



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 03:56 PM UTC

PDB ID : 6ZFX / pdb_00006zfx
EMDB ID : EMD-11187
Title : hSARM1 GraFix-ed
Authors : Sporny, M.; Guez-Haddad, J.; Khazma, T.; Yaron, A.; Dessau, M.; Mim, C.;
Isupov, M.N.; Zalk, R.; Hons, M.; Opatowsky, Y.
Deposited on : 2020-06-18
Resolution : 2.88 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:

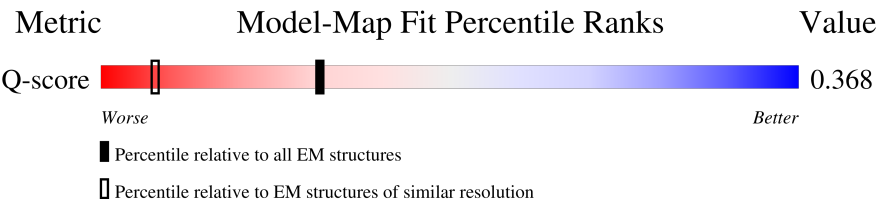
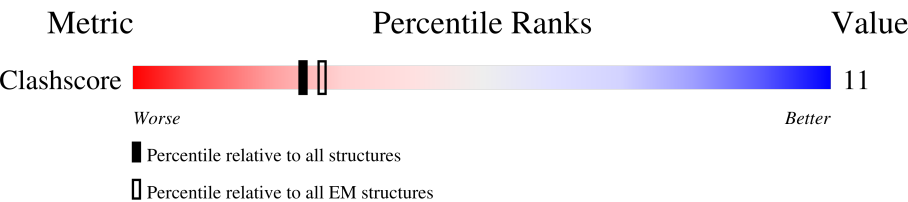
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
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 2.88 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	-
Q-score	-	25397	12111 (2.38 - 3.38)

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	726	 24% 63% 23% • 13%
1	B	726	 24% 63% 24% • 13%
1	C	726	 24% 64% 23% • 13%
1	D	726	 24% 63% 23% • 13%
1	E	726	 24% 63% 23% • 13%
1	F	726	 24% 64% 23% • 13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	726	24% 64% 23% • 13%
1	H	726	24% 63% 23% • 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 39856 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 NAD(+) hydrolase SARM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	635	Total 4959	C 3128	N 890	O 918	S 23	0	0
1	B	635	Total 4959	C 3128	N 890	O 918	S 23	0	0
1	C	635	Total 4959	C 3128	N 890	O 918	S 23	0	0
1	D	635	Total 4959	C 3128	N 890	O 918	S 23	0	0
1	E	635	Total 4959	C 3128	N 890	O 918	S 23	0	0
1	F	635	Total 4959	C 3128	N 890	O 918	S 23	0	0
1	G	635	Total 4959	C 3128	N 890	O 918	S 23	0	0
1	H	635	Total 4959	C 3128	N 890	O 918	S 23	0	0

There are 224 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP Q6SZW1
A	0	SER	-	expression tag	UNP Q6SZW1
A	1	TYR	-	expression tag	UNP Q6SZW1
A	2	HIS	-	expression tag	UNP Q6SZW1
A	3	HIS	-	expression tag	UNP Q6SZW1
A	4	HIS	-	expression tag	UNP Q6SZW1
A	5	HIS	-	expression tag	UNP Q6SZW1
A	6	HIS	-	expression tag	UNP Q6SZW1
A	7	HIS	-	expression tag	UNP Q6SZW1
A	8	ASP	-	expression tag	UNP Q6SZW1
A	9	TYR	-	expression tag	UNP Q6SZW1
A	10	ASP	-	expression tag	UNP Q6SZW1
A	11	ILE	-	expression tag	UNP Q6SZW1
A	12	PRO	-	expression tag	UNP Q6SZW1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	THR	-	expression tag	UNP Q6SZW1
A	14	THR	-	expression tag	UNP Q6SZW1
A	15	GLU	-	expression tag	UNP Q6SZW1
A	16	ASN	-	expression tag	UNP Q6SZW1
A	17	LEU	-	expression tag	UNP Q6SZW1
A	18	TYR	-	expression tag	UNP Q6SZW1
A	19	PHE	-	expression tag	UNP Q6SZW1
A	20	GLN	-	expression tag	UNP Q6SZW1
A	21	GLY	-	expression tag	UNP Q6SZW1
A	22	ALA	-	expression tag	UNP Q6SZW1
A	23	MET	-	expression tag	UNP Q6SZW1
A	24	GLY	-	expression tag	UNP Q6SZW1
A	25	SER	-	expression tag	UNP Q6SZW1
A	642	GLN	GLU	engineered mutation	UNP Q6SZW1
B	-1	MET	-	initiating methionine	UNP Q6SZW1
B	0	SER	-	expression tag	UNP Q6SZW1
B	1	TYR	-	expression tag	UNP Q6SZW1
B	2	HIS	-	expression tag	UNP Q6SZW1
B	3	HIS	-	expression tag	UNP Q6SZW1
B	4	HIS	-	expression tag	UNP Q6SZW1
B	5	HIS	-	expression tag	UNP Q6SZW1
B	6	HIS	-	expression tag	UNP Q6SZW1
B	7	HIS	-	expression tag	UNP Q6SZW1
B	8	ASP	-	expression tag	UNP Q6SZW1
B	9	TYR	-	expression tag	UNP Q6SZW1
B	10	ASP	-	expression tag	UNP Q6SZW1
B	11	ILE	-	expression tag	UNP Q6SZW1
B	12	PRO	-	expression tag	UNP Q6SZW1
B	13	THR	-	expression tag	UNP Q6SZW1
B	14	THR	-	expression tag	UNP Q6SZW1
B	15	GLU	-	expression tag	UNP Q6SZW1
B	16	ASN	-	expression tag	UNP Q6SZW1
B	17	LEU	-	expression tag	UNP Q6SZW1
B	18	TYR	-	expression tag	UNP Q6SZW1
B	19	PHE	-	expression tag	UNP Q6SZW1
B	20	GLN	-	expression tag	UNP Q6SZW1
B	21	GLY	-	expression tag	UNP Q6SZW1
B	22	ALA	-	expression tag	UNP Q6SZW1
B	23	MET	-	expression tag	UNP Q6SZW1
B	24	GLY	-	expression tag	UNP Q6SZW1
B	25	SER	-	expression tag	UNP Q6SZW1
B	642	GLN	GLU	engineered mutation	UNP Q6SZW1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	MET	-	initiating methionine	UNP Q6SZW1
C	0	SER	-	expression tag	UNP Q6SZW1
C	1	TYR	-	expression tag	UNP Q6SZW1
C	2	HIS	-	expression tag	UNP Q6SZW1
C	3	HIS	-	expression tag	UNP Q6SZW1
C	4	HIS	-	expression tag	UNP Q6SZW1
C	5	HIS	-	expression tag	UNP Q6SZW1
C	6	HIS	-	expression tag	UNP Q6SZW1
C	7	HIS	-	expression tag	UNP Q6SZW1
C	8	ASP	-	expression tag	UNP Q6SZW1
C	9	TYR	-	expression tag	UNP Q6SZW1
C	10	ASP	-	expression tag	UNP Q6SZW1
C	11	ILE	-	expression tag	UNP Q6SZW1
C	12	PRO	-	expression tag	UNP Q6SZW1
C	13	THR	-	expression tag	UNP Q6SZW1
C	14	THR	-	expression tag	UNP Q6SZW1
C	15	GLU	-	expression tag	UNP Q6SZW1
C	16	ASN	-	expression tag	UNP Q6SZW1
C	17	LEU	-	expression tag	UNP Q6SZW1
C	18	TYR	-	expression tag	UNP Q6SZW1
C	19	PHE	-	expression tag	UNP Q6SZW1
C	20	GLN	-	expression tag	UNP Q6SZW1
C	21	GLY	-	expression tag	UNP Q6SZW1
C	22	ALA	-	expression tag	UNP Q6SZW1
C	23	MET	-	expression tag	UNP Q6SZW1
C	24	GLY	-	expression tag	UNP Q6SZW1
C	25	SER	-	expression tag	UNP Q6SZW1
C	642	GLN	GLU	engineered mutation	UNP Q6SZW1
D	-1	MET	-	initiating methionine	UNP Q6SZW1
D	0	SER	-	expression tag	UNP Q6SZW1
D	1	TYR	-	expression tag	UNP Q6SZW1
D	2	HIS	-	expression tag	UNP Q6SZW1
D	3	HIS	-	expression tag	UNP Q6SZW1
D	4	HIS	-	expression tag	UNP Q6SZW1
D	5	HIS	-	expression tag	UNP Q6SZW1
D	6	HIS	-	expression tag	UNP Q6SZW1
D	7	HIS	-	expression tag	UNP Q6SZW1
D	8	ASP	-	expression tag	UNP Q6SZW1
D	9	TYR	-	expression tag	UNP Q6SZW1
D	10	ASP	-	expression tag	UNP Q6SZW1
D	11	ILE	-	expression tag	UNP Q6SZW1
D	12	PRO	-	expression tag	UNP Q6SZW1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	13	THR	-	expression tag	UNP Q6SZW1
D	14	THR	-	expression tag	UNP Q6SZW1
D	15	GLU	-	expression tag	UNP Q6SZW1
D	16	ASN	-	expression tag	UNP Q6SZW1
D	17	LEU	-	expression tag	UNP Q6SZW1
D	18	TYR	-	expression tag	UNP Q6SZW1
D	19	PHE	-	expression tag	UNP Q6SZW1
D	20	GLN	-	expression tag	UNP Q6SZW1
D	21	GLY	-	expression tag	UNP Q6SZW1
D	22	ALA	-	expression tag	UNP Q6SZW1
D	23	MET	-	expression tag	UNP Q6SZW1
D	24	GLY	-	expression tag	UNP Q6SZW1
D	25	SER	-	expression tag	UNP Q6SZW1
D	642	GLN	GLU	engineered mutation	UNP Q6SZW1
E	-1	MET	-	initiating methionine	UNP Q6SZW1
E	0	SER	-	expression tag	UNP Q6SZW1
E	1	TYR	-	expression tag	UNP Q6SZW1
E	2	HIS	-	expression tag	UNP Q6SZW1
E	3	HIS	-	expression tag	UNP Q6SZW1
E	4	HIS	-	expression tag	UNP Q6SZW1
E	5	HIS	-	expression tag	UNP Q6SZW1
E	6	HIS	-	expression tag	UNP Q6SZW1
E	7	HIS	-	expression tag	UNP Q6SZW1
E	8	ASP	-	expression tag	UNP Q6SZW1
E	9	TYR	-	expression tag	UNP Q6SZW1
E	10	ASP	-	expression tag	UNP Q6SZW1
E	11	ILE	-	expression tag	UNP Q6SZW1
E	12	PRO	-	expression tag	UNP Q6SZW1
E	13	THR	-	expression tag	UNP Q6SZW1
E	14	THR	-	expression tag	UNP Q6SZW1
E	15	GLU	-	expression tag	UNP Q6SZW1
E	16	ASN	-	expression tag	UNP Q6SZW1
E	17	LEU	-	expression tag	UNP Q6SZW1
E	18	TYR	-	expression tag	UNP Q6SZW1
E	19	PHE	-	expression tag	UNP Q6SZW1
E	20	GLN	-	expression tag	UNP Q6SZW1
E	21	GLY	-	expression tag	UNP Q6SZW1
E	22	ALA	-	expression tag	UNP Q6SZW1
E	23	MET	-	expression tag	UNP Q6SZW1
E	24	GLY	-	expression tag	UNP Q6SZW1
E	25	SER	-	expression tag	UNP Q6SZW1
E	642	GLN	GLU	engineered mutation	UNP Q6SZW1

Continued on next page...

Continued from previous page...

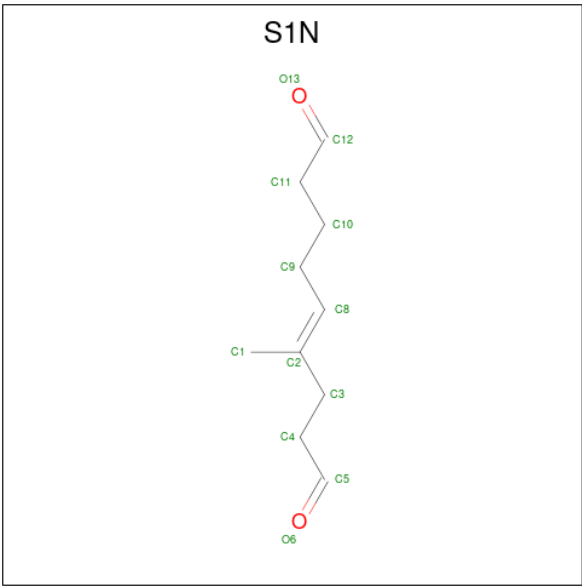
Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	MET	-	initiating methionine	UNP Q6SZW1
F	0	SER	-	expression tag	UNP Q6SZW1
F	1	TYR	-	expression tag	UNP Q6SZW1
F	2	HIS	-	expression tag	UNP Q6SZW1
F	3	HIS	-	expression tag	UNP Q6SZW1
F	4	HIS	-	expression tag	UNP Q6SZW1
F	5	HIS	-	expression tag	UNP Q6SZW1
F	6	HIS	-	expression tag	UNP Q6SZW1
F	7	HIS	-	expression tag	UNP Q6SZW1
F	8	ASP	-	expression tag	UNP Q6SZW1
F	9	TYR	-	expression tag	UNP Q6SZW1
F	10	ASP	-	expression tag	UNP Q6SZW1
F	11	ILE	-	expression tag	UNP Q6SZW1
F	12	PRO	-	expression tag	UNP Q6SZW1
F	13	THR	-	expression tag	UNP Q6SZW1
F	14	THR	-	expression tag	UNP Q6SZW1
F	15	GLU	-	expression tag	UNP Q6SZW1
F	16	ASN	-	expression tag	UNP Q6SZW1
F	17	LEU	-	expression tag	UNP Q6SZW1
F	18	TYR	-	expression tag	UNP Q6SZW1
F	19	PHE	-	expression tag	UNP Q6SZW1
F	20	GLN	-	expression tag	UNP Q6SZW1
F	21	GLY	-	expression tag	UNP Q6SZW1
F	22	ALA	-	expression tag	UNP Q6SZW1
F	23	MET	-	expression tag	UNP Q6SZW1
F	24	GLY	-	expression tag	UNP Q6SZW1
F	25	SER	-	expression tag	UNP Q6SZW1
F	642	GLN	GLU	engineered mutation	UNP Q6SZW1
G	-1	MET	-	initiating methionine	UNP Q6SZW1
G	0	SER	-	expression tag	UNP Q6SZW1
G	1	TYR	-	expression tag	UNP Q6SZW1
G	2	HIS	-	expression tag	UNP Q6SZW1
G	3	HIS	-	expression tag	UNP Q6SZW1
G	4	HIS	-	expression tag	UNP Q6SZW1
G	5	HIS	-	expression tag	UNP Q6SZW1
G	6	HIS	-	expression tag	UNP Q6SZW1
G	7	HIS	-	expression tag	UNP Q6SZW1
G	8	ASP	-	expression tag	UNP Q6SZW1
G	9	TYR	-	expression tag	UNP Q6SZW1
G	10	ASP	-	expression tag	UNP Q6SZW1
G	11	ILE	-	expression tag	UNP Q6SZW1
G	12	PRO	-	expression tag	UNP Q6SZW1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	13	THR	-	expression tag	UNP Q6SZW1
G	14	THR	-	expression tag	UNP Q6SZW1
G	15	GLU	-	expression tag	UNP Q6SZW1
G	16	ASN	-	expression tag	UNP Q6SZW1
G	17	LEU	-	expression tag	UNP Q6SZW1
G	18	TYR	-	expression tag	UNP Q6SZW1
G	19	PHE	-	expression tag	UNP Q6SZW1
G	20	GLN	-	expression tag	UNP Q6SZW1
G	21	GLY	-	expression tag	UNP Q6SZW1
G	22	ALA	-	expression tag	UNP Q6SZW1
G	23	MET	-	expression tag	UNP Q6SZW1
G	24	GLY	-	expression tag	UNP Q6SZW1
G	25	SER	-	expression tag	UNP Q6SZW1
G	642	GLN	GLU	engineered mutation	UNP Q6SZW1
H	-1	MET	-	initiating methionine	UNP Q6SZW1
H	0	SER	-	expression tag	UNP Q6SZW1
H	1	TYR	-	expression tag	UNP Q6SZW1
H	2	HIS	-	expression tag	UNP Q6SZW1
H	3	HIS	-	expression tag	UNP Q6SZW1
H	4	HIS	-	expression tag	UNP Q6SZW1
H	5	HIS	-	expression tag	UNP Q6SZW1
H	6	HIS	-	expression tag	UNP Q6SZW1
H	7	HIS	-	expression tag	UNP Q6SZW1
H	8	ASP	-	expression tag	UNP Q6SZW1
H	9	TYR	-	expression tag	UNP Q6SZW1
H	10	ASP	-	expression tag	UNP Q6SZW1
H	11	ILE	-	expression tag	UNP Q6SZW1
H	12	PRO	-	expression tag	UNP Q6SZW1
H	13	THR	-	expression tag	UNP Q6SZW1
H	14	THR	-	expression tag	UNP Q6SZW1
H	15	GLU	-	expression tag	UNP Q6SZW1
H	16	ASN	-	expression tag	UNP Q6SZW1
H	17	LEU	-	expression tag	UNP Q6SZW1
H	18	TYR	-	expression tag	UNP Q6SZW1
H	19	PHE	-	expression tag	UNP Q6SZW1
H	20	GLN	-	expression tag	UNP Q6SZW1
H	21	GLY	-	expression tag	UNP Q6SZW1
H	22	ALA	-	expression tag	UNP Q6SZW1
H	23	MET	-	expression tag	UNP Q6SZW1
H	24	GLY	-	expression tag	UNP Q6SZW1
H	25	SER	-	expression tag	UNP Q6SZW1
H	642	GLN	GLU	engineered mutation	UNP Q6SZW1

- Molecule 2 is ({E})-4-methylnon-4-enedial (CCD ID: S1N) (formula: C₁₀H₁₆O₂).



Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			12	10	2	
2	A	1	Total	C	O	0
			11	10	1	
2	B	1	Total	C	O	0
			12	10	2	
2	B	1	Total	C	O	0
			11	10	1	
2	C	1	Total	C	O	0
			12	10	2	
2	C	1	Total	C	O	0
			11	10	1	
2	D	1	Total	C	O	0
			12	10	2	
2	D	1	Total	C	O	0
			11	10	1	
2	E	1	Total	C	O	0
			12	10	2	
2	E	1	Total	C	O	0
			11	10	1	
2	F	1	Total	C	O	0
			12	10	2	
2	F	1	Total	C	O	0
			11	10	1	
2	G	1	Total	C	O	0
			12	10	2	

Continued on next page...

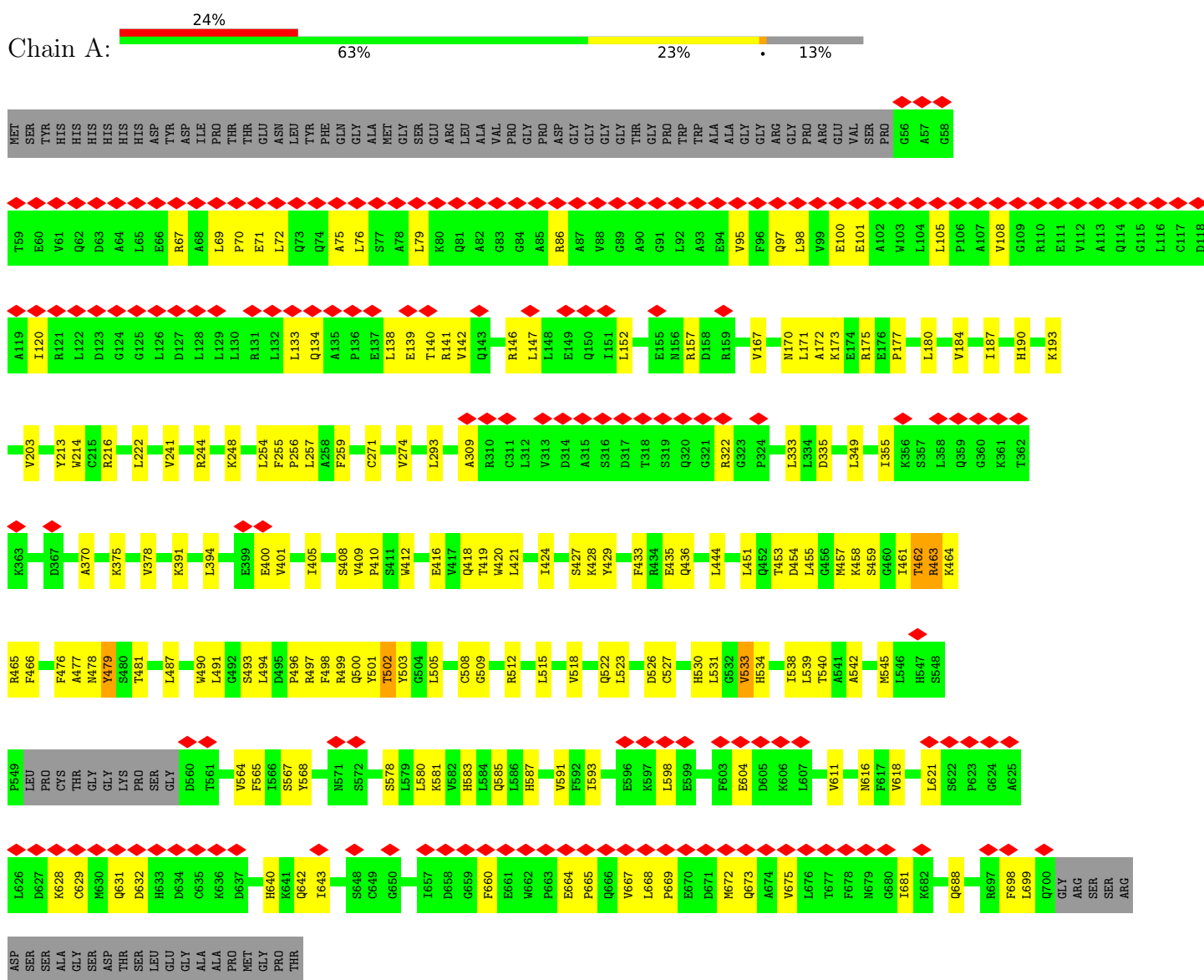
Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
2	G	1	Total	C	O	0
			11	10	1	
2	H	1	Total	C	O	0
			12	10	2	
2	H	1	Total	C	O	0
			11	10	1	

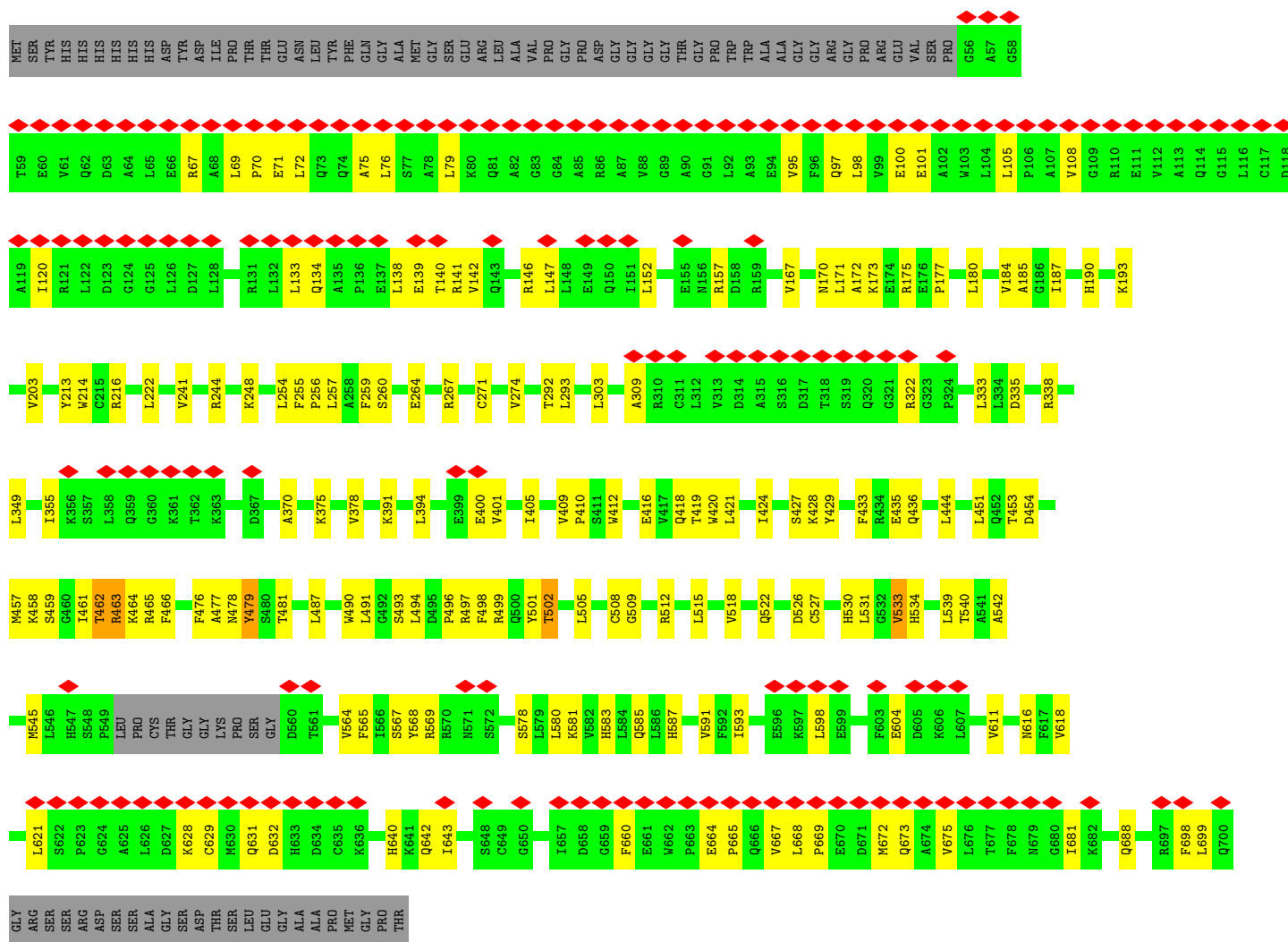
3 Residue-property plots

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.

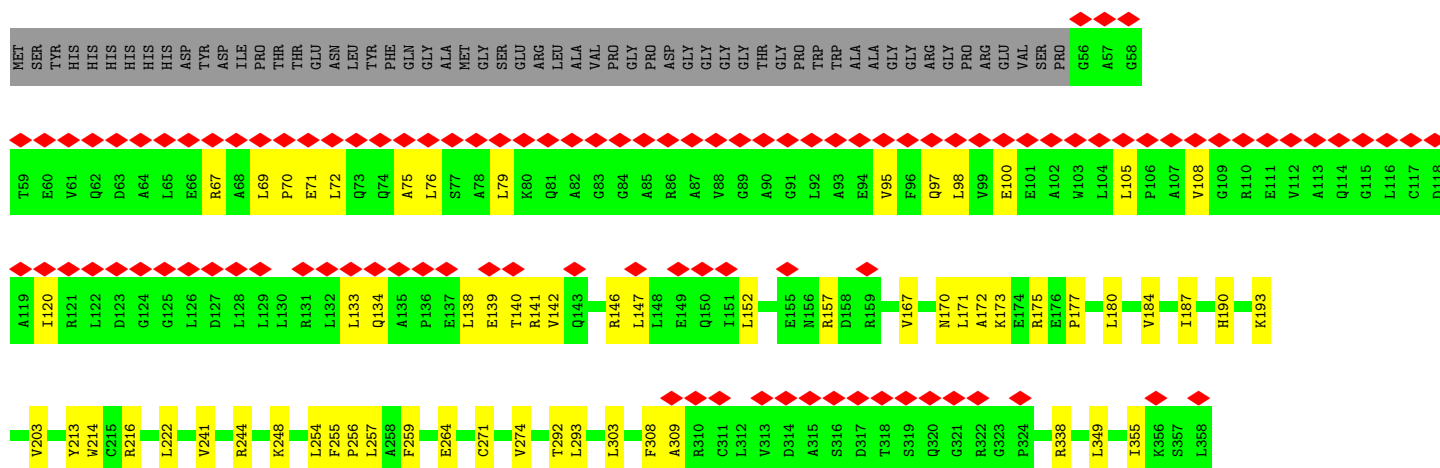
• Molecule 1: NAD(+) hydrolase SARM1

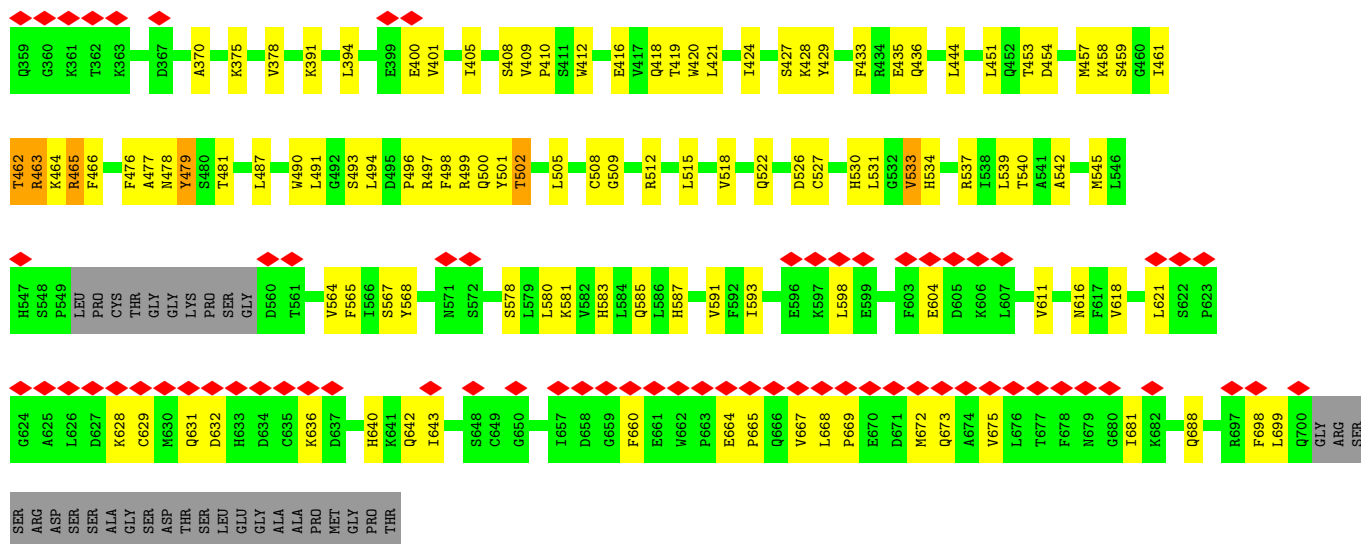


• Molecule 1: NAD(+) hydrolase SARM1

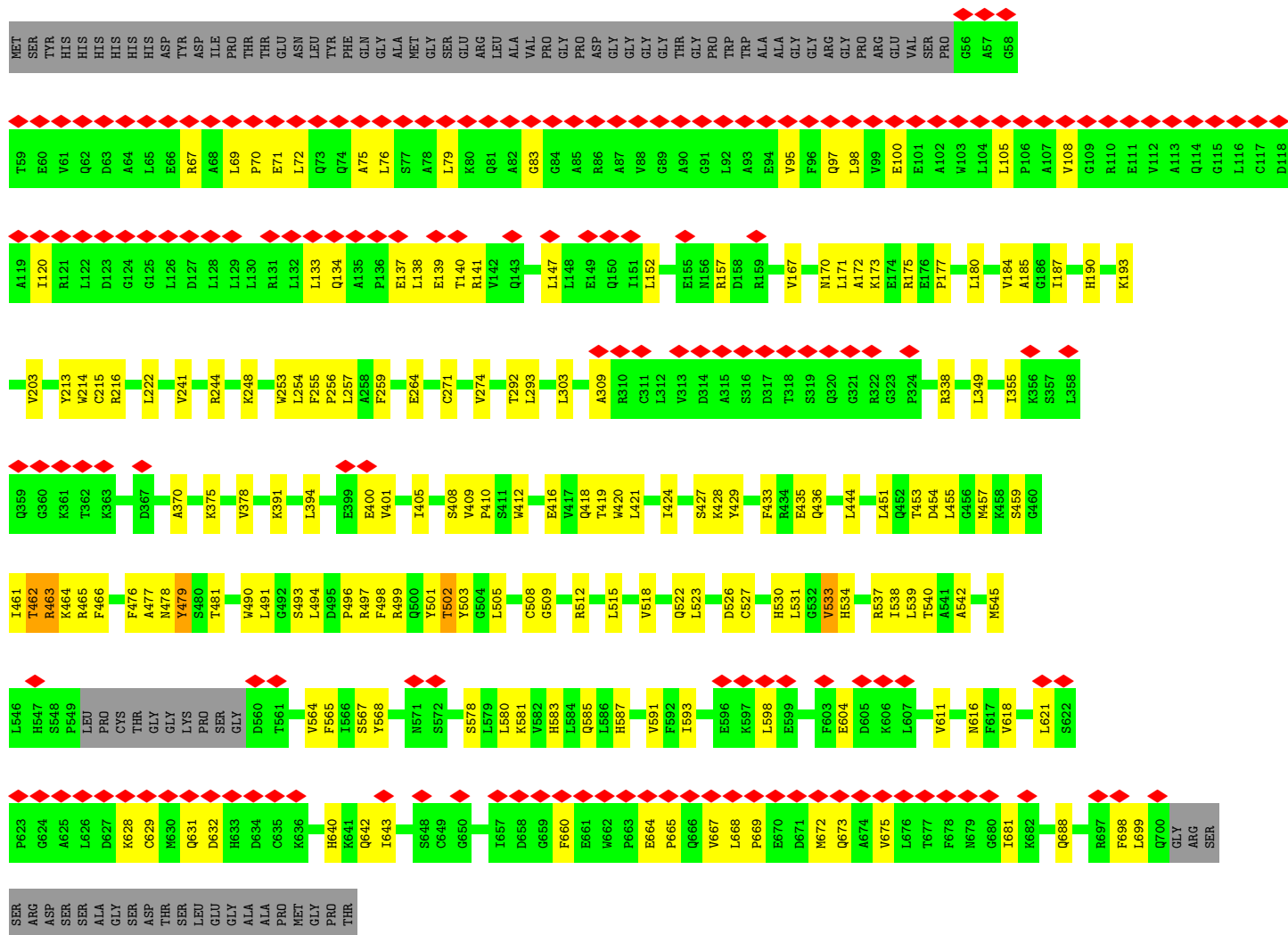


• Molecule 1: NAD(+) hydrolase SARM1

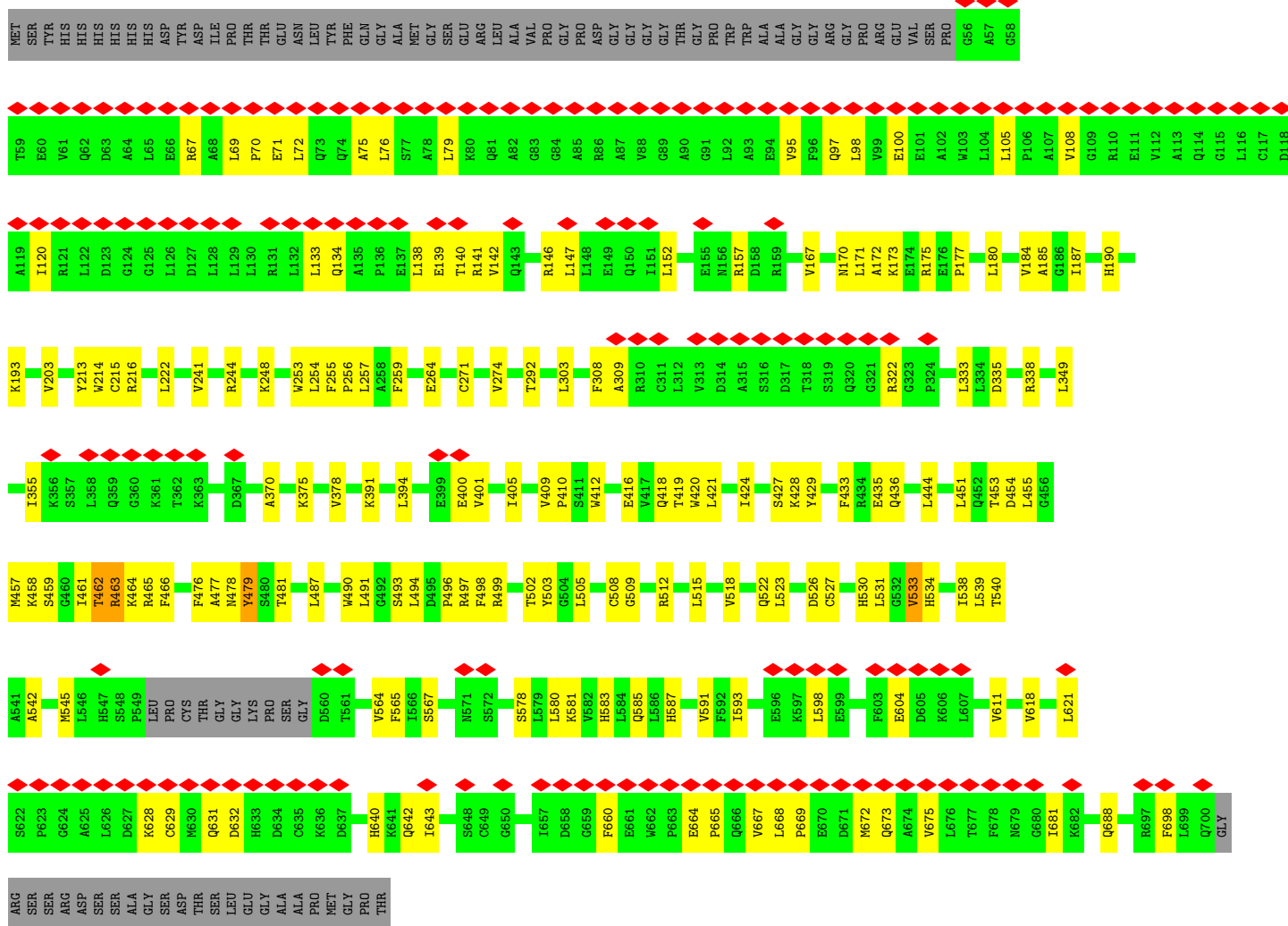




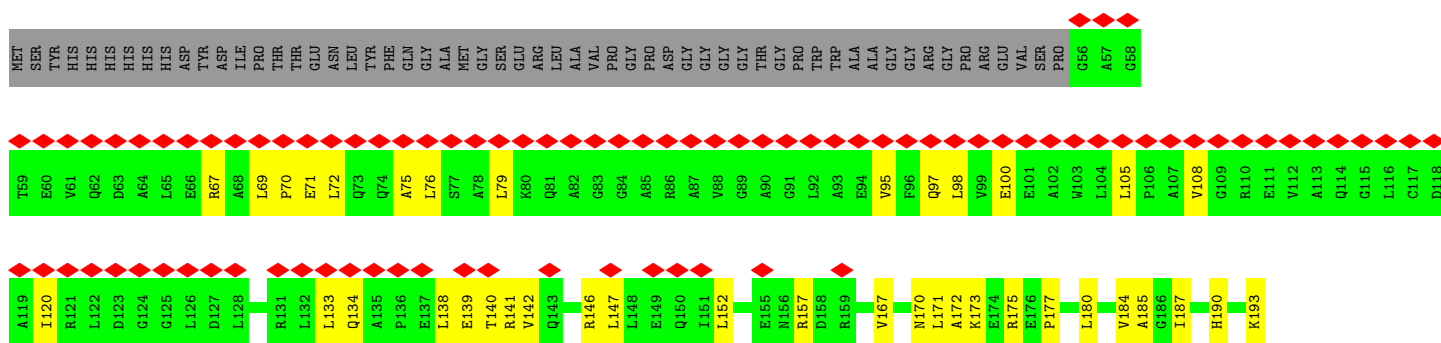
• Molecule 1: NAD(+) hydrolase SARM1



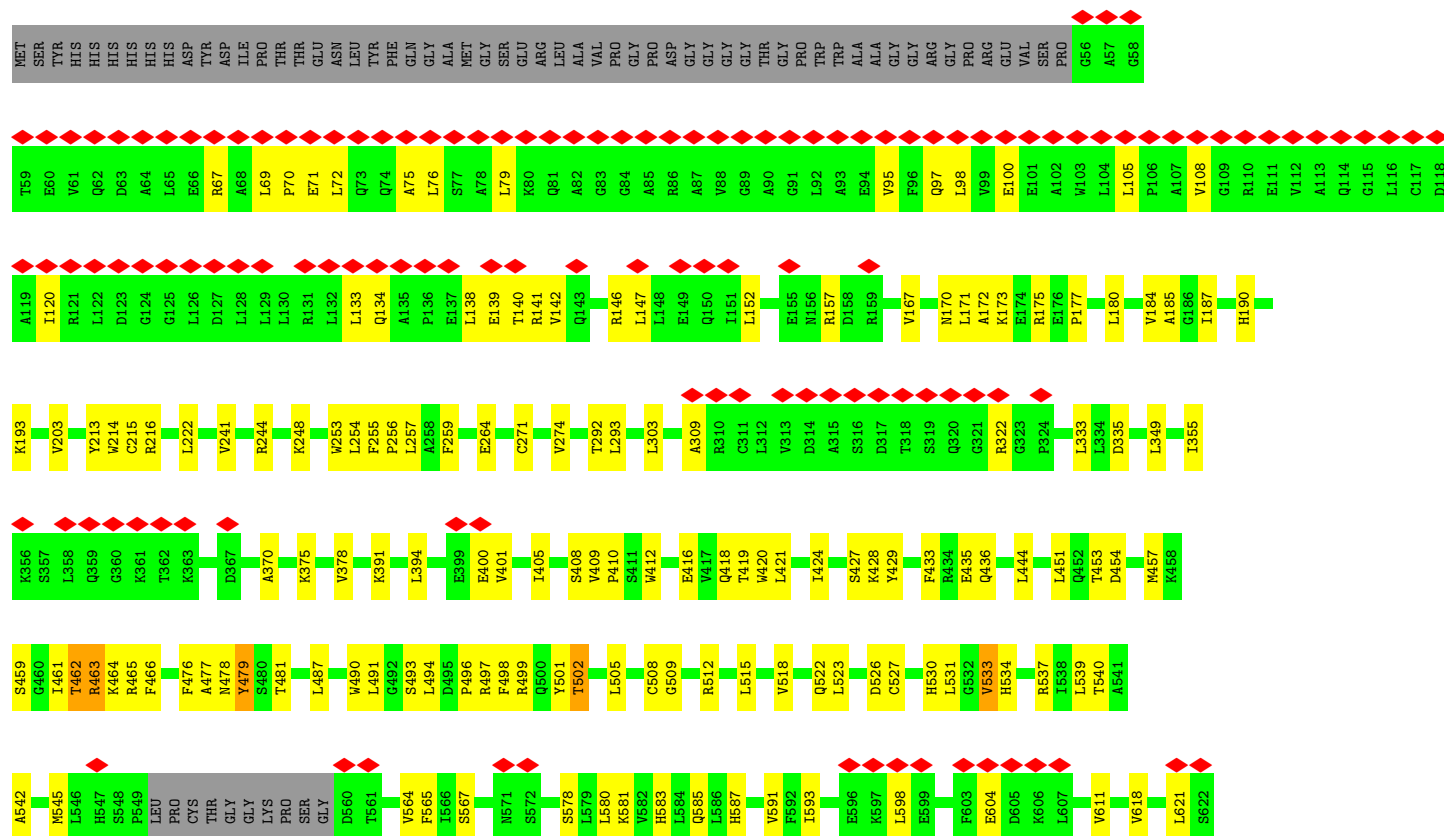
• Molecule 1: NAD(+) hydrolase SARM1

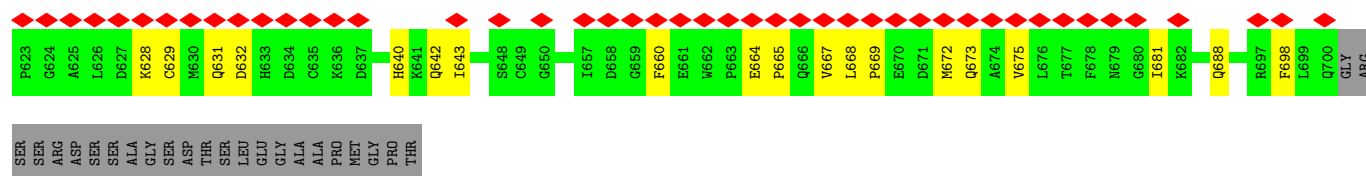


• Molecule 1: NAD(+) hydrolase SARM1

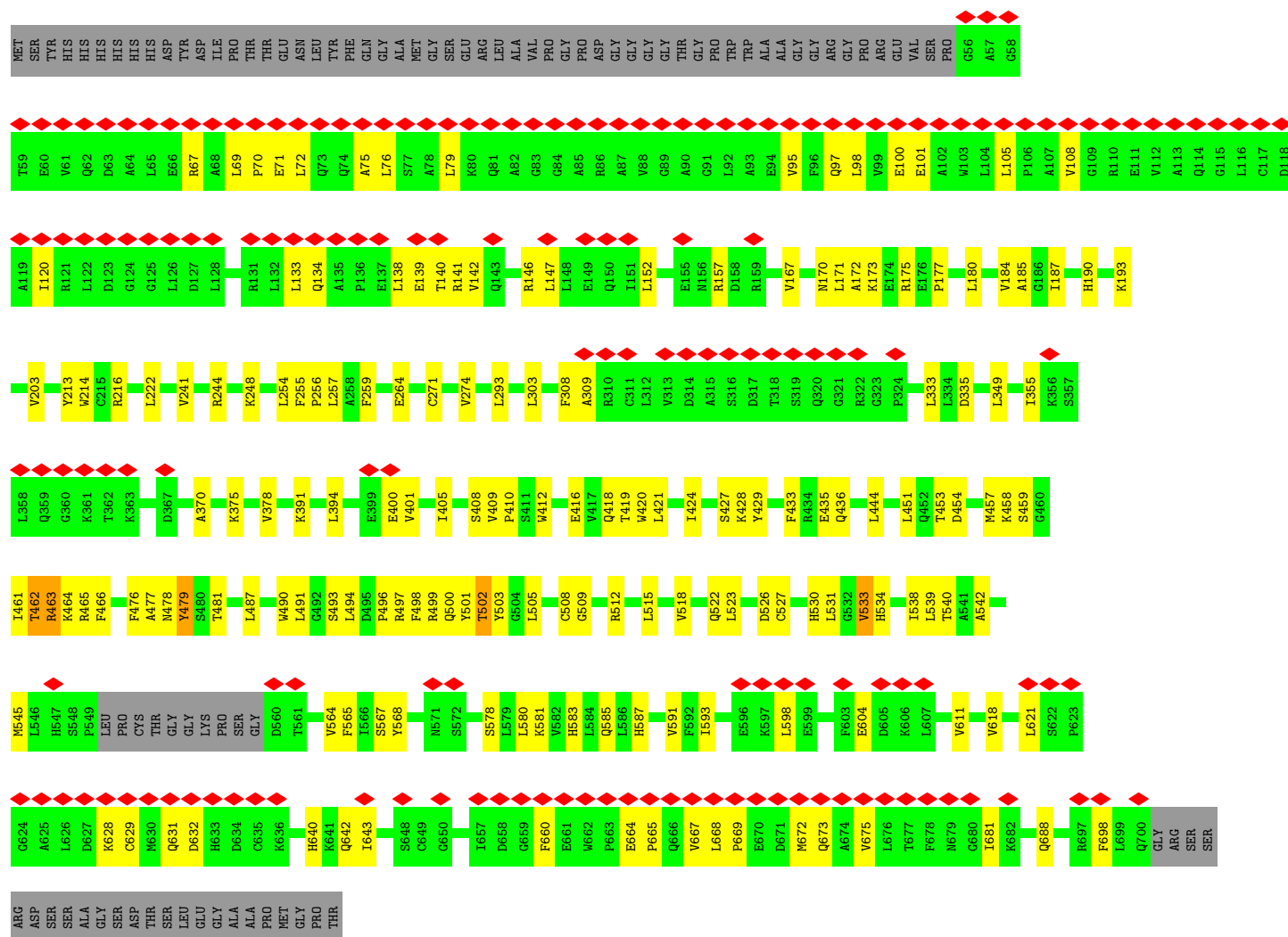


- Molecule 1: NAD(+) hydrolase SARM1





• Molecule 1: NAD(+) hydrolase SARM1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	145000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50, 50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k), GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.645	Depositor
Minimum map value	-0.213	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.1	Depositor
Map size ($\text{\AA}$)	289.45, 289.45, 289.45	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.827, 0.827, 0.827	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: S1N

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	0.57	0/5041	1.40	33/6816 (0.5%)
1	B	0.57	0/5041	1.39	32/6816 (0.5%)
1	C	0.56	0/5041	1.39	30/6816 (0.4%)
1	D	0.56	0/5041	1.39	34/6816 (0.5%)
1	E	0.57	0/5041	1.40	34/6816 (0.5%)
1	F	0.57	0/5041	1.39	32/6816 (0.5%)
1	G	0.57	0/5041	1.39	32/6816 (0.5%)
1	H	0.57	0/5041	1.39	34/6816 (0.5%)
All	All	0.57	0/40328	1.40	261/54528 (0.5%)

There are no bond length outliers.

All (261) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	462	THR	CA-CB-OG1	-12.71	90.54	109.60
1	B	462	THR	CA-CB-OG1	-12.70	90.56	109.60
1	E	462	THR	CA-CB-OG1	-12.68	90.58	109.60
1	H	462	THR	CA-CB-OG1	-12.68	90.58	109.60
1	F	462	THR	CA-CB-OG1	-12.67	90.59	109.60
1	D	462	THR	CA-CB-OG1	-12.67	90.60	109.60
1	C	462	THR	CA-CB-OG1	-12.64	90.63	109.60
1	G	462	THR	CA-CB-OG1	-12.64	90.64	109.60
1	B	424	ILE	N-CA-C	-9.77	103.44	112.43
1	D	424	ILE	N-CA-C	-9.77	103.44	112.43
1	A	424	ILE	N-CA-C	-9.76	103.45	112.43
1	F	424	ILE	N-CA-C	-9.76	103.45	112.43
1	C	424	ILE	N-CA-C	-9.75	103.46	112.43
1	G	424	ILE	N-CA-C	-9.73	103.47	112.43
1	E	424	ILE	N-CA-C	-9.73	103.48	112.43
1	H	424	ILE	N-CA-C	-9.71	103.50	112.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	ARG	CG-CD-NE	8.71	131.17	112.00
1	D	436	GLN	CB-CG-CD	-7.42	99.98	112.60
1	F	436	GLN	CB-CG-CD	-7.41	100.01	112.60
1	A	436	GLN	CB-CG-CD	-7.40	100.02	112.60
1	B	436	GLN	CB-CG-CD	-7.40	100.03	112.60
1	H	436	GLN	CB-CG-CD	-7.38	100.05	112.60
1	C	436	GLN	CB-CG-CD	-7.38	100.05	112.60
1	E	436	GLN	CB-CG-CD	-7.37	100.08	112.60
1	G	436	GLN	CB-CG-CD	-7.36	100.08	112.60
1	E	419	THR	CA-CB-OG1	-7.28	98.69	109.60
1	A	419	THR	CA-CB-OG1	-7.27	98.69	109.60
1	G	419	THR	CA-CB-OG1	-7.27	98.70	109.60
1	F	419	THR	CA-CB-OG1	-7.27	98.70	109.60
1	B	419	THR	CA-CB-OG1	-7.26	98.72	109.60
1	D	419	THR	CA-CB-OG1	-7.25	98.73	109.60
1	C	419	THR	CA-CB-OG1	-7.24	98.74	109.60
1	H	419	THR	CA-CB-OG1	-7.22	98.77	109.60
1	H	418	GLN	CA-C-N	-7.01	110.33	120.29
1	H	418	GLN	C-N-CA	-7.01	110.33	120.29
1	C	418	GLN	CA-C-N	-7.01	110.34	120.29
1	C	418	GLN	C-N-CA	-7.01	110.34	120.29
1	G	418	GLN	CA-C-N	-7.01	110.34	120.29
1	G	418	GLN	C-N-CA	-7.01	110.34	120.29
1	A	418	GLN	CA-C-N	-6.99	110.36	120.29
1	A	418	GLN	C-N-CA	-6.99	110.36	120.29
1	D	418	GLN	CA-C-N	-6.97	110.39	120.29
1	D	418	GLN	C-N-CA	-6.97	110.39	120.29
1	B	418	GLN	CA-C-N	-6.96	110.40	120.29
1	B	418	GLN	C-N-CA	-6.96	110.40	120.29
1	F	418	GLN	CA-C-N	-6.96	110.40	120.29
1	F	418	GLN	C-N-CA	-6.96	110.40	120.29
1	E	418	GLN	CA-C-N	-6.96	110.40	120.29
1	E	418	GLN	C-N-CA	-6.96	110.40	120.29
1	H	465	ARG	CB-CA-C	-6.88	96.34	110.38
1	A	465	ARG	CB-CA-C	-6.87	96.36	110.38
1	G	465	ARG	CB-CA-C	-6.86	96.39	110.38
1	C	465	ARG	CB-CA-C	-6.86	96.40	110.38
1	E	465	ARG	CB-CA-C	-6.86	96.40	110.38
1	D	465	ARG	CB-CA-C	-6.84	96.42	110.38
1	F	465	ARG	CB-CA-C	-6.84	96.42	110.38
1	B	465	ARG	CB-CA-C	-6.83	96.44	110.38
1	D	502	THR	CA-CB-OG1	-6.33	100.11	109.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	502	THR	CA-CB-OG1	-6.33	100.11	109.60
1	C	502	THR	CA-CB-OG1	-6.33	100.11	109.60
1	E	502	THR	CA-CB-OG1	-6.32	100.12	109.60
1	G	502	THR	CA-CB-OG1	-6.32	100.12	109.60
1	F	502	THR	CA-CB-OG1	-6.31	100.13	109.60
1	A	502	THR	CA-CB-OG1	-6.31	100.14	109.60
1	B	502	THR	CA-CB-OG1	-6.30	100.14	109.60
1	D	465	ARG	N-CA-CB	6.24	119.90	110.30
1	H	465	ARG	N-CA-CB	6.22	119.88	110.30
1	A	465	ARG	N-CA-CB	6.21	119.87	110.30
1	C	465	ARG	N-CA-CB	6.21	119.87	110.30
1	E	465	ARG	N-CA-CB	6.21	119.87	110.30
1	G	465	ARG	N-CA-CB	6.21	119.87	110.30
1	B	465	ARG	N-CA-CB	6.20	119.85	110.30
1	F	465	ARG	N-CA-CB	6.19	119.83	110.30
1	A	453	THR	CA-CB-OG1	-6.09	100.47	109.60
1	H	453	THR	CA-CB-OG1	-6.09	100.47	109.60
1	D	453	THR	CA-CB-OG1	-6.08	100.48	109.60
1	A	499	ARG	CB-CG-CD	-6.07	97.33	111.30
1	C	499	ARG	CB-CG-CD	-6.07	97.34	111.30
1	E	453	THR	CA-CB-OG1	-6.06	100.50	109.60
1	B	499	ARG	CB-CG-CD	-6.06	97.36	111.30
1	F	499	ARG	CB-CG-CD	-6.05	97.38	111.30
1	E	499	ARG	CB-CG-CD	-6.05	97.38	111.30
1	G	499	ARG	CB-CG-CD	-6.05	97.38	111.30
1	D	499	ARG	CB-CG-CD	-6.04	97.40	111.30
1	A	476	PHE	CA-CB-CG	6.04	119.84	113.80
1	H	499	ARG	CB-CG-CD	-6.04	97.41	111.30
1	E	476	PHE	CA-CB-CG	6.03	119.83	113.80
1	F	476	PHE	CA-CB-CG	6.02	119.82	113.80
1	B	476	PHE	CA-CB-CG	6.02	119.82	113.80
1	D	476	PHE	CA-CB-CG	6.02	119.82	113.80
1	H	476	PHE	CA-CB-CG	6.02	119.82	113.80
1	G	453	THR	CA-CB-OG1	-6.01	100.58	109.60
1	B	453	THR	CA-CB-OG1	-6.01	100.59	109.60
1	F	453	THR	CA-CB-OG1	-6.01	100.59	109.60
1	C	453	THR	CA-CB-OG1	-6.00	100.59	109.60
1	C	476	PHE	CA-CB-CG	6.00	119.80	113.80
1	G	476	PHE	CA-CB-CG	6.00	119.80	113.80
1	E	481	THR	CA-C-N	-5.99	112.94	122.29
1	E	481	THR	C-N-CA	-5.99	112.94	122.29
1	E	496	PRO	N-CD-CG	-5.98	94.23	103.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	481	THR	CA-C-N	-5.97	112.98	122.29
1	D	481	THR	C-N-CA	-5.97	112.98	122.29
1	D	496	PRO	N-CD-CG	-5.97	94.25	103.20
1	B	496	PRO	N-CD-CG	-5.96	94.26	103.20
1	A	496	PRO	N-CD-CG	-5.95	94.27	103.20
1	H	496	PRO	N-CD-CG	-5.95	94.27	103.20
1	A	481	THR	CA-C-N	-5.95	113.01	122.29
1	A	481	THR	C-N-CA	-5.95	113.01	122.29
1	C	481	THR	CA-C-N	-5.95	113.01	122.29
1	C	481	THR	C-N-CA	-5.95	113.01	122.29
1	G	481	THR	CA-C-N	-5.95	113.01	122.29
1	G	481	THR	C-N-CA	-5.95	113.01	122.29
1	F	496	PRO	N-CD-CG	-5.95	94.28	103.20
1	F	481	THR	CA-C-N	-5.94	113.02	122.29
1	F	481	THR	C-N-CA	-5.94	113.02	122.29
1	H	481	THR	CA-C-N	-5.94	113.02	122.29
1	H	481	THR	C-N-CA	-5.94	113.02	122.29
1	B	481	THR	CA-C-N	-5.94	113.02	122.29
1	B	481	THR	C-N-CA	-5.94	113.02	122.29
1	C	496	PRO	N-CD-CG	-5.93	94.30	103.20
1	G	496	PRO	N-CD-CG	-5.93	94.30	103.20
1	G	540	THR	CA-CB-OG1	-5.92	100.73	109.60
1	C	540	THR	CA-CB-OG1	-5.91	100.74	109.60
1	F	479	TYR	N-CA-CB	-5.88	101.63	110.91
1	C	479	TYR	N-CA-CB	-5.88	101.63	110.91
1	E	479	TYR	N-CA-CB	-5.87	101.63	110.91
1	G	479	TYR	N-CA-CB	-5.87	101.63	110.91
1	F	540	THR	CA-CB-OG1	-5.87	100.80	109.60
1	D	479	TYR	N-CA-CB	-5.86	101.65	110.91
1	B	540	THR	CA-CB-OG1	-5.85	100.83	109.60
1	D	540	THR	CA-CB-OG1	-5.85	100.83	109.60
1	H	540	THR	CA-CB-OG1	-5.85	100.83	109.60
1	A	479	TYR	N-CA-CB	-5.85	101.67	110.91
1	B	479	TYR	N-CA-CB	-5.84	101.68	110.91
1	E	540	THR	CA-CB-OG1	-5.83	100.85	109.60
1	H	479	TYR	N-CA-CB	-5.83	101.70	110.91
1	A	540	THR	CA-CB-OG1	-5.80	100.91	109.60
1	B	499	ARG	CG-CD-NE	-5.71	99.44	112.00
1	A	499	ARG	CG-CD-NE	-5.70	99.46	112.00
1	C	499	ARG	CG-CD-NE	-5.70	99.46	112.00
1	D	499	ARG	CG-CD-NE	-5.70	99.47	112.00
1	G	499	ARG	CG-CD-NE	-5.69	99.48	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	499	ARG	CG-CD-NE	-5.68	99.50	112.00
1	H	499	ARG	CG-CD-NE	-5.68	99.50	112.00
1	E	499	ARG	CG-CD-NE	-5.68	99.51	112.00
1	B	533	VAL	N-CA-C	-5.48	105.18	110.72
1	F	533	VAL	N-CA-C	-5.48	105.18	110.72
1	H	533	VAL	N-CA-C	-5.48	105.18	110.72
1	C	533	VAL	N-CA-C	-5.48	105.18	110.72
1	C	478	ASN	CA-C-N	-5.47	114.41	122.83
1	C	478	ASN	C-N-CA	-5.47	114.41	122.83
1	G	478	ASN	CA-C-N	-5.47	114.41	122.83
1	G	478	ASN	C-N-CA	-5.47	114.41	122.83
1	G	533	VAL	N-CA-C	-5.47	105.20	110.72
1	A	533	VAL	N-CA-C	-5.46	105.20	110.72
1	F	478	ASN	CA-C-N	-5.46	114.43	122.83
1	F	478	ASN	C-N-CA	-5.46	114.43	122.83
1	D	533	VAL	N-CA-C	-5.45	105.21	110.72
1	A	464	LYS	CA-C-N	-5.44	111.42	120.68
1	A	464	LYS	C-N-CA	-5.44	111.42	120.68
1	C	464	LYS	CA-C-N	-5.44	111.42	120.68
1	C	464	LYS	C-N-CA	-5.44	111.42	120.68
1	E	464	LYS	CA-C-N	-5.44	111.42	120.68
1	E	464	LYS	C-N-CA	-5.44	111.42	120.68
1	G	464	LYS	CA-C-N	-5.44	111.42	120.68
1	G	464	LYS	C-N-CA	-5.44	111.42	120.68
1	B	464	LYS	CA-C-N	-5.44	111.43	120.68
1	B	464	LYS	C-N-CA	-5.44	111.43	120.68
1	A	478	ASN	CA-C-N	-5.44	114.45	122.83
1	A	478	ASN	C-N-CA	-5.44	114.45	122.83
1	D	478	ASN	CA-C-N	-5.44	114.45	122.83
1	D	478	ASN	C-N-CA	-5.44	114.45	122.83
1	E	478	ASN	CA-C-N	-5.44	114.45	122.83
1	E	478	ASN	C-N-CA	-5.44	114.45	122.83
1	F	464	LYS	CA-C-N	-5.44	111.44	120.68
1	F	464	LYS	C-N-CA	-5.44	111.44	120.68
1	H	464	LYS	CA-C-N	-5.43	111.45	120.68
1	H	464	LYS	C-N-CA	-5.43	111.45	120.68
1	B	478	ASN	CA-C-N	-5.43	114.47	122.83
1	B	478	ASN	C-N-CA	-5.43	114.47	122.83
1	H	478	ASN	CA-C-N	-5.43	114.47	122.83
1	H	478	ASN	C-N-CA	-5.43	114.47	122.83
1	A	530	HIS	CA-CB-CG	-5.42	108.38	113.80
1	E	533	VAL	N-CA-C	-5.42	105.25	110.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	464	LYS	CA-C-N	-5.41	111.49	120.68
1	D	464	LYS	C-N-CA	-5.41	111.49	120.68
1	H	530	HIS	CA-CB-CG	-5.38	108.42	113.80
1	E	530	HIS	CA-CB-CG	-5.37	108.43	113.80
1	D	530	HIS	CA-CB-CG	-5.34	108.46	113.80
1	B	530	HIS	CA-CB-CG	-5.33	108.47	113.80
1	F	530	HIS	CA-CB-CG	-5.33	108.47	113.80
1	C	530	HIS	CA-CB-CG	-5.28	108.52	113.80
1	G	530	HIS	CA-CB-CG	-5.27	108.53	113.80
1	H	400	GLU	CA-C-N	-5.20	118.85	122.59
1	H	400	GLU	C-N-CA	-5.20	118.85	122.59
1	E	400	GLU	CA-C-N	-5.17	118.87	122.59
1	E	400	GLU	C-N-CA	-5.17	118.87	122.59
1	B	400	GLU	CA-C-N	-5.16	118.88	122.59
1	B	400	GLU	C-N-CA	-5.16	118.88	122.59
1	D	400	GLU	CA-C-N	-5.16	118.88	122.59
1	D	400	GLU	C-N-CA	-5.16	118.88	122.59
1	C	400	GLU	CA-C-N	-5.14	118.89	122.59
1	C	400	GLU	C-N-CA	-5.14	118.89	122.59
1	D	416	GLU	CA-C-N	-5.14	111.87	120.30
1	D	416	GLU	C-N-CA	-5.14	111.87	120.30
1	A	400	GLU	CA-C-N	-5.14	118.89	122.59
1	A	400	GLU	C-N-CA	-5.14	118.89	122.59
1	C	416	GLU	CA-C-N	-5.13	111.88	120.30
1	C	416	GLU	C-N-CA	-5.13	111.88	120.30
1	B	435	GLU	N-CA-C	-5.13	105.87	111.82
1	H	435	GLU	N-CA-C	-5.12	105.88	111.82
1	A	416	GLU	CA-C-N	-5.12	111.90	120.30
1	A	416	GLU	C-N-CA	-5.12	111.90	120.30
1	E	416	GLU	CA-C-N	-5.12	111.90	120.30
1	E	416	GLU	C-N-CA	-5.12	111.90	120.30
1	E	538	ILE	N-CA-C	-5.12	105.72	110.53
1	F	416	GLU	CA-C-N	-5.12	111.91	120.30
1	F	416	GLU	C-N-CA	-5.12	111.91	120.30
1	H	416	GLU	CA-C-N	-5.12	111.91	120.30
1	H	416	GLU	C-N-CA	-5.12	111.91	120.30
1	G	416	GLU	CA-C-N	-5.11	111.92	120.30
1	G	416	GLU	C-N-CA	-5.11	111.92	120.30
1	E	435	GLU	N-CA-C	-5.11	105.89	111.82
1	G	435	GLU	N-CA-C	-5.11	105.89	111.82
1	F	400	GLU	CA-C-N	-5.10	118.92	122.59
1	F	400	GLU	C-N-CA	-5.10	118.92	122.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	416	GLU	CA-C-N	-5.10	111.94	120.30
1	B	416	GLU	C-N-CA	-5.10	111.94	120.30
1	D	435	GLU	N-CA-C	-5.09	105.91	111.82
1	A	538	ILE	N-CA-C	-5.09	105.75	110.53
1	C	435	GLU	N-CA-C	-5.09	105.91	111.82
1	D	503	TYR	CB-CA-C	-5.09	102.34	110.79
1	H	503	TYR	CB-CA-C	-5.09	102.34	110.79
1	D	463	ARG	CG-CD-NE	-5.09	100.81	112.00
1	B	463	ARG	CG-CD-NE	-5.08	100.83	112.00
1	D	538	ILE	N-CA-C	-5.08	105.76	110.53
1	H	463	ARG	CG-CD-NE	-5.08	100.83	112.00
1	A	503	TYR	CB-CA-C	-5.08	102.36	110.79
1	E	463	ARG	CG-CD-NE	-5.08	100.83	112.00
1	E	503	TYR	CB-CA-C	-5.08	102.36	110.79
1	G	400	GLU	CA-C-N	-5.08	118.94	122.59
1	G	400	GLU	C-N-CA	-5.08	118.94	122.59
1	F	435	GLU	N-CA-C	-5.06	105.95	111.82
1	C	463	ARG	CG-CD-NE	-5.06	100.86	112.00
1	G	463	ARG	CG-CD-NE	-5.06	100.86	112.00
1	F	185	ALA	CA-C-N	5.06	125.56	119.94
1	F	185	ALA	C-N-CA	5.06	125.56	119.94
1	G	185	ALA	CA-C-N	5.06	125.56	119.94
1	G	185	ALA	C-N-CA	5.06	125.56	119.94
1	A	435	GLU	N-CA-C	-5.06	105.95	111.82
1	F	463	ARG	CG-CD-NE	-5.06	100.87	112.00
1	A	463	ARG	CG-CD-NE	-5.05	100.88	112.00
1	H	185	ALA	CA-C-N	5.05	125.55	119.94
1	H	185	ALA	C-N-CA	5.05	125.55	119.94
1	H	538	ILE	N-CA-C	-5.05	105.78	110.53
1	D	185	ALA	CA-C-N	5.05	125.54	119.94
1	D	185	ALA	C-N-CA	5.05	125.54	119.94
1	E	185	ALA	CA-C-N	5.03	125.53	119.94
1	E	185	ALA	C-N-CA	5.03	125.53	119.94
1	B	185	ALA	CA-C-N	5.03	125.52	119.94
1	B	185	ALA	C-N-CA	5.03	125.52	119.94

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	4959	0	5024	117	0
1	B	4959	0	5024	116	0
1	C	4959	0	5024	116	0
1	D	4959	0	5024	114	0
1	E	4959	0	5024	114	0
1	F	4959	0	5024	114	0
1	G	4959	0	5024	113	0
1	H	4959	0	5024	112	0
2	A	23	0	0	0	0
2	B	23	0	0	0	0
2	C	23	0	0	0	0
2	D	23	0	0	0	0
2	E	23	0	0	0	0
2	F	23	0	0	0	0
2	G	23	0	0	0	0
2	H	23	0	0	0	0
All	All	39856	0	40192	854	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 11.

All (854) 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:H:213:TYR:HE1	1:H:216:ARG:HH21	1.21	0.88
1:G:213:TYR:HE1	1:G:216:ARG:HH21	1.21	0.88
1:B:213:TYR:HE1	1:B:216:ARG:HH21	1.21	0.88
1:A:213:TYR:HE1	1:A:216:ARG:HH21	1.22	0.88
1:C:213:TYR:HE1	1:C:216:ARG:HH21	1.21	0.88
1:E:213:TYR:HE1	1:E:216:ARG:HH21	1.22	0.88
1:D:213:TYR:HE1	1:D:216:ARG:HH21	1.22	0.88
1:F:213:TYR:HE1	1:F:216:ARG:HH21	1.22	0.87
1:E:170:ASN:OD1	1:E:173:LYS:HE3	1.79	0.83
1:G:170:ASN:OD1	1:G:173:LYS:HE3	1.79	0.82
1:A:170:ASN:OD1	1:A:173:LYS:HE3	1.79	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ASN:OD1	1:B:173:LYS:HE3	1.79	0.82
1:C:170:ASN:OD1	1:C:173:LYS:HE3	1.79	0.82
1:C:203:VAL:HG21	1:C:241:VAL:HG13	1.63	0.81
1:H:170:ASN:OD1	1:H:173:LYS:HE3	1.79	0.81
1:E:203:VAL:HG21	1:E:241:VAL:HG13	1.63	0.81
1:A:203:VAL:HG21	1:A:241:VAL:HG13	1.63	0.81
1:B:203:VAL:HG21	1:B:241:VAL:HG13	1.63	0.81
1:D:170:ASN:OD1	1:D:173:LYS:HE3	1.79	0.81
1:H:203:VAL:HG21	1:H:241:VAL:HG13	1.63	0.81
1:F:203:VAL:HG21	1:F:241:VAL:HG13	1.63	0.81
1:G:203:VAL:HG21	1:G:241:VAL:HG13	1.63	0.81
1:D:203:VAL:HG21	1:D:241:VAL:HG13	1.63	0.81
1:F:170:ASN:OD1	1:F:173:LYS:HE3	1.79	0.80
1:A:522:GLN:HG2	1:H:533:VAL:CG2	2.15	0.77
1:C:533:VAL:CG2	1:D:522:GLN:HG2	2.15	0.77
1:G:533:VAL:CG2	1:H:522:GLN:HG2	2.15	0.77
1:D:533:VAL:CG2	1:E:522:GLN:HG2	2.15	0.77
1:A:533:VAL:CG2	1:B:522:GLN:HG2	2.14	0.77
1:E:533:VAL:CG2	1:F:522:GLN:HG2	2.14	0.76
1:B:533:VAL:CG2	1:C:522:GLN:HG2	2.15	0.76
1:F:533:VAL:CG2	1:G:522:GLN:HG2	2.15	0.76
1:B:76:LEU:HA	1:B:79:LEU:HD12	1.69	0.75
1:C:76:LEU:HA	1:C:79:LEU:HD12	1.69	0.74
1:G:76:LEU:HA	1:G:79:LEU:HD12	1.68	0.74
1:D:76:LEU:HA	1:D:79:LEU:HD12	1.69	0.74
1:B:72:LEU:HD13	1:B:120:ILE:HG12	1.70	0.74
1:C:72:LEU:HD13	1:C:120:ILE:HG12	1.70	0.74
1:D:533:VAL:HG22	1:E:522:GLN:HG2	1.70	0.73
1:D:72:LEU:HD13	1:D:120:ILE:HG12	1.70	0.73
1:F:76:LEU:HA	1:F:79:LEU:HD12	1.69	0.73
1:H:76:LEU:HA	1:H:79:LEU:HD12	1.69	0.73
1:A:522:GLN:HG2	1:H:533:VAL:HG22	1.70	0.73
1:A:76:LEU:HA	1:A:79:LEU:HD12	1.69	0.72
1:A:72:LEU:HD13	1:A:120:ILE:HG12	1.70	0.72
1:E:76:LEU:HA	1:E:79:LEU:HD12	1.69	0.72
1:G:533:VAL:HG22	1:H:522:GLN:HG2	1.70	0.72
1:G:72:LEU:HD13	1:G:120:ILE:HG12	1.70	0.72
1:E:72:LEU:HD13	1:E:120:ILE:HG12	1.70	0.72
1:E:533:VAL:HG22	1:F:522:GLN:HG2	1.70	0.72
1:F:72:LEU:HD13	1:F:120:ILE:HG12	1.70	0.72
1:B:533:VAL:HG22	1:C:522:GLN:HG2	1.70	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:VAL:HG22	1:B:522:GLN:HG2	1.70	0.71
1:F:533:VAL:HG22	1:G:522:GLN:HG2	1.70	0.71
1:C:533:VAL:HG22	1:D:522:GLN:HG2	1.70	0.71
1:H:72:LEU:HD13	1:H:120:ILE:HG12	1.70	0.71
1:G:213:TYR:HE1	1:G:216:ARG:NH2	1.90	0.70
1:F:213:TYR:HE1	1:F:216:ARG:NH2	1.90	0.69
1:H:213:TYR:HE1	1:H:216:ARG:NH2	1.89	0.69
1:B:213:TYR:HE1	1:B:216:ARG:NH2	1.89	0.69
1:D:213:TYR:HE1	1:D:216:ARG:NH2	1.90	0.69
1:C:213:TYR:HE1	1:C:216:ARG:NH2	1.90	0.69
1:E:213:TYR:HE1	1:E:216:ARG:NH2	1.90	0.68
1:A:213:TYR:HE1	1:A:216:ARG:NH2	1.90	0.68
1:C:665:PRO:O	1:C:673:GLN:HG2	1.94	0.68
1:E:665:PRO:O	1:E:673:GLN:HG2	1.94	0.68
1:D:665:PRO:O	1:D:673:GLN:HG2	1.94	0.68
1:F:665:PRO:O	1:F:673:GLN:HG2	1.94	0.68
1:B:665:PRO:O	1:B:673:GLN:HG2	1.94	0.67
1:G:665:PRO:O	1:G:673:GLN:HG2	1.94	0.67
1:A:665:PRO:O	1:A:673:GLN:HG2	1.94	0.67
1:E:611:VAL:HG21	1:E:642:GLN:HG2	1.78	0.66
1:H:665:PRO:O	1:H:673:GLN:HG2	1.94	0.66
1:A:611:VAL:HG21	1:A:642:GLN:HG2	1.78	0.65
1:B:611:VAL:HG21	1:B:642:GLN:HG2	1.78	0.65
1:H:611:VAL:HG21	1:H:642:GLN:HG2	1.78	0.65
1:D:611:VAL:HG21	1:D:642:GLN:HG2	1.78	0.65
1:F:611:VAL:HG21	1:F:642:GLN:HG2	1.78	0.65
1:C:611:VAL:HG21	1:C:642:GLN:HG2	1.78	0.65
1:G:611:VAL:HG21	1:G:642:GLN:HG2	1.78	0.65
1:A:688:GLN:HE22	1:H:216:ARG:HB2	1.63	0.63
1:D:429:TYR:CE1	1:D:457:MET:HG3	2.34	0.63
1:B:497:ARG:HH22	1:C:509:GLY:HA2	1.64	0.63
1:F:429:TYR:CE1	1:F:457:MET:HG3	2.34	0.63
1:H:429:TYR:CE1	1:H:457:MET:HG3	2.34	0.63
1:C:216:ARG:HB2	1:D:688:GLN:HE22	1.63	0.63
1:A:216:ARG:HB2	1:B:688:GLN:HE22	1.63	0.63
1:D:216:ARG:HB2	1:E:688:GLN:HE22	1.63	0.63
1:E:429:TYR:CE1	1:E:457:MET:HG3	2.34	0.63
1:C:429:TYR:CE1	1:C:457:MET:HG3	2.34	0.63
1:B:429:TYR:CE1	1:B:457:MET:HG3	2.34	0.63
1:C:497:ARG:HH22	1:D:509:GLY:HA2	1.64	0.63
1:D:497:ARG:HH22	1:E:509:GLY:HA2	1.64	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:429:TYR:CE1	1:G:457:MET:HG3	2.34	0.63
1:G:497:ARG:HH22	1:H:509:GLY:HA2	1.64	0.63
1:E:497:ARG:HH22	1:F:509:GLY:HA2	1.64	0.63
1:A:629:CYS:HA	1:A:640:HIS:HB2	1.81	0.62
1:B:216:ARG:HB2	1:C:688:GLN:HE22	1.64	0.62
1:G:216:ARG:HB2	1:H:688:GLN:HE22	1.64	0.62
1:H:629:CYS:HA	1:H:640:HIS:HB2	1.81	0.62
1:F:497:ARG:HH22	1:G:509:GLY:HA2	1.64	0.62
1:A:509:GLY:HA2	1:H:497:ARG:HH22	1.64	0.62
1:A:429:TYR:CE1	1:A:457:MET:HG3	2.34	0.62
1:B:629:CYS:HA	1:B:640:HIS:HB2	1.81	0.62
1:A:497:ARG:HH22	1:B:509:GLY:HA2	1.64	0.62
1:E:491:LEU:HD11	1:E:505:LEU:HD12	1.82	0.62
1:F:216:ARG:HB2	1:G:688:GLN:HE22	1.64	0.62
1:A:491:LEU:HD11	1:A:505:LEU:HD12	1.82	0.62
1:F:629:CYS:HA	1:F:640:HIS:HB2	1.81	0.62
1:G:629:CYS:HA	1:G:640:HIS:HB2	1.81	0.62
1:C:629:CYS:HA	1:C:640:HIS:HB2	1.81	0.61
1:D:491:LEU:HD11	1:D:505:LEU:HD12	1.82	0.61
1:C:491:LEU:HD11	1:C:505:LEU:HD12	1.82	0.61
1:F:491:LEU:HD11	1:F:505:LEU:HD12	1.82	0.61
1:H:491:LEU:HD11	1:H:505:LEU:HD12	1.82	0.61
1:B:491:LEU:HD11	1:B:505:LEU:HD12	1.82	0.61
1:E:216:ARG:HB2	1:F:688:GLN:HE22	1.63	0.61
1:G:491:LEU:HD11	1:G:505:LEU:HD12	1.82	0.61
1:D:629:CYS:HA	1:D:640:HIS:HB2	1.81	0.61
1:E:629:CYS:HA	1:E:640:HIS:HB2	1.81	0.61
1:C:391:LYS:HG2	1:C:401:VAL:HG21	1.84	0.60
1:G:391:LYS:HG2	1:G:401:VAL:HG21	1.84	0.60
1:E:581:LYS:HB2	1:E:593:ILE:HD11	1.84	0.60
1:F:391:LYS:HG2	1:F:401:VAL:HG21	1.84	0.60
1:F:581:LYS:HB2	1:F:593:ILE:HD11	1.84	0.60
1:A:533:VAL:HG23	1:B:522:GLN:HG2	1.84	0.60
1:B:391:LYS:HG2	1:B:401:VAL:HG21	1.84	0.60
1:A:391:LYS:HG2	1:A:401:VAL:HG21	1.84	0.59
1:D:391:LYS:HG2	1:D:401:VAL:HG21	1.84	0.59
1:H:391:LYS:HG2	1:H:401:VAL:HG21	1.84	0.59
1:E:391:LYS:HG2	1:E:401:VAL:HG21	1.84	0.59
1:G:581:LYS:HB2	1:G:593:ILE:HD11	1.84	0.59
1:B:533:VAL:HG23	1:C:522:GLN:HG2	1.84	0.59
1:A:190:HIS:HA	1:A:193:LYS:HE2	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:LEU:HA	1:D:141:ARG:HD3	1.85	0.59
1:E:138:LEU:HA	1:E:141:ARG:HD3	1.85	0.59
1:H:581:LYS:HB2	1:H:593:ILE:HD11	1.84	0.59
1:B:190:HIS:HA	1:B:193:LYS:HE2	1.85	0.59
1:C:581:LYS:HB2	1:C:593:ILE:HD11	1.84	0.59
1:D:581:LYS:HB2	1:D:593:ILE:HD11	1.84	0.59
1:H:244:ARG:O	1:H:248:LYS:HG2	2.03	0.59
1:C:138:LEU:HA	1:C:141:ARG:HD3	1.85	0.59
1:F:244:ARG:O	1:F:248:LYS:HG2	2.03	0.59
1:A:522:GLN:HG2	1:H:533:VAL:HG23	1.85	0.58
1:E:533:VAL:HG23	1:F:522:GLN:HG2	1.84	0.58
1:F:138:LEU:HA	1:F:141:ARG:HD3	1.85	0.58
1:H:190:HIS:HA	1:H:193:LYS:HE2	1.85	0.58
1:A:581:LYS:HB2	1:A:593:ILE:HD11	1.84	0.58
1:D:409:VAL:N	1:D:410:PRO:CD	2.67	0.58
1:F:533:VAL:HG23	1:G:522:GLN:HG2	1.84	0.58
1:B:244:ARG:O	1:B:248:LYS:HG2	2.03	0.58
1:B:409:VAL:N	1:B:410:PRO:CD	2.67	0.58
1:C:190:HIS:HA	1:C:193:LYS:HE2	1.85	0.58
1:B:138:LEU:HA	1:B:141:ARG:HD3	1.85	0.58
1:C:533:VAL:HG23	1:D:522:GLN:HG2	1.85	0.58
1:G:138:LEU:HA	1:G:141:ARG:HD3	1.85	0.58
1:A:409:VAL:N	1:A:410:PRO:CD	2.67	0.58
1:D:244:ARG:O	1:D:248:LYS:HG2	2.04	0.58
1:E:190:HIS:HA	1:E:193:LYS:HE2	1.85	0.58
1:F:409:VAL:N	1:F:410:PRO:CD	2.67	0.58
1:A:138:LEU:HA	1:A:141:ARG:HD3	1.85	0.58
1:E:244:ARG:O	1:E:248:LYS:HG2	2.03	0.58
1:G:533:VAL:HG23	1:H:522:GLN:HG2	1.84	0.58
1:H:409:VAL:N	1:H:410:PRO:CD	2.67	0.58
1:B:581:LYS:HB2	1:B:593:ILE:HD11	1.84	0.58
1:H:138:LEU:HA	1:H:141:ARG:HD3	1.85	0.58
1:D:533:VAL:HG23	1:E:522:GLN:HG2	1.85	0.58
1:G:409:VAL:N	1:G:410:PRO:CD	2.67	0.58
1:D:190:HIS:HA	1:D:193:LYS:HE2	1.85	0.57
1:G:244:ARG:O	1:G:248:LYS:HG2	2.03	0.57
1:C:409:VAL:N	1:C:410:PRO:CD	2.67	0.57
1:F:190:HIS:HA	1:F:193:LYS:HE2	1.85	0.57
1:E:409:VAL:N	1:E:410:PRO:CD	2.67	0.57
1:A:244:ARG:O	1:A:248:LYS:HG2	2.03	0.57
1:C:244:ARG:O	1:C:248:LYS:HG2	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:190:HIS:HA	1:G:193:LYS:HE2	1.85	0.57
1:C:134:GLN:NE2	1:C:167:VAL:HG21	2.20	0.56
1:B:421:LEU:HD11	1:B:433:PHE:CG	2.41	0.56
1:E:421:LEU:HD11	1:E:433:PHE:CG	2.41	0.56
1:G:421:LEU:HD11	1:G:433:PHE:CG	2.41	0.56
1:B:134:GLN:NE2	1:B:167:VAL:HG21	2.20	0.56
1:F:134:GLN:NE2	1:F:167:VAL:HG21	2.20	0.56
1:G:134:GLN:NE2	1:G:167:VAL:HG21	2.20	0.56
1:G:451:LEU:HD21	1:G:466:PHE:CD2	2.41	0.56
1:H:421:LEU:HD11	1:H:433:PHE:CG	2.41	0.56
1:B:451:LEU:HD21	1:B:466:PHE:CD2	2.41	0.56
1:E:134:GLN:NE2	1:E:167:VAL:HG21	2.20	0.56
1:F:75:ALA:O	1:F:79:LEU:HG	2.06	0.56
1:H:451:LEU:HD21	1:H:466:PHE:CD2	2.41	0.56
1:A:461:ILE:HD12	1:B:454:ASP:HB2	1.88	0.56
1:C:461:ILE:HD12	1:D:454:ASP:HB2	1.88	0.56
1:C:493:SER:O	1:C:494:LEU:C	2.49	0.56
1:E:461:ILE:HD12	1:F:454:ASP:HB2	1.88	0.56
1:F:421:LEU:HD11	1:F:433:PHE:CG	2.41	0.56
1:H:134:GLN:NE2	1:H:167:VAL:HG21	2.20	0.56
1:D:421:LEU:HD11	1:D:433:PHE:CG	2.41	0.56
1:G:461:ILE:HD12	1:H:454:ASP:HB2	1.88	0.56
1:H:75:ALA:O	1:H:79:LEU:HG	2.06	0.56
1:A:421:LEU:HD11	1:A:433:PHE:CG	2.41	0.55
1:A:451:LEU:HD21	1:A:466:PHE:CD2	2.41	0.55
1:C:664:GLU:O	1:C:667:VAL:HG22	2.07	0.55
1:D:451:LEU:HD21	1:D:466:PHE:CD2	2.41	0.55
1:E:451:LEU:HD21	1:E:466:PHE:CD2	2.41	0.55
1:D:134:GLN:NE2	1:D:167:VAL:HG21	2.20	0.55
1:A:134:GLN:NE2	1:A:167:VAL:HG21	2.20	0.55
1:C:75:ALA:O	1:C:79:LEU:HG	2.06	0.55
1:C:421:LEU:HD11	1:C:433:PHE:CG	2.41	0.55
1:D:493:SER:O	1:D:494:LEU:C	2.49	0.55
1:C:214:TRP:HB3	1:C:222:LEU:HD11	1.88	0.55
1:D:75:ALA:O	1:D:79:LEU:HG	2.06	0.55
1:D:214:TRP:HB3	1:D:222:LEU:HD11	1.88	0.55
1:D:664:GLU:O	1:D:667:VAL:HG22	2.07	0.55
1:G:214:TRP:HB3	1:G:222:LEU:HD11	1.88	0.55
1:B:75:ALA:O	1:B:79:LEU:HG	2.06	0.55
1:B:664:GLU:O	1:B:667:VAL:HG22	2.07	0.55
1:E:493:SER:O	1:E:494:LEU:C	2.49	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ALA:O	1:A:79:LEU:HG	2.06	0.55
1:F:451:LEU:HD21	1:F:466:PHE:CD2	2.41	0.55
1:H:214:TRP:HB3	1:H:222:LEU:HD11	1.88	0.55
1:A:568:TYR:HH	1:H:259:PHE:HZ	1.55	0.55
1:C:451:LEU:HD21	1:C:466:PHE:CD2	2.41	0.55
1:F:461:ILE:HD12	1:G:454:ASP:HB2	1.88	0.55
1:G:75:ALA:O	1:G:79:LEU:HG	2.06	0.54
1:E:664:GLU:O	1:E:667:VAL:HG22	2.07	0.54
1:F:214:TRP:HB3	1:F:222:LEU:HD11	1.88	0.54
1:F:493:SER:O	1:F:494:LEU:C	2.49	0.54
1:G:213:TYR:CE1	1:G:216:ARG:NH2	2.72	0.54
1:E:75:ALA:O	1:E:79:LEU:HG	2.06	0.54
1:G:664:GLU:O	1:G:667:VAL:HG22	2.07	0.54
1:A:214:TRP:HB3	1:A:222:LEU:HD11	1.88	0.54
1:B:461:ILE:HD12	1:C:454:ASP:HB2	1.88	0.54
1:D:461:ILE:HD12	1:E:454:ASP:HB2	1.88	0.54
1:B:214:TRP:HB3	1:B:222:LEU:HD11	1.88	0.54
1:A:454:ASP:HB2	1:H:461:ILE:HD12	1.88	0.54
1:B:515:LEU:O	1:B:518:VAL:HG12	2.08	0.54
1:G:493:SER:O	1:G:494:LEU:C	2.49	0.54
1:E:214:TRP:HB3	1:E:222:LEU:HD11	1.88	0.54
1:G:515:LEU:O	1:G:518:VAL:HG12	2.08	0.54
1:H:664:GLU:O	1:H:667:VAL:HG22	2.07	0.54
1:A:213:TYR:CE1	1:A:216:ARG:NH2	2.72	0.53
1:A:664:GLU:O	1:A:667:VAL:HG22	2.07	0.53
1:F:515:LEU:O	1:F:518:VAL:HG12	2.08	0.53
1:F:664:GLU:O	1:F:667:VAL:HG22	2.07	0.53
1:E:515:LEU:O	1:E:518:VAL:HG12	2.08	0.53
1:A:259:PHE:HZ	1:B:568:TYR:HH	1.56	0.53
1:G:259:PHE:HZ	1:H:568:TYR:HH	1.56	0.53
1:C:515:LEU:O	1:C:518:VAL:HG12	2.09	0.53
1:F:67:ARG:O	1:F:71:GLU:HG2	2.09	0.53
1:H:493:SER:O	1:H:494:LEU:C	2.49	0.53
1:A:175:ARG:HD3	1:A:213:TYR:CD2	2.44	0.53
1:E:175:ARG:HD3	1:E:213:TYR:CD2	2.44	0.53
1:A:515:LEU:O	1:A:518:VAL:HG12	2.08	0.53
1:C:67:ARG:O	1:C:71:GLU:HG2	2.09	0.53
1:D:67:ARG:O	1:D:71:GLU:HG2	2.09	0.53
1:D:175:ARG:HD3	1:D:213:TYR:CD2	2.44	0.53
1:A:67:ARG:O	1:A:71:GLU:HG2	2.09	0.53
1:C:175:ARG:HD3	1:C:213:TYR:CD2	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:67:ARG:O	1:E:71:GLU:HG2	2.09	0.53
1:E:72:LEU:CD1	1:E:120:ILE:HG12	2.39	0.53
1:F:175:ARG:HD3	1:F:213:TYR:CD2	2.44	0.53
1:H:515:LEU:O	1:H:518:VAL:HG12	2.09	0.53
1:B:67:ARG:O	1:B:71:GLU:HG2	2.09	0.52
1:A:493:SER:O	1:A:494:LEU:C	2.49	0.52
1:G:175:ARG:HD3	1:G:213:TYR:CD2	2.44	0.52
1:H:175:ARG:HD3	1:H:213:TYR:CD2	2.44	0.52
1:C:72:LEU:CD1	1:C:120:ILE:HG12	2.39	0.52
1:D:515:LEU:O	1:D:518:VAL:HG12	2.09	0.52
1:G:508:CYS:SG	1:G:526:ASP:HB3	2.50	0.52
1:H:67:ARG:O	1:H:71:GLU:HG2	2.09	0.52
1:H:72:LEU:CD1	1:H:120:ILE:HG12	2.39	0.52
1:B:175:ARG:HD3	1:B:213:TYR:CD2	2.44	0.52
1:B:213:TYR:CE1	1:B:216:ARG:NH2	2.72	0.52
1:B:508:CYS:SG	1:B:526:ASP:HB3	2.50	0.52
1:C:254:LEU:HD23	1:C:257:LEU:HD12	1.92	0.52
1:F:213:TYR:CE1	1:F:216:ARG:NH2	2.72	0.52
1:F:508:CYS:SG	1:F:526:ASP:HB3	2.50	0.52
1:H:508:CYS:SG	1:H:526:ASP:HB3	2.50	0.52
1:A:508:CYS:SG	1:A:526:ASP:HB3	2.50	0.52
1:E:254:LEU:HD23	1:E:257:LEU:HD12	1.92	0.52
1:G:67:ARG:O	1:G:71:GLU:HG2	2.09	0.52
1:B:254:LEU:HD23	1:B:257:LEU:HD12	1.92	0.52
1:B:493:SER:O	1:B:494:LEU:C	2.49	0.52
1:C:508:CYS:SG	1:C:526:ASP:HB3	2.50	0.52
1:D:254:LEU:HD23	1:D:257:LEU:HD12	1.92	0.52
1:F:254:LEU:HD23	1:F:257:LEU:HD12	1.92	0.52
1:D:539:LEU:O	1:D:542:ALA:HB3	2.10	0.52
1:E:539:LEU:O	1:E:542:ALA:HB3	2.10	0.52
1:G:539:LEU:O	1:G:542:ALA:HB3	2.10	0.52
1:B:539:LEU:O	1:B:542:ALA:HB3	2.10	0.51
1:H:539:LEU:O	1:H:542:ALA:HB3	2.10	0.51
1:A:254:LEU:HD23	1:A:257:LEU:HD12	1.92	0.51
1:C:539:LEU:O	1:C:542:ALA:HB3	2.10	0.51
1:F:72:LEU:CD1	1:F:120:ILE:HG12	2.39	0.51
1:F:349:LEU:HD21	1:F:370:ALA:HB1	1.93	0.51
1:G:349:LEU:HD21	1:G:370:ALA:HB1	1.93	0.51
1:E:508:CYS:SG	1:E:526:ASP:HB3	2.50	0.51
1:B:349:LEU:HD21	1:B:370:ALA:HB1	1.93	0.51
1:C:349:LEU:HD21	1:C:370:ALA:HB1	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:508:CYS:SG	1:D:526:ASP:HB3	2.50	0.51
1:E:213:TYR:CE1	1:E:216:ARG:NH2	2.72	0.51
1:G:254:LEU:HD23	1:G:257:LEU:HD12	1.92	0.51
1:A:72:LEU:CD1	1:A:120:ILE:HG12	2.39	0.51
1:H:213:TYR:CE1	1:H:216:ARG:NH2	2.72	0.51
1:H:349:LEU:HD21	1:H:370:ALA:HB1	1.93	0.51
1:F:539:LEU:O	1:F:542:ALA:HB3	2.10	0.51
1:A:349:LEU:HD21	1:A:370:ALA:HB1	1.93	0.51
1:D:349:LEU:HD21	1:D:370:ALA:HB1	1.93	0.51
1:A:170:ASN:O	1:A:173:LYS:HG2	2.11	0.51
1:B:170:ASN:O	1:B:173:LYS:HG2	2.11	0.51
1:H:254:LEU:HD23	1:H:257:LEU:HD12	1.92	0.51
1:B:180:LEU:O	1:B:184:VAL:HG23	2.12	0.50
1:C:180:LEU:O	1:C:184:VAL:HG23	2.11	0.50
1:E:349:LEU:HD21	1:E:370:ALA:HB1	1.93	0.50
1:A:180:LEU:O	1:A:184:VAL:HG23	2.12	0.50
1:A:539:LEU:O	1:A:542:ALA:HB3	2.10	0.50
1:G:180:LEU:O	1:G:184:VAL:HG23	2.12	0.50
1:A:95:VAL:HA	1:A:98:LEU:HB2	1.94	0.50
1:E:170:ASN:O	1:E:173:LYS:HG2	2.11	0.50
1:D:170:ASN:O	1:D:173:LYS:HG2	2.11	0.50
1:D:213:TYR:CE1	1:D:216:ARG:NH2	2.72	0.50
1:D:271:CYS:HA	1:D:274:VAL:HG12	1.94	0.50
1:B:95:VAL:HA	1:B:98:LEU:HB2	1.94	0.50
1:D:180:LEU:O	1:D:184:VAL:HG23	2.12	0.50
1:F:180:LEU:O	1:F:184:VAL:HG23	2.11	0.50
1:G:170:ASN:O	1:G:173:LYS:HG2	2.11	0.50
1:H:170:ASN:O	1:H:173:LYS:HG2	2.11	0.50
1:H:180:LEU:O	1:H:184:VAL:HG23	2.11	0.50
1:C:95:VAL:HA	1:C:98:LEU:HB2	1.94	0.50
1:C:170:ASN:O	1:C:173:LYS:HG2	2.11	0.50
1:E:271:CYS:HA	1:E:274:VAL:HG12	1.94	0.50
1:E:180:LEU:O	1:E:184:VAL:HG23	2.12	0.49
1:D:72:LEU:CD1	1:D:120:ILE:HG12	2.39	0.49
1:H:95:VAL:HA	1:H:98:LEU:HB2	1.94	0.49
1:E:95:VAL:HA	1:E:98:LEU:HB2	1.94	0.49
1:F:170:ASN:O	1:F:173:LYS:HG2	2.11	0.49
1:H:271:CYS:HA	1:H:274:VAL:HG12	1.94	0.49
1:B:271:CYS:HA	1:B:274:VAL:HG12	1.94	0.49
1:B:498:PHE:HE1	1:B:534:HIS:CD2	2.31	0.49
1:A:498:PHE:HE1	1:A:534:HIS:CD2	2.31	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:VAL:HA	1:D:98:LEU:HB2	1.94	0.49
1:G:498:PHE:HE1	1:G:534:HIS:CD2	2.31	0.49
1:A:427:SER:C	1:A:429:TYR:N	2.70	0.49
1:H:668:LEU:HD13	1:H:672:MET:HE2	1.95	0.49
1:C:427:SER:C	1:C:429:TYR:N	2.70	0.48
1:E:427:SER:C	1:E:429:TYR:N	2.70	0.48
1:F:95:VAL:HA	1:F:98:LEU:HB2	1.94	0.48
1:H:498:PHE:HE1	1:H:534:HIS:CD2	2.31	0.48
1:A:271:CYS:HA	1:A:274:VAL:HG12	1.94	0.48
1:A:309:ALA:O	1:A:355:ILE:HD11	2.13	0.48
1:B:72:LEU:CD1	1:B:120:ILE:HG12	2.39	0.48
1:G:95:VAL:HA	1:G:98:LEU:HB2	1.93	0.48
1:A:578:SER:HB3	1:H:259:PHE:HD2	1.79	0.48
1:A:668:LEU:HD13	1:A:672:MET:HE2	1.95	0.48
1:C:259:PHE:HD2	1:D:578:SER:HB3	1.79	0.48
1:C:271:CYS:HA	1:C:274:VAL:HG12	1.94	0.48
1:C:69:LEU:HB3	1:C:70:PRO:HD3	1.96	0.48
1:C:498:PHE:HE1	1:C:534:HIS:CD2	2.31	0.48
1:F:427:SER:C	1:F:429:TYR:N	2.70	0.48
1:G:72:LEU:CD1	1:G:120:ILE:HG12	2.39	0.48
1:G:668:LEU:HD13	1:G:672:MET:HE2	1.95	0.48
1:B:322:ARG:H	1:B:322:ARG:HG3	1.41	0.48
1:C:477:ALA:HB3	1:C:479:TYR:CE2	2.49	0.48
1:D:170:ASN:OD1	1:D:173:LYS:CE	2.58	0.48
1:H:477:ALA:HB3	1:H:479:TYR:CE2	2.48	0.48
1:D:477:ALA:HB3	1:D:479:TYR:CE2	2.48	0.48
1:G:309:ALA:O	1:G:355:ILE:HD11	2.14	0.48
1:B:668:LEU:HD13	1:B:672:MET:HE2	1.95	0.48
1:C:213:TYR:CE1	1:C:216:ARG:NH2	2.72	0.48
1:F:170:ASN:OD1	1:F:173:LYS:CE	2.58	0.48
1:F:498:PHE:HE1	1:F:534:HIS:CD2	2.31	0.48
1:G:271:CYS:HA	1:G:274:VAL:HG12	1.94	0.48
1:B:477:ALA:HB3	1:B:479:TYR:CE2	2.48	0.48
1:G:69:LEU:HB3	1:G:70:PRO:HD3	1.96	0.48
1:F:271:CYS:HA	1:F:274:VAL:HG12	1.94	0.48
1:D:498:PHE:HE1	1:D:534:HIS:CD2	2.31	0.48
1:H:672:MET:O	1:H:675:VAL:HG12	2.14	0.48
1:A:672:MET:O	1:A:675:VAL:HG12	2.14	0.47
1:C:309:ALA:O	1:C:355:ILE:HD11	2.13	0.47
1:C:498:PHE:CE1	1:C:534:HIS:CD2	3.02	0.47
1:C:672:MET:O	1:C:675:VAL:HG12	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:477:ALA:HB3	1:E:479:TYR:CE2	2.49	0.47
1:E:498:PHE:HE1	1:E:534:HIS:CD2	2.31	0.47
1:F:498:PHE:CE1	1:F:534:HIS:CD2	3.02	0.47
1:F:668:LEU:HD13	1:F:672:MET:HE2	1.95	0.47
1:F:672:MET:O	1:F:675:VAL:HG12	2.14	0.47
1:A:259:PHE:HD2	1:B:578:SER:HB3	1.79	0.47
1:B:672:MET:O	1:B:675:VAL:HG12	2.14	0.47
1:D:498:PHE:CE1	1:D:534:HIS:CD2	3.02	0.47
1:D:672:MET:O	1:D:675:VAL:HG12	2.14	0.47
1:E:498:PHE:CE1	1:E:534:HIS:CD2	3.02	0.47
1:G:498:PHE:CE1	1:G:534:HIS:CD2	3.02	0.47
1:A:512:ARG:HD3	1:A:545:MET:HE1	1.97	0.47
1:B:259:PHE:HD2	1:C:578:SER:HB3	1.79	0.47
1:E:69:LEU:HB3	1:E:70:PRO:HD3	1.97	0.47
1:F:259:PHE:HD2	1:G:578:SER:HB3	1.78	0.47
1:F:477:ALA:HB3	1:F:479:TYR:CE2	2.48	0.47
1:H:512:ARG:HD3	1:H:545:MET:HE1	1.97	0.47
1:A:69:LEU:HB3	1:A:70:PRO:HD3	1.97	0.47
1:B:512:ARG:HD3	1:B:545:MET:HE1	1.96	0.47
1:D:309:ALA:O	1:D:355:ILE:HD11	2.13	0.47
1:E:309:ALA:O	1:E:355:ILE:HD11	2.13	0.47
1:E:427:SER:O	1:E:428:LYS:C	2.58	0.47
1:E:512:ARG:HD3	1:E:545:MET:HE1	1.96	0.47
1:G:477:ALA:HB3	1:G:479:TYR:CE2	2.49	0.47
1:H:309:ALA:O	1:H:355:ILE:HD11	2.13	0.47
1:B:498:PHE:CE1	1:B:534:HIS:CD2	3.02	0.47
1:D:259:PHE:HD2	1:E:578:SER:HB3	1.79	0.47
1:D:427:SER:O	1:D:428:LYS:C	2.58	0.47
1:D:668:LEU:HD13	1:D:672:MET:HE2	1.95	0.47
1:E:170:ASN:OD1	1:E:173:LYS:CE	2.58	0.47
1:H:427:SER:O	1:H:428:LYS:C	2.58	0.47
1:E:259:PHE:HD2	1:F:578:SER:HB3	1.79	0.47
1:A:477:ALA:HB3	1:A:479:TYR:CE2	2.49	0.47
1:A:498:PHE:CE1	1:A:534:HIS:CD2	3.02	0.47
1:C:668:LEU:HD13	1:C:672:MET:HE2	1.95	0.47
1:D:69:LEU:HB3	1:D:70:PRO:HD3	1.96	0.47
1:E:672:MET:O	1:E:675:VAL:HG12	2.14	0.47
1:H:498:PHE:CE1	1:H:534:HIS:CD2	3.03	0.47
1:A:405:ILE:HD13	1:A:420:TRP:HD1	1.80	0.47
1:B:309:ALA:O	1:B:355:ILE:HD11	2.13	0.47
1:B:427:SER:C	1:B:429:TYR:N	2.70	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:512:ARG:HD3	1:C:545:MET:HE1	1.96	0.47
1:D:427:SER:C	1:D:429:TYR:N	2.70	0.47
1:B:170:ASN:OD1	1:B:173:LYS:CE	2.58	0.47
1:B:405:ILE:HD13	1:B:420:TRP:HD1	1.80	0.47
1:C:427:SER:O	1:C:428:LYS:C	2.58	0.47
1:F:309:ALA:O	1:F:355:ILE:HD11	2.13	0.47
1:G:170:ASN:OD1	1:G:173:LYS:CE	2.58	0.47
1:G:672:MET:O	1:G:675:VAL:HG12	2.14	0.47
1:H:405:ILE:HD13	1:H:420:TRP:HD1	1.80	0.47
1:C:170:ASN:OD1	1:C:173:LYS:CE	2.58	0.47
1:C:405:ILE:HD13	1:C:420:TRP:HD1	1.80	0.47
1:F:512:ARG:HD3	1:F:545:MET:HE1	1.97	0.47
1:G:427:SER:O	1:G:428:LYS:C	2.58	0.47
1:H:69:LEU:HB3	1:H:70:PRO:HD3	1.96	0.47
1:D:512:ARG:HD3	1:D:545:MET:HE1	1.96	0.46
1:G:259:PHE:HD2	1:H:578:SER:HB3	1.79	0.46
1:G:405:ILE:HD13	1:G:420:TRP:HD1	1.80	0.46
1:G:427:SER:C	1:G:429:TYR:N	2.70	0.46
1:G:512:ARG:HD3	1:G:545:MET:HE1	1.96	0.46
1:B:69:LEU:HB3	1:B:70:PRO:HD3	1.96	0.46
1:E:668:LEU:HD13	1:E:672:MET:HE2	1.95	0.46
1:A:565:PHE:HE1	1:A:567:SER:HB2	1.80	0.46
1:E:405:ILE:HD13	1:E:420:TRP:HD1	1.80	0.46
1:F:69:LEU:HB3	1:F:70:PRO:HD3	1.96	0.46
1:D:405:ILE:HD13	1:D:420:TRP:HD1	1.80	0.46
1:D:581:LYS:O	1:D:585:GLN:HG3	2.16	0.46
1:F:405:ILE:HD13	1:F:420:TRP:HD1	1.80	0.46
1:G:565:PHE:HE1	1:G:567:SER:HB2	1.80	0.46
1:C:581:LYS:O	1:C:585:GLN:HG3	2.16	0.46
1:H:565:PHE:HE1	1:H:567:SER:HB2	1.80	0.46
1:C:95:VAL:HG13	1:C:147:LEU:HD22	1.98	0.46
1:D:565:PHE:HE1	1:D:567:SER:HB2	1.80	0.46
1:B:581:LYS:O	1:B:585:GLN:HG3	2.16	0.46
1:E:133:LEU:O	1:E:141:ARG:HD2	2.16	0.46
1:E:565:PHE:HE1	1:E:567:SER:HB2	1.80	0.46
1:E:581:LYS:O	1:E:585:GLN:HG3	2.16	0.46
1:F:133:LEU:O	1:F:141:ARG:HD2	2.16	0.46
1:F:581:LYS:O	1:F:585:GLN:HG3	2.16	0.46
1:H:505:LEU:HD23	1:H:527:CYS:HB3	1.98	0.46
1:A:505:LEU:HD23	1:A:527:CYS:HB3	1.98	0.46
1:B:427:SER:O	1:B:428:LYS:C	2.58	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:505:LEU:HD23	1:G:527:CYS:HB3	1.98	0.46
1:G:581:LYS:O	1:G:585:GLN:HG3	2.16	0.46
1:C:152:LEU:HD21	1:C:187:ILE:HG13	1.99	0.45
1:D:133:LEU:O	1:D:141:ARG:HD2	2.16	0.45
1:F:308:PHE:HD1	1:F:308:PHE:HA	1.61	0.45
1:E:643:ILE:HG21	1:E:672:MET:HB2	1.99	0.45
1:F:565:PHE:HE1	1:F:567:SER:HB2	1.80	0.45
1:B:531:LEU:HD12	1:B:534:HIS:CE1	2.51	0.45
1:F:427:SER:O	1:F:428:LYS:C	2.58	0.45
1:G:157:ARG:NH2	1:G:193:LYS:HE3	2.32	0.45
1:G:531:LEU:HD12	1:G:534:HIS:CE1	2.51	0.45
1:H:531:LEU:HD12	1:H:534:HIS:CE1	2.51	0.45
1:A:458:LYS:H	1:A:458:LYS:HG2	1.52	0.45
1:A:581:LYS:O	1:A:585:GLN:HG3	2.16	0.45
1:B:505:LEU:HD23	1:B:527:CYS:HB3	1.98	0.45
1:C:133:LEU:O	1:C:141:ARG:HD2	2.16	0.45
1:F:505:LEU:HD23	1:F:527:CYS:HB3	1.98	0.45
1:A:531:LEU:HD12	1:A:534:HIS:CE1	2.51	0.45
1:D:139:GLU:HG3	1:D:140:THR:HG23	1.98	0.45
1:F:643:ILE:HG21	1:F:672:MET:HB2	1.99	0.45
1:G:133:LEU:O	1:G:141:ARG:HD2	2.16	0.45
1:H:157:ARG:NH2	1:H:193:LYS:HE3	2.32	0.45
1:H:462:THR:O	1:H:463:ARG:C	2.59	0.45
1:C:565:PHE:HE1	1:C:567:SER:HB2	1.80	0.45
1:F:462:THR:O	1:F:463:ARG:C	2.59	0.45
1:A:95:VAL:HG13	1:A:147:LEU:HD22	1.98	0.45
1:A:462:THR:O	1:A:463:ARG:C	2.59	0.45
1:B:133:LEU:O	1:B:141:ARG:HD2	2.16	0.45
1:D:95:VAL:HG13	1:D:147:LEU:HD22	1.98	0.45
1:D:537:ARG:HE	1:D:537:ARG:HB3	1.52	0.45
1:E:139:GLU:HG3	1:E:140:THR:HG23	1.99	0.45
1:E:152:LEU:HD21	1:E:187:ILE:HG13	1.99	0.45
1:E:487:LEU:HD12	1:E:487:LEU:HA	1.71	0.45
1:A:152:LEU:HD21	1:A:187:ILE:HG13	1.99	0.45
1:B:95:VAL:HG13	1:B:147:LEU:HD22	1.98	0.45
1:B:565:PHE:HE1	1:B:567:SER:HB2	1.80	0.45
1:C:531:LEU:HD12	1:C:534:HIS:CE1	2.51	0.45
1:D:157:ARG:NH2	1:D:193:LYS:HE3	2.32	0.45
1:G:487:LEU:HD12	1:G:487:LEU:HA	1.71	0.45
1:B:487:LEU:HD12	1:B:487:LEU:HA	1.71	0.45
1:C:157:ARG:NH2	1:C:193:LYS:HE3	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:LEU:HD21	1:D:187:ILE:HG13	1.99	0.45
1:G:462:THR:O	1:G:463:ARG:C	2.59	0.45
1:H:643:ILE:HG21	1:H:672:MET:HB2	1.99	0.45
1:A:583:HIS:O	1:A:587:HIS:HD2	2.00	0.45
1:A:643:ILE:HG21	1:A:672:MET:HB2	1.99	0.45
1:C:583:HIS:O	1:C:587:HIS:HD2	2.00	0.45
1:D:583:HIS:O	1:D:587:HIS:HD2	2.00	0.45
1:D:643:ILE:HG21	1:D:672:MET:HB2	1.99	0.45
1:F:152:LEU:HD21	1:F:187:ILE:HG13	1.99	0.45
1:G:139:GLU:HG3	1:G:140:THR:HG23	1.98	0.45
1:G:501:TYR:O	1:G:502:THR:C	2.60	0.45
1:G:643:ILE:HG21	1:G:672:MET:HB2	1.99	0.45
1:H:95:VAL:HG13	1:H:147:LEU:HD22	1.98	0.45
1:H:487:LEU:HD12	1:H:487:LEU:HA	1.71	0.45
1:A:157:ARG:NH2	1:A:193:LYS:HE3	2.32	0.44
1:F:583:HIS:O	1:F:587:HIS:HD2	2.00	0.44
1:E:95:VAL:HG13	1:E:147:LEU:HD22	1.98	0.44
1:F:501:TYR:O	1:F:502:THR:C	2.60	0.44
1:F:531:LEU:HD12	1:F:534:HIS:CE1	2.51	0.44
1:H:170:ASN:OD1	1:H:173:LYS:CE	2.58	0.44
1:H:293:LEU:HD12	1:H:293:LEU:HA	1.87	0.44
1:H:429:TYR:CZ	1:H:457:MET:HG3	2.53	0.44
1:H:581:LYS:O	1:H:585:GLN:HG3	2.16	0.44
1:A:293:LEU:HD12	1:A:293:LEU:HA	1.88	0.44
1:B:139:GLU:HG3	1:B:140:THR:HG23	1.99	0.44
1:B:429:TYR:CZ	1:B:457:MET:HG3	2.53	0.44
1:B:490:TRP:CZ3	1:B:515:LEU:HD21	2.53	0.44
1:C:505:LEU:HD23	1:C:527:CYS:HB3	1.98	0.44
1:E:505:LEU:HD23	1:E:527:CYS:HB3	1.98	0.44
1:F:157:ARG:NH2	1:F:193:LYS:HE3	2.32	0.44
1:F:429:TYR:CZ	1:F:457:MET:HG3	2.52	0.44
1:G:152:LEU:HD21	1:G:187:ILE:HG13	1.99	0.44
1:G:420:TRP:O	1:G:421:LEU:C	2.59	0.44
1:H:133:LEU:O	1:H:141:ARG:HD2	2.16	0.44
1:A:133:LEU:O	1:A:141:ARG:HD2	2.16	0.44
1:A:139:GLU:HG3	1:A:140:THR:HG23	1.99	0.44
1:B:583:HIS:O	1:B:587:HIS:HD2	2.00	0.44
1:D:490:TRP:CZ3	1:D:515:LEU:HD21	2.53	0.44
1:D:531:LEU:HD12	1:D:534:HIS:CE1	2.51	0.44
1:F:95:VAL:HG13	1:F:147:LEU:HD22	1.98	0.44
1:H:308:PHE:HD1	1:H:308:PHE:HA	1.61	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:458:LYS:H	1:H:458:LYS:HG2	1.52	0.44
1:H:501:TYR:O	1:H:502:THR:C	2.60	0.44
1:H:583:HIS:O	1:H:587:HIS:HD2	2.00	0.44
1:A:643:ILE:CG2	1:A:672:MET:HB2	2.48	0.44
1:B:157:ARG:NH2	1:B:193:LYS:HE3	2.32	0.44
1:B:375:LYS:O	1:B:378:VAL:HG12	2.18	0.44
1:C:375:LYS:O	1:C:378:VAL:HG12	2.18	0.44
1:D:505:LEU:HD23	1:D:527:CYS:HB3	1.98	0.44
1:D:643:ILE:CG2	1:D:672:MET:HB2	2.48	0.44
1:E:157:ARG:NH2	1:E:193:LYS:HE3	2.32	0.44
1:E:490:TRP:CZ3	1:E:515:LEU:HD21	2.53	0.44
1:E:531:LEU:HD12	1:E:534:HIS:CE1	2.51	0.44
1:G:95:VAL:HG13	1:G:147:LEU:HD22	1.98	0.44
1:A:427:SER:O	1:A:428:LYS:C	2.58	0.44
1:B:643:ILE:HG21	1:B:672:MET:HB2	1.99	0.44
1:C:643:ILE:HG21	1:C:672:MET:HB2	1.99	0.44
1:D:429:TYR:CZ	1:D:457:MET:HG3	2.53	0.44
1:E:429:TYR:CZ	1:E:457:MET:HG3	2.53	0.44
1:E:643:ILE:CG2	1:E:672:MET:HB2	2.48	0.44
1:G:375:LYS:O	1:G:378:VAL:HG12	2.18	0.44
1:H:139:GLU:HG3	1:H:140:THR:HG23	1.98	0.44
1:D:293:LEU:HD12	1:D:293:LEU:HA	1.87	0.44
1:F:375:LYS:O	1:F:378:VAL:HG12	2.18	0.44
1:C:444:LEU:HD23	1:C:444:LEU:HA	1.81	0.44
1:E:462:THR:O	1:E:463:ARG:C	2.59	0.44
1:F:564:VAL:HB	1:F:591:VAL:HG13	2.00	0.44
1:G:429:TYR:CZ	1:G:457:MET:HG3	2.52	0.44
1:A:429:TYR:CZ	1:A:457:MET:HG3	2.53	0.44
1:A:490:TRP:CZ3	1:A:515:LEU:HD21	2.53	0.44
1:A:564:VAL:HB	1:A:591:VAL:HG13	2.00	0.44
1:B:152:LEU:HD21	1:B:187:ILE:HG13	1.99	0.44
1:B:293:LEU:HD12	1:B:293:LEU:HA	1.88	0.44
1:C:490:TRP:CZ3	1:C:515:LEU:HD21	2.53	0.44
1:C:643:ILE:CG2	1:C:672:MET:HB2	2.48	0.44
1:E:564:VAL:HB	1:E:591:VAL:HG13	2.00	0.44
1:F:139:GLU:HG3	1:F:140:THR:HG23	1.99	0.44
1:F:490:TRP:CZ3	1:F:515:LEU:HD21	2.53	0.44
1:G:643:ILE:CG2	1:G:672:MET:HB2	2.48	0.44
1:H:490:TRP:CZ3	1:H:515:LEU:HD21	2.53	0.44
1:A:322:ARG:H	1:A:322:ARG:HG3	1.41	0.43
1:C:409:VAL:N	1:C:410:PRO:HD2	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:420:TRP:O	1:H:421:LEU:C	2.59	0.43
1:H:628:LYS:O	1:H:632:ASP:HB2	2.18	0.43
1:B:643:ILE:CG2	1:B:672:MET:HB2	2.48	0.43
1:C:139:GLU:HG3	1:C:140:THR:HG23	1.99	0.43
1:E:583:HIS:O	1:E:587:HIS:HD2	2.00	0.43
1:F:628:LYS:O	1:F:632:ASP:HB2	2.18	0.43
1:F:643:ILE:CG2	1:F:672:MET:HB2	2.48	0.43
1:G:490:TRP:CZ3	1:G:515:LEU:HD21	2.53	0.43
1:A:501:TYR:O	1:A:502:THR:C	2.60	0.43
1:B:462:THR:O	1:B:463:ARG:C	2.59	0.43
1:B:564:VAL:HB	1:B:591:VAL:HG13	2.00	0.43
1:C:308:PHE:HD1	1:C:308:PHE:HA	1.61	0.43
1:C:564:VAL:HB	1:C:591:VAL:HG13	2.00	0.43
1:D:375:LYS:O	1:D:378:VAL:HG12	2.18	0.43
1:D:420:TRP:O	1:D:421:LEU:C	2.59	0.43
1:H:133:LEU:HD22	1:H:171:LEU:HD22	2.00	0.43
1:C:293:LEU:HD12	1:C:293:LEU:HA	1.88	0.43
1:D:628:LYS:O	1:D:632:ASP:HB2	2.18	0.43
1:E:375:LYS:O	1:E:378:VAL:HG12	2.18	0.43
1:G:133:LEU:HD22	1:G:171:LEU:HD22	2.01	0.43
1:G:583:HIS:O	1:G:587:HIS:HD2	2.00	0.43
1:G:628:LYS:O	1:G:632:ASP:HB2	2.19	0.43
1:H:375:LYS:O	1:H:378:VAL:HG12	2.18	0.43
1:A:375:LYS:O	1:A:378:VAL:HG12	2.18	0.43
1:B:409:VAL:N	1:B:410:PRO:HD2	2.34	0.43
1:E:259:PHE:HZ	1:F:568:TYR:HH	1.66	0.43
1:F:133:LEU:HD22	1:F:171:LEU:HD22	2.01	0.43
1:G:564:VAL:HB	1:G:591:VAL:HG13	2.00	0.43
1:H:427:SER:C	1:H:429:TYR:N	2.70	0.43
1:A:628:LYS:O	1:A:632:ASP:HB2	2.18	0.43
1:C:628:LYS:O	1:C:632:ASP:HB2	2.18	0.43
1:H:643:ILE:CG2	1:H:672:MET:HB2	2.48	0.43
1:A:420:TRP:O	1:A:421:LEU:C	2.59	0.43
1:D:255:PHE:HB3	1:D:256:PRO:HD3	2.00	0.43
1:D:523:LEU:HD23	1:D:523:LEU:HA	1.75	0.43
1:E:177:PRO:HG2	1:E:180:LEU:HD23	2.01	0.43
1:E:338:ARG:HA	1:E:338:ARG:HD2	1.80	0.43
1:F:322:ARG:H	1:F:322:ARG:HG3	1.41	0.43
1:F:338:ARG:HA	1:F:338:ARG:HD2	1.80	0.43
1:H:152:LEU:HD21	1:H:187:ILE:HG13	1.99	0.43
1:A:133:LEU:HD22	1:A:171:LEU:HD22	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:ARG:HA	1:C:338:ARG:HD2	1.80	0.43
1:D:564:VAL:HB	1:D:591:VAL:HG13	2.00	0.43
1:E:458:LYS:H	1:E:458:LYS:HG2	1.52	0.43
1:F:177:PRO:HG2	1:F:180:LEU:HD23	2.01	0.43
1:A:105:LEU:HA	1:A:108:VAL:HB	2.01	0.43
1:A:405:ILE:CG2	1:A:412:TRP:HZ2	2.32	0.43
1:A:459:SER:HB3	1:A:462:THR:HB	2.01	0.43
1:C:255:PHE:HB3	1:C:256:PRO:HD3	2.01	0.43
1:D:409:VAL:N	1:D:410:PRO:HD2	2.33	0.43
1:E:105:LEU:HA	1:E:108:VAL:HB	2.01	0.43
1:A:170:ASN:OD1	1:A:173:LYS:CE	2.58	0.43
1:B:105:LEU:HA	1:B:108:VAL:HB	2.01	0.43
1:B:405:ILE:CG2	1:B:412:TRP:HZ2	2.32	0.43
1:C:429:TYR:CZ	1:C:457:MET:HG3	2.53	0.43
1:C:621:LEU:HB3	1:C:660:PHE:CG	2.54	0.43
1:D:405:ILE:CG2	1:D:412:TRP:HZ2	2.32	0.43
1:E:133:LEU:HD22	1:E:171:LEU:HD22	2.01	0.43
1:G:255:PHE:HB3	1:G:256:PRO:HD3	2.01	0.43
1:G:459:SER:HB3	1:G:462:THR:HB	2.01	0.43
1:H:255:PHE:HB3	1:H:256:PRO:HD3	2.00	0.43
1:H:564:VAL:HB	1:H:591:VAL:HG13	2.00	0.43
1:A:444:LEU:HD23	1:A:444:LEU:HA	1.81	0.42
1:B:133:LEU:HD22	1:B:171:LEU:HD22	2.01	0.42
1:B:628:LYS:O	1:B:632:ASP:HB2	2.18	0.42
1:C:405:ILE:CG2	1:C:412:TRP:HZ2	2.32	0.42
1:D:177:PRO:HG2	1:D:180:LEU:HD23	2.01	0.42
1:E:405:ILE:CG2	1:E:412:TRP:HZ2	2.32	0.42
1:F:523:LEU:HD23	1:F:523:LEU:HA	1.75	0.42
1:F:621:LEU:HB3	1:F:660:PHE:CG	2.54	0.42
1:A:621:LEU:HB3	1:A:660:PHE:CG	2.54	0.42
1:C:105:LEU:HA	1:C:108:VAL:HB	2.00	0.42
1:C:459:SER:HB3	1:C:462:THR:HB	2.01	0.42
1:C:462:THR:O	1:C:463:ARG:C	2.59	0.42
1:D:462:THR:O	1:D:463:ARG:C	2.59	0.42
1:E:621:LEU:HB3	1:E:660:PHE:CG	2.54	0.42
1:F:409:VAL:N	1:F:410:PRO:HD2	2.34	0.42
1:F:420:TRP:O	1:F:421:LEU:C	2.59	0.42
1:H:405:ILE:CG2	1:H:412:TRP:HZ2	2.32	0.42
1:H:621:LEU:HB3	1:H:660:PHE:CG	2.54	0.42
1:B:501:TYR:O	1:B:502:THR:C	2.60	0.42
1:D:133:LEU:HD22	1:D:171:LEU:HD22	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:455:LEU:HD23	1:D:455:LEU:HA	1.92	0.42
1:D:621:LEU:HB3	1:D:660:PHE:CG	2.54	0.42
1:E:444:LEU:HD23	1:E:444:LEU:HA	1.81	0.42
1:G:105:LEU:HA	1:G:108:VAL:HB	2.00	0.42
1:G:293:LEU:HD12	1:G:293:LEU:HA	1.88	0.42
1:G:409:VAL:N	1:G:410:PRO:HD2	2.33	0.42
1:B:255:PHE:HB3	1:B:256:PRO:HD3	2.01	0.42
1:A:598:LEU:O	1:A:604:GLU:HG3	2.20	0.42
1:D:105:LEU:HA	1:D:108:VAL:HB	2.00	0.42
1:D:501:TYR:O	1:D:502:THR:C	2.60	0.42
1:E:459:SER:HB3	1:E:462:THR:HB	2.01	0.42
1:E:628:LYS:O	1:E:632:ASP:HB2	2.18	0.42
1:F:255:PHE:HB3	1:F:256:PRO:HD3	2.01	0.42
1:E:420:TRP:O	1:E:421:LEU:C	2.59	0.42
1:H:459:SER:HB3	1:H:462:THR:HB	2.01	0.42
1:B:621:LEU:HB3	1:B:660:PHE:CG	2.54	0.42
1:C:133:LEU:HD22	1:C:171:LEU:HD22	2.01	0.42
1:C:420:TRP:O	1:C:421:LEU:C	2.59	0.42
1:F:405:ILE:CG2	1:F:412:TRP:HZ2	2.32	0.42
1:F:459:SER:HB3	1:F:462:THR:HB	2.01	0.42
1:F:598:LEU:O	1:F:604:GLU:HG3	2.20	0.42
1:H:105:LEU:HA	1:H:108:VAL:HB	2.00	0.42
1:A:255:PHE:HB3	1:A:256:PRO:HD3	2.01	0.42
1:B:177:PRO:HG2	1:B:180:LEU:HD23	2.01	0.42
1:C:427:SER:C	1:C:429:TYR:H	2.28	0.42
1:E:97:GLN:HA	1:E:100:GLU:HB3	2.02	0.42
1:F:451:LEU:HD12	1:F:451:LEU:HA	1.90	0.42
1:G:621:LEU:HB3	1:G:660:PHE:CG	2.54	0.42
1:A:142:VAL:HG22	1:A:146:ARG:HE	1.85	0.42
1:C:636:LYS:HD3	1:C:636:LYS:HA	1.92	0.42
1:D:427:SER:C	1:D:429:TYR:H	2.28	0.42
1:D:631:GLN:H	1:D:669:PRO:HD3	1.85	0.42
1:E:523:LEU:HD23	1:E:523:LEU:HA	1.75	0.42
1:F:105:LEU:HA	1:F:108:VAL:HB	2.01	0.42
1:F:264:GLU:HB3	1:F:303:LEU:HD21	2.02	0.42
1:H:444:LEU:HA	1:H:444:LEU:HD23	1.81	0.42
1:A:177:PRO:HG2	1:A:180:LEU:HD23	2.01	0.41
1:A:333:LEU:C	1:A:335:ASP:H	2.28	0.41
1:B:420:TRP:O	1:B:421:LEU:C	2.59	0.41
1:C:177:PRO:HG2	1:C:180:LEU:HD23	2.01	0.41
1:D:444:LEU:HA	1:D:444:LEU:HD23	1.81	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:598:LEU:O	1:E:604:GLU:HG3	2.20	0.41
1:G:97:GLN:HA	1:G:100:GLU:HB3	2.02	0.41
1:G:405:ILE:CG2	1:G:412:TRP:HZ2	2.32	0.41
1:H:142:VAL:HG22	1:H:146:ARG:HE	1.85	0.41
1:H:409:VAL:N	1:H:410:PRO:HD2	2.33	0.41
1:H:631:GLN:H	1:H:669:PRO:HD3	1.85	0.41
1:A:455:LEU:HD23	1:A:455:LEU:HA	1.92	0.41
1:B:172:ALA:HA	1:B:184:VAL:HG11	2.02	0.41
1:B:427:SER:C	1:B:429:TYR:H	2.28	0.41
1:C:631:GLN:H	1:C:669:PRO:HD3	1.85	0.41
1:D:338:ARG:HA	1:D:338:ARG:HD2	1.80	0.41
1:E:255:PHE:HB3	1:E:256:PRO:HD3	2.01	0.41
1:E:427:SER:C	1:E:429:TYR:H	2.28	0.41
1:E:631:GLN:H	1:E:669:PRO:HD3	1.85	0.41
1:F:580:LEU:HD13	1:F:618:VAL:HG11	2.02	0.41
1:F:681:ILE:HD11	1:F:698:PHE:CG	2.55	0.41
1:G:177:PRO:HG2	1:G:180:LEU:HD23	2.01	0.41
1:G:598:LEU:O	1:G:604:GLU:HG3	2.20	0.41
1:H:264:GLU:HB3	1:H:303:LEU:HD21	2.02	0.41
1:H:598:LEU:O	1:H:604:GLU:HG3	2.20	0.41
1:A:375:LYS:HG3	1:A:394:LEU:HD21	2.03	0.41
1:A:409:VAL:N	1:A:410:PRO:HD2	2.34	0.41
1:B:459:SER:HB3	1:B:462:THR:HB	2.01	0.41
1:E:308:PHE:HD1	1:E:308:PHE:HA	1.61	0.41
1:F:455:LEU:HD23	1:F:455:LEU:HA	1.92	0.41
1:F:631:GLN:H	1:F:669:PRO:HD3	1.85	0.41
1:H:333:LEU:C	1:H:335:ASP:H	2.28	0.41
1:A:487:LEU:HD12	1:A:487:LEU:HA	1.71	0.41
1:A:631:GLN:H	1:A:669:PRO:HD3	1.85	0.41
1:D:598:LEU:O	1:D:604:GLU:HG3	2.20	0.41
1:E:375:LYS:HG3	1:E:394:LEU:HD21	2.03	0.41
1:G:333:LEU:C	1:G:335:ASP:H	2.29	0.41
1:G:523:LEU:HA	1:G:523:LEU:HD23	1.75	0.41
1:H:97:GLN:HA	1:H:100:GLU:HB3	2.02	0.41
1:H:523:LEU:HA	1:H:523:LEU:HD23	1.75	0.41
1:A:451:LEU:HD12	1:A:451:LEU:HA	1.90	0.41
1:B:421:LEU:HD23	1:B:421:LEU:HA	1.93	0.41
1:C:375:LYS:HG3	1:C:394:LEU:HD21	2.03	0.41
1:E:264:GLU:HB3	1:E:303:LEU:HD21	2.02	0.41
1:E:409:VAL:N	1:E:410:PRO:HD2	2.34	0.41
1:E:681:ILE:HD11	1:E:698:PHE:CG	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:322:ARG:H	1:G:322:ARG:HG3	1.41	0.41
1:G:631:GLN:H	1:G:669:PRO:HD3	1.85	0.41
1:A:97:GLN:HA	1:A:100:GLU:HB3	2.02	0.41
1:B:142:VAL:HG22	1:B:146:ARG:HE	1.85	0.41
1:B:681:ILE:HD11	1:B:698:PHE:CG	2.55	0.41
1:C:259:PHE:HZ	1:D:568:TYR:HH	1.69	0.41
1:C:598:LEU:O	1:C:604:GLU:HG3	2.20	0.41
1:D:459:SER:HB3	1:D:462:THR:HB	2.01	0.41
1:D:681:ILE:HD11	1:D:698:PHE:CG	2.56	0.41
1:E:142:VAL:HG22	1:E:146:ARG:HE	1.85	0.41
1:F:333:LEU:C	1:F:335:ASP:H	2.29	0.41
1:G:580:LEU:HD13	1:G:618:VAL:HG11	2.02	0.41
1:G:681:ILE:HD11	1:G:698:PHE:CG	2.56	0.41
1:H:172:ALA:HA	1:H:184:VAL:HG11	2.02	0.41
1:A:681:ILE:HD11	1:A:698:PHE:CG	2.56	0.41
1:B:444:LEU:HD23	1:B:444:LEU:HA	1.81	0.41
1:B:569:ARG:HD3	1:B:569:ARG:HA	1.95	0.41
1:C:97:GLN:HA	1:C:100:GLU:HB3	2.02	0.41
1:C:465:ARG:HH21	1:C:465:ARG:HD3	1.69	0.41
1:C:681:ILE:HD11	1:C:698:PHE:CG	2.56	0.41
1:G:264:GLU:HB3	1:G:303:LEU:HD21	2.02	0.41
1:G:375:LYS:HG3	1:G:394:LEU:HD21	2.03	0.41
1:H:177:PRO:HG2	1:H:180:LEU:HD23	2.01	0.41
1:H:408:SER:C	1:H:410:PRO:HD2	2.46	0.41
1:H:498:PHE:C	1:H:500:GLN:N	2.78	0.41
1:A:172:ALA:HA	1:A:184:VAL:HG11	2.02	0.41
1:A:408:SER:C	1:A:410:PRO:HD2	2.46	0.41
1:B:580:LEU:HD13	1:B:618:VAL:HG11	2.02	0.41
1:B:598:LEU:O	1:B:604:GLU:HG3	2.20	0.41
1:C:501:TYR:O	1:C:502:THR:C	2.60	0.41
1:C:537:ARG:HE	1:C:537:ARG:HB3	1.52	0.41
1:C:580:LEU:HD13	1:C:618:VAL:HG11	2.02	0.41
1:D:274:VAL:HG11	1:D:292:THR:HG22	2.03	0.41
1:D:375:LYS:HG3	1:D:394:LEU:HD21	2.02	0.41
1:E:172:ALA:HA	1:E:184:VAL:HG11	2.02	0.41
1:E:322:ARG:H	1:E:322:ARG:HG3	1.41	0.41
1:F:97:GLN:HA	1:F:100:GLU:HB3	2.02	0.41
1:F:375:LYS:HG3	1:F:394:LEU:HD21	2.02	0.41
1:G:172:ALA:HA	1:G:184:VAL:HG11	2.02	0.41
1:G:408:SER:C	1:G:410:PRO:HD2	2.46	0.41
1:G:444:LEU:HD23	1:G:444:LEU:HA	1.81	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:LEU:HA	1:A:523:LEU:HD23	1.75	0.41
1:B:631:GLN:H	1:B:669:PRO:HD3	1.86	0.41
1:C:142:VAL:HG22	1:C:146:ARG:HE	1.85	0.41
1:D:172:ALA:HA	1:D:184:VAL:HG11	2.02	0.41
1:D:408:SER:C	1:D:410:PRO:HD2	2.46	0.41
1:E:580:LEU:HD13	1:E:618:VAL:HG11	2.02	0.41
1:F:427:SER:C	1:F:429:TYR:H	2.28	0.41
1:G:427:SER:C	1:G:429:TYR:H	2.28	0.41
1:A:427:SER:C	1:A:429:TYR:H	2.28	0.41
1:B:259:PHE:HZ	1:C:568:TYR:HH	1.69	0.41
1:B:458:LYS:H	1:B:458:LYS:HG2	1.52	0.41
1:C:487:LEU:HD12	1:C:487:LEU:HA	1.71	0.41
1:D:616:ASN:HB3	1:D:699:LEU:HD22	2.03	0.41
1:F:152:LEU:HD12	1:F:152:LEU:HA	1.93	0.41
1:F:172:ALA:HA	1:F:184:VAL:HG11	2.02	0.41
1:F:274:VAL:HG11	1:F:292:THR:HG22	2.03	0.41
1:G:537:ARG:HE	1:G:537:ARG:HB3	1.53	0.41
1:B:264:GLU:HB3	1:B:303:LEU:HD21	2.02	0.40
1:B:375:LYS:HG3	1:B:394:LEU:HD21	2.02	0.40
1:C:274:VAL:HG11	1:C:292:THR:HG22	2.03	0.40
1:C:458:LYS:H	1:C:458:LYS:HG2	1.52	0.40
1:C:616:ASN:HB3	1:C:699:LEU:HD22	2.03	0.40
1:D:97:GLN:HA	1:D:100:GLU:HB3	2.02	0.40
1:D:433:PHE:CZ	1:D:455:LEU:HD13	2.56	0.40
1:D:494:LEU:N	1:D:494:LEU:HD12	2.36	0.40
1:E:333:LEU:C	1:E:335:ASP:H	2.29	0.40
1:E:433:PHE:CZ	1:E:455:LEU:HD13	2.56	0.40
1:F:408:SER:C	1:F:410:PRO:HD2	2.46	0.40
1:H:681:ILE:HD11	1:H:698:PHE:CG	2.56	0.40
1:A:498:PHE:C	1:A:500:GLN:N	2.78	0.40
1:A:580:LEU:HD13	1:A:618:VAL:HG11	2.02	0.40
1:C:408:SER:C	1:C:410:PRO:HD2	2.46	0.40
1:C:498:PHE:C	1:C:500:GLN:N	2.78	0.40
1:D:264:GLU:HB3	1:D:303:LEU:HD21	2.02	0.40
1:E:215:CYS:SG	1:E:253:TRP:O	2.80	0.40
1:E:274:VAL:HG11	1:E:292:THR:HG22	2.03	0.40
1:A:421:LEU:HD23	1:A:421:LEU:HA	1.93	0.40
1:B:260:SER:H	1:B:267:ARG:HE	1.69	0.40
1:C:264:GLU:HB3	1:C:303:LEU:HD21	2.02	0.40
1:D:580:LEU:HD13	1:D:618:VAL:HG11	2.02	0.40
1:F:142:VAL:HG22	1:F:146:ARG:HE	1.85	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:494:LEU:N	1:G:494:LEU:HD12	2.36	0.40
1:B:97:GLN:HA	1:B:100:GLU:HB3	2.02	0.40
1:B:274:VAL:HG11	1:B:292:THR:HG22	2.03	0.40
1:B:338:ARG:HA	1:B:338:ARG:HD2	1.80	0.40
1:B:616:ASN:HB3	1:B:699:LEU:HD22	2.03	0.40
1:E:421:LEU:HD23	1:E:421:LEU:HA	1.93	0.40
1:E:494:LEU:N	1:E:494:LEU:HD12	2.36	0.40
1:G:142:VAL:HG22	1:G:146:ARG:HE	1.85	0.40
1:H:375:LYS:HG3	1:H:394:LEU:HD21	2.02	0.40
1:A:71:GLU:HB3	1:A:98:LEU:HD13	2.04	0.40
1:A:97:GLN:O	1:A:101:GLU:HG3	2.22	0.40
1:A:616:ASN:HB3	1:A:699:LEU:HD22	2.03	0.40
1:B:97:GLN:O	1:B:101:GLU:HG3	2.22	0.40
1:B:333:LEU:C	1:B:335:ASP:H	2.28	0.40
1:C:172:ALA:HA	1:C:184:VAL:HG11	2.02	0.40
1:D:83:GLY:H	1:D:137:GLU:HG3	1.87	0.40
1:D:215:CYS:SG	1:D:253:TRP:O	2.80	0.40
1:F:293:LEU:HD12	1:F:293:LEU:HA	1.88	0.40
1:F:537:ARG:HE	1:F:537:ARG:HB3	1.53	0.40
1:G:215:CYS:SG	1:G:253:TRP:O	2.80	0.40
1:G:274:VAL:HG11	1:G:292:THR:HG22	2.03	0.40
1:H:97:GLN:O	1:H:101:GLU:HG3	2.22	0.40
1:H:580:LEU:HD13	1:H:618:VAL:HG11	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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

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](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	S1N	H	801	1	9,11,11	0.64	0	10,11,11	1.84	2 (20%)
2	S1N	A	801	1	9,11,11	0.64	0	10,11,11	1.85	2 (20%)
2	S1N	G	801	1	9,11,11	0.64	0	10,11,11	1.86	2 (20%)
2	S1N	D	801	1	9,11,11	0.64	0	10,11,11	1.85	2 (20%)
2	S1N	D	802	1	9,10,11	0.66	0	8,10,11	1.20	1 (12%)
2	S1N	G	802	1	9,10,11	0.65	0	8,10,11	1.20	1 (12%)
2	S1N	H	802	1	9,10,11	0.65	0	8,10,11	1.18	1 (12%)
2	S1N	E	801	1	9,11,11	0.64	0	10,11,11	1.85	2 (20%)
2	S1N	F	801	1	9,11,11	0.65	0	10,11,11	1.85	2 (20%)
2	S1N	F	802	1	9,10,11	0.66	0	8,10,11	1.19	1 (12%)
2	S1N	B	801	1	9,11,11	0.65	0	10,11,11	1.85	2 (20%)
2	S1N	C	802	1	9,10,11	0.67	0	8,10,11	1.22	1 (12%)
2	S1N	E	802	1	9,10,11	0.67	0	8,10,11	1.22	1 (12%)
2	S1N	B	802	1	9,10,11	0.66	0	8,10,11	1.19	1 (12%)
2	S1N	A	802	1	9,10,11	0.65	0	8,10,11	1.20	1 (12%)
2	S1N	C	801	1	9,11,11	0.65	0	10,11,11	1.86	2 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	S1N	H	801	1	-	4/10/10/10	-
2	S1N	A	801	1	-	4/10/10/10	-
2	S1N	G	801	1	-	4/10/10/10	-
2	S1N	D	801	1	-	4/10/10/10	-
2	S1N	D	802	1	-	1/9/9/10	-
2	S1N	G	802	1	-	1/9/9/10	-
2	S1N	H	802	1	-	1/9/9/10	-
2	S1N	E	801	1	-	4/10/10/10	-
2	S1N	F	801	1	-	4/10/10/10	-
2	S1N	F	802	1	-	1/9/9/10	-
2	S1N	B	801	1	-	4/10/10/10	-
2	S1N	C	802	1	-	1/9/9/10	-
2	S1N	E	802	1	-	1/9/9/10	-
2	S1N	B	802	1	-	1/9/9/10	-
2	S1N	A	802	1	-	1/9/9/10	-
2	S1N	C	801	1	-	4/10/10/10	-

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	S1N	C1-C2-C3	4.67	123.33	115.23
2	G	801	S1N	C1-C2-C3	4.67	123.33	115.23
2	B	801	S1N	C1-C2-C3	4.65	123.30	115.23
2	F	801	S1N	C1-C2-C3	4.65	123.30	115.23
2	C	801	S1N	C1-C2-C3	4.65	123.30	115.23
2	A	801	S1N	C1-C2-C3	4.65	123.30	115.23
2	E	801	S1N	C1-C2-C3	4.65	123.30	115.23
2	H	801	S1N	C1-C2-C3	4.64	123.28	115.23
2	C	802	S1N	C1-C2-C3	2.52	119.60	115.23
2	E	802	S1N	C1-C2-C3	2.52	119.59	115.23
2	A	802	S1N	C1-C2-C3	2.46	119.50	115.23
2	G	802	S1N	C1-C2-C3	2.46	119.50	115.23
2	D	802	S1N	C1-C2-C3	2.46	119.49	115.23
2	B	802	S1N	C1-C2-C3	2.44	119.46	115.23
2	F	802	S1N	C1-C2-C3	2.43	119.45	115.23
2	H	802	S1N	C1-C2-C3	2.43	119.45	115.23
2	E	801	S1N	C3-C2-C8	-2.33	115.93	121.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	S1N	C3-C2-C8	-2.33	115.93	121.17
2	B	801	S1N	C3-C2-C8	-2.33	115.93	121.17
2	F	801	S1N	C3-C2-C8	-2.33	115.93	121.17
2	G	801	S1N	C3-C2-C8	-2.33	115.94	121.17
2	D	801	S1N	C3-C2-C8	-2.33	115.94	121.17
2	A	801	S1N	C3-C2-C8	-2.32	115.97	121.17
2	H	801	S1N	C3-C2-C8	-2.31	115.97	121.17

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	S1N	C2-C3-C4-C5
2	B	801	S1N	C2-C3-C4-C5
2	C	801	S1N	C2-C3-C4-C5
2	D	801	S1N	C2-C3-C4-C5
2	E	801	S1N	C2-C3-C4-C5
2	F	801	S1N	C2-C3-C4-C5
2	G	801	S1N	C2-C3-C4-C5
2	H	801	S1N	C2-C3-C4-C5
2	B	801	S1N	C1-C2-C3-C4
2	D	801	S1N	C1-C2-C3-C4
2	F	801	S1N	C1-C2-C3-C4
2	H	801	S1N	C1-C2-C3-C4
2	A	801	S1N	C1-C2-C3-C4
2	E	801	S1N	C1-C2-C3-C4
2	G	801	S1N	C1-C2-C3-C4
2	A	802	S1N	C11-C10-C9-C8
2	B	802	S1N	C11-C10-C9-C8
2	C	802	S1N	C11-C10-C9-C8
2	D	802	S1N	C11-C10-C9-C8
2	E	802	S1N	C11-C10-C9-C8
2	F	802	S1N	C11-C10-C9-C8
2	G	802	S1N	C11-C10-C9-C8
2	H	802	S1N	C11-C10-C9-C8
2	C	801	S1N	C1-C2-C3-C4
2	B	801	S1N	C8-C2-C3-C4
2	C	801	S1N	C8-C2-C3-C4
2	D	801	S1N	C8-C2-C3-C4
2	F	801	S1N	C8-C2-C3-C4
2	G	801	S1N	C8-C2-C3-C4
2	H	801	S1N	C8-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	801	S1N	C8-C2-C3-C4
2	E	801	S1N	C8-C2-C3-C4
2	C	801	S1N	C11-C10-C9-C8
2	E	801	S1N	C11-C10-C9-C8
2	G	801	S1N	C11-C10-C9-C8
2	A	801	S1N	C11-C10-C9-C8
2	B	801	S1N	C11-C10-C9-C8
2	D	801	S1N	C11-C10-C9-C8
2	F	801	S1N	C11-C10-C9-C8
2	H	801	S1N	C11-C10-C9-C8

There are no ring outliers.

No monomer is involved in short contacts.

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.

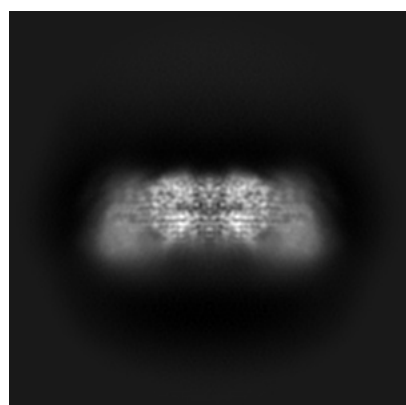
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11187. These allow visual inspection of the internal detail of the map and identification of artifacts.

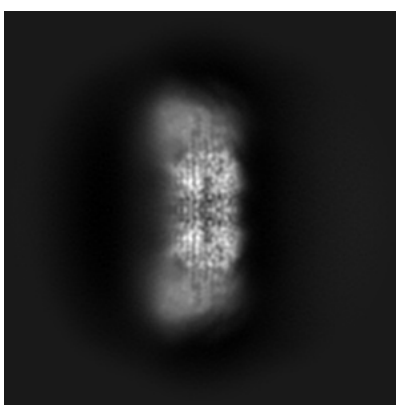
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

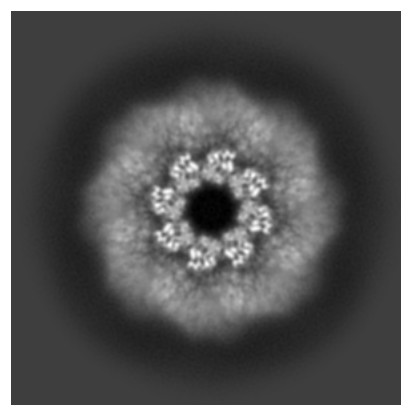
6.1.1 Primary map



X



Y

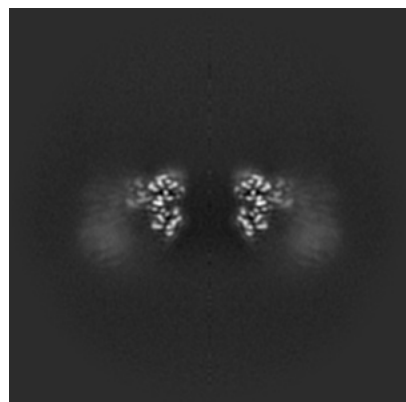


Z

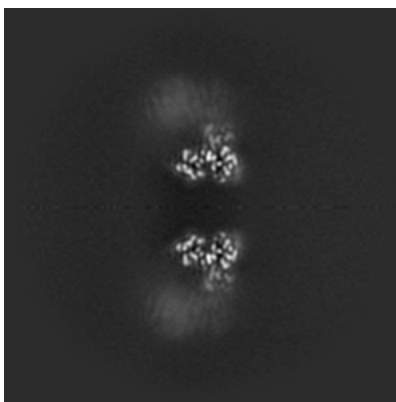
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

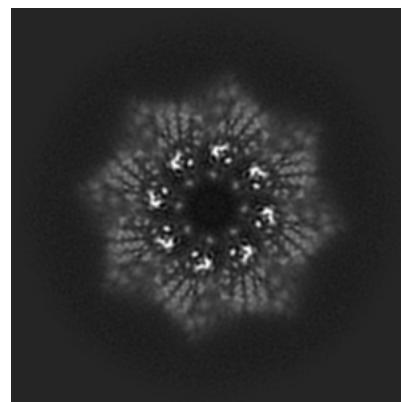
6.2.1 Primary map



X Index: 175



Y Index: 175

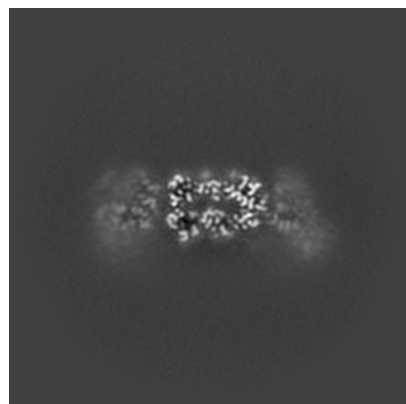


Z Index: 175

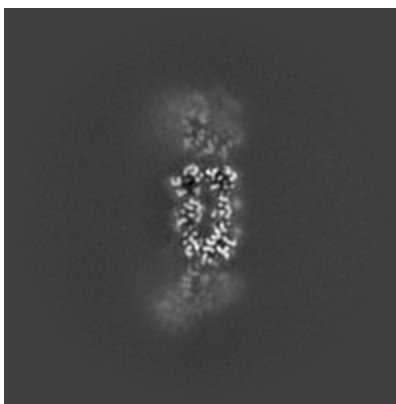
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

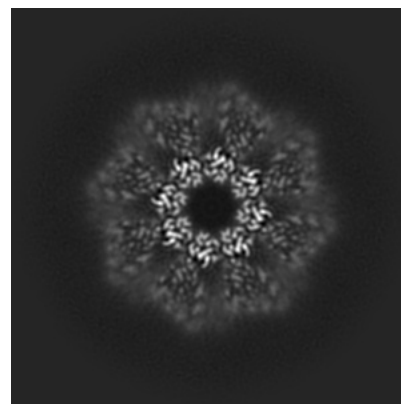
6.3.1 Primary map



X Index: 145



Y Index: 145

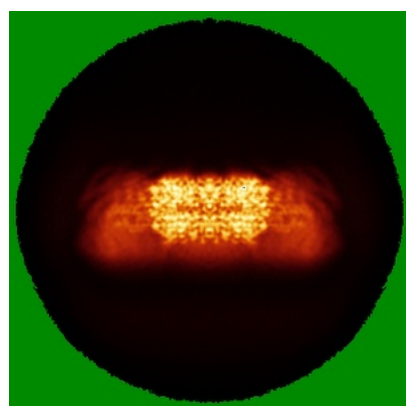


Z Index: 169

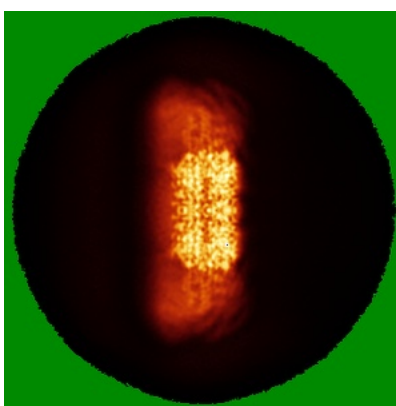
The images above show the largest variance slices of the map in three orthogonal directions.

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

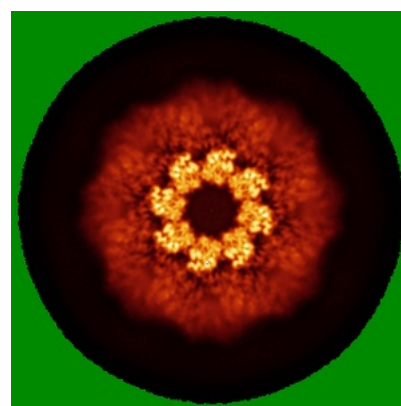
6.4.1 Primary map



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

This section was not generated.

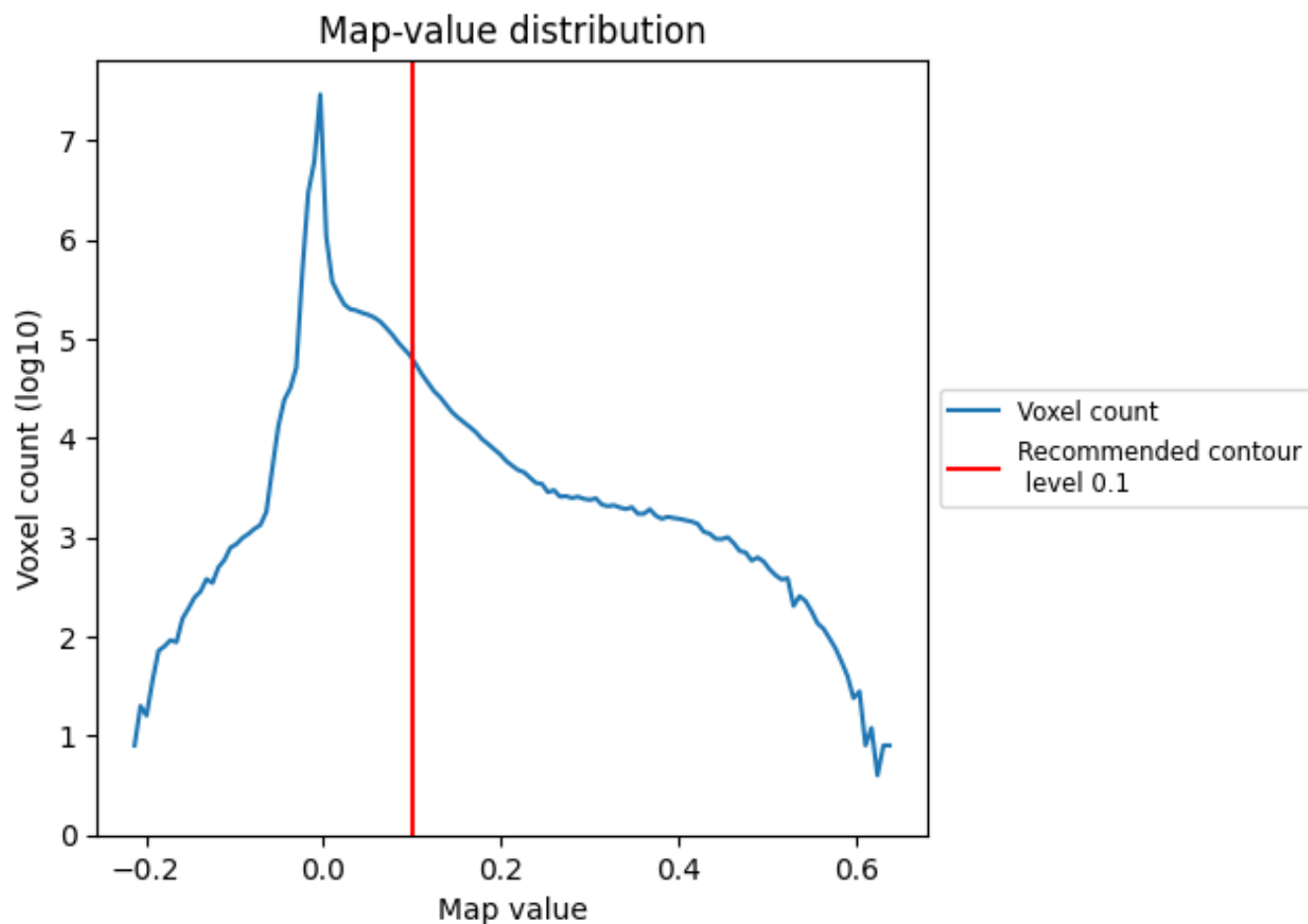
6.6 Mask visualisation

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

7 Map analysis [i](#)

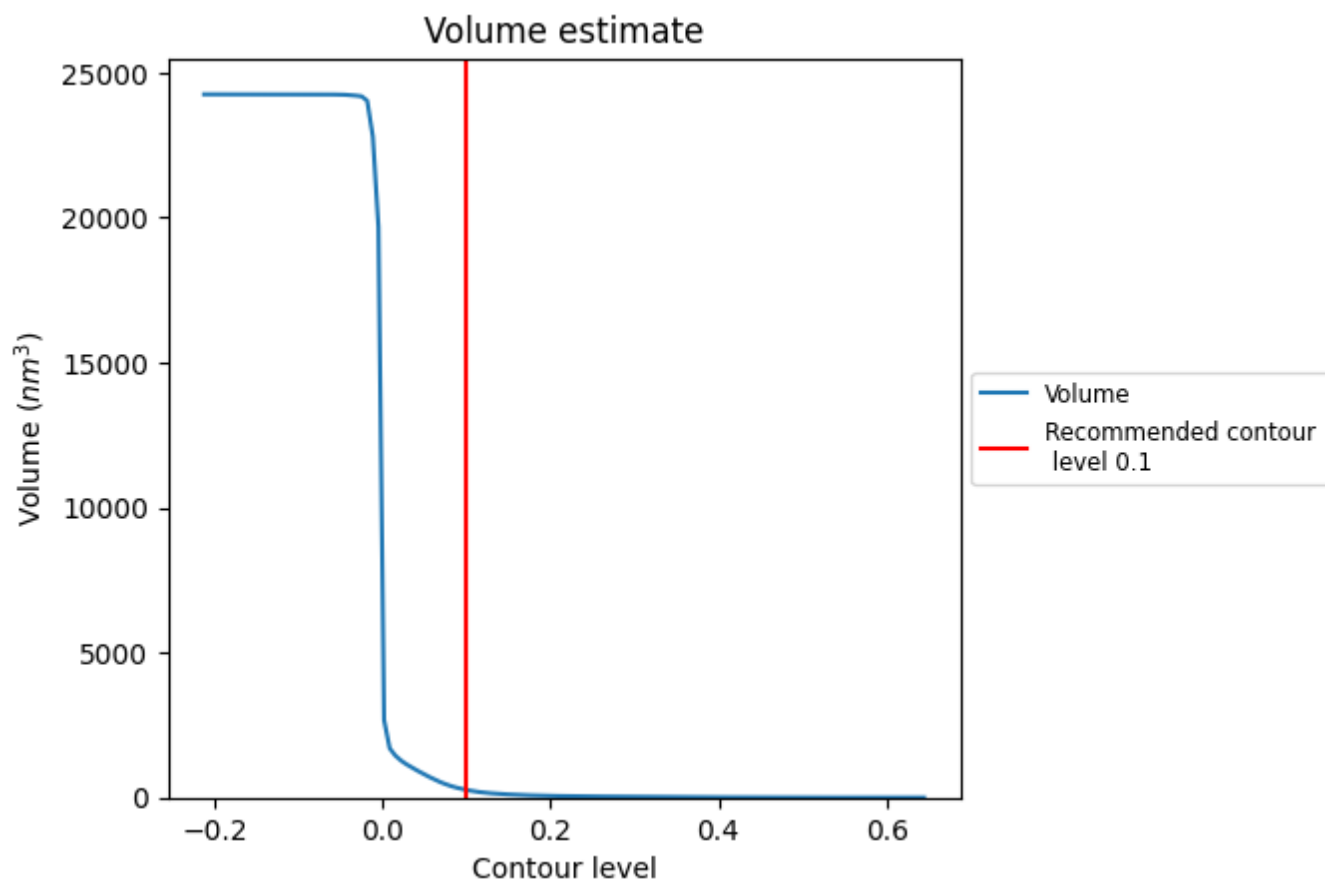
This section contains the results of statistical analysis of the map.

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.

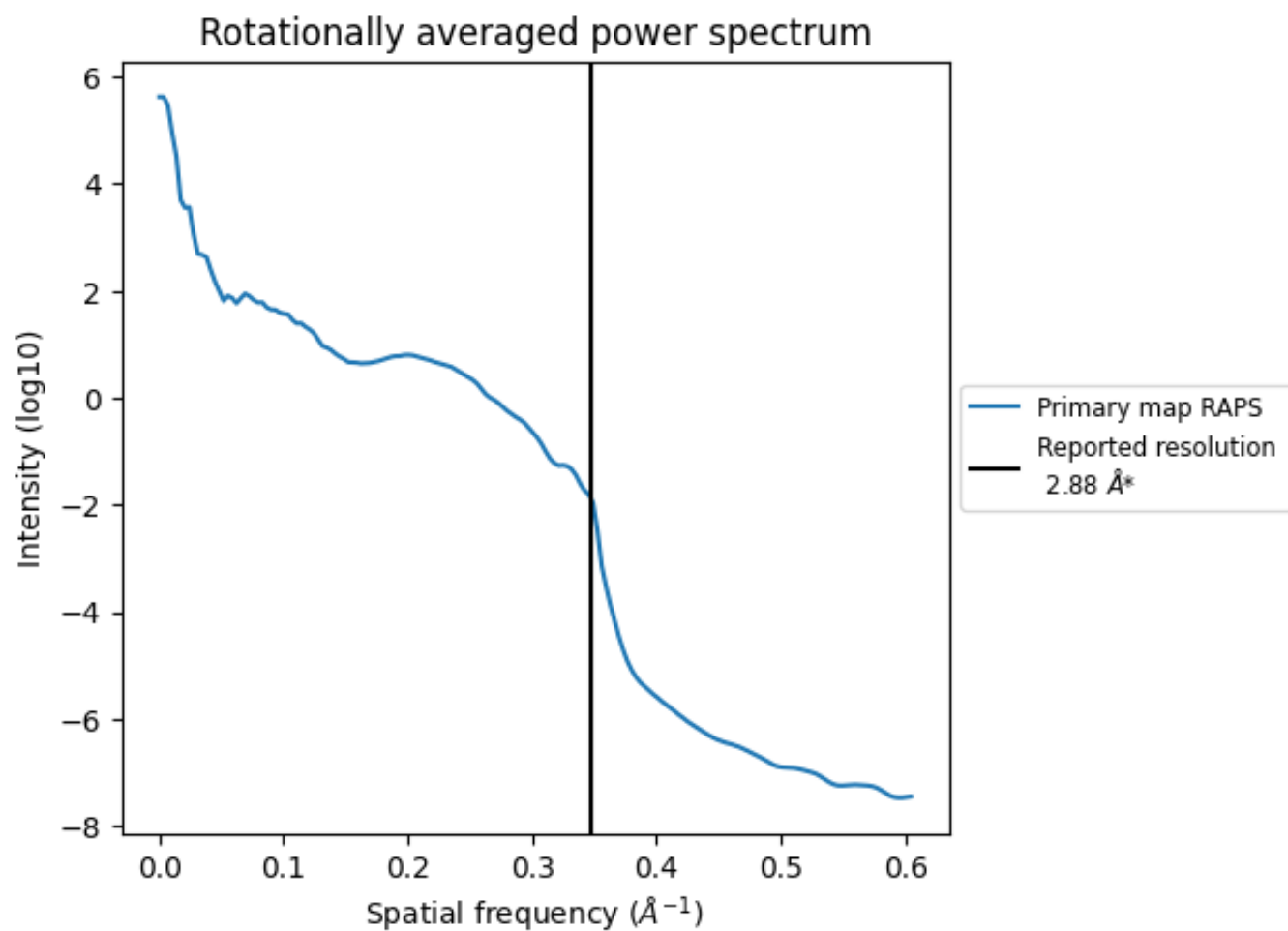
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 261 nm³; this corresponds to an approximate mass of 235 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 0.347 Å⁻¹

8 Fourier-Shell correlation ⓘ

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

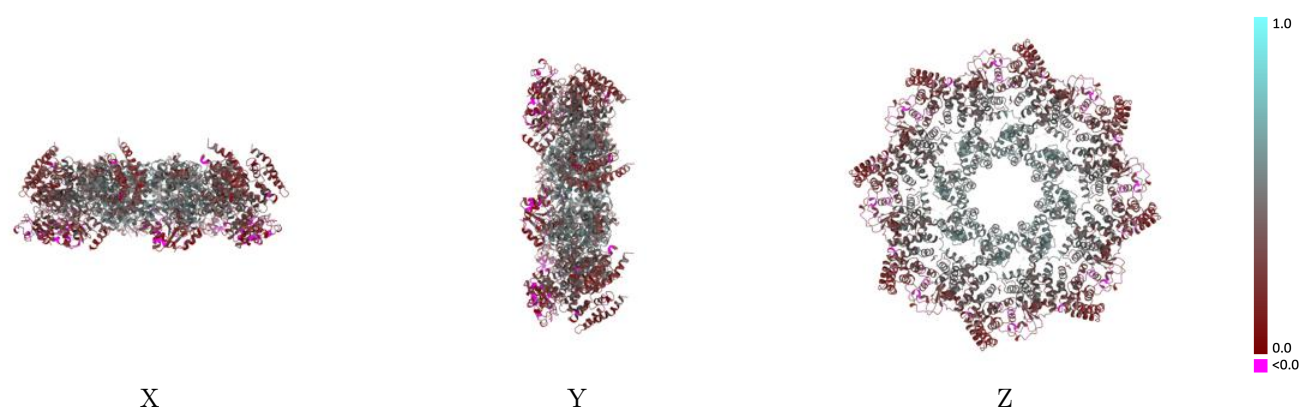
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11187 and PDB model 6ZFX. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)

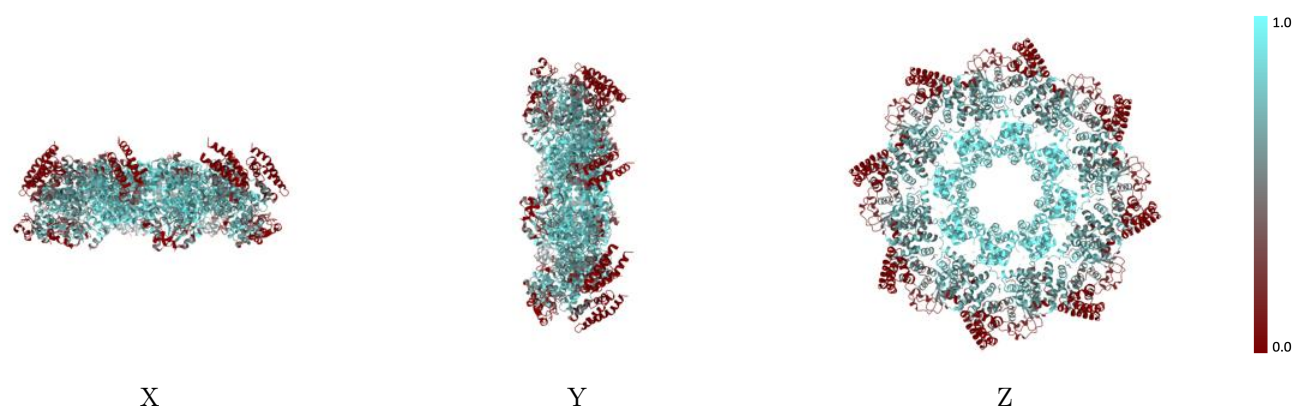
This section was not generated.

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



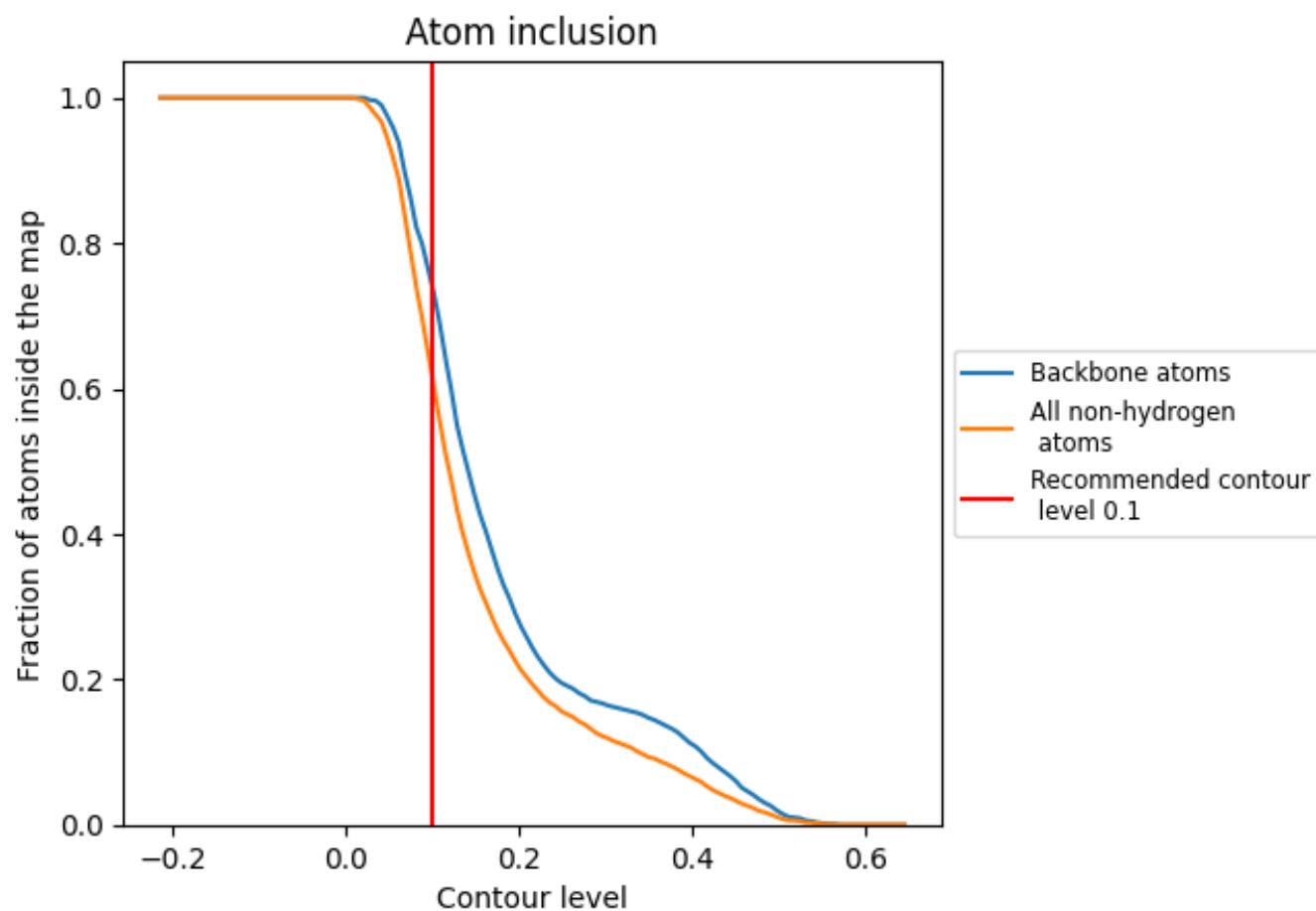
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 62% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6170	0.3680
A	0.6160	0.3680
B	0.6190	0.3680
C	0.6160	0.3680
D	0.6190	0.3680
E	0.6160	0.3670
F	0.6190	0.3690
G	0.6160	0.3680
H	0.6190	0.3690

1.0

0.0

<0.0