187:HIS:O	1:B:191:ILE:HG12	1.97	0.65
1:A:682:ALA:HB3	1:A:685:GLU:HB2	1.78	0.65
1:B:529:LYS:HD2	1:B:627:HIS:ND1	2.09	0.65
1:A:817:THR:OG1	1:A:820:GLY:HA3	1.96	0.65
1:C:32:PHE:CE2	1:C:36:LEU:HD11	2.31	0.65
1:B:560:ASN:HD21	1:B:566:ILE:CG1	2.09	0.65
1:A:309:GLU:OE2	1:A:609:LYS:CE	2.42	0.65
1:A:929:ARG:HG2	1:A:931:LYS:HE3	1.79	0.65
1:A:372:GLU:OE2	1:A:377:PRO:CB	2.45	0.64
1:A:780:ILE:HG13	1:A:849:PHE:CE1	2.31	0.64
1:C:114:LEU:HB2	1:C:135:LEU:HD11	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:GLU:CG	1:A:109:SER:HB3	2.27	0.64
1:B:667:SER:OG	1:B:769:ILE:HD11	1.97	0.64
1:B:963:LYS:HA	1:B:968:SER:HA	1.78	0.64
1:B:124:VAL:HG22	1:B:135:LEU:HD22	1.78	0.64
1:B:958:ALA:HB1	1:B:1018:VAL:HG11	1.80	0.64
1:B:946:LEU:HD21	1:B:1007:LEU:HD11	1.79	0.64
1:C:66:THR:HG22	1:C:68:LYS:HG3	1.77	0.64
1:B:592:TYR:CZ	1:B:630:LEU:CD1	2.81	0.64
1:D:52:THR:HB	1:D:60:ASN:ND2	2.10	0.64
1:A:737:LYS:O	1:A:740:ILE:HG12	1.98	0.64
1:A:45:LEU:HD11	1:A:75:ARG:NH1	2.13	0.63
1:A:862:ARG:HG2	1:A:869:LEU:CD1	2.27	0.63
1:C:6:VAL:HG13	1:C:132:LEU:HD23	1.80	0.63
1:B:3:LEU:HD21	1:B:130:GLY:CA	2.18	0.63
1:B:452:ARG:HB3	1:B:464:ASN:HD21	1.62	0.63
1:A:188:PHE:CZ	1:A:208:MET:CE	2.81	0.63
1:A:747:PRO:HD3	1:A:804:LEU:HD12	1.80	0.63
1:B:243:ALA:O	1:B:247:LYS:HG3	1.98	0.63
1:B:645:VAL:HG21	1:B:666:TYR:HB3	1.81	0.63
1:B:1006:LEU:HD11	1:B:1010:VAL:HG21	1.78	0.63
1:B:336:GLU:HB2	1:B:442:VAL:HA	1.81	0.63
1:A:153:ALA:CB	1:A:265:ILE:HD13	2.23	0.62
1:B:731:LYS:HG2	1:B:732:SER:H	1.63	0.62
1:A:48:ILE:HD12	1:D:20:GLY:CA	2.30	0.62
1:A:357:LYS:O	1:A:357:LYS:HG2	2.00	0.62
1:B:150:PHE:HB2	1:B:272:ILE:CD1	2.28	0.62
1:A:591:TRP:HB3	1:A:618:PHE:HB3	1.81	0.61
1:C:69:ASP:CG	1:C:70:SER:N	2.45	0.61
1:B:807:LYS:HE2	2:G:8:DT:C6	2.34	0.61
1:A:762:MET:HE1	2:E:5:DC:C5	2.35	0.61
1:C:32:PHE:CD2	1:C:36:LEU:HD11	2.36	0.61
1:A:309:GLU:HG2	1:A:609:LYS:HG3	1.81	0.61
1:B:138:LEU:C	1:B:138:LEU:CD1	2.74	0.61
1:B:807:LYS:CE	2:G:8:DT:H2''	2.31	0.61
1:D:69:ASP:CG	1:D:70:SER:H	2.07	0.61
1:A:519:ILE:HG22	1:A:630:LEU:CD1	2.31	0.61
1:A:116:GLN:CD	1:A:142:PHE:CD1	2.80	0.60
1:C:13:LEU:CD1	1:C:28:VAL:HG22	2.32	0.60
1:D:118:GLY:O	1:D:119:GLU:CG	2.49	0.60
1:A:928:ALA:HB2	1:A:996:PHE:HB2	1.84	0.60
1:A:48:ILE:HD11	1:D:20:GLY:N	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:LEU:CD1	1:B:330:LEU:C	2.75	0.60
1:B:467:TYR:HB2	1:B:470:ILE:HG22	1.83	0.60
1:A:746:ARG:HA	1:A:804:LEU:HD12	1.83	0.60
1:B:3:LEU:CD2	1:B:130:GLY:CA	2.77	0.60
1:B:592:TYR:CG	1:B:621:ILE:HD11	2.37	0.60
1:A:83:GLU:HB3	1:A:110:ARG:CZ	2.32	0.60
1:A:560:ASN:HB2	1:A:564:ASP:HA	1.84	0.60
1:A:209:LEU:CD1	1:A:245:PHE:CZ	2.81	0.60
1:B:363:LYS:HA	1:B:367:GLU:HB2	1.84	0.59
1:B:509:ILE:HG22	1:B:576:VAL:CB	2.29	0.59
1:A:487:THR:HG21	3:F:24:DG:C5'	2.31	0.59
1:B:164:LEU:HD13	1:B:261:TYR:HD2	1.65	0.59
1:A:408:LEU:O	1:A:470:ILE:CG1	2.50	0.59
1:A:905:TYR:HB2	1:A:1012:THR:CG2	2.32	0.59
1:B:510:VAL:HG23	1:B:510:VAL:O	2.02	0.59
1:B:803:ASP:OD1	1:B:803:ASP:O	2.21	0.59
1:A:116:GLN:NE2	1:A:142:PHE:CE1	2.71	0.59
1:A:528:ARG:HA	1:A:531:VAL:HG22	1.84	0.59
1:B:556:ARG:HG3	1:B:597:ASP:CG	2.27	0.59
1:A:555:LYS:HB3	1:A:598:PHE:CE1	2.37	0.59
1:B:543:MET:SD	1:B:608:LEU:HD13	2.41	0.59
1:A:408:LEU:HB3	1:A:470:ILE:HG13	1.84	0.59
1:A:519:ILE:HG22	1:A:630:LEU:HD11	1.85	0.59
1:C:95:LEU:HD11	1:C:115:MET:HE1	1.85	0.59
1:B:403:VAL:CG1	1:B:405:VAL:CG2	2.75	0.59
1:A:336:GLU:HB2	1:A:442:VAL:HA	1.85	0.59
1:B:589:LYS:HA	1:B:620:HIS:HE1	1.68	0.58
1:A:83:GLU:HB3	1:A:110:ARG:HE	1.68	0.58
1:A:184:GLU:OE1	1:A:244:THR:CG2	2.51	0.58
1:B:20:GLY:HA3	1:C:48:ILE:HD13	1.84	0.58
1:A:504:LEU:HD22	1:A:510:VAL:HG23	1.85	0.58
1:B:333:LYS:HG3	1:B:362:GLN:CD	2.28	0.58
1:B:357:LYS:HG3	1:B:392:LYS:HE3	1.85	0.58
1:C:48:ILE:HG22	1:C:51:VAL:CG2	2.33	0.58
1:A:8:LYS:HG2	1:A:12:ARG:HE	1.69	0.58
1:B:274:ASP:OD2	1:B:277:GLU:HG2	2.02	0.58
1:A:188:PHE:CE2	1:A:208:MET:SD	2.97	0.58
1:B:543:MET:CE	1:B:561:VAL:CB	2.82	0.58
1:A:519:ILE:HG12	1:A:540:ILE:HD13	1.85	0.58
1:A:710:SER:HG	1:A:712:ASN:HD21	1.52	0.57
1:A:681:ARG:NH1	1:A:751:LEU:HD21	2.12	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:LEU:HD21	1:B:75:ARG:NE	2.19	0.57
1:B:433:ARG:HA	1:B:436:ARG:HD3	1.85	0.57
1:D:71:LEU:N	1:D:71:LEU:CD1	2.67	0.57
1:A:309:GLU:HG2	1:A:609:LYS:CD	2.33	0.57
1:A:588:THR:CG2	1:A:589:LYS:H	2.17	0.57
1:B:309:GLU:HB3	1:B:609:LYS:HB2	1.85	0.57
1:C:124:VAL:HG22	1:C:135:LEU:HD22	1.85	0.57
1:A:452:ARG:HH22	1:A:462:ASN:HB3	1.68	0.57
1:A:45:LEU:HD11	1:A:75:ARG:CZ	2.34	0.57
1:A:668:LEU:HD23	1:A:809:GLN:HA	1.86	0.57
1:A:762:MET:HE2	2:E:6:DC:C5	2.38	0.57
1:C:122:GLN:HB3	1:C:135:LEU:HD13	1.86	0.57
1:A:146:GLN:NE2	1:A:271:GLN:OE1	2.37	0.57
1:A:403:VAL:HG12	1:A:404:LEU:N	2.20	0.57
1:B:529:LYS:CE	1:B:627:HIS:CE1	2.88	0.57
1:B:543:MET:CE	1:B:608:LEU:HD12	2.32	0.57
1:B:643:LEU:CG	1:B:875:ARG:CZ	2.81	0.57
1:B:700:ILE:O	1:B:708:LEU:HD21	2.05	0.56
1:A:881:GLU:OE1	1:A:884:ARG:HD2	2.05	0.56
1:A:178:LYS:NZ	1:A:245:PHE:HA	2.21	0.56
1:B:777:ASN:HD22	1:B:816:TYR:HE1	1.54	0.56
1:A:855:VAL:HG11	1:A:877:PRO:HD2	1.86	0.56
1:B:750:VAL:HG23	1:B:750:VAL:O	2.05	0.56
1:A:161:MET:O	1:A:165:LEU:HG	2.06	0.56
1:A:803:ASP:OD1	1:A:803:ASP:O	2.22	0.56
1:A:203:ARG:NH1	1:A:204:ASP:OD1	2.39	0.56
1:A:762:MET:HE1	2:E:5:DC:H6	1.60	0.56
1:A:49:THR:O	1:D:27:SER:OG	2.22	0.56
1:A:203:ARG:O	1:A:203:ARG:HG2	2.05	0.56
1:A:328:LYS:HD3	1:A:443:ARG:HH12	1.71	0.56
1:B:52:THR:HG22	1:B:62:ARG:HE	1.71	0.55
1:B:922:LEU:HD12	1:B:949:LEU:HD11	1.88	0.55
1:A:724:ILE:O	1:A:728:GLN:HG3	2.07	0.55
1:A:153:ALA:HB1	1:A:265:ILE:CD1	2.25	0.55
1:B:215:THR:CG2	1:B:219:PHE:CZ	2.89	0.55
1:A:214:LEU:HD12	1:A:262:TYR:OH	2.07	0.55
1:A:652:GLN:CD	1:A:664:LYS:HE3	2.32	0.55
1:A:924:LEU:HD21	1:A:927:LYS:HZ1	1.72	0.55
1:B:4:GLN:HG2	1:B:8:LYS:HZ2	1.72	0.55
1:B:813:PHE:HZ	1:B:846:GLU:HG2	1.70	0.55
1:A:116:GLN:NE2	1:A:142:PHE:HD1	2.03	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:VAL:HG22	1:B:123:ARG:HG3	1.89	0.55
1:B:642:PHE:CZ	1:B:830:ALA:HA	2.40	0.55
1:A:519:ILE:CG2	1:A:630:LEU:CD1	2.85	0.55
1:A:587:ASP:OD1	1:A:588:THR:N	2.40	0.55
1:A:474:ILE:HD11	1:A:495:ARG:HA	1.89	0.55
1:B:406:ASP:HB3	1:B:409:ASP:HB2	1.89	0.55
1:B:807:LYS:HE3	2:G:8:DT:C5	2.36	0.54
1:A:45:LEU:CD2	1:A:75:ARG:HD3	2.37	0.54
1:A:639:TRP:CH2	1:A:869:LEU:HD23	2.42	0.54
1:B:234:ILE:CD1	1:B:404:LEU:HD22	2.37	0.54
1:A:233:ASN:HB2	1:A:427:THR:HG21	1.90	0.54
1:A:929:ARG:HG2	1:A:931:LYS:CE	2.37	0.54
1:B:403:VAL:HG22	1:B:433:ARG:HB3	1.89	0.54
1:B:858:HIS:CE1	1:B:1025:PRO:HG2	2.43	0.54
1:A:780:ILE:HG13	1:A:849:PHE:CZ	2.41	0.54
1:A:986:THR:O	1:A:986:THR:HG22	2.07	0.54
1:B:973:VAL:CG2	1:B:977:HIS:CD2	2.90	0.54
1:B:592:TYR:CB	1:B:621:ILE:HD11	2.38	0.54
1:A:83:GLU:HG2	1:A:109:SER:CB	2.37	0.54
1:A:825:ASN:O	1:A:826:ILE:C	2.50	0.54
1:B:807:LYS:CE	2:G:8:DT:C2'	2.83	0.54
1:B:996:PHE:CE1	1:B:1003:VAL:HG21	2.42	0.54
1:A:850:HIS:CE1	1:A:893:MET:SD	3.00	0.53
1:C:13:LEU:CD1	1:C:28:VAL:CG1	2.80	0.53
1:A:153:ALA:C	1:A:265:ILE:CD1	2.81	0.53
1:B:534:ASP:OD1	1:B:577:ARG:CZ	2.57	0.53
1:B:731:LYS:HG2	1:B:732:SER:N	2.24	0.53
1:B:797:ASP:OD1	1:B:797:ASP:O	2.27	0.53
1:B:814:TYR:HB3	1:B:822:ARG:HG3	1.91	0.53
1:A:45:LEU:HD13	1:A:75:ARG:HD3	1.86	0.53
1:A:787:ALA:HB3	1:A:870:ARG:HG2	1.91	0.53
1:B:198:PRO:HD2	1:B:465:ARG:HH21	1.74	0.53
1:A:652:GLN:OE1	1:A:664:LYS:HE3	2.08	0.53
1:A:895:LEU:CD1	1:A:902:VAL:CG2	2.79	0.53
1:B:896:HIS:C	1:B:898:GLY:N	2.64	0.53
1:A:185:ARG:NH1	1:A:186:ASP:OD1	2.41	0.53
1:B:238:LEU:CD1	1:B:375:LEU:HD21	2.39	0.52
1:D:8:LYS:HE3	1:D:11:LYS:HD2	1.91	0.52
1:B:54:LYS:CE	1:B:58:GLY:CA	2.86	0.52
1:A:164:LEU:HD13	1:A:261:TYR:CD2	2.43	0.52
1:A:403:VAL:HG11	1:A:434:ALA:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:824:ASN:HD22	1:A:845:ARG:HG3	1.75	0.52
1:B:238:LEU:CD1	1:B:375:LEU:CD2	2.87	0.52
1:B:766:MET:HE2	1:B:800:PRO:HD2	1.91	0.52
1:A:157:PHE:O	1:A:161:MET:CG	2.46	0.52
1:A:650:THR:CG2	1:A:666:TYR:CD1	2.92	0.52
1:A:119:GLU:OE1	1:A:121:VAL:HG12	2.09	0.52
1:A:372:GLU:CD	1:A:377:PRO:HB2	2.33	0.52
1:A:450:PRO:HA	2:E:11:DA:H62	1.75	0.52
1:B:701:ILE:HG13	1:B:731:LYS:O	2.10	0.52
1:B:974:LEU:CD2	1:B:1007:LEU:HD21	2.40	0.52
1:A:83:GLU:HA	1:A:108:ASP:O	2.10	0.52
1:A:176:GLU:O	1:A:176:GLU:HG2	2.09	0.52
1:A:666:TYR:HE2	1:A:809:GLN:HB3	1.75	0.52
1:A:527:PHE:CZ	1:A:531:VAL:HG11	2.45	0.51
1:A:650:THR:CG2	1:A:666:TYR:HD1	2.23	0.51
1:B:643:LEU:CG	1:B:875:ARG:NE	2.73	0.51
1:C:132:LEU:HG	1:C:136:LEU:CD1	2.40	0.51
1:A:209:LEU:CD2	1:A:245:PHE:CE2	2.80	0.51
1:A:487:THR:CG2	3:F:24:DG:H5'	2.36	0.51
1:B:150:PHE:CG	1:B:272:ILE:CD1	2.94	0.51
1:A:540:ILE:HD11	1:A:629:TRP:CZ3	2.46	0.51
1:A:826:ILE:HG22	1:A:845:ARG:HH21	1.76	0.51
1:B:974:LEU:HD21	1:B:1007:LEU:HD21	1.93	0.51
1:A:543:MET:HB3	1:A:561:VAL:HG21	1.91	0.51
1:A:750:VAL:CG2	1:A:899:PHE:HZ	2.23	0.51
1:B:536:ASP:H	1:B:577:ARG:HA	1.75	0.51
1:B:643:LEU:HG	1:B:875:ARG:NH2	2.25	0.51
1:A:666:TYR:HA	1:A:812:PRO:HD3	1.93	0.51
1:B:899:PHE:HD2	1:B:1006:LEU:CD1	2.23	0.51
1:A:73:GLN:NE2	1:A:146:GLN:HE22	2.09	0.51
1:B:54:LYS:HE2	1:B:58:GLY:CA	2.31	0.51
1:B:739:SER:OG	1:B:754:TYR:CE1	2.64	0.51
1:B:996:PHE:HE1	1:B:1003:VAL:HG21	1.75	0.51
1:A:675:ASP:HA	1:A:678:VAL:HG12	1.92	0.51
1:A:865:TYR:O	1:A:869:LEU:HG	2.11	0.51
1:A:895:LEU:CD2	1:A:1016:GLU:HB3	2.40	0.51
1:B:164:LEU:CD1	1:B:261:TYR:CD2	2.90	0.51
1:A:45:LEU:HD21	1:A:75:ARG:CD	2.40	0.51
1:A:650:THR:HG21	1:A:666:TYR:CE1	2.46	0.50
1:B:621:ILE:HG21	1:B:629:TRP:HB3	1.93	0.50
1:B:977:HIS:CG	1:B:999:HIS:NE2	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:ASP:OD1	1:B:123:ARG:NH1	2.44	0.50
1:B:556:ARG:HG3	1:B:597:ASP:OD1	2.09	0.50
1:B:180:ASP:O	1:B:184:GLU:HG2	2.10	0.50
1:A:16:ILE:HG21	1:A:27:SER:O	2.12	0.50
1:A:710:SER:HG	1:A:712:ASN:ND2	2.08	0.50
1:B:519:ILE:CG2	1:B:630:LEU:CG	2.90	0.50
1:B:975:GLU:HA	1:B:978:LYS:CD	2.40	0.50
1:D:106:PHE:HB2	1:D:113:VAL:HG22	1.92	0.50
1:A:491:ASP:OD1	1:A:493:TYR:HD2	1.92	0.50
1:A:45:LEU:HD11	1:A:75:ARG:NE	2.26	0.50
1:A:849:PHE:HE2	1:A:893:MET:HG3	1.76	0.50
1:B:311:VAL:HG21	1:B:346:THR:HG22	1.94	0.50
1:B:333:LYS:HG3	1:B:362:GLN:HE22	1.75	0.50
1:B:287:GLU:OE2	1:B:305:TYR:HD1	1.94	0.49
1:B:880:PRO:O	1:B:881:GLU:HG3	2.12	0.49
1:A:556:ARG:HB3	1:A:597:ASP:OD2	2.12	0.49
1:A:968:SER:OG	1:A:971:GLU:CD	2.55	0.49
1:B:150:PHE:CD1	1:B:272:ILE:CD1	2.94	0.49
1:B:697:TYR:CZ	1:B:701:ILE:HD11	2.47	0.49
1:C:4:GLN:HG2	1:C:5:LEU:H	1.75	0.49
1:C:95:LEU:HD22	1:C:101:ARG:HG2	1.94	0.49
1:A:24:ASN:HB3	2:G:24:DC:H5''	1.95	0.49
1:B:899:PHE:CD2	1:B:1006:LEU:CD1	2.96	0.49
1:B:914:PRO:HG3	1:B:922:LEU:HD13	1.94	0.49
1:A:777:ASN:HD21	1:A:814:TYR:H	1.58	0.49
1:B:147:VAL:O	1:B:151:ARG:HG3	2.11	0.49
1:C:113:VAL:HG13	1:C:120:GLU:HG3	1.93	0.49
1:A:116:GLN:CG	1:A:142:PHE:CE1	2.96	0.49
1:A:700:ILE:O	1:A:703:LEU:HB2	2.13	0.49
1:B:960:TRP:CD1	1:B:960:TRP:H	2.30	0.49
1:D:118:GLY:C	1:D:119:GLU:HG3	2.38	0.49
1:A:78:TRP:CZ2	1:A:80:SER:HB2	2.48	0.49
1:A:693:PHE:C	1:A:695:GLY:N	2.69	0.49
1:A:242:ALA:C	1:A:244:THR:N	2.70	0.49
1:B:667:SER:OG	1:B:769:ILE:CD1	2.60	0.49
1:B:164:LEU:HD11	1:B:258:THR:HG22	1.93	0.49
1:B:219:PHE:HA	1:B:223:PHE:HB2	1.95	0.49
1:C:45:LEU:HD22	1:C:67:LEU:HG	1.94	0.49
1:A:650:THR:HG21	1:A:666:TYR:CD1	2.47	0.49
1:B:488:LYS:NZ	2:G:8:DT:H1'	2.28	0.49
1:B:858:HIS:HE1	1:B:1025:PRO:HG2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:899:PHE:CD2	1:B:1006:LEU:HD13	2.48	0.48
1:D:105:ILE:HG12	1:D:114:LEU:HD13	1.94	0.48
1:A:519:ILE:HD11	1:A:540:ILE:HG21	1.96	0.48
1:A:668:LEU:HD21	1:A:809:GLN:HE21	1.79	0.48
1:B:243:ALA:O	1:B:247:LYS:HE3	2.13	0.48
1:A:20:GLY:HA2	1:D:68:LYS:HD3	1.95	0.48
1:A:847:ASP:HB3	1:A:882:PHE:HE2	1.78	0.48
1:B:519:ILE:CG2	1:B:630:LEU:HG	2.42	0.48
1:B:543:MET:HE1	1:B:608:LEU:HD12	1.93	0.48
1:A:109:SER:O	1:A:110:ARG:HG3	2.14	0.48
1:A:164:LEU:HD13	1:A:261:TYR:HB2	1.95	0.48
1:A:403:VAL:CG1	1:A:404:LEU:N	2.77	0.48
1:B:652:GLN:HG3	1:B:658:GLN:HB3	1.95	0.48
1:B:782:LEU:HD22	1:B:793:VAL:HG12	1.72	0.48
1:B:813:PHE:CZ	1:B:846:GLU:HG2	2.47	0.48
1:B:928:ALA:HB2	1:B:996:PHE:HB2	1.95	0.48
1:A:408:LEU:O	1:A:470:ILE:HD11	2.13	0.48
1:A:475:LYS:HA	1:A:479:VAL:HB	1.94	0.48
1:B:529:LYS:NZ	1:B:627:HIS:CE1	2.81	0.48
1:B:556:ARG:CG	1:B:597:ASP:CG	2.83	0.48
1:B:642:PHE:HD1	1:B:878:PHE:CZ	2.31	0.48
1:A:467:TYR:HE2	1:A:492:MET:HE1	1.77	0.48
1:B:973:VAL:HG21	1:B:1006:LEU:HD23	0.65	0.48
1:A:445:ILE:HD11	1:A:503:ARG:HB3	1.96	0.48
1:A:747:PRO:HB3	1:A:964:LEU:HD23	1.96	0.48
1:B:896:HIS:C	1:B:898:GLY:H	2.22	0.48
1:B:962:TYR:O	1:B:963:LYS:C	2.57	0.48
1:A:924:LEU:HD22	1:A:927:LYS:HZ2	1.77	0.47
1:A:976:ARG:HD2	1:A:976:ARG:HA	1.54	0.47
1:B:803:ASP:OD2	3:H:19:DC:H5	1.97	0.47
1:A:741:VAL:HG11	1:A:773:GLY:HA3	1.96	0.47
1:A:789:LYS:HB2	1:A:806:GLU:HG3	1.95	0.47
1:A:792:GLN:HG3	1:A:805:LEU:HD13	1.95	0.47
1:B:769:ILE:HD13	1:B:812:PRO:HG3	1.96	0.47
1:A:711:ARG:HE	1:A:711:ARG:HB3	1.45	0.47
4:A:1101:SAM:HB1	4:A:1101:SAM:HE2	1.60	0.47
1:B:445:ILE:O	1:B:445:ILE:HG22	2.13	0.47
1:A:343:GLY:HA3	4:A:1101:SAM:HG2	1.96	0.47
1:B:535:PHE:CD1	1:B:577:ARG:HB2	2.50	0.47
1:A:189:VAL:O	1:A:193:LYS:HG3	2.14	0.47
1:A:362:GLN:HE21	1:A:363:LYS:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:ARG:HD2	1:A:464:ASN:HD21	1.79	0.47
1:A:746:ARG:C	1:A:804:LEU:CD1	2.88	0.47
1:A:895:LEU:O	1:A:895:LEU:CG	2.63	0.47
1:B:150:PHE:HA	1:B:268:ALA:HB1	1.95	0.47
1:B:203:ARG:O	1:B:207:GLU:HG3	2.15	0.47
1:B:686:LEU:HD23	1:B:740:ILE:HG23	1.97	0.47
1:B:973:VAL:HG23	1:B:977:HIS:NE2	2.29	0.47
1:B:116:GLN:HE21	1:B:142:PHE:HB2	1.79	0.47
1:B:899:PHE:O	1:B:1009:ARG:HB3	2.15	0.47
1:A:325:HIS:CD2	1:A:576:VAL:HG21	2.50	0.47
1:B:507:ASP:OD1	1:B:507:ASP:O	2.33	0.47
1:B:531:VAL:HG12	1:B:538:ILE:HD11	1.97	0.47
1:A:552:GLU:HB3	1:A:556:ARG:HH21	1.80	0.47
1:B:45:LEU:HD21	1:B:75:ARG:CZ	2.45	0.47
3:H:5:DG:H2"	3:H:6:DG:C8	2.50	0.47
1:A:541:LEU:HD11	1:A:607:TRP:HH2	1.81	0.46
1:A:862:ARG:HA	1:A:869:LEU:CD1	2.45	0.46
1:B:899:PHE:CE2	1:B:1006:LEU:HD13	2.50	0.46
1:B:930:LEU:O	1:B:931:LYS:HG3	2.15	0.46
1:C:13:LEU:HD12	1:C:28:VAL:HG22	1.96	0.46
1:A:83:GLU:HG3	1:A:109:SER:HB3	1.98	0.46
1:A:666:TYR:CE2	1:A:809:GLN:HB3	2.50	0.46
1:B:961:ALA:C	1:B:963:LYS:H	2.23	0.46
1:A:445:ILE:HD13	1:A:500:ALA:HA	1.98	0.46
1:A:680:SER:HB3	1:A:686:LEU:HD13	1.97	0.46
1:A:865:TYR:HB3	1:A:868:ASN:HB2	1.97	0.46
1:B:237:GLN:OE1	1:B:427:THR:HG22	2.15	0.46
1:B:700:ILE:HA	1:B:703:LEU:HD11	1.98	0.46
1:B:922:LEU:CD1	1:B:926:LYS:HE3	2.30	0.46
2:E:16:DG:H2"	2:E:17:DA:C8	2.50	0.46
1:A:119:GLU:OE1	1:A:121:VAL:CG1	2.64	0.46
1:A:762:MET:CE	2:E:5:DC:C5	2.97	0.46
1:B:220:THR:HG22	1:B:226:ALA:HA	1.97	0.46
1:C:66:THR:O	1:C:66:THR:CG2	2.48	0.46
1:C:102:ASP:O	1:C:116:GLN:HA	2.15	0.46
1:B:232:ASN:HD21	1:B:378:TYR:HE2	1.62	0.46
1:B:813:PHE:HB2	1:B:849:PHE:CE1	2.51	0.46
1:A:736:GLU:C	1:A:738:ASN:N	2.72	0.46
1:C:48:ILE:HG22	1:C:51:VAL:HG23	1.97	0.46
1:A:116:GLN:CD	1:A:142:PHE:CE1	2.94	0.46
1:B:6:VAL:HG11	1:B:129:ALA:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:654:LYS:H	1:B:654:LYS:HG2	1.54	0.46
1:B:893:MET:O	1:B:897:ILE:HB	2.15	0.46
1:A:561:VAL:HG12	1:A:561:VAL:O	2.16	0.46
1:B:222:VAL:HG12	1:B:266:GLN:HG2	1.97	0.46
1:B:649:ASP:O	1:B:652:GLN:HB3	2.16	0.46
1:A:188:PHE:CZ	1:A:208:MET:SD	3.09	0.46
1:B:560:ASN:HB3	1:B:564:ASP:HA	1.98	0.45
1:B:922:LEU:CD1	1:B:949:LEU:HD11	2.47	0.45
1:C:45:LEU:HD21	1:C:75:ARG:HD3	1.98	0.45
1:D:59:ASN:HD21	2:G:26:DC:H5'	1.82	0.45
1:A:871:GLN:HE21	1:A:871:GLN:HB2	1.55	0.45
1:B:352:ILE:HA	1:B:360:LEU:HD13	1.98	0.45
1:D:94:LYS:HA	1:D:94:LYS:HD3	1.68	0.45
1:A:662:ILE:HA	1:A:830:ALA:HB2	1.97	0.45
1:B:592:TYR:HB2	1:B:621:ILE:CD1	2.47	0.45
1:B:701:ILE:HD13	1:B:701:ILE:HA	1.67	0.45
1:B:282:LEU:HD22	1:B:380:ILE:HG23	1.99	0.45
1:B:807:LYS:CG	2:G:8:DT:H72	2.43	0.45
1:A:73:GLN:HE21	1:A:146:GLN:HE22	1.63	0.45
1:B:895:LEU:HB3	1:B:1013:VAL:HG13	1.99	0.45
1:D:69:ASP:CG	1:D:70:SER:N	2.68	0.45
1:A:161:MET:SD	1:A:288:ASN:CB	3.04	0.45
1:B:233:ASN:ND2	1:B:429:GLU:HB3	2.31	0.45
1:A:239:GLN:O	1:A:240:GLN:C	2.60	0.45
1:B:272:ILE:HG21	1:B:277:GLU:HB2	1.99	0.45
1:B:475:LYS:HA	1:B:479:VAL:HB	1.99	0.45
1:B:973:VAL:CG2	1:B:977:HIS:NE2	2.80	0.45
2:G:18:DA:H2''	2:G:19:DC:H5'	1.98	0.45
1:A:588:THR:CG2	1:A:589:LYS:N	2.66	0.45
1:B:510:VAL:HG23	1:B:575:LEU:HB2	1.86	0.45
1:D:37:SER:O	1:D:41:GLU:HG3	2.17	0.45
1:A:233:ASN:HB3	1:A:429:GLU:OE1	2.17	0.45
1:B:592:TYR:CZ	1:B:630:LEU:HD21	2.51	0.45
1:A:372:GLU:HG2	1:A:378:TYR:HB2	1.99	0.44
1:B:324:LYS:HB3	1:B:324:LYS:HE3	1.41	0.44
1:B:341:ALA:HB1	4:B:1101:SAM:H5'2	1.99	0.44
1:B:855:VAL:HG11	1:B:877:PRO:HD2	1.98	0.44
1:C:120:GLU:OE2	1:C:123:ARG:HB2	2.17	0.44
1:C:126:MET:HB3	1:C:126:MET:HE2	1.55	0.44
1:A:789:LYS:H	1:A:806:GLU:HG3	1.82	0.44
1:A:898:GLY:O	1:A:902:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:536:ASP:O	1:B:537:HIS:CG	2.70	0.44
1:B:984:ASP:O	1:B:985:ALA:C	2.60	0.44
1:C:2:SER:HB2	1:C:4:GLN:OE1	2.17	0.44
1:C:5:LEU:HD21	1:C:38:ASP:HB2	1.99	0.44
1:A:445:ILE:HG22	1:A:445:ILE:O	2.16	0.44
1:A:747:PRO:CD	1:A:804:LEU:HD12	2.47	0.44
1:A:45:LEU:HD21	1:A:75:ARG:HD3	1.97	0.44
1:B:33:GLN:NE2	1:C:30:ALA:HB1	2.31	0.44
1:D:111:LEU:HA	1:D:125:ASP:HA	1.98	0.44
1:B:518:PHE:CD1	1:B:519:ILE:HD12	2.53	0.44
1:B:681:ARG:H	1:B:681:ARG:HG2	1.41	0.44
1:A:451:TYR:CE1	1:A:514:SER:HA	2.53	0.44
1:A:910:THR:O	1:A:910:THR:OG1	2.29	0.44
1:B:188:PHE:CZ	1:B:238:LEU:HD21	2.53	0.44
1:B:520:ASP:CG	1:B:520:ASP:O	2.61	0.44
1:B:509:ILE:HG21	1:B:576:VAL:CG2	2.25	0.44
1:A:164:LEU:HD21	1:A:262:TYR:CE1	2.53	0.44
1:A:193:LYS:HE2	1:A:200:PHE:O	2.18	0.44
1:B:658:GLN:O	1:B:659:GLU:C	2.61	0.44
1:B:958:ALA:O	1:B:959:ALA:C	2.61	0.44
1:D:111:LEU:N	1:D:126:MET:HG3	2.32	0.44
1:A:181:TYR:CE1	1:A:245:PHE:CE2	3.06	0.43
1:A:723:THR:O	1:A:724:ILE:C	2.60	0.43
1:A:847:ASP:HB3	1:A:882:PHE:CE2	2.53	0.43
1:A:935:ASP:C	1:A:937:ALA:N	2.76	0.43
1:B:932:VAL:HA	1:B:944:VAL:HG22	1.99	0.43
1:B:952:LEU:HD12	1:B:952:LEU:HA	1.89	0.43
1:A:457:ASN:HB2	1:A:718:LYS:HE2	1.99	0.43
1:A:659:GLU:O	1:A:659:GLU:HG3	2.17	0.43
1:B:427:THR:OG1	1:B:430:ASN:HB2	2.18	0.43
1:B:543:MET:HE1	1:B:561:VAL:CB	2.48	0.43
1:A:696:ARG:HH22	1:A:714:GLU:HB2	1.84	0.43
1:B:333:LYS:HG3	1:B:362:GLN:OE1	2.19	0.43
1:B:920:GLU:HA	1:D:92:GLN:HE21	1.82	0.43
1:B:977:HIS:HB3	1:B:999:HIS:NE2	2.33	0.43
1:D:66:THR:O	1:D:67:LEU:C	2.61	0.43
1:A:188:PHE:CZ	1:A:208:MET:HE1	2.42	0.43
1:A:197:ASN:HB3	1:A:200:PHE:HD1	1.82	0.43
1:A:651:LYS:HA	1:A:651:LYS:HD3	1.63	0.43
1:A:826:ILE:O	1:A:845:ARG:NH2	2.51	0.43
1:B:746:ARG:HG3	1:B:976:ARG:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:936:ALA:O	1:B:939:GLN:HG3	2.18	0.43
1:A:22:THR:HB	1:A:27:SER:OG	2.19	0.43
1:A:486:LYS:HB3	2:E:8:DT:H5'	2.00	0.43
1:C:25:GLU:O	1:C:26:SER:C	2.61	0.43
1:A:45:LEU:HD21	1:A:75:ARG:HD2	2.00	0.43
1:A:678:VAL:O	1:A:686:LEU:HD21	2.19	0.43
1:A:846:GLU:O	1:A:849:PHE:HB3	2.18	0.43
1:B:198:PRO:HD2	1:B:465:ARG:NH2	2.33	0.43
1:B:376:LEU:HB3	1:B:377:PRO:HD3	2.00	0.43
1:B:448:ASN:HD21	2:G:11:DA:H61	1.66	0.43
1:B:753:MET:HE2	1:B:753:MET:HB3	1.94	0.43
1:C:114:LEU:CB	1:C:135:LEU:HD11	2.47	0.43
1:A:309:GLU:CG	1:A:609:LYS:CG	2.91	0.43
1:A:528:ARG:O	1:A:531:VAL:HG22	2.19	0.43
1:A:736:GLU:O	1:A:738:ASN:N	2.52	0.43
1:A:777:ASN:ND2	1:A:814:TYR:H	2.17	0.43
1:A:884:ARG:NE	1:A:888:TRP:CH2	2.87	0.43
1:B:371:ASN:CB	1:B:407:THR:HG22	2.49	0.43
1:B:403:VAL:HG11	1:B:405:VAL:CG2	2.48	0.43
1:B:865:TYR:O	1:B:869:LEU:HG	2.18	0.43
1:D:66:THR:HG23	1:D:77:TYR:CE1	2.54	0.43
1:A:658:GLN:O	1:A:659:GLU:C	2.62	0.43
1:C:13:LEU:HD11	1:C:28:VAL:HG22	2.01	0.43
1:A:641:GLU:HB3	1:A:642:PHE:H	1.69	0.43
1:A:641:GLU:H	1:A:875:ARG:HD3	1.84	0.43
1:A:961:ALA:O	1:A:963:LYS:HG3	2.19	0.43
1:B:150:PHE:CB	1:B:272:ILE:CD1	2.92	0.43
1:B:472:ARG:HE	1:B:472:ARG:HB3	1.58	0.43
1:B:518:PHE:CE1	1:B:519:ILE:HD12	2.54	0.43
1:B:987:ILE:HG23	1:B:991:PHE:HB2	2.00	0.43
1:A:786:PRO:HA	1:A:870:ARG:O	2.18	0.42
1:B:279:GLN:HA	1:B:282:LEU:HD12	2.00	0.42
1:B:674:ARG:HH12	1:B:720:THR:HG22	1.84	0.42
1:D:124:VAL:HB	1:D:131:ALA:HB1	2.00	0.42
1:A:178:LYS:HZ2	1:A:245:PHE:HA	1.84	0.42
1:A:445:ILE:HG21	1:A:500:ALA:HB1	2.00	0.42
1:A:646:ALA:H	1:A:649:ASP:HB2	1.83	0.42
1:B:403:VAL:HG12	1:B:404:LEU:N	2.34	0.42
1:B:527:PHE:CZ	1:B:531:VAL:HG21	2.53	0.42
1:A:681:ARG:HH22	1:A:976:ARG:NH1	2.17	0.42
1:A:705:LEU:O	1:A:709:MET:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:777:ASN:HD21	1:A:813:PHE:H	1.66	0.42
1:B:54:LYS:HG2	1:B:55:ALA:N	2.34	0.42
1:B:974:LEU:HD21	1:B:1007:LEU:CD2	2.49	0.42
1:A:814:TYR:HD1	1:A:824:ASN:HA	1.83	0.42
1:B:20:GLY:HA3	1:C:48:ILE:HD11	1.97	0.42
1:B:605:LEU:HA	1:B:605:LEU:HD23	1.77	0.42
1:C:82:ASP:OD1	1:C:83:GLU:N	2.52	0.42
1:A:181:TYR:HE1	1:A:245:PHE:CE2	2.37	0.42
1:A:964:LEU:HD12	1:A:964:LEU:HA	1.79	0.42
1:B:34:GLN:HG3	1:B:38:ASP:OD2	2.19	0.42
1:A:755:PHE:HA	1:A:760:ASN:ND2	2.34	0.42
1:B:176:GLU:O	1:B:176:GLU:HG3	2.19	0.42
1:B:642:PHE:CD1	1:B:878:PHE:CZ	3.07	0.42
1:B:852:VAL:HG13	1:B:876:ILE:HG21	2.02	0.42
1:C:132:LEU:O	1:C:133:ALA:C	2.63	0.42
1:A:693:PHE:C	1:A:695:GLY:H	2.27	0.42
1:A:755:PHE:HA	1:A:760:ASN:HD21	1.84	0.42
1:B:81:LYS:NZ	1:B:90:GLU:HB3	2.35	0.42
1:B:404:LEU:HD12	1:B:404:LEU:HA	1.86	0.42
1:B:782:LEU:HD13	1:B:874:PRO:HG3	2.01	0.42
1:B:1029:MET:HE3	1:B:1029:MET:HB2	1.89	0.42
1:D:54:LYS:CG	1:D:55:ALA:N	2.58	0.42
1:A:528:ARG:CA	1:A:531:VAL:HG22	2.49	0.42
1:B:858:HIS:ND1	1:B:885:TRP:HH2	2.18	0.42
1:A:67:LEU:HD12	1:A:67:LEU:HA	1.88	0.42
1:B:504:LEU:HD11	1:B:507:ASP:O	2.19	0.42
1:A:165:LEU:HB2	1:A:169:ARG:HH21	1.85	0.41
1:A:519:ILE:CD1	1:A:540:ILE:HG21	2.50	0.41
1:A:802:LEU:HD12	1:A:802:LEU:HA	1.91	0.41
1:B:392:LYS:HE3	1:B:392:LYS:HB3	1.89	0.41
1:B:731:LYS:CG	1:B:732:SER:H	2.33	0.41
1:A:330:LEU:HD23	1:A:330:LEU:HA	1.93	0.41
1:A:376:LEU:HB3	1:A:377:PRO:HD3	2.02	0.41
1:A:893:MET:HE2	1:A:893:MET:HB3	1.84	0.41
1:B:227:GLN:O	1:B:228:TYR:C	2.62	0.41
1:B:682:ALA:HB3	1:B:685:GLU:HB3	2.02	0.41
1:B:970:LEU:HD23	1:B:970:LEU:HA	1.84	0.41
1:A:460:ASP:O	1:A:461:ASN:HB2	2.19	0.41
1:A:782:LEU:HD11	1:A:856:LEU:HD13	2.02	0.41
1:B:33:GLN:NE2	1:C:30:ALA:CB	2.83	0.41
1:A:25:GLU:C	1:A:27:SER:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:PHE:HE2	1:A:208:MET:SD	2.40	0.41
1:A:607:TRP:O	1:A:611:THR:HB	2.21	0.41
1:A:782:LEU:HD22	1:A:811:LEU:HD11	2.01	0.41
1:A:895:LEU:HD22	1:A:1016:GLU:CB	2.44	0.41
1:A:935:ASP:C	1:A:937:ALA:H	2.26	0.41
1:B:52:THR:HG22	1:B:62:ARG:NE	2.35	0.41
1:B:237:GLN:HB2	1:B:427:THR:CG2	2.51	0.41
1:B:451:TYR:CE1	1:B:514:SER:HA	2.54	0.41
1:B:451:TYR:HA	1:B:493:TYR:HD2	1.84	0.41
1:B:804:LEU:HG	1:B:805:LEU:HG	2.03	0.41
1:A:78:TRP:CE2	1:A:80:SER:HB2	2.55	0.41
1:B:238:LEU:CD1	1:B:375:LEU:HD22	2.50	0.41
1:B:704:PRO:O	1:B:705:LEU:C	2.63	0.41
1:C:94:LYS:HA	1:C:94:LYS:HD3	1.85	0.41
1:A:713:TRP:HB2	1:A:714:GLU:H	1.67	0.41
1:B:437:GLN:HE21	1:B:437:GLN:HB3	1.61	0.41
1:B:803:ASP:OD2	3:H:19:DC:C5	2.73	0.41
1:A:45:LEU:HD11	1:A:75:ARG:HH11	1.80	0.41
1:A:528:ARG:HH11	1:A:629:TRP:H	1.68	0.41
1:A:639:TRP:HH2	1:A:874:PRO:HA	1.85	0.41
1:A:736:GLU:C	1:A:738:ASN:H	2.28	0.41
1:A:895:LEU:HD22	1:A:1016:GLU:HB3	2.01	0.41
1:B:592:TYR:CE2	1:B:630:LEU:HD22	2.53	0.41
1:A:503:ARG:HD2	1:A:503:ARG:HA	1.88	0.41
1:A:528:ARG:HA	1:A:531:VAL:CG2	2.49	0.41
1:A:608:LEU:HD23	1:A:608:LEU:HA	1.72	0.41
1:A:792:GLN:HE21	1:A:805:LEU:HD22	1.84	0.41
1:A:990:LYS:HE2	1:A:990:LYS:HB2	1.86	0.41
1:B:161:MET:HB3	1:B:162:PRO:HD3	2.03	0.41
1:B:20:GLY:O	1:B:21:GLY:C	2.63	0.41
1:B:290:TYR:HB3	1:B:298:ALA:HB2	2.02	0.41
1:B:338:LEU:HB2	1:B:442:VAL:HG11	2.03	0.41
1:B:602:ARG:H	1:B:602:ARG:HG2	1.58	0.41
1:C:138:LEU:HA	1:C:138:LEU:HD23	1.82	0.41
1:D:102:ASP:HA	1:D:117:ASN:HA	2.03	0.41
1:A:445:ILE:HG21	1:A:500:ALA:CB	2.51	0.41
1:A:656:LEU:HD22	1:A:656:LEU:HA	1.88	0.41
1:B:36:LEU:HD23	1:B:36:LEU:HA	1.75	0.41
1:A:323:GLU:H	1:A:323:GLU:HG3	1.52	0.40
1:A:889:GLY:O	1:A:893:MET:HB2	2.21	0.40
1:B:2:SER:OG	1:B:5:LEU:HG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:LEU:O	1:B:302:GLY:C	2.62	0.40
1:B:465:ARG:NH1	1:B:467:TYR:CD1	2.89	0.40
1:B:881:GLU:O	1:B:882:PHE:C	2.65	0.40
1:A:93:LYS:HE2	1:A:93:LYS:HB3	1.86	0.40
1:A:329:GLU:O	1:A:330:LEU:C	2.64	0.40
1:A:746:ARG:CA	1:A:804:LEU:HD12	2.50	0.40
1:B:333:LYS:CE	1:B:362:GLN:NE2	2.71	0.40
1:B:543:MET:HE1	1:B:561:VAL:HB	2.03	0.40
1:B:662:ILE:O	1:B:827:THR:HG23	2.21	0.40
1:B:835:GLN:HG3	1:B:843:ILE:HB	2.02	0.40
1:C:132:LEU:HG	1:C:136:LEU:HD11	2.03	0.40
1:A:57:ALA:HB3	1:A:59:ASN:HD22	1.87	0.40
1:A:467:TYR:HE2	1:A:492:MET:SD	2.45	0.40
1:A:639:TRP:HH2	1:A:869:LEU:HD23	1.84	0.40
1:A:750:VAL:HG23	1:A:899:PHE:CZ	2.47	0.40
1:C:66:THR:O	1:C:67:LEU:C	2.63	0.40
1:A:128:ASP:OD1	1:A:129:ALA:N	2.54	0.40
1:B:672:THR:OG1	1:B:675:ASP:OD1	2.39	0.40
1:B:677:TRP:CD2	1:B:987:ILE:HD11	2.56	0.40
1:B:977:HIS:HB3	1:B:999:HIS:CD2	2.56	0.40
1:C:87:LEU:HD13	1:C:108:ASP:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1005/1029 (98%)	895 (89%)	98 (10%)	12 (1%)	10	36
1	B	1006/1029 (98%)	883 (88%)	112 (11%)	11 (1%)	11	38
1	C	141/1029 (14%)	124 (88%)	14 (10%)	3 (2%)	5	25
1	D	144/1029 (14%)	127 (88%)	13 (9%)	4 (3%)	4	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2296/4116 (56%)	2029 (88%)	237 (10%)	30 (1%)	12	34

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	737	LYS
1	B	959	ALA
1	B	990	LYS
1	A	327	GLN
1	A	822	ARG
1	B	656	LEU
1	B	963	LYS
1	C	118	GLY
1	A	110	ARG
1	A	456	ALA
1	A	1025	PRO
1	B	643	LEU
1	C	50	GLU
1	D	103	ASN
1	A	644	PRO
1	A	812	PRO
1	B	874	PRO
1	B	906	PRO
1	B	999	HIS
1	B	1025	PRO
1	C	45	LEU
1	A	874	PRO
1	B	198	PRO
1	D	95	LEU
1	A	394	GLY
1	A	678	VAL
1	D	98	GLY
1	A	826	ILE
1	B	956	PRO
1	D	121	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	860/872 (99%)	725 (84%)	135 (16%)	2	11
1	B	860/872 (99%)	748 (87%)	112 (13%)	4	17
1	C	119/872 (14%)	106 (89%)	13 (11%)	6	23
1	D	122/872 (14%)	108 (88%)	14 (12%)	5	21
All	All	1961/3488 (56%)	1687 (86%)	274 (14%)	5	15

All (274) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	THR
1	A	37	SER
1	A	46	ARG
1	A	47	LEU
1	A	52	THR
1	A	60	ASN
1	A	62	ARG
1	A	68	LYS
1	A	70	SER
1	A	101	ARG
1	A	104	ILE
1	A	105	ILE
1	A	107	GLU
1	A	111	LEU
1	A	113	VAL
1	A	136	LEU
1	A	147	VAL
1	A	148	LEU
1	A	158	LYS
1	A	166	LYS
1	A	167	ILE
1	A	168	LEU
1	A	185	ARG
1	A	191	ILE
1	A	194	GLU
1	A	210	ILE
1	A	215	THR
1	A	233	ASN
1	A	237	GLN
1	A	238	LEU

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Mol	Chain	Res	Type
1	A	241	LEU
1	A	250	VAL
1	A	256	GLU
1	A	272	ILE
1	A	300	ARG
1	A	323	GLU
1	A	324	LYS
1	A	328	LYS
1	A	329	GLU
1	A	346	THR
1	A	351	LEU
1	A	362	GLN
1	A	365	ARG
1	A	366	GLU
1	A	383	LEU
1	A	392	LYS
1	A	393	MET
1	A	395	ARG
1	A	411	THR
1	A	433	ARG
1	A	440	ARG
1	A	442	VAL
1	A	451	TYR
1	A	452	ARG
1	A	455	GLN
1	A	474	ILE
1	A	494	SER
1	A	497	LEU
1	A	509	ILE
1	A	523	THR
1	A	544	LYS
1	A	552	GLU
1	A	570	VAL
1	A	575	LEU
1	A	576	VAL
1	A	578	SER
1	A	589	LYS
1	A	600	ARG
1	A	608	LEU
1	A	611	THR
1	A	619	ASP
1	A	641	GLU

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Mol	Chain	Res	Type
1	A	645	VAL
1	A	647	ASP
1	A	651	LYS
1	A	654	LYS
1	A	656	LEU
1	A	660	ARG
1	A	671	VAL
1	A	674	ARG
1	A	678	VAL
1	A	680	SER
1	A	684	ASP
1	A	685	GLU
1	A	686	LEU
1	A	691	ARG
1	A	694	ILE
1	A	696	ARG
1	A	699	GLU
1	A	700	ILE
1	A	701	ILE
1	A	723	THR
1	A	726	ASP
1	A	732	SER
1	A	734	SER
1	A	736	GLU
1	A	751	LEU
1	A	753	MET
1	A	759	LEU
1	A	765	GLN
1	A	766	MET
1	A	779	VAL
1	A	782	LEU
1	A	783	SER
1	A	785	SER
1	A	792	GLN
1	A	793	VAL
1	A	796	THR
1	A	798	ILE
1	A	805	LEU
1	A	811	LEU
1	A	815	ARG
1	A	822	ARG
1	A	826	ILE

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Mol	Chain	Res	Type
1	A	846	GLU
1	A	848	ILE
1	A	871	GLN
1	A	872	GLU
1	A	893	MET
1	A	900	GLU
1	A	901	SER
1	A	912	GLU
1	A	916	ASN
1	A	917	ASP
1	A	933	GLN
1	A	938	LYS
1	A	976	ARG
1	A	978	LYS
1	A	983	LYS
1	A	987	ILE
1	A	988	ARG
1	A	993	THR
1	A	1001	GLU
1	A	1019	ARG
1	A	1028	THR
1	B	8	LYS
1	B	11	LYS
1	B	14	GLU
1	B	16	ILE
1	B	25	GLU
1	B	36	LEU
1	B	47	LEU
1	B	93	LYS
1	B	105	ILE
1	B	121	VAL
1	B	132	LEU
1	B	138	LEU
1	B	145	PRO
1	B	154	VAL
1	B	159	ASP
1	B	167	ILE
1	B	209	LEU
1	B	213	ILE
1	B	214	LEU
1	B	222	VAL
1	B	225	ASN

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Mol	Chain	Res	Type
1	B	246	TYR
1	B	250	VAL
1	B	256	GLU
1	B	291	ARG
1	B	310	ILE
1	B	311	VAL
1	B	312	ARG
1	B	315	ILE
1	B	322	LEU
1	B	324	LYS
1	B	330	LEU
1	B	350	GLU
1	B	351	LEU
1	B	372	GLU
1	B	392	LYS
1	B	436	ARG
1	B	437	GLN
1	B	448	ASN
1	B	452	ARG
1	B	458	GLU
1	B	459	ASN
1	B	470	ILE
1	B	472	ARG
1	B	473	ARG
1	B	475	LYS
1	B	491	ASP
1	B	492	MET
1	B	505	LYS
1	B	512	PHE
1	B	521	SER
1	B	523	THR
1	B	589	LYS
1	B	590	ILE
1	B	599	TRP
1	B	600	ARG
1	B	602	ARG
1	B	609	LYS
1	B	616	ILE
1	B	617	GLU
1	B	635	GLU
1	B	649	ASP
1	B	652	GLN

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Mol	Chain	Res	Type
1	B	654	LYS
1	B	656	LEU
1	B	659	GLU
1	B	662	ILE
1	B	664	LYS
1	B	670	VAL
1	B	681	ARG
1	B	689	LYS
1	B	690	VAL
1	B	691	ARG
1	B	694	ILE
1	B	700	ILE
1	B	705	LEU
1	B	724	ILE
1	B	740	ILE
1	B	761	GLU
1	B	772	LYS
1	B	779	VAL
1	B	792	GLN
1	B	798	ILE
1	B	801	SER
1	B	802	LEU
1	B	804	LEU
1	B	810	CYS
1	B	815	ARG
1	B	821	GLU
1	B	826	ILE
1	B	831	LEU
1	B	843	ILE
1	B	857	HIS
1	B	870	ARG
1	B	876	ILE
1	B	890	ARG
1	B	897	ILE
1	B	909	ARG
1	B	927	LYS
1	B	932	VAL
1	B	945	GLU
1	B	955	ILE
1	B	967	ARG
1	B	974	LEU
1	B	975	GLU

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Mol	Chain	Res	Type
1	B	983	LYS
1	B	984	ASP
1	B	986	THR
1	B	987	ILE
1	B	1004	ILE
1	B	1018	VAL
1	B	1021	VAL
1	C	2	SER
1	C	3	LEU
1	C	14	GLU
1	C	25	GLU
1	C	45	LEU
1	C	46	ARG
1	C	60	ASN
1	C	67	LEU
1	C	92	GLN
1	C	105	ILE
1	C	111	LEU
1	C	121	VAL
1	C	143	GLU
1	D	46	ARG
1	D	47	LEU
1	D	68	LYS
1	D	73	GLN
1	D	82	ASP
1	D	86	THR
1	D	88	ASP
1	D	90	GLU
1	D	93	LYS
1	D	94	LYS
1	D	104	ILE
1	D	105	ILE
1	D	107	GLU
1	D	111	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	73	GLN
1	A	116	GLN
1	A	117	ASN

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Mol	Chain	Res	Type
1	A	146	GLN
1	A	197	ASN
1	A	229	HIS
1	A	232	ASN
1	A	279	GLN
1	A	288	ASN
1	A	325	HIS
1	A	362	GLN
1	A	384	ASN
1	A	391	GLN
1	A	437	GLN
1	A	448	ASN
1	A	464	ASN
1	A	627	HIS
1	A	637	ASN
1	A	673	ASN
1	A	712	ASN
1	A	763	GLN
1	A	777	ASN
1	A	792	GLN
1	A	809	GLN
1	A	850	HIS
1	A	966	ASN
1	B	33	GLN
1	B	34	GLN
1	B	59	ASN
1	B	116	GLN
1	B	117	ASN
1	B	197	ASN
1	B	212	HIS
1	B	229	HIS
1	B	232	ASN
1	B	276	HIS
1	B	371	ASN
1	B	437	GLN
1	B	454	ASN
1	B	459	ASN
1	B	464	ASN
1	B	560	ASN
1	B	563	ASN
1	B	620	HIS
1	B	627	HIS

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Mol	Chain	Res	Type
1	B	758	ASN
1	B	763	GLN
1	B	809	GLN
1	B	824	ASN
1	B	857	HIS
1	C	34	GLN
1	C	59	ASN
1	C	92	GLN
1	D	10	GLN
1	D	24	ASN
1	D	59	ASN
1	D	60	ASN
1	D	92	GLN
1	D	116	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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
4	SAM	A	1101	-	27,29,29	0.47	0	34,42,42	0.62	0
4	SAM	B	1101	-	27,29,29	0.48	0	34,42,42	0.54	0

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
4	SAM	A	1101	-	-	6/17/33/33	0/3/3/3
4	SAM	B	1101	-	-	7/17/33/33	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1101	SAM	N-CA-CB-CG
4	A	1101	SAM	C-CA-CB-CG
4	A	1101	SAM	CA-CB-CG-SD
4	A	1101	SAM	O4'-C4'-C5'-SD
4	A	1101	SAM	C3'-C4'-C5'-SD
4	B	1101	SAM	N-CA-CB-CG
4	B	1101	SAM	C-CA-CB-CG
4	B	1101	SAM	O4'-C4'-C5'-SD
4	B	1101	SAM	C3'-C4'-C5'-SD
4	B	1101	SAM	CA-CB-CG-SD
4	A	1101	SAM	CB-CG-SD-C5'
4	B	1101	SAM	CB-CG-SD-C5'
4	B	1101	SAM	O4'-C1'-N9-C8

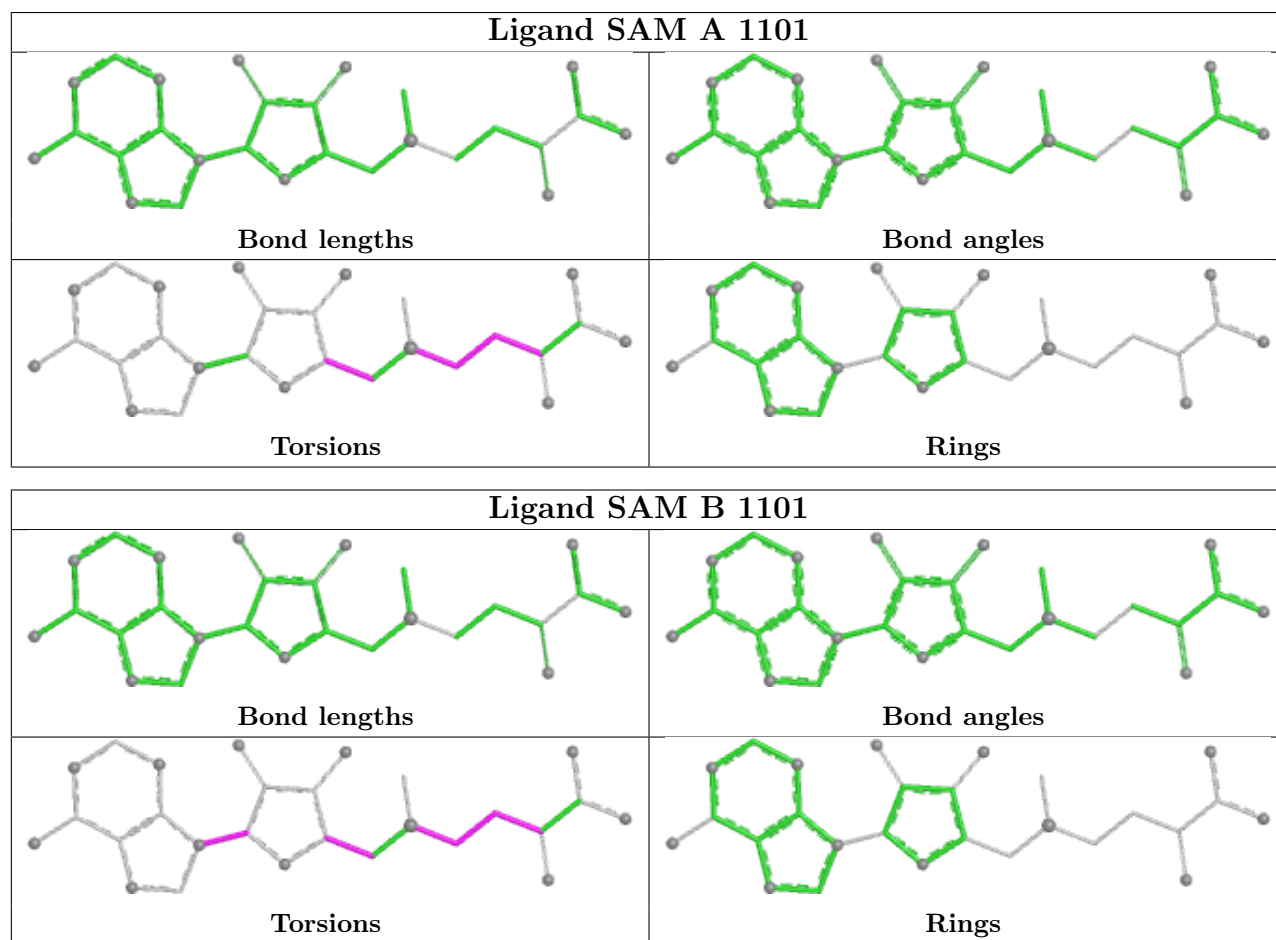
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1101	SAM	2	0
4	B	1101	SAM	1	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.

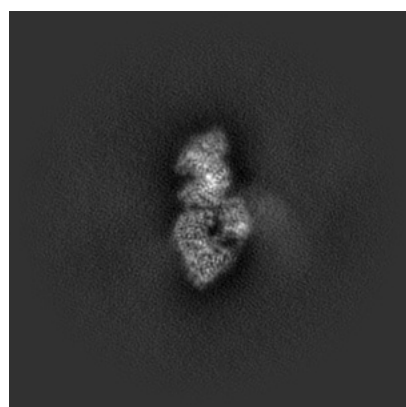
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23543. These allow visual inspection of the internal detail of the map and identification of artifacts.

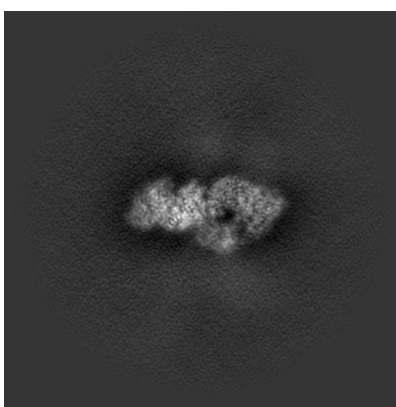
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

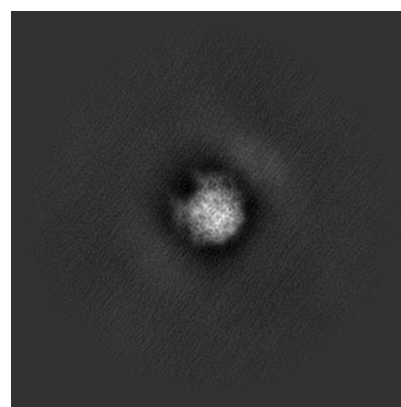
6.1.1 Primary map



X



Y

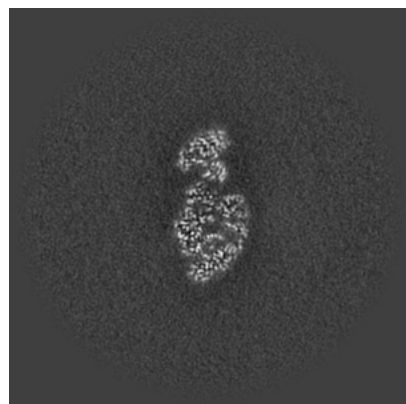


Z

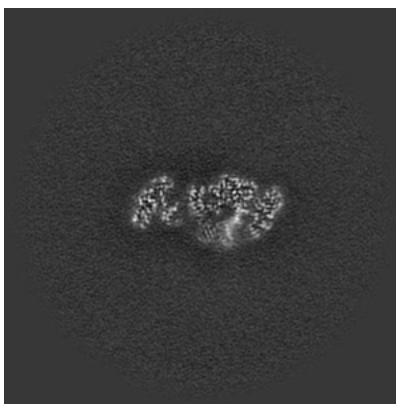
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

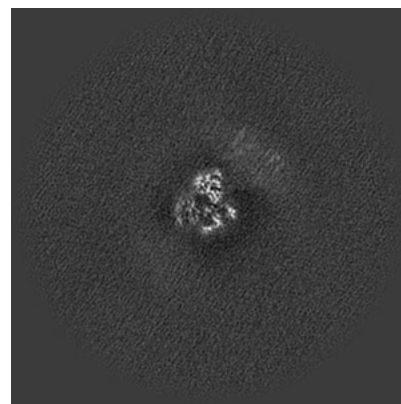
6.2.1 Primary map



X Index: 200



Y Index: 200

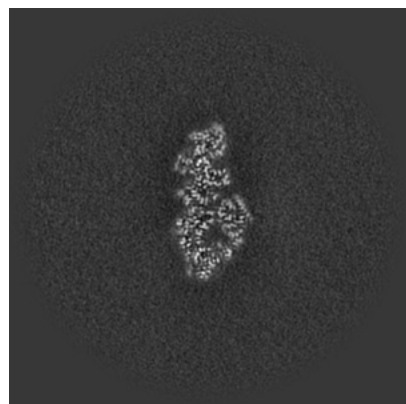


Z Index: 200

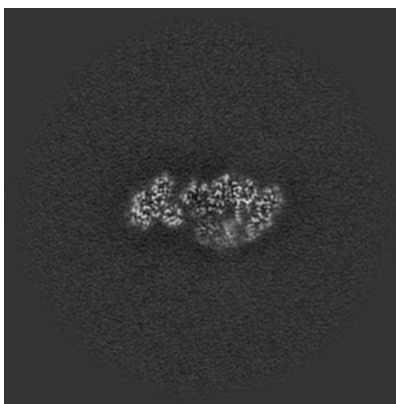
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

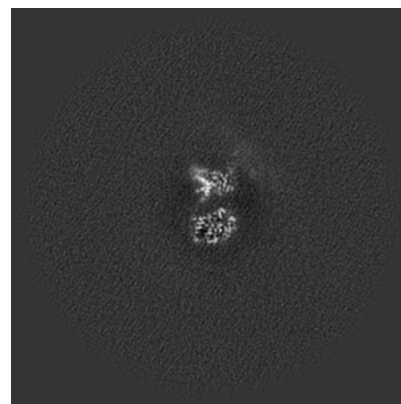
6.3.1 Primary map



X Index: 208



Y Index: 197

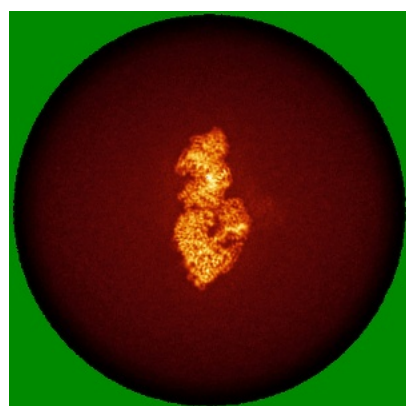


Z Index: 181

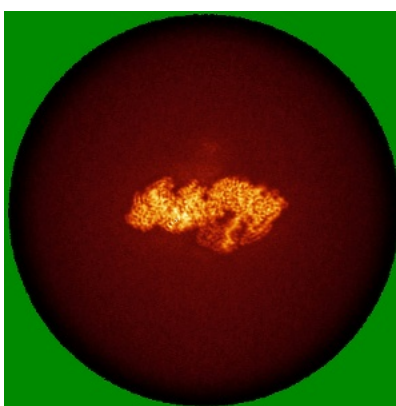
The images above show the largest variance slices of the map in three orthogonal directions.

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

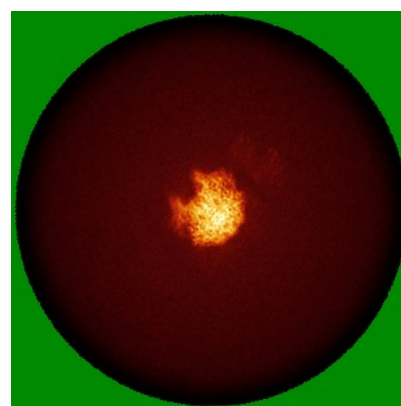
6.4.1 Primary map



X



Y

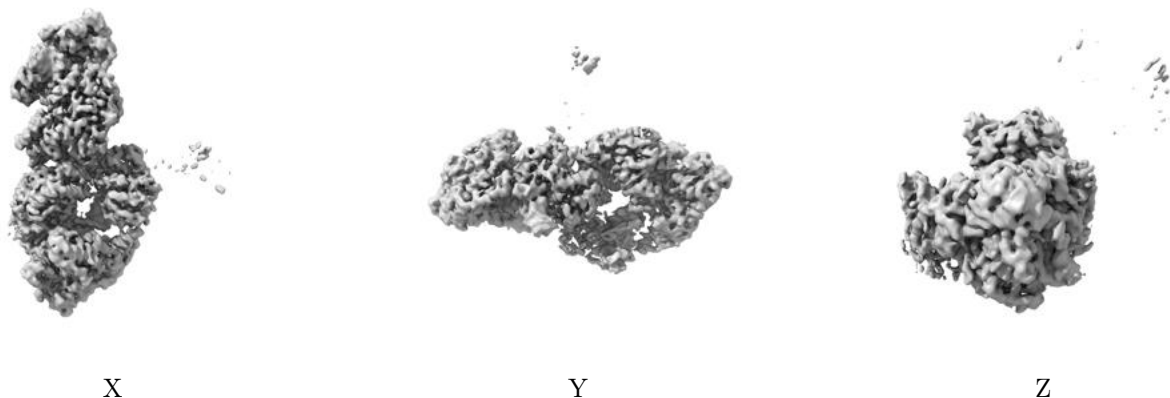


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.375. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

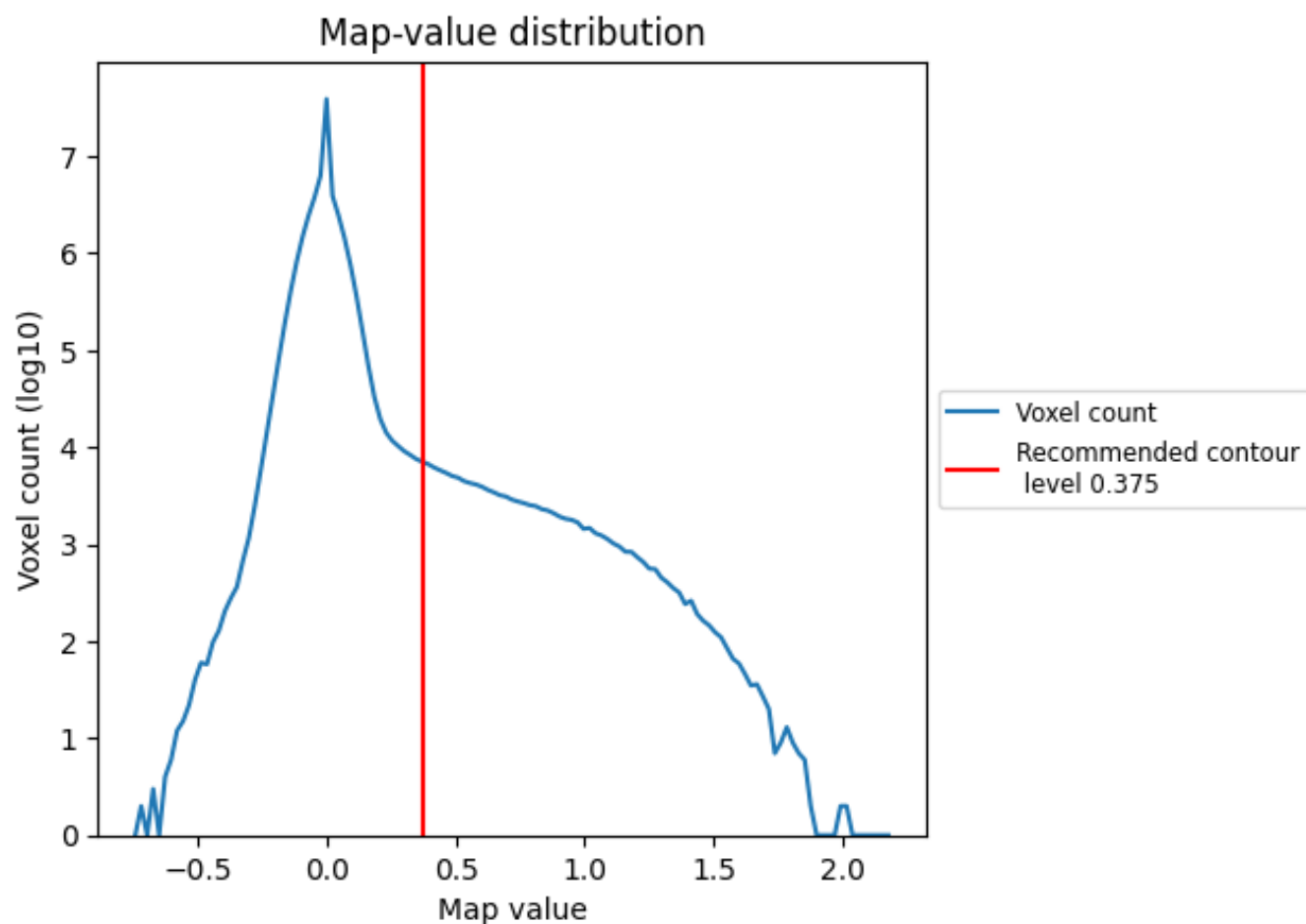
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

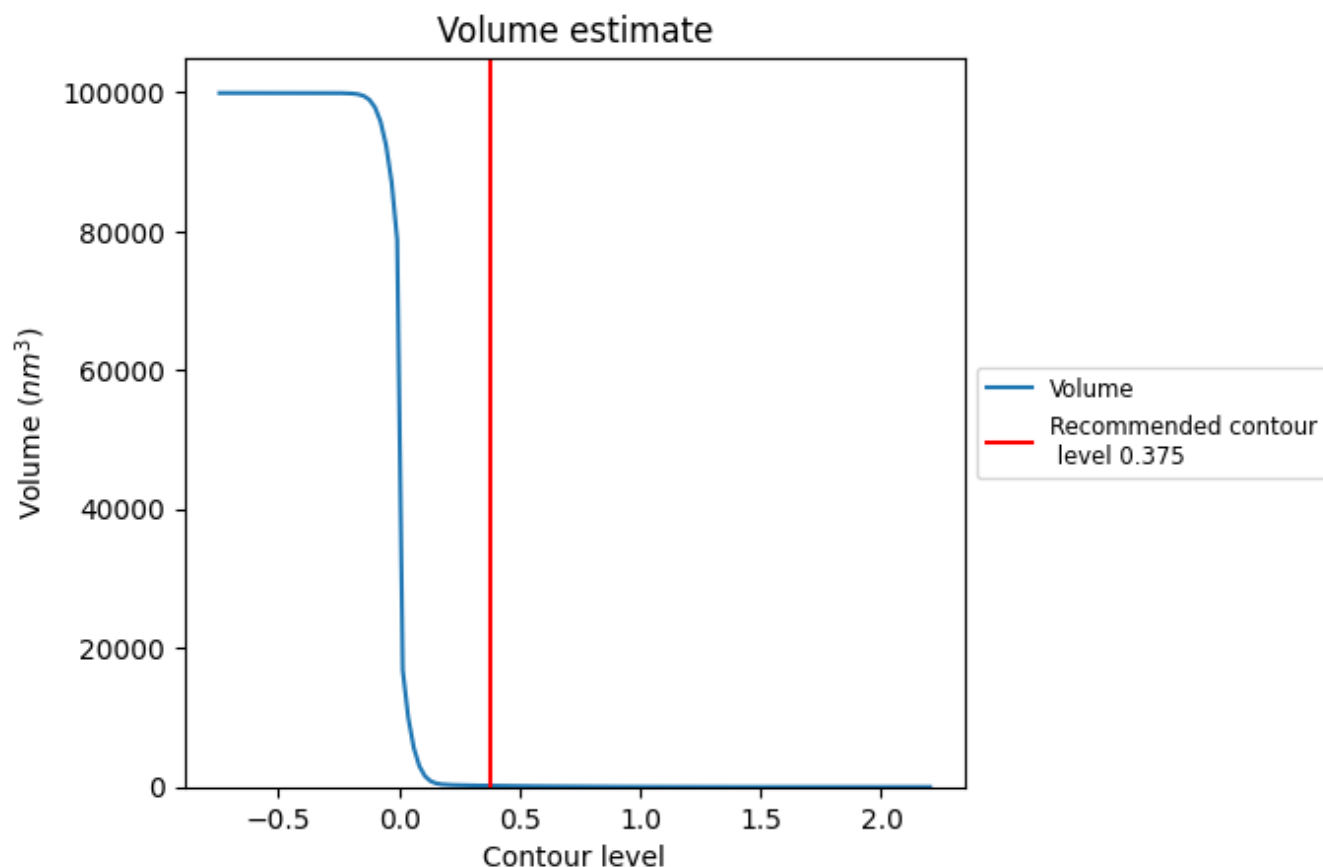
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

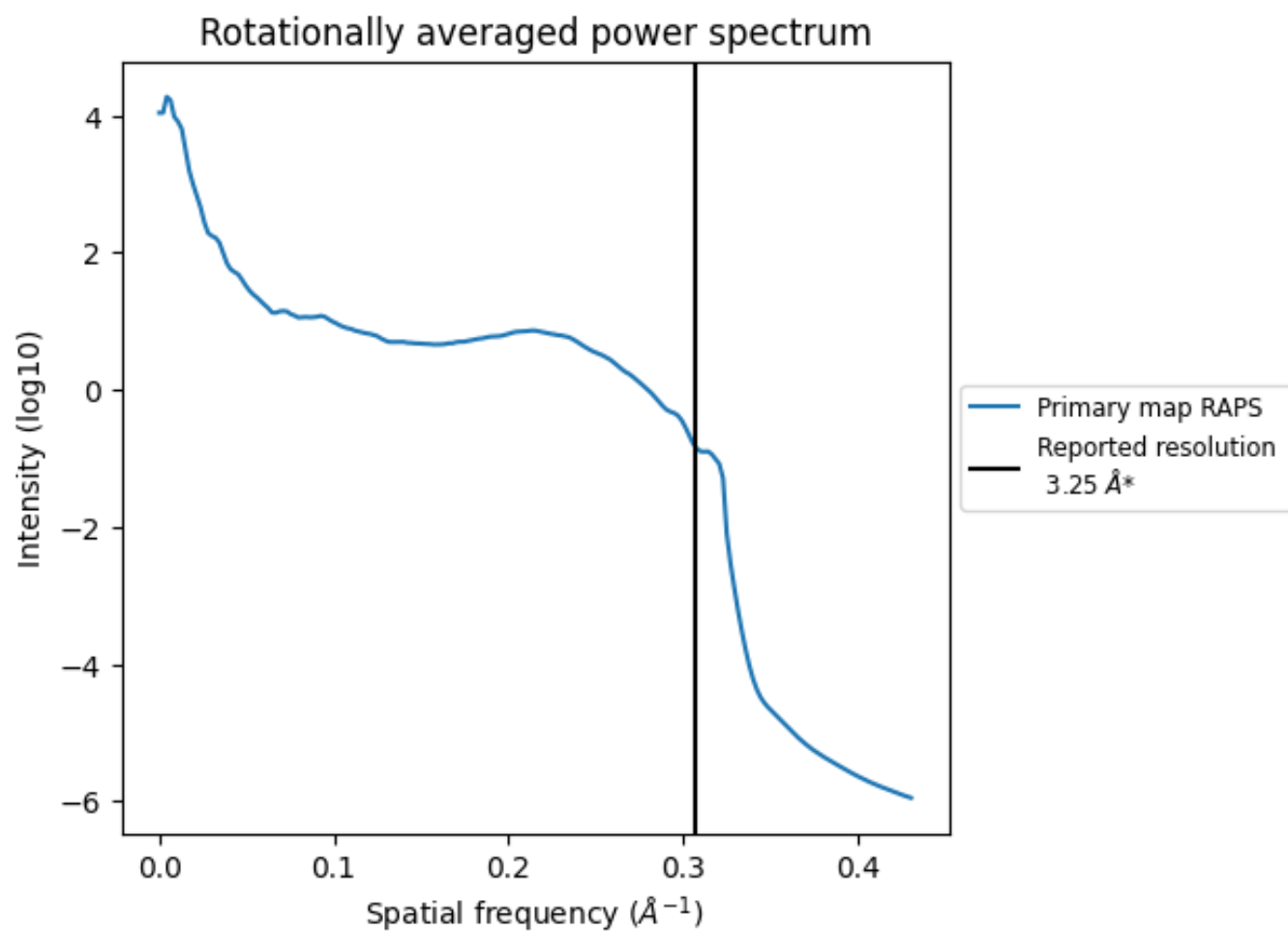
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 176 nm^3 ; this corresponds to an approximate mass of 159 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 0.308 Å⁻¹

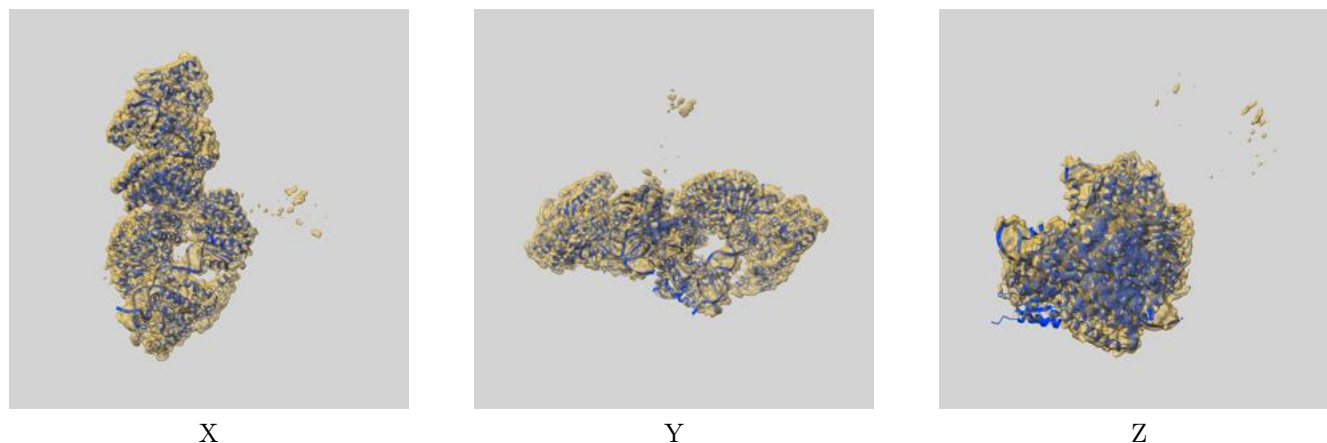
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

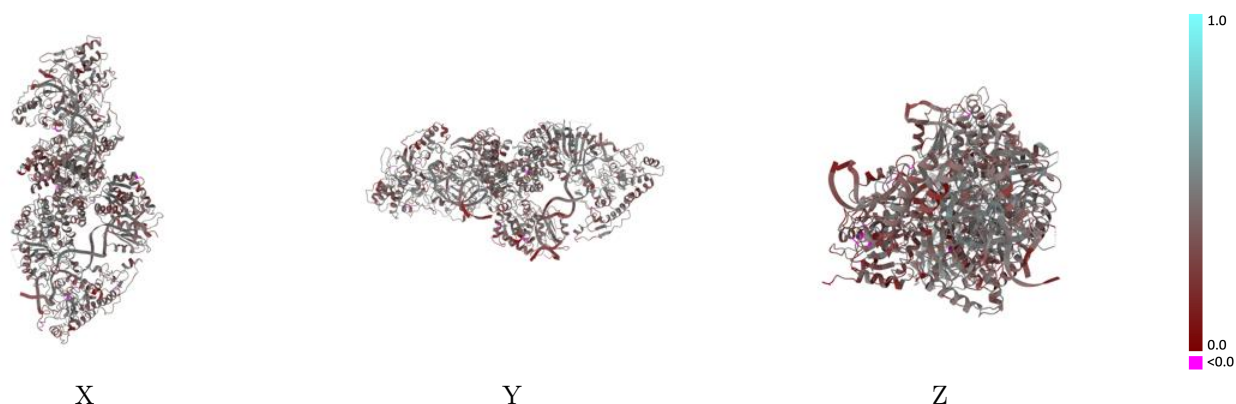
This section contains information regarding the fit between EMDB map EMD-23543 and PDB model 7LVV. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



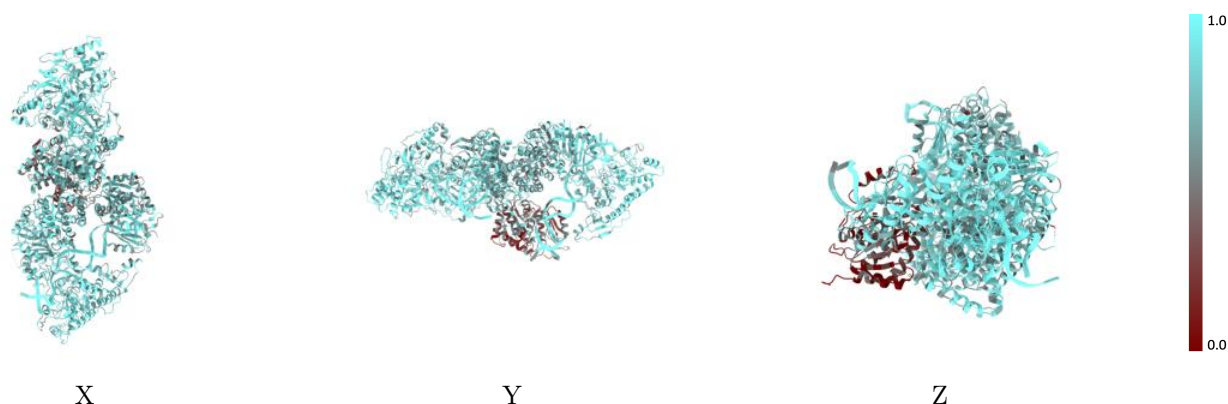
The images above show the 3D surface view of the map at the recommended contour level 0.375 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



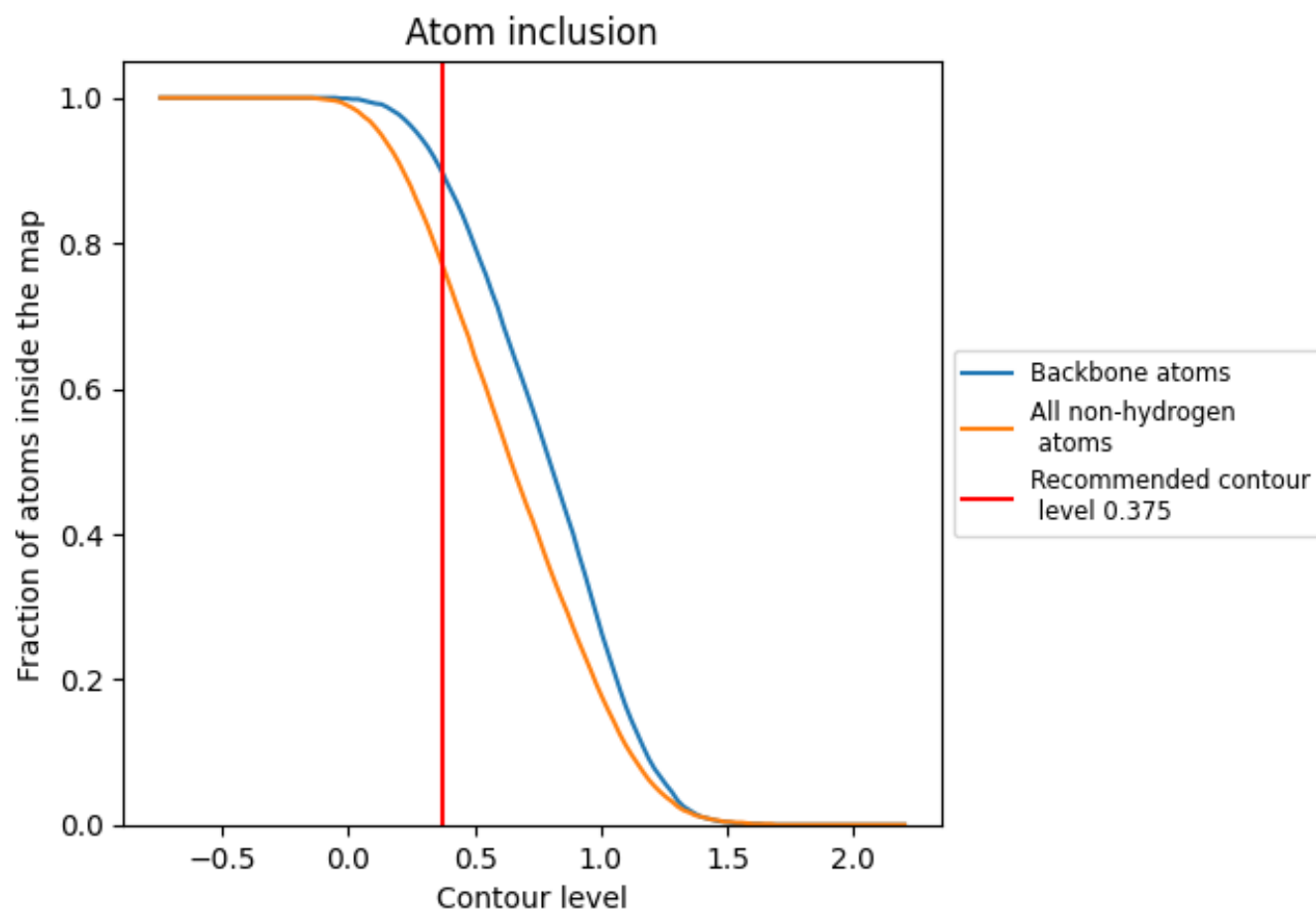
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.375).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 77% 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 (0.375) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7670	0.3940
A	0.7550	0.3950
B	0.7960	0.4010
C	0.7280	0.3940
D	0.3190	0.3150
E	0.9730	0.4240
F	0.9630	0.4220
G	0.9320	0.3840
H	0.9490	0.3820

1.0

0.0

<0.0