



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 04:13 PM UTC

PDB ID : 7TAW / pdb_00007taw
EMDB ID : EMD-25788
Title : Cryo-EM structure of the Csy-AcrIF24-promoter DNA dimer
Authors : Mukherjee, I.A.; Chang, L.
Deposited on : 2021-12-21
Resolution : 2.70 Å (reported)
Based on initial model : 7JZW

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

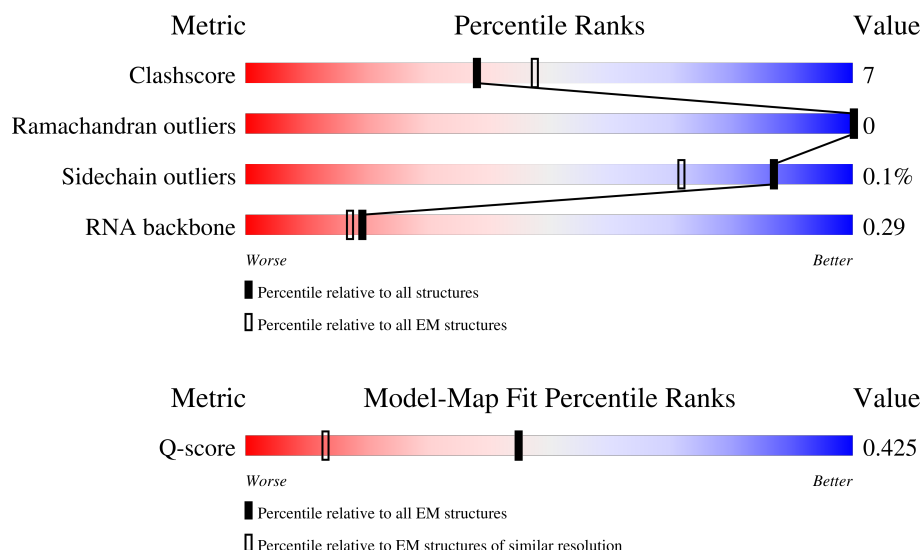
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.70 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	10327 (2.20 - 3.20)

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	434	
1	a	434	
2	B	327	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	b	327	
3	C	187	
3	c	187	
4	D	360	
4	E	360	
4	F	360	
4	G	360	
4	H	360	
4	I	360	
4	d	360	
4	e	360	
4	f	360	
4	g	360	
4	h	360	
4	i	360	
5	J	228	
5	K	228	
6	M	61	
6	m	61	
7	Y	19	
8	X	19	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 51399 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 CRISPR-associated protein Csy1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	427	Total	C	N	O	S	0	0
			3145	1982	593	567	3		
1	a	427	Total	C	N	O	S	0	0
			3145	1982	593	567	3		

- Molecule 2 is a protein called CRISPR type I-F/YPEST-associated protein Csy2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	306	Total	C	N	O	S	0	0
			2411	1529	445	432	5		
2	b	306	Total	C	N	O	S	0	0
			2411	1529	445	432	5		

- Molecule 3 is a protein called CRISPR-associated endonuclease Cas6/Csy4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	187	Total	C	N	O	S	1	0
			1448	922	264	257	5		
3	c	187	Total	C	N	O	S	1	0
			1448	922	264	257	5		

- Molecule 4 is a protein called CRISPR type I-F/YPEST-associated protein Csy3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	298	Total	C	N	O	S	0	0
			2307	1453	415	437	2		
4	E	335	Total	C	N	O	S	0	0
			2592	1626	471	493	2		
4	F	335	Total	C	N	O	S	0	0
			2592	1626	471	493	2		
4	G	335	Total	C	N	O	S	0	0
			2592	1626	471	493	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	335	Total	C	N	O	S	0	0
			2592	1626	471	493	2		
4	I	335	Total	C	N	O	S	0	0
			2592	1626	471	493	2		
4	d	298	Total	C	N	O	S	0	0
			2307	1453	415	437	2		
4	e	335	Total	C	N	O	S	0	0
			2592	1626	471	493	2		
4	f	335	Total	C	N	O	S	0	0
			2592	1626	471	493	2		
4	g	335	Total	C	N	O	S	0	0
			2592	1626	471	493	2		
4	h	335	Total	C	N	O	S	0	0
			2592	1626	471	493	2		
4	i	335	Total	C	N	O	S	0	0
			2592	1626	471	493	2		

There are 228 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	2	MET	-	initiating methionine	UNP A0A444M080
D	3	LYS	-	expression tag	UNP A0A444M080
D	4	SER	-	expression tag	UNP A0A444M080
D	5	SER	-	expression tag	UNP A0A444M080
D	6	HIS	-	expression tag	UNP A0A444M080
D	7	HIS	-	expression tag	UNP A0A444M080
D	8	HIS	-	expression tag	UNP A0A444M080
D	9	HIS	-	expression tag	UNP A0A444M080
D	10	HIS	-	expression tag	UNP A0A444M080
D	11	HIS	-	expression tag	UNP A0A444M080
D	12	GLU	-	expression tag	UNP A0A444M080
D	13	ASN	-	expression tag	UNP A0A444M080
D	14	LEU	-	expression tag	UNP A0A444M080
D	15	TYR	-	expression tag	UNP A0A444M080
D	16	PHE	-	expression tag	UNP A0A444M080
D	17	GLN	-	expression tag	UNP A0A444M080
D	18	SER	-	expression tag	UNP A0A444M080
D	19	ASN	-	expression tag	UNP A0A444M080
D	20	ALA	-	expression tag	UNP A0A444M080
E	2	MET	-	initiating methionine	UNP A0A444M080
E	3	LYS	-	expression tag	UNP A0A444M080
E	4	SER	-	expression tag	UNP A0A444M080
E	5	SER	-	expression tag	UNP A0A444M080

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	6	HIS	-	expression tag	UNP A0A444M080
E	7	HIS	-	expression tag	UNP A0A444M080
E	8	HIS	-	expression tag	UNP A0A444M080
E	9	HIS	-	expression tag	UNP A0A444M080
E	10	HIS	-	expression tag	UNP A0A444M080
E	11	HIS	-	expression tag	UNP A0A444M080
E	12	GLU	-	expression tag	UNP A0A444M080
E	13	ASN	-	expression tag	UNP A0A444M080
E	14	LEU	-	expression tag	UNP A0A444M080
E	15	TYR	-	expression tag	UNP A0A444M080
E	16	PHE	-	expression tag	UNP A0A444M080
E	17	GLN	-	expression tag	UNP A0A444M080
E	18	SER	-	expression tag	UNP A0A444M080
E	19	ASN	-	expression tag	UNP A0A444M080
E	20	ALA	-	expression tag	UNP A0A444M080
F	2	MET	-	initiating methionine	UNP A0A444M080
F	3	LYS	-	expression tag	UNP A0A444M080
F	4	SER	-	expression tag	UNP A0A444M080
F	5	SER	-	expression tag	UNP A0A444M080
F	6	HIS	-	expression tag	UNP A0A444M080
F	7	HIS	-	expression tag	UNP A0A444M080
F	8	HIS	-	expression tag	UNP A0A444M080
F	9	HIS	-	expression tag	UNP A0A444M080
F	10	HIS	-	expression tag	UNP A0A444M080
F	11	HIS	-	expression tag	UNP A0A444M080
F	12	GLU	-	expression tag	UNP A0A444M080
F	13	ASN	-	expression tag	UNP A0A444M080
F	14	LEU	-	expression tag	UNP A0A444M080
F	15	TYR	-	expression tag	UNP A0A444M080
F	16	PHE	-	expression tag	UNP A0A444M080
F	17	GLN	-	expression tag	UNP A0A444M080
F	18	SER	-	expression tag	UNP A0A444M080
F	19	ASN	-	expression tag	UNP A0A444M080
F	20	ALA	-	expression tag	UNP A0A444M080
G	2	MET	-	initiating methionine	UNP A0A444M080
G	3	LYS	-	expression tag	UNP A0A444M080
G	4	SER	-	expression tag	UNP A0A444M080
G	5	SER	-	expression tag	UNP A0A444M080
G	6	HIS	-	expression tag	UNP A0A444M080
G	7	HIS	-	expression tag	UNP A0A444M080
G	8	HIS	-	expression tag	UNP A0A444M080
G	9	HIS	-	expression tag	UNP A0A444M080

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	10	HIS	-	expression tag	UNP A0A444M080
G	11	HIS	-	expression tag	UNP A0A444M080
G	12	GLU	-	expression tag	UNP A0A444M080
G	13	ASN	-	expression tag	UNP A0A444M080
G	14	LEU	-	expression tag	UNP A0A444M080
G	15	TYR	-	expression tag	UNP A0A444M080
G	16	PHE	-	expression tag	UNP A0A444M080
G	17	GLN	-	expression tag	UNP A0A444M080
G	18	SER	-	expression tag	UNP A0A444M080
G	19	ASN	-	expression tag	UNP A0A444M080
G	20	ALA	-	expression tag	UNP A0A444M080
H	2	MET	-	initiating methionine	UNP A0A444M080
H	3	LYS	-	expression tag	UNP A0A444M080
H	4	SER	-	expression tag	UNP A0A444M080
H	5	SER	-	expression tag	UNP A0A444M080
H	6	HIS	-	expression tag	UNP A0A444M080
H	7	HIS	-	expression tag	UNP A0A444M080
H	8	HIS	-	expression tag	UNP A0A444M080
H	9	HIS	-	expression tag	UNP A0A444M080
H	10	HIS	-	expression tag	UNP A0A444M080
H	11	HIS	-	expression tag	UNP A0A444M080
H	12	GLU	-	expression tag	UNP A0A444M080
H	13	ASN	-	expression tag	UNP A0A444M080
H	14	LEU	-	expression tag	UNP A0A444M080
H	15	TYR	-	expression tag	UNP A0A444M080
H	16	PHE	-	expression tag	UNP A0A444M080
H	17	GLN	-	expression tag	UNP A0A444M080
H	18	SER	-	expression tag	UNP A0A444M080
H	19	ASN	-	expression tag	UNP A0A444M080
H	20	ALA	-	expression tag	UNP A0A444M080
I	2	MET	-	initiating methionine	UNP A0A444M080
I	3	LYS	-	expression tag	UNP A0A444M080
I	4	SER	-	expression tag	UNP A0A444M080
I	5	SER	-	expression tag	UNP A0A444M080
I	6	HIS	-	expression tag	UNP A0A444M080
I	7	HIS	-	expression tag	UNP A0A444M080
I	8	HIS	-	expression tag	UNP A0A444M080
I	9	HIS	-	expression tag	UNP A0A444M080
I	10	HIS	-	expression tag	UNP A0A444M080
I	11	HIS	-	expression tag	UNP A0A444M080
I	12	GLU	-	expression tag	UNP A0A444M080
I	13	ASN	-	expression tag	UNP A0A444M080

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	14	LEU	-	expression tag	UNP A0A444M080
I	15	TYR	-	expression tag	UNP A0A444M080
I	16	PHE	-	expression tag	UNP A0A444M080
I	17	GLN	-	expression tag	UNP A0A444M080
I	18	SER	-	expression tag	UNP A0A444M080
I	19	ASN	-	expression tag	UNP A0A444M080
I	20	ALA	-	expression tag	UNP A0A444M080
d	2	MET	-	initiating methionine	UNP A0A444M080
d	3	LYS	-	expression tag	UNP A0A444M080
d	4	SER	-	expression tag	UNP A0A444M080
d	5	SER	-	expression tag	UNP A0A444M080
d	6	HIS	-	expression tag	UNP A0A444M080
d	7	HIS	-	expression tag	UNP A0A444M080
d	8	HIS	-	expression tag	UNP A0A444M080
d	9	HIS	-	expression tag	UNP A0A444M080
d	10	HIS	-	expression tag	UNP A0A444M080
d	11	HIS	-	expression tag	UNP A0A444M080
d	12	GLU	-	expression tag	UNP A0A444M080
d	13	ASN	-	expression tag	UNP A0A444M080
d	14	LEU	-	expression tag	UNP A0A444M080
d	15	TYR	-	expression tag	UNP A0A444M080
d	16	PHE	-	expression tag	UNP A0A444M080
d	17	GLN	-	expression tag	UNP A0A444M080
d	18	SER	-	expression tag	UNP A0A444M080
d	19	ASN	-	expression tag	UNP A0A444M080
d	20	ALA	-	expression tag	UNP A0A444M080
e	2	MET	-	initiating methionine	UNP A0A444M080
e	3	LYS	-	expression tag	UNP A0A444M080
e	4	SER	-	expression tag	UNP A0A444M080
e	5	SER	-	expression tag	UNP A0A444M080
e	6	HIS	-	expression tag	UNP A0A444M080
e	7	HIS	-	expression tag	UNP A0A444M080
e	8	HIS	-	expression tag	UNP A0A444M080
e	9	HIS	-	expression tag	UNP A0A444M080
e	10	HIS	-	expression tag	UNP A0A444M080
e	11	HIS	-	expression tag	UNP A0A444M080
e	12	GLU	-	expression tag	UNP A0A444M080
e	13	ASN	-	expression tag	UNP A0A444M080
e	14	LEU	-	expression tag	UNP A0A444M080
e	15	TYR	-	expression tag	UNP A0A444M080
e	16	PHE	-	expression tag	UNP A0A444M080
e	17	GLN	-	expression tag	UNP A0A444M080

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
e	18	SER	-	expression tag	UNP A0A444M080
e	19	ASN	-	expression tag	UNP A0A444M080
e	20	ALA	-	expression tag	UNP A0A444M080
f	2	MET	-	initiating methionine	UNP A0A444M080
f	3	LYS	-	expression tag	UNP A0A444M080
f	4	SER	-	expression tag	UNP A0A444M080
f	5	SER	-	expression tag	UNP A0A444M080
f	6	HIS	-	expression tag	UNP A0A444M080
f	7	HIS	-	expression tag	UNP A0A444M080
f	8	HIS	-	expression tag	UNP A0A444M080
f	9	HIS	-	expression tag	UNP A0A444M080
f	10	HIS	-	expression tag	UNP A0A444M080
f	11	HIS	-	expression tag	UNP A0A444M080
f	12	GLU	-	expression tag	UNP A0A444M080
f	13	ASN	-	expression tag	UNP A0A444M080
f	14	LEU	-	expression tag	UNP A0A444M080
f	15	TYR	-	expression tag	UNP A0A444M080
f	16	PHE	-	expression tag	UNP A0A444M080
f	17	GLN	-	expression tag	UNP A0A444M080
f	18	SER	-	expression tag	UNP A0A444M080
f	19	ASN	-	expression tag	UNP A0A444M080
f	20	ALA	-	expression tag	UNP A0A444M080
g	2	MET	-	initiating methionine	UNP A0A444M080
g	3	LYS	-	expression tag	UNP A0A444M080
g	4	SER	-	expression tag	UNP A0A444M080
g	5	SER	-	expression tag	UNP A0A444M080
g	6	HIS	-	expression tag	UNP A0A444M080
g	7	HIS	-	expression tag	UNP A0A444M080
g	8	HIS	-	expression tag	UNP A0A444M080
g	9	HIS	-	expression tag	UNP A0A444M080
g	10	HIS	-	expression tag	UNP A0A444M080
g	11	HIS	-	expression tag	UNP A0A444M080
g	12	GLU	-	expression tag	UNP A0A444M080
g	13	ASN	-	expression tag	UNP A0A444M080
g	14	LEU	-	expression tag	UNP A0A444M080
g	15	TYR	-	expression tag	UNP A0A444M080
g	16	PHE	-	expression tag	UNP A0A444M080
g	17	GLN	-	expression tag	UNP A0A444M080
g	18	SER	-	expression tag	UNP A0A444M080
g	19	ASN	-	expression tag	UNP A0A444M080
g	20	ALA	-	expression tag	UNP A0A444M080
h	2	MET	-	initiating methionine	UNP A0A444M080

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
h	3	LYS	-	expression tag	UNP A0A444M080
h	4	SER	-	expression tag	UNP A0A444M080
h	5	SER	-	expression tag	UNP A0A444M080
h	6	HIS	-	expression tag	UNP A0A444M080
h	7	HIS	-	expression tag	UNP A0A444M080
h	8	HIS	-	expression tag	UNP A0A444M080
h	9	HIS	-	expression tag	UNP A0A444M080
h	10	HIS	-	expression tag	UNP A0A444M080
h	11	HIS	-	expression tag	UNP A0A444M080
h	12	GLU	-	expression tag	UNP A0A444M080
h	13	ASN	-	expression tag	UNP A0A444M080
h	14	LEU	-	expression tag	UNP A0A444M080
h	15	TYR	-	expression tag	UNP A0A444M080
h	16	PHE	-	expression tag	UNP A0A444M080
h	17	GLN	-	expression tag	UNP A0A444M080
h	18	SER	-	expression tag	UNP A0A444M080
h	19	ASN	-	expression tag	UNP A0A444M080
h	20	ALA	-	expression tag	UNP A0A444M080
i	2	MET	-	initiating methionine	UNP A0A444M080
i	3	LYS	-	expression tag	UNP A0A444M080
i	4	SER	-	expression tag	UNP A0A444M080
i	5	SER	-	expression tag	UNP A0A444M080
i	6	HIS	-	expression tag	UNP A0A444M080
i	7	HIS	-	expression tag	UNP A0A444M080
i	8	HIS	-	expression tag	UNP A0A444M080
i	9	HIS	-	expression tag	UNP A0A444M080
i	10	HIS	-	expression tag	UNP A0A444M080
i	11	HIS	-	expression tag	UNP A0A444M080
i	12	GLU	-	expression tag	UNP A0A444M080
i	13	ASN	-	expression tag	UNP A0A444M080
i	14	LEU	-	expression tag	UNP A0A444M080
i	15	TYR	-	expression tag	UNP A0A444M080
i	16	PHE	-	expression tag	UNP A0A444M080
i	17	GLN	-	expression tag	UNP A0A444M080
i	18	SER	-	expression tag	UNP A0A444M080
i	19	ASN	-	expression tag	UNP A0A444M080
i	20	ALA	-	expression tag	UNP A0A444M080

- Molecule 5 is a protein called AcrIF24.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	228	Total	C	N	O	S	0	0
			1766	1129	309	324	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	228	Total	C	N	O	S	0	0
			1766	1129	309	324	4		

- Molecule 6 is a RNA chain called RNA (61-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	61	Total	C	N	O	P	0	0
			1273	569	223	421	60		
6	m	61	Total	C	N	O	P	0	0
			1273	569	223	421	60		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	41	A	G	conflict	GB 313291946
M	53	A	G	conflict	GB 313291946
m	41	A	G	conflict	GB 313291946
m	53	A	G	conflict	GB 313291946

- Molecule 7 is a DNA chain called DNA (5'-D(P*AP*TP*AP*GP*CP*TP*CP*GP*AP*TP*TP*CP*GP*AP*GP*CP*TP*AP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	19	Total	C	N	O	P	0	0
			390	186	72	113	19		

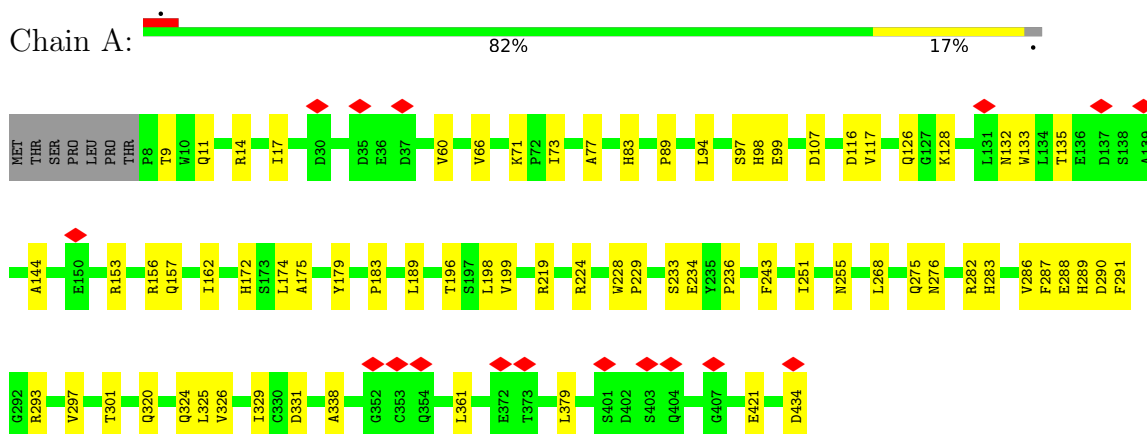
- Molecule 8 is a DNA chain called DNA (5'-D(P*TP*TP*AP*GP*CP*TP*CP*GP*AP*AP*TP*CP*GP*AP*GP*CP*TP*AP*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
8	X	19	Total	C	N	O	P	0	0
			389	186	69	115	19		

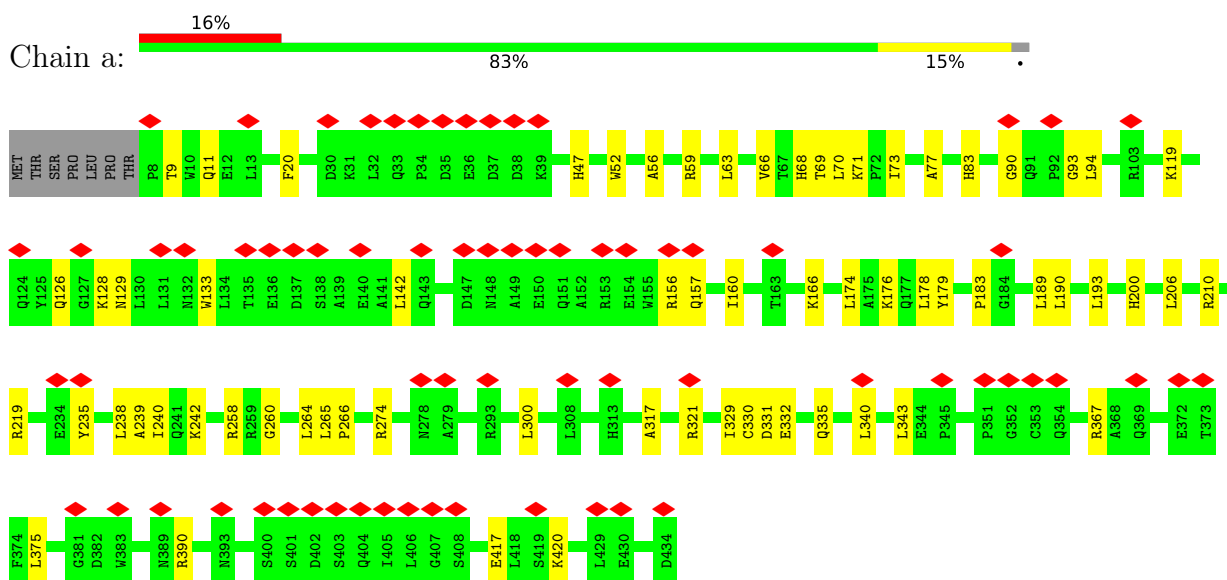
3 Residue-property plots

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: CRISPR-associated protein Csy1

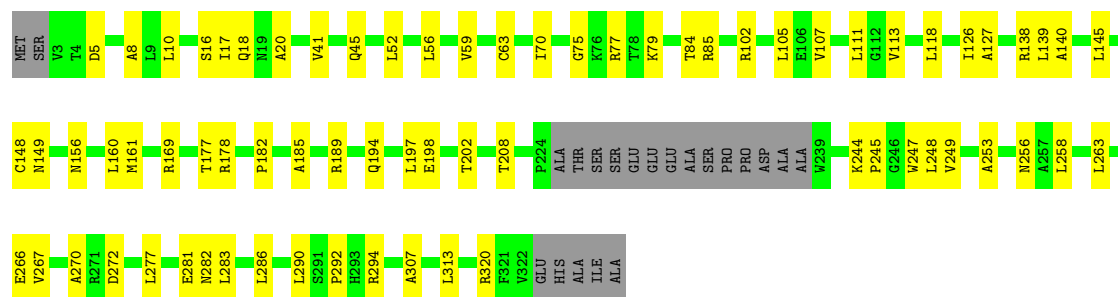


- Molecule 1: CRISPR-associated protein Csy1

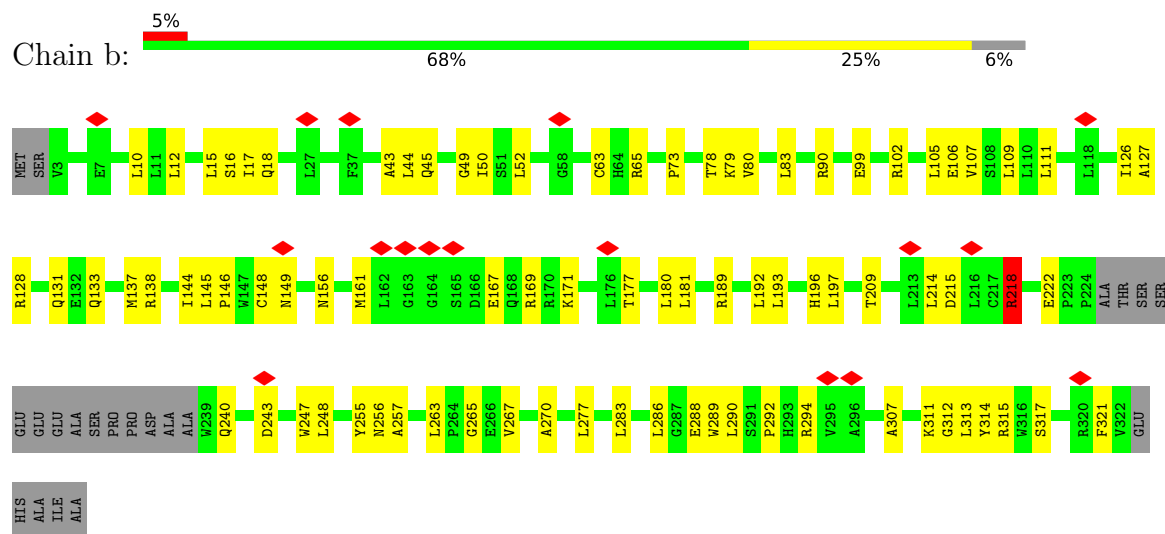


- Molecule 2: CRISPR type I-F/YPEST-associated protein Csy2

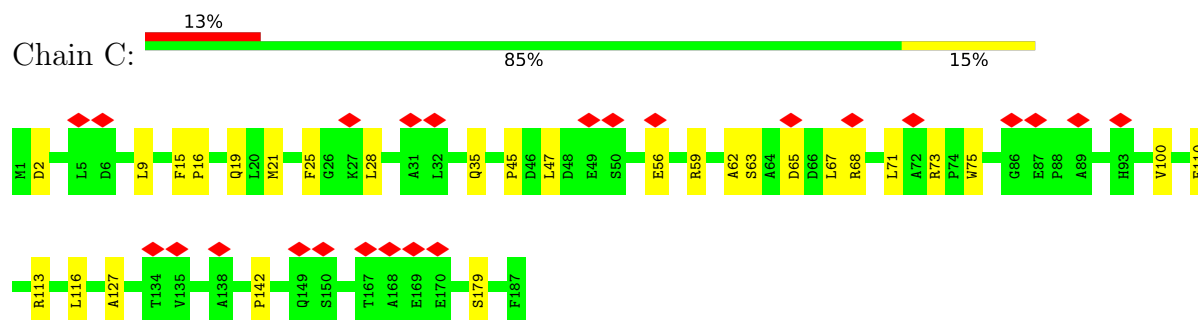




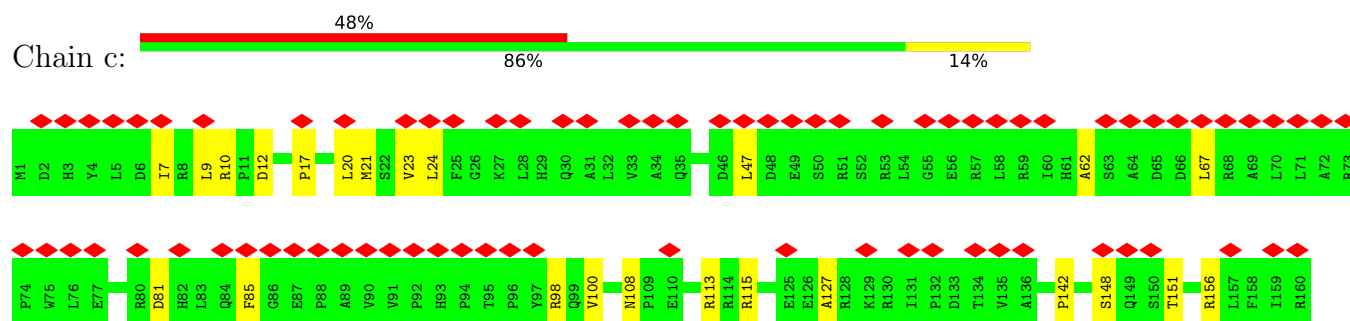
• Molecule 2: CRISPR type I-F/YPEST-associated protein Csy2

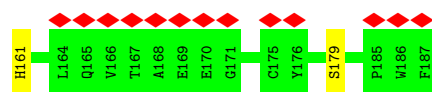


• Molecule 3: CRISPR-associated endonuclease Cas6/Csy4



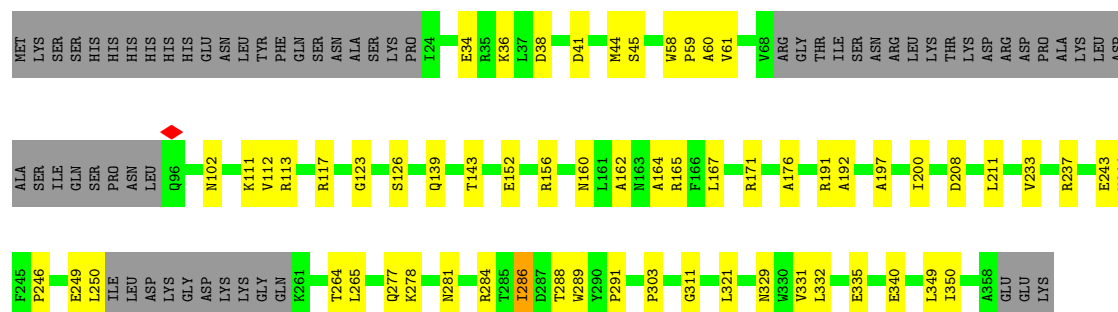
• Molecule 3: CRISPR-associated endonuclease Cas6/Csy4





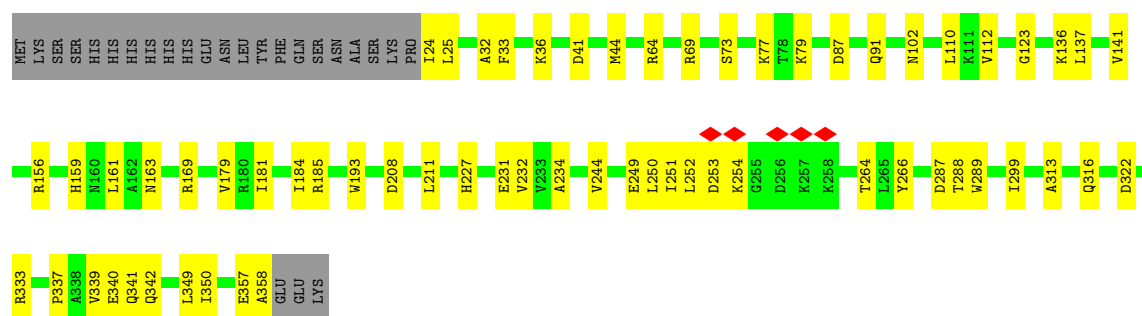
- Molecule 4: CRISPR type I-F/YPEST-associated protein Csy3

Chain D: 66% 17% 17%



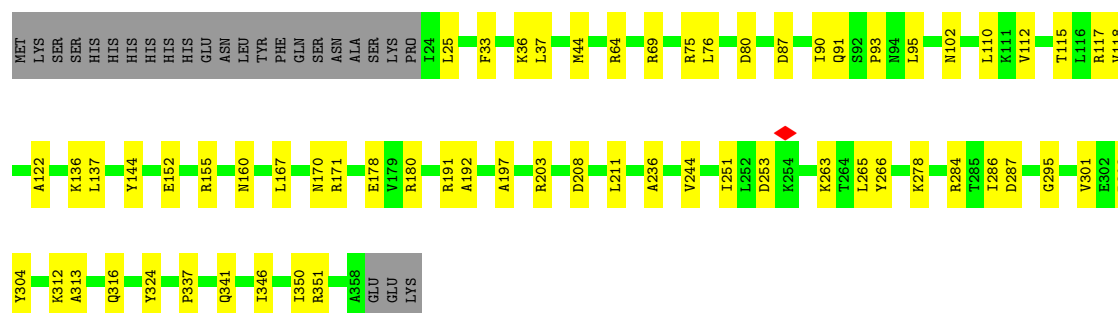
- Molecule 4: CRISPR type I-F/YPEST-associated protein Csy3

Chain E: 76% 18% 7%



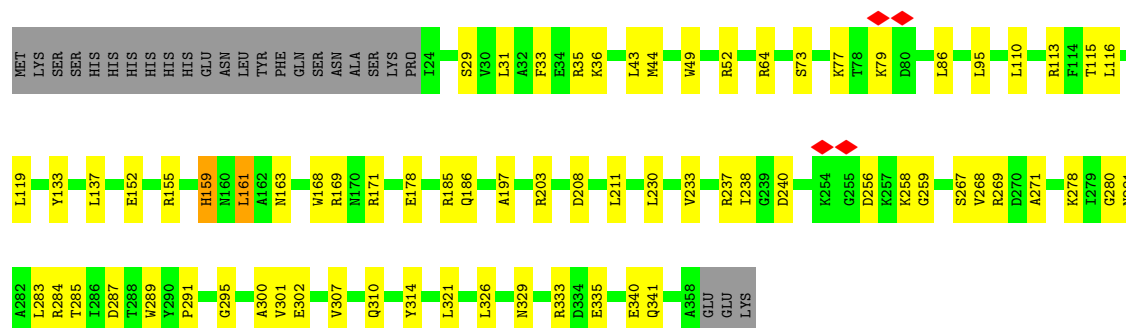
- Molecule 4: CRISPR type I-F/YPEST-associated protein Csy3

Chain F: 76% 18% 7%



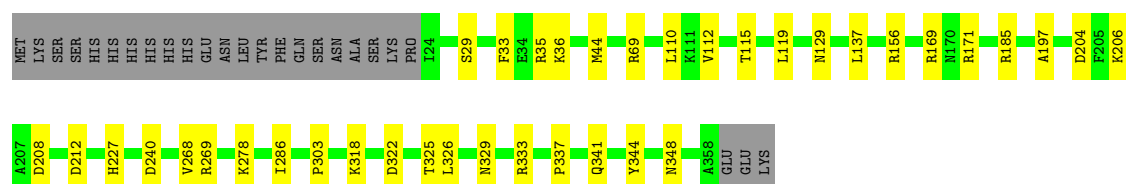
- Molecule 4: CRISPR type I-F/YPEST-associated protein Csy3

Chain G: 73% 19% 7%



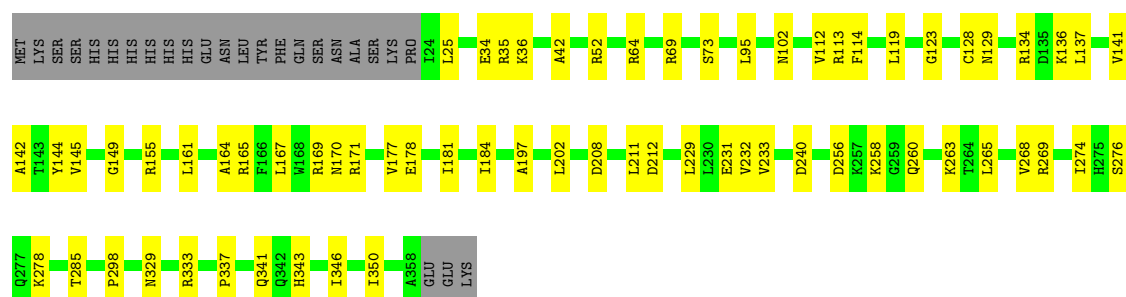
• Molecule 4: CRISPR type I-F/YPEST-associated protein Csy3

Chain H: 82% 11% 7%



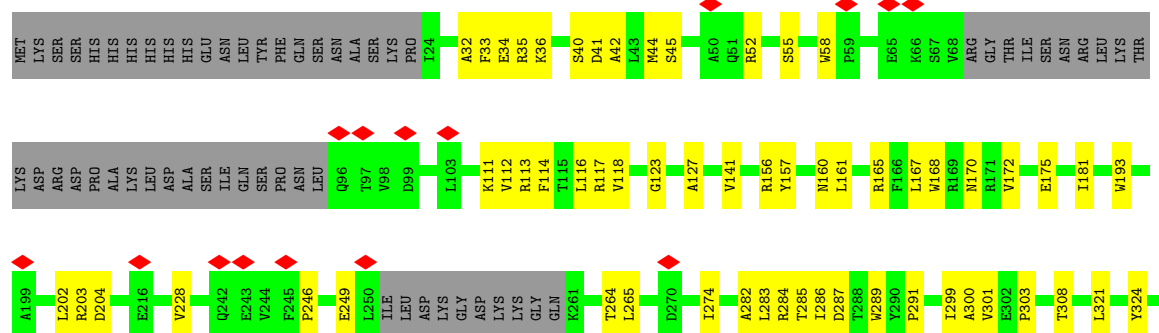
• Molecule 4: CRISPR type I-F/YPEST-associated protein Csy3

Chain I: 74% 19% 7%



• Molecule 4: CRISPR type I-F/YPEST-associated protein Csy3

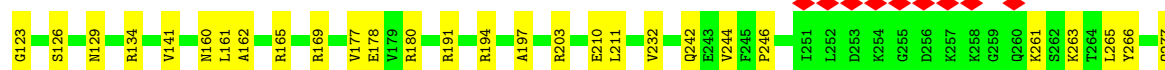
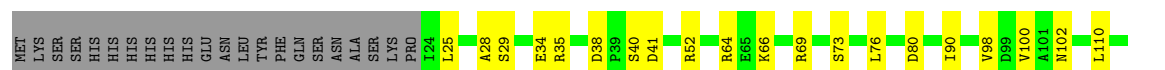
Chain d: 64% 19% 17%





• Molecule 4: CRISPR type I-F/YPEST-associated protein Csy3

Chain e: 75% 18% 7%



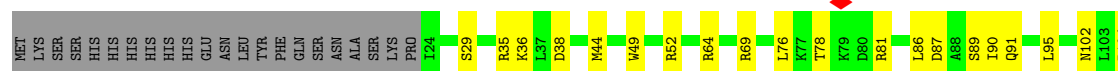
• Molecule 4: CRISPR type I-F/YPEST-associated protein Csy3

Chain f: 70% 23% 7%



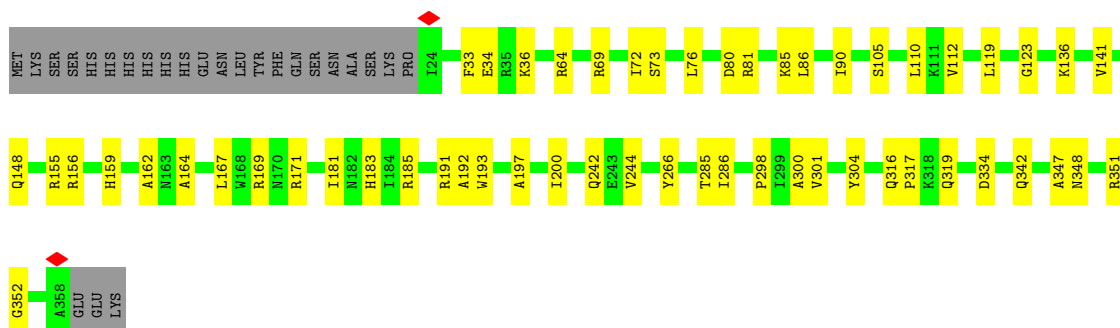
• Molecule 4: CRISPR type I-F/YPEST-associated protein Csy3

Chain g: 71% 21% 7%



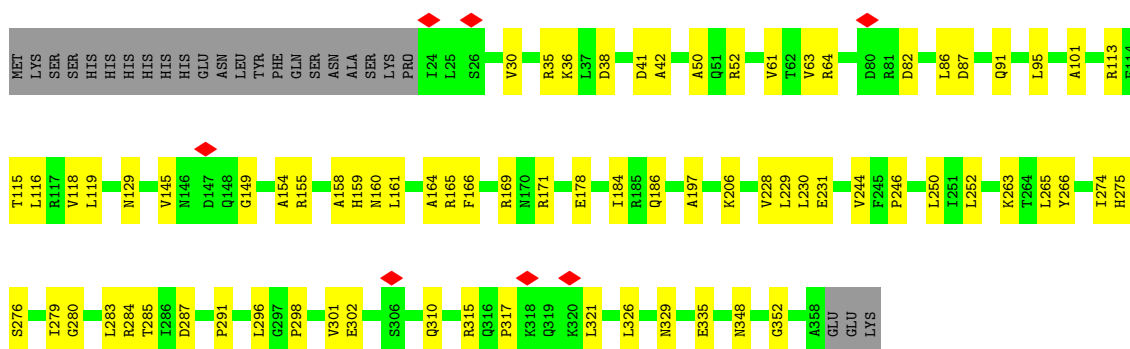
• Molecule 4: CRISPR type I-F/YPEST-associated protein Csy3

Chain h: 78% 15% 7%



- Molecule 4: CRISPR type I-F/YPEST-associated protein Csy3

Chain i: 72% 21% 7%



- Molecule 5: AcrIF24

Chain J: 90% 10%



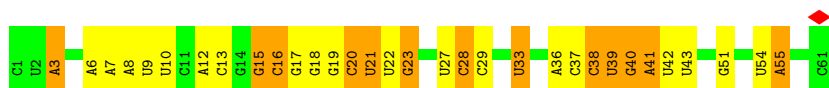
- Molecule 5: AcrIF24

Chain K: 87% 13%



- Molecule 6: RNA (61-MER)

Chain M: 48% 31% 21%



- Molecule 6: RNA (61-MER)

Chain m: 5% 38% 49% 13%



- Molecule 7: DNA (5'-D(P*AP*TP*AP*GP*CP*TP*CP*GP*AP*TP*TP*CP*GP*AP*GP*CP*TP*AP*A)-3')

Chain Y: 89% 11%



- Molecule 8: DNA (5'-D(P*TP*TP*AP*GP*CP*TP*CP*GP*AP*AP*TP*CP*GP*AP*GP*CP*TP*AP*T)-3')

Chain X: 79% 21%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	406243	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	54	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.287	Depositor
Minimum map value	-0.508	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.06	Depositor
Map size ($\text{\AA}$)	337.28, 337.28, 337.28	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.054, 1.054, 1.054	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.16	0/3218	0.42	0/4389
1	a	0.14	0/3218	0.39	0/4389
2	B	0.15	0/2471	0.39	0/3365
2	b	0.18	0/2471	0.45	1/3365 (0.0%)
3	C	0.12	0/1490	0.33	0/2024
3	c	0.11	0/1490	0.30	0/2024
4	D	0.14	0/2350	0.39	1/3190 (0.0%)
4	E	0.14	0/2639	0.38	0/3579
4	F	0.14	0/2639	0.37	0/3579
4	G	0.33	2/2639 (0.1%)	0.49	4/3579 (0.1%)
4	H	0.13	0/2639	0.35	0/3579
4	I	0.13	0/2639	0.35	0/3579
4	d	0.13	0/2350	0.39	0/3190
4	e	0.15	0/2639	0.38	0/3579
4	f	0.13	0/2639	0.35	0/3579
4	g	0.14	0/2639	0.38	0/3579
4	h	0.14	0/2639	0.39	0/3579
4	i	0.12	0/2639	0.34	0/3579
5	J	0.14	0/1817	0.39	0/2484
5	K	0.17	0/1817	0.40	0/2484
6	M	0.10	0/1421	0.24	0/2211
6	m	0.09	0/1421	0.22	0/2211
7	Y	0.22	0/437	0.38	0/672
8	X	0.21	0/435	0.39	0/669
All	All	0.16	2/52796 (0.0%)	0.38	6/72457 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	271	ALA	CA-C	-5.49	1.46	1.52
4	G	159	HIS	C-O	-5.11	1.18	1.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	161	LEU	N-CA-C	-9.41	102.37	114.04
2	b	218	ARG	N-CA-C	6.37	120.00	110.14
4	G	267	SER	O-C-N	5.83	130.38	123.33
4	G	161	LEU	CA-C-N	-5.29	111.68	120.68
4	G	161	LEU	C-N-CA	-5.29	111.68	120.68
4	D	286	ILE	N-CA-C	-5.15	108.25	113.20

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	3145	0	2874	47	0
1	a	3145	0	2874	44	0
2	B	2411	0	2408	53	0
2	b	2411	0	2408	70	0
3	C	1448	0	1394	17	0
3	c	1448	0	1394	17	0
4	D	2307	0	2275	39	0
4	E	2592	0	2581	42	0
4	F	2592	0	2581	43	0
4	G	2592	0	2581	46	0
4	H	2592	0	2581	26	0
4	I	2592	0	2581	47	0
4	d	2307	0	2275	48	0
4	e	2592	0	2581	51	0
4	f	2592	0	2581	60	0
4	g	2592	0	2581	54	0
4	h	2592	0	2581	38	0
4	i	2592	0	2581	60	0
5	J	1766	0	1732	15	0
5	K	1766	0	1732	20	0
6	M	1273	0	646	31	0
6	m	1273	0	646	33	0
7	Y	390	0	215	2	0
8	X	389	0	216	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	51399	0	48899	743	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 7.

All (743) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:18:GLN:HE22	4:i:276:SER:HB3	1.49	0.76
4:e:310:GLN:HG3	4:e:312:LYS:H	1.51	0.75
4:G:268:VAL:HG23	4:G:269:ARG:H	1.50	0.73
2:b:63:CYS:H	2:b:107:VAL:HG13	1.54	0.72
4:g:36:LYS:HG3	4:g:119:LEU:HB2	1.72	0.71
4:d:168:TRP:HE1	4:d:282:ALA:HB2	1.55	0.71
4:d:291:PRO:HD3	4:d:321:LEU:HD11	1.73	0.70
4:G:113:ARG:HG3	4:G:233:VAL:HG22	1.74	0.70
4:I:164:ALA:HB1	4:I:167:LEU:HD13	1.73	0.69
1:a:242:LYS:HD3	1:a:260:GLY:HA3	1.74	0.69
4:h:69:ARG:NH2	6:m:21:U:O2'	2.24	0.69
2:b:15:LEU:HB3	2:b:144:ILE:HD11	1.74	0.68
4:f:177:VAL:HG13	4:f:197:ALA:HB3	1.74	0.67
4:E:161:LEU:HD11	4:E:232:VAL:HG21	1.78	0.66
4:d:181:ILE:HB	4:d:193:TRP:HB2	1.78	0.66
4:g:177:VAL:HG13	4:g:197:ALA:HB3	1.78	0.65
2:B:263:LEU:HB2	2:B:266:GLU:HG3	1.79	0.65
4:E:357:GLU:HB2	4:F:75:ARG:HB2	1.79	0.64
2:B:149:ASN:ND2	4:I:231:GLU:OE2	2.29	0.64
4:D:249:GLU:HB3	4:D:264:THR:HG23	1.78	0.64
1:A:128:LYS:HZ1	1:A:132:ASN:HB3	1.61	0.64
1:A:224:ARG:O	5:J:67:ARG:NH2	2.31	0.64
4:D:113:ARG:HG3	4:D:233:VAL:HG22	1.79	0.63
4:g:222:LEU:HD22	4:g:350:ILE:HD11	1.79	0.63
4:i:287:ASP:HB2	4:i:301:VAL:HG22	1.79	0.63
4:I:167:LEU:HB3	4:I:170:ASN:HB2	1.80	0.63
4:d:160:ASN:OD1	4:d:165:ARG:NH2	2.30	0.63
4:g:156:ARG:HA	4:g:159:HIS:HD2	1.64	0.63
4:i:291:PRO:HD3	4:i:321:LEU:HD22	1.80	0.63
1:a:332:GLU:HA	1:a:335:GLN:HB2	1.79	0.63
4:F:284:ARG:HD3	4:F:351:ARG:HG3	1.79	0.62
4:G:95:LEU:HD12	4:G:258:LYS:HD3	1.81	0.62
1:a:70:LEU:HD12	1:a:73:ILE:HD13	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:9:LEU:HD21	3:c:21:MET:HB2	1.80	0.62
4:e:289:TRP:NE1	4:e:340:GLU:OE2	2.32	0.62
1:a:63:LEU:O	1:a:166:LYS:NZ	2.33	0.62
2:b:161:MET:SD	2:b:169:ARG:NH1	2.73	0.62
4:g:64:ARG:HH12	4:g:102:ASN:HB2	1.64	0.62
2:b:263:LEU:HD23	2:b:265:GLY:H	1.63	0.62
4:e:64:ARG:HH12	4:e:102:ASN:HB2	1.65	0.62
4:g:181:ILE:HG22	4:g:232:VAL:HA	1.81	0.62
2:B:16:SER:HB3	2:B:145:LEU:HB2	1.81	0.62
1:A:60:VAL:HG13	1:A:162:ILE:HD12	1.81	0.62
4:D:164:ALA:HB1	4:D:167:LEU:HD13	1.81	0.62
4:f:115:THR:HG22	4:f:231:GLU:HG2	1.82	0.62
4:f:115:THR:HG21	4:g:240:ASP:HB3	1.82	0.62
1:a:69:THR:HG22	1:a:71:LYS:H	1.65	0.62
1:A:153:ARG:O	1:A:157:GLN:NE2	2.33	0.62
4:E:250:LEU:HD11	4:F:95:LEU:HD12	1.82	0.61
4:I:278:LYS:NZ	6:M:8:A:N3	2.47	0.61
4:f:162:ALA:HB2	4:f:211:LEU:HD21	1.82	0.61
1:A:77:ALA:HB2	1:A:174:LEU:HB2	1.82	0.61
5:K:138:PRO:HB3	5:K:227:ALA:HB3	1.81	0.61
1:a:93:GLY:HA2	2:b:193:LEU:HD22	1.82	0.61
4:D:36:LYS:HB2	4:D:350:ILE:HG23	1.82	0.61
4:E:251:ILE:HG22	4:E:253:ASP:H	1.65	0.61
4:e:325:THR:O	4:e:329:ASN:ND2	2.33	0.61
4:D:156:ARG:HD3	4:D:286:ILE:HB	1.83	0.61
1:a:240:ILE:HB	2:b:80:VAL:HG12	1.81	0.61
4:g:113:ARG:NH2	4:h:105:SER:OG	2.33	0.61
2:b:267:VAL:HG21	2:b:277:LEU:HB3	1.81	0.61
4:h:181:ILE:HB	4:h:193:TRP:HB2	1.83	0.61
1:A:287:PHE:HA	1:A:291:PHE:HB3	1.82	0.60
2:b:197:LEU:HD21	2:b:209:THR:HA	1.83	0.60
4:d:34:GLU:OE1	4:e:169:ARG:NE	2.33	0.60
4:F:171:ARG:NH2	4:F:197:ALA:O	2.34	0.60
4:G:281:ASN:ND2	6:M:20:C:O2	2.34	0.60
4:g:29:SER:OG	4:g:129:ASN:ND2	2.34	0.60
1:A:219:ARG:NH2	1:A:233:SER:O	2.34	0.60
4:E:36:LYS:HB2	4:E:350:ILE:HG23	1.84	0.60
4:f:128:CYS:O	4:f:134:ARG:NH2	2.34	0.60
2:B:10:LEU:HB3	2:B:111:LEU:HB2	1.83	0.60
2:B:75:GLY:HA3	4:I:258:LYS:HG3	1.83	0.60
4:F:278:LYS:NZ	6:M:28:C:OP1	2.33	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:171:ARG:NH2	4:H:197:ALA:O	2.34	0.60
4:I:169:ARG:NH2	6:M:12:A:OP1	2.34	0.60
1:a:142:LEU:HD21	1:a:156:ARG:HD2	1.84	0.60
2:b:270:ALA:O	4:i:129:ASN:ND2	2.35	0.60
4:G:208:ASP:HB3	4:G:211:LEU:HB2	1.82	0.60
4:g:281:ASN:ND2	6:m:20:C:O2	2.34	0.60
4:D:152:GLU:OE2	4:D:156:ARG:NH1	2.35	0.60
5:J:138:PRO:HB3	5:J:227:ALA:HB3	1.82	0.60
4:E:159:HIS:O	4:E:163:ASN:ND2	2.34	0.60
4:H:29:SER:HB3	4:H:129:ASN:HD21	1.66	0.60
4:E:266:TYR:HH	4:F:64:ARG:HH21	1.48	0.59
2:b:248:LEU:HB3	2:b:286:LEU:HD12	1.84	0.59
6:m:51:G:H21	6:m:55:A:H62	1.50	0.59
4:G:171:ARG:NH2	4:G:197:ALA:O	2.36	0.59
1:a:128:LYS:NZ	1:a:129:ASN:O	2.34	0.59
4:f:278:LYS:NZ	6:m:26:G:N3	2.50	0.59
1:a:300:LEU:HD21	1:a:329:ILE:HG12	1.85	0.59
4:E:181:ILE:HB	4:E:193:TRP:HB2	1.84	0.59
4:i:35:ARG:HB2	6:m:6:A:H5''	1.84	0.59
4:i:250:LEU:HB2	6:m:9:U:H5''	1.85	0.59
1:A:89:PRO:HB3	2:B:313:LEU:HD21	1.84	0.59
4:d:41:ASP:OD2	4:e:102:ASN:ND2	2.36	0.59
4:F:167:LEU:HG	4:F:170:ASN:HB2	1.85	0.59
4:e:69:ARG:NH2	6:m:39:U:O2	2.31	0.59
4:i:155:ARG:O	4:i:159:HIS:ND1	2.36	0.59
4:i:246:PRO:HG2	4:i:265:LEU:HD22	1.84	0.59
4:d:308:THR:HG22	4:e:90:ILE:HB	1.84	0.59
2:b:248:LEU:HD23	2:b:288:GLU:HB2	1.84	0.58
4:f:36:LYS:HB2	4:f:350:ILE:HG23	1.85	0.58
4:F:191:ARG:NH1	4:F:192:ALA:O	2.36	0.58
4:i:36:LYS:HG3	4:i:119:LEU:HB2	1.83	0.58
2:b:133:GLN:NE2	2:b:137:MET:SD	2.76	0.58
4:F:203:ARG:NH1	4:F:295:GLY:O	2.34	0.58
4:i:284:ARG:NH2	4:i:302:GLU:OE2	2.36	0.58
4:D:278:LYS:NZ	6:M:40:G:OP1	2.35	0.58
4:G:280:GLY:O	4:G:284:ARG:HB2	2.03	0.58
4:d:156:ARG:NH2	4:d:286:ILE:O	2.31	0.58
4:D:277:GLN:NE2	6:M:39:U:OP1	2.37	0.58
4:D:311:GLY:O	4:E:91:GLN:NE2	2.37	0.58
4:F:266:TYR:OH	4:G:64:ARG:NH1	2.36	0.58
4:H:35:ARG:NH1	6:M:13:C:OP2	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:157:TYR:OH	4:d:284:ARG:NH1	2.37	0.57
4:e:123:GLY:HA3	4:e:141:VAL:HG11	1.85	0.57
4:f:87:ASP:HA	4:f:90:ILE:HD12	1.86	0.57
1:A:288:GLU:O	1:A:293:ARG:NH1	2.36	0.57
2:B:5:ASP:HA	2:B:320:ARG:HH12	1.69	0.57
1:a:239:ALA:HB3	1:a:264:LEU:HB2	1.87	0.57
4:g:35:ARG:HB2	6:m:18:G:H5"	1.87	0.57
4:h:348:ASN:HA	4:h:351:ARG:HB3	1.86	0.57
3:C:9:LEU:HD11	3:C:21:MET:HE2	1.86	0.57
4:i:118:VAL:HB	4:i:228:VAL:HB	1.87	0.57
4:H:36:LYS:HG3	4:H:119:LEU:HB2	1.87	0.57
4:g:35:ARG:NH1	6:m:19:G:OP2	2.38	0.57
2:B:270:ALA:O	4:I:129:ASN:ND2	2.30	0.56
4:f:208:ASP:HB3	4:f:211:LEU:HB2	1.87	0.56
4:I:123:GLY:HA3	4:I:141:VAL:HG11	1.88	0.56
4:D:191:ARG:NH1	4:D:192:ALA:O	2.39	0.56
4:d:165:ARG:HD3	4:d:202:LEU:HD22	1.87	0.56
4:f:315:ARG:NH2	4:f:341:GLN:OE1	2.38	0.56
4:g:266:TYR:OH	4:h:64:ARG:NH2	2.38	0.56
2:b:146:PRO:HG2	4:i:229:LEU:HD13	1.88	0.56
1:A:326:VAL:HG13	1:A:421:GLU:HG3	1.88	0.56
2:B:18:GLN:HE22	4:I:276:SER:HB3	1.71	0.56
2:B:161:MET:O	2:B:169:ARG:NH1	2.39	0.55
4:E:249:GLU:HB2	4:E:264:THR:HG23	1.87	0.55
4:f:181:ILE:HG22	4:f:230:LEU:HD12	1.86	0.55
4:f:155:ARG:O	4:f:159:HIS:ND1	2.38	0.55
2:B:41:VAL:HG21	2:B:59:VAL:HB	1.87	0.55
4:D:102:ASN:HB3	4:D:243:GLU:HG3	1.88	0.55
4:H:329:ASN:OD1	4:H:333:ARG:NH2	2.37	0.55
4:e:110:LEU:HD13	4:e:244:VAL:HG11	1.88	0.55
4:h:169:ARG:NH2	6:m:18:G:OP1	2.40	0.55
3:C:35:GLN:OE1	3:C:73:ARG:NH2	2.40	0.55
2:B:148:CYS:HB3	4:I:229:LEU:HD21	1.89	0.55
4:I:128:CYS:HB3	4:I:134:ARG:HD3	1.89	0.55
5:J:168:ARG:HA	5:J:171:VAL:HG12	1.89	0.55
4:d:284:ARG:HH22	4:d:350:ILE:HG22	1.72	0.55
4:h:171:ARG:NH2	4:h:197:ALA:O	2.39	0.55
3:C:47:LEU:HD11	3:C:142:PRO:HG3	1.88	0.55
4:I:256:ASP:OD2	4:I:260:GLN:NE2	2.40	0.55
1:a:317:ALA:HB1	1:a:321:ARG:HH12	1.71	0.55
3:c:100:VAL:O	3:c:179:SER:OG	2.25	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:f:117:ARG:HH21	4:f:119:LEU:HD11	1.72	0.55
4:g:171:ARG:NH2	4:g:197:ALA:O	2.40	0.55
4:G:268:VAL:HG23	4:G:269:ARG:N	2.22	0.54
4:H:69:ARG:NH1	6:M:21:U:O2'	2.40	0.54
4:I:263:LYS:HE2	4:I:265:LEU:HD21	1.88	0.54
1:a:190:LEU:HD11	2:b:314:TYR:HD2	1.72	0.54
1:A:243:PHE:HB2	1:A:255:ASN:HD21	1.72	0.54
2:b:193:LEU:HD12	2:b:286:LEU:HD23	1.89	0.54
4:h:110:LEU:HD21	4:h:244:VAL:HG21	1.88	0.54
1:A:126:GLN:H	1:A:133:TRP:HH2	1.54	0.54
4:D:156:ARG:NH2	4:D:288:THR:OG1	2.41	0.54
4:E:25:LEU:HD21	4:E:136:LYS:HG2	1.88	0.54
4:e:41:ASP:OD2	4:f:64:ARG:NH2	2.39	0.54
4:g:203:ARG:NH2	4:g:295:GLY:O	2.38	0.54
4:h:191:ARG:NH1	4:h:192:ALA:O	2.40	0.54
1:a:56:ALA:HA	1:a:59:ARG:HD2	1.90	0.54
4:E:185:ARG:NH1	4:E:227:HIS:O	2.41	0.54
4:d:117:ARG:HB2	4:e:242:GLN:HE22	1.72	0.54
4:h:266:TYR:OH	4:i:64:ARG:NH2	2.40	0.54
4:F:37:LEU:HD23	4:F:118:VAL:HG22	1.90	0.54
4:G:329:ASN:OD1	4:G:333:ARG:NH1	2.40	0.54
4:I:165:ARG:NH2	4:I:202:LEU:O	2.37	0.54
4:d:44:MET:HE3	4:d:274:ILE:HD11	1.90	0.54
4:h:156:ARG:NH1	4:h:286:ILE:O	2.40	0.54
2:b:83:LEU:HD12	4:i:252:LEU:HD23	1.89	0.54
7:Y:4:DG:H1	8:X:16:DC:H42	1.54	0.54
4:F:152:GLU:OE2	4:F:155:ARG:NH2	2.41	0.54
4:g:317:PRO:HB2	4:h:81:ARG:HD3	1.89	0.54
5:K:106:ARG:NH2	4:e:25:LEU:O	2.41	0.54
4:g:329:ASN:HB3	4:g:335:GLU:HB2	1.90	0.54
4:G:287:ASP:HB2	4:G:301:VAL:HG12	1.88	0.53
1:a:126:GLN:H	1:a:133:TRP:HH2	1.56	0.53
2:b:138:ARG:O	6:m:2:U:N3	2.41	0.53
3:c:23:VAL:HG11	4:d:172:VAL:HG12	1.90	0.53
1:A:183:PRO:HD3	2:B:307:ALA:HB3	1.90	0.53
4:D:284:ARG:NH2	6:M:38:C:OP2	2.38	0.53
4:I:145:VAL:HA	4:I:149:GLY:HA2	1.90	0.53
4:f:167:LEU:HG	4:f:170:ASN:HB2	1.91	0.53
3:C:9:LEU:HD12	3:C:56:GLU:HA	1.90	0.53
5:J:112:LEU:HD23	5:J:120:GLY:HA3	1.89	0.53
4:f:287:ASP:HB2	4:f:301:VAL:HG22	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:i:63:VAL:HG12	4:i:101:ALA:HB2	1.89	0.53
4:F:33:PHE:HZ	4:F:137:LEU:HD21	1.74	0.53
4:h:155:ARG:O	4:h:159:HIS:ND1	2.35	0.53
1:A:282:ARG:O	1:A:283:HIS:ND1	2.41	0.53
4:E:357:GLU:H	4:F:75:ARG:HD2	1.74	0.53
1:a:9:THR:HG22	1:a:11:GLN:H	1.73	0.53
4:f:36:LYS:HE3	4:f:122:ALA:HA	1.91	0.53
4:f:284:ARG:HD3	4:f:351:ARG:HG3	1.89	0.53
4:D:45:SER:HB3	4:D:111:LYS:HB3	1.90	0.53
4:I:52:ARG:NH1	4:I:178:GLU:OE1	2.40	0.53
1:a:94:LEU:HD11	2:b:313:LEU:HD11	1.90	0.53
4:g:69:ARG:NE	6:m:26:G:O2'	2.39	0.53
4:h:34:GLU:OE1	4:i:169:ARG:NE	2.42	0.53
4:h:316:GLN:OE1	4:h:319:GLN:NE2	2.41	0.53
1:A:97:SER:HA	1:A:198:LEU:HD21	1.91	0.53
4:E:169:ARG:NH2	6:M:36:A:OP1	2.42	0.53
2:b:52:LEU:HD22	2:b:126:ILE:HG22	1.91	0.53
4:F:287:ASP:HB2	4:F:301:VAL:HG22	1.91	0.53
1:a:179:TYR:HB2	6:m:1:C:H3'	1.91	0.53
4:d:123:GLY:HA3	4:d:141:VAL:HG11	1.91	0.53
4:d:328:ASP:OD2	4:d:333:ARG:NH1	2.36	0.53
4:i:41:ASP:OD2	4:i:266:TYR:OH	2.25	0.53
4:i:171:ARG:HH12	4:i:197:ALA:HB1	1.74	0.53
2:B:258:LEU:HD13	2:B:281:GLU:HG2	1.91	0.52
4:I:64:ARG:HH12	4:I:102:ASN:HB2	1.74	0.52
3:C:15:PHE:HB3	3:C:19:GLN:HE21	1.74	0.52
4:D:162:ALA:HB1	4:D:200:ILE:HD13	1.91	0.52
4:f:34:GLU:OE2	4:g:169:ARG:NH2	2.42	0.52
4:i:145:VAL:HA	4:i:149:GLY:HA2	1.91	0.52
4:D:176:ALA:HB3	4:D:237:ARG:HG3	1.91	0.52
2:b:16:SER:HB2	2:b:145:LEU:HB2	1.90	0.52
4:e:134:ARG:NH2	4:f:310:GLN:OE1	2.41	0.52
1:A:283:HIS:HD2	1:A:289:HIS:HB3	1.75	0.52
2:b:138:ARG:NH2	6:m:6:A:OP1	2.41	0.52
4:e:34:GLU:HG3	4:e:126:SER:HB3	1.92	0.52
4:D:58:TRP:HE3	4:D:59:PRO:HD2	1.75	0.52
4:E:156:ARG:NH1	4:E:288:THR:OG1	2.36	0.52
4:F:324:TYR:OH	4:G:73:SER:O	2.26	0.52
4:I:42:ALA:HB3	4:I:274:ILE:HB	1.92	0.52
5:K:170:VAL:O	5:K:177:THR:OG1	2.24	0.52
1:A:9:THR:HG22	1:A:11:GLN:H	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:44:MET:HG2	4:D:112:VAL:HG22	1.92	0.52
1:a:200:HIS:HB2	1:a:258:ARG:HH21	1.75	0.52
4:d:55:SER:O	4:d:113:ARG:NH2	2.42	0.52
4:g:110:LEU:HD13	4:g:244:VAL:HG11	1.92	0.52
4:g:118:VAL:HB	4:g:228:VAL:HB	1.92	0.52
1:A:320:GLN:NE2	1:A:324:GLN:OE1	2.43	0.52
5:K:21:GLY:N	4:i:95:LEU:O	2.35	0.52
4:I:42:ALA:HA	4:I:114:PHE:HB3	1.91	0.52
2:b:247:TRP:HE3	2:b:289:TRP:HB2	1.73	0.52
4:d:249:GLU:N	4:d:264:THR:O	2.39	0.52
1:a:157:GLN:HA	1:a:160:ILE:HG22	1.92	0.51
3:C:73:ARG:HB3	3:C:75:TRP:HD1	1.76	0.51
4:E:123:GLY:HA2	4:E:349:LEU:HD23	1.93	0.51
5:J:26:HIS:ND1	5:J:44:ASP:OD1	2.35	0.51
2:b:167:GLU:HG3	2:b:171:LYS:HE2	1.91	0.51
4:d:165:ARG:HH21	4:d:285:THR:HB	1.75	0.51
4:D:45:SER:HA	4:D:60:ALA:HA	1.93	0.51
4:g:208:ASP:HB3	4:g:211:LEU:HB2	1.91	0.51
4:E:333:ARG:NH2	5:J:105:ASP:OD1	2.37	0.51
4:H:44:MET:HB2	4:H:110:LEU:HD11	1.92	0.51
4:G:284:ARG:NH2	4:G:302:GLU:OE2	2.43	0.51
4:H:35:ARG:HB2	6:M:12:A:H5"	1.93	0.51
4:e:266:TYR:OH	4:f:64:ARG:NH2	2.43	0.51
4:I:155:ARG:NH1	4:I:212:ASP:OD1	2.44	0.51
2:b:256:ASN:HB2	2:b:283:LEU:HD21	1.93	0.51
4:g:52:ARG:NH1	4:g:178:GLU:OE1	2.43	0.51
4:F:251:ILE:HG22	4:F:253:ASP:H	1.76	0.51
4:G:329:ASN:HB3	4:G:335:GLU:HB2	1.91	0.51
4:I:95:LEU:HD12	5:J:18:LEU:HD13	1.92	0.51
4:g:115:THR:HG22	4:g:231:GLU:HG2	1.93	0.51
4:e:277:GLN:NE2	6:m:33:U:OP1	2.44	0.51
2:B:113:VAL:HG12	2:B:118:LEU:HD11	1.93	0.50
1:a:330:CYS:SG	2:b:294:ARG:NH2	2.81	0.50
4:f:339:VAL:O	4:f:343:HIS:ND1	2.44	0.50
4:F:115:THR:HG21	4:G:240:ASP:HB3	1.93	0.50
4:E:250:LEU:HD21	4:F:95:LEU:HB3	1.93	0.50
4:F:110:LEU:HD13	4:F:244:VAL:HG11	1.94	0.50
2:b:45:GLN:HE21	2:b:50:ILE:HG23	1.77	0.50
4:d:42:ALA:HB1	4:d:112:VAL:HG13	1.93	0.50
4:D:331:VAL:HG23	4:D:332:LEU:HD12	1.92	0.50
2:b:44:LEU:O	2:b:49:GLY:N	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:222:GLU:OE2	2:b:240:GLN:NE2	2.45	0.50
1:A:179:TYR:OH	2:B:272:ASP:OD2	2.24	0.50
1:a:77:ALA:HB2	1:a:174:LEU:HB2	1.94	0.50
4:F:167:LEU:HD21	4:F:236:ALA:HB2	1.93	0.50
4:f:275:HIS:ND1	6:m:27:U:OP1	2.45	0.50
5:J:75:LEU:HD13	5:J:111:LEU:HD21	1.94	0.50
2:b:90:ARG:HD2	4:i:317:PRO:HG3	1.92	0.50
2:B:138:ARG:NH1	4:I:34:GLU:OE2	2.45	0.50
4:H:185:ARG:NH2	4:H:227:HIS:O	2.44	0.50
4:I:208:ASP:HB3	4:I:211:LEU:HB2	1.92	0.50
4:f:76:LEU:HB3	4:f:80:ASP:HB2	1.94	0.50
4:i:82:ASP:OD1	4:i:82:ASP:N	2.45	0.50
4:E:64:ARG:NH2	4:E:102:ASN:OD1	2.45	0.50
4:F:64:ARG:HH12	4:F:102:ASN:HB2	1.77	0.50
4:e:263:LYS:HE3	4:e:265:LEU:HD21	1.93	0.50
4:h:36:LYS:HG3	4:h:119:LEU:HB2	1.93	0.50
2:B:177:THR:HG23	2:B:292:PRO:HB2	1.94	0.49
1:a:68:HIS:HB3	1:a:193:LEU:HB3	1.93	0.49
4:i:35:ARG:NH1	6:m:7:A:OP2	2.45	0.49
2:B:17:ILE:HB	2:B:105:LEU:HB2	1.94	0.49
4:G:52:ARG:NE	4:G:178:GLU:OE2	2.34	0.49
6:M:51:G:H21	6:M:55:A:H62	1.59	0.49
2:b:146:PRO:HB2	4:i:229:LEU:HD22	1.93	0.49
4:h:164:ALA:HB3	4:h:171:ARG:HG3	1.93	0.49
1:a:417:GLU:HA	1:a:420:LYS:HG2	1.94	0.49
4:e:177:VAL:HB	4:e:197:ALA:HB3	1.94	0.49
4:E:77:LYS:HG3	4:E:79:LYS:HG2	1.92	0.49
5:K:103:PRO:HG3	5:K:112:LEU:HD11	1.95	0.49
2:b:148:CYS:O	4:i:113:ARG:NH2	2.46	0.49
4:d:118:VAL:HB	4:d:228:VAL:HB	1.92	0.49
4:g:95:LEU:HD12	4:g:258:LYS:HD3	1.94	0.49
4:h:112:VAL:HG21	4:h:167:LEU:HD21	1.95	0.49
4:D:38:ASP:OD2	4:D:117:ARG:NH2	2.45	0.49
4:e:203:ARG:NH1	4:e:296:LEU:O	2.46	0.49
4:f:307:VAL:HG12	4:f:310:GLN:H	1.78	0.49
1:A:331:ASP:OD1	2:B:294:ARG:NH1	2.46	0.49
1:a:331:ASP:O	1:a:335:GLN:N	2.40	0.49
4:i:329:ASN:HB3	4:i:335:GLU:HB2	1.95	0.49
4:G:203:ARG:NH2	4:G:295:GLY:O	2.33	0.49
4:d:246:PRO:HG2	4:d:265:LEU:HD22	1.94	0.49
5:K:30:LEU:HG	5:K:37:MET:HE3	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:149:ASN:ND2	4:i:231:GLU:OE1	2.42	0.49
2:b:65:ARG:HG2	2:b:106:GLU:HB3	1.95	0.49
4:h:80:ASP:HA	4:h:85:LYS:HE2	1.95	0.49
4:D:289:TRP:CG	4:D:340:GLU:HB3	2.47	0.49
4:e:28:ALA:HB1	4:e:129:ASN:HB2	1.94	0.49
4:f:164:ALA:HB1	4:f:167:LEU:HB3	1.94	0.49
4:E:41:ASP:OD2	4:F:64:ARG:NH2	2.46	0.48
2:b:148:CYS:HB3	4:i:229:LEU:HD21	1.94	0.48
4:d:339:VAL:O	4:d:343:HIS:ND1	2.44	0.48
4:h:72:ILE:HD13	4:h:90:ILE:HD13	1.95	0.48
4:G:49:TRP:CG	4:G:237:ARG:HH21	2.31	0.48
4:e:180:ARG:HG2	4:e:194:ARG:HG2	1.94	0.48
4:f:284:ARG:HD2	4:f:300:ALA:HB1	1.94	0.48
4:F:263:LYS:HE2	4:F:265:LEU:HD21	1.95	0.48
4:e:311:GLY:HA3	4:f:91:GLN:HE21	1.78	0.48
4:h:136:LYS:NZ	4:h:334:ASP:OD1	2.40	0.48
4:E:33:PHE:HZ	4:E:137:LEU:HD21	1.78	0.48
2:b:18:GLN:NE2	4:i:41:ASP:OD1	2.40	0.48
1:a:210:ARG:HA	1:a:219:ARG:HH12	1.78	0.48
3:c:47:LEU:HD11	3:c:142:PRO:HG3	1.96	0.48
1:A:66:VAL:HA	1:A:83:HIS:HB2	1.96	0.48
1:A:128:LYS:HZ2	1:A:133:TRP:CD1	2.31	0.48
4:G:326:LEU:HD21	4:G:341:GLN:HB3	1.95	0.48
2:b:315:ARG:NH2	2:b:317:SER:OG	2.46	0.48
4:g:324:TYR:OH	4:h:73:SER:O	2.32	0.48
3:C:110:GLU:HA	3:C:113:ARG:HD2	1.95	0.48
1:a:340:LEU:HD13	1:a:343:LEU:HD12	1.95	0.48
2:b:214:LEU:HD23	2:b:218:ARG:HH12	1.78	0.48
4:e:351:ARG:NH2	6:m:30:G:O2'	2.46	0.48
4:i:296:LEU:HD11	4:i:310:GLN:HG3	1.96	0.48
4:H:268:VAL:HG23	4:H:269:ARG:H	1.79	0.48
5:K:95:PRO:HD2	5:K:98:LEU:HD11	1.96	0.48
4:d:42:ALA:HB3	4:d:274:ILE:HB	1.95	0.48
4:f:277:GLN:NE2	6:m:27:U:OP2	2.36	0.48
4:h:162:ALA:HB1	4:h:200:ILE:HD13	1.96	0.48
1:A:71:LYS:HG2	1:A:251:ILE:HA	1.95	0.48
4:F:87:ASP:O	4:F:91:GLN:HG2	2.14	0.48
4:g:253:ASP:OD1	4:g:260:GLN:NE2	2.46	0.48
1:A:196:THR:HA	1:A:199:VAL:HG22	1.95	0.47
3:C:100:VAL:O	3:C:179:SER:OG	2.27	0.47
4:D:208:ASP:HB3	4:D:211:LEU:HB2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:291:PRO:HD3	4:D:321:LEU:HD13	1.96	0.47
4:F:304:TYR:HB3	4:G:86:LEU:HD21	1.95	0.47
4:G:289:TRP:CD1	4:G:340:GLU:HB3	2.48	0.47
1:A:189:LEU:HB2	2:B:277:LEU:HA	1.96	0.47
4:D:171:ARG:NH2	4:D:197:ALA:O	2.47	0.47
4:H:33:PHE:HZ	4:H:137:LEU:HD21	1.78	0.47
4:d:204:ASP:OD1	4:d:204:ASP:N	2.47	0.47
4:e:35:ARG:HB2	6:m:30:G:H5''	1.96	0.47
4:E:313:ALA:HB2	4:F:90:ILE:HD11	1.96	0.47
4:F:178:GLU:OE1	4:F:180:ARG:NE	2.44	0.47
1:A:325:LEU:O	1:A:329:ILE:HD12	2.15	0.47
4:E:357:GLU:HG3	4:E:358:ALA:H	1.80	0.47
1:a:20:PHE:HZ	1:a:119:LYS:HG3	1.79	0.47
1:a:176:LYS:HG3	6:m:3:A:H1'	1.96	0.47
4:f:326:LEU:HD22	4:f:337:PRO:HB3	1.97	0.47
4:f:329:ASN:OD1	4:f:333:ARG:NH1	2.42	0.47
4:g:35:ARG:NE	4:g:38:ASP:OD1	2.45	0.47
4:h:285:THR:HG22	4:h:298:PRO:HB2	1.95	0.47
4:G:29:SER:OG	5:J:16:ARG:NH1	2.48	0.47
4:G:161:LEU:HD13	4:G:283:LEU:HD21	1.97	0.47
4:f:216:GLU:HA	4:f:219:ALA:HB3	1.95	0.47
4:h:148:GLN:OE1	4:h:342:GLN:NE2	2.47	0.47
4:h:183:HIS:CE1	4:h:185:ARG:HE	2.33	0.47
1:A:286:VAL:HG23	1:A:290:ASP:HB3	1.96	0.47
4:E:287:ASP:HB3	4:E:299:ILE:HG13	1.96	0.47
4:G:31:LEU:HD11	4:G:133:TYR:HE2	1.80	0.47
2:B:45:GLN:HG3	2:B:56:LEU:H	1.78	0.47
4:I:113:ARG:HG3	4:I:233:VAL:HG22	1.97	0.47
4:g:104:PRO:HD2	4:g:107:ALA:HB3	1.97	0.47
2:B:253:ALA:N	2:B:283:LEU:O	2.41	0.47
4:f:181:ILE:HG23	4:f:232:VAL:HG22	1.97	0.47
5:J:8:PRO:HG3	5:J:169:HIS:HA	1.97	0.47
1:a:66:VAL:HA	1:a:83:HIS:HB2	1.96	0.47
2:b:12:LEU:HB2	2:b:109:LEU:HB2	1.97	0.47
4:f:44:MET:HG2	4:f:112:VAL:HG12	1.96	0.47
4:h:123:GLY:HA3	4:h:141:VAL:HG21	1.97	0.47
4:D:246:PRO:HG2	4:D:265:LEU:HD12	1.97	0.47
4:H:156:ARG:NH1	4:H:286:ILE:O	2.48	0.47
2:b:73:PRO:HD2	2:b:79:LYS:HA	1.97	0.47
4:g:156:ARG:NH1	4:g:286:ILE:O	2.48	0.47
2:B:52:LEU:HD22	2:B:126:ILE:HG22	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:35:ARG:NH1	6:M:19:G:OP2	2.48	0.46
4:G:159:HIS:O	4:G:163:ASN:ND2	2.49	0.46
4:d:33:PHE:HB2	4:d:352:GLY:HA2	1.96	0.46
4:e:160:ASN:ND2	4:e:282:ALA:O	2.48	0.46
4:f:65:GLU:OE2	4:f:97:THR:OG1	2.28	0.46
4:d:175:GLU:N	4:d:175:GLU:OE2	2.48	0.46
2:B:185:ALA:N	2:B:290:LEU:O	2.49	0.46
4:F:303:PRO:HG2	4:G:73:SER:HB2	1.97	0.46
4:E:322:ASP:OD1	4:E:322:ASP:N	2.45	0.46
4:H:44:MET:HB3	4:H:112:VAL:HG22	1.96	0.46
5:K:20:TYR:HB3	5:K:25:HIS:CD2	2.50	0.46
2:b:148:CYS:HB2	4:i:184:ILE:HG13	1.97	0.46
4:d:324:TYR:OH	4:e:73:SER:O	2.29	0.46
4:H:185:ARG:HH12	4:H:227:HIS:HB3	1.80	0.46
4:i:30:VAL:N	4:i:129:ASN:OD1	2.44	0.46
1:a:238:LEU:HB2	2:b:78:THR:HG22	1.98	0.46
2:b:10:LEU:HB3	2:b:111:LEU:HB2	1.97	0.46
4:g:113:ARG:HG3	4:g:233:VAL:HG22	1.96	0.46
4:i:155:ARG:NH1	4:i:206:LYS:O	2.48	0.46
2:B:63:CYS:HA	2:B:107:VAL:HG12	1.96	0.46
4:I:164:ALA:HB3	4:I:171:ARG:HG3	1.98	0.46
3:c:21:MET:HA	3:c:24:LEU:HB3	1.97	0.46
4:d:40:SER:HB2	4:d:114:PHE:HB2	1.97	0.46
4:e:284:ARG:NH2	6:m:32:G:OP2	2.49	0.46
8:X:6:DT:H2''	8:X:7:DC:H5'	1.97	0.46
1:A:116:ASP:OD1	1:A:117:VAL:N	2.49	0.46
2:B:127:ALA:O	2:B:156:ASN:ND2	2.49	0.46
4:G:44:MET:HE3	4:G:110:LEU:HD21	1.98	0.46
4:f:284:ARG:HG2	4:f:301:VAL:H	1.81	0.46
4:F:44:MET:HG2	4:F:112:VAL:HG22	1.97	0.46
2:B:194:GLN:O	2:B:198:GLU:HG2	2.16	0.46
4:G:256:ASP:OD1	4:G:259:GLY:N	2.42	0.46
3:C:63:SER:OG	3:C:65:ASP:OD1	2.28	0.45
5:K:173:GLU:N	7:Y:2:DT:OP1	2.49	0.45
4:i:263:LYS:HE2	4:i:265:LEU:HD21	1.98	0.45
4:f:171:ARG:NH2	4:f:197:ALA:O	2.47	0.45
4:f:313:ALA:HB3	4:f:316:GLN:HE21	1.81	0.45
4:i:161:LEU:HD22	4:i:283:LEU:HD22	1.98	0.45
1:A:268:LEU:O	2:B:247:TRP:NE1	2.49	0.45
1:A:275:GLN:HG2	1:A:276:ASN:H	1.81	0.45
4:D:34:GLU:HG3	4:D:126:SER:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:43:LEU:CD2	4:G:268:VAL:HG21	2.46	0.45
4:G:307:VAL:HG12	4:G:310:GLN:H	1.82	0.45
1:a:206:LEU:HA	1:a:235:TYR:HE2	1.80	0.45
2:b:17:ILE:N	2:b:105:LEU:O	2.43	0.45
4:d:35:ARG:HB2	6:m:36:A:H5''	1.99	0.45
4:d:289:TRP:CD1	4:d:340:GLU:HB3	2.52	0.45
4:e:69:ARG:O	6:m:37:C:O2'	2.34	0.45
3:C:113:ARG:HG2	3:C:127:ALA:HB1	1.98	0.45
3:c:115:ARG:NH2	6:m:50:C:OP2	2.38	0.45
4:f:249:GLU:OE2	4:f:275:HIS:NE2	2.44	0.45
3:C:62:ALA:HB3	3:C:67:LEU:HG	1.99	0.45
4:F:69:ARG:HH21	4:F:93:PRO:HG3	1.81	0.45
4:G:185:ARG:HG2	4:G:186:GLN:OE1	2.16	0.45
4:e:351:ARG:HH21	6:m:31:C:H5'	1.82	0.45
4:F:36:LYS:HB2	4:F:350:ILE:HG23	1.98	0.45
3:c:108:ASN:ND2	6:m:47:U:OP2	2.38	0.45
4:e:161:LEU:HD22	4:e:232:VAL:HG21	1.98	0.45
4:g:76:LEU:HD11	4:g:86:LEU:HD12	1.98	0.45
4:g:351:ARG:NH2	6:m:18:G:O2'	2.50	0.45
1:A:73:ILE:HG21	1:A:175:ALA:HA	1.99	0.45
1:A:297:VAL:O	1:A:301:THR:HG23	2.17	0.45
4:E:184:ILE:HD11	4:E:231:GLU:HG2	1.98	0.45
5:J:171:VAL:HG11	5:J:199:THR:HG21	1.99	0.45
1:a:178:LEU:N	1:a:189:LEU:O	2.47	0.45
4:f:251:ILE:HG22	4:f:253:ASP:H	1.82	0.45
4:g:168:TRP:CD1	4:g:278:LYS:HE3	2.52	0.45
4:g:292:ASP:OD2	4:g:312:LYS:NZ	2.45	0.45
4:G:285:THR:HA	4:G:300:ALA:HA	1.99	0.45
2:b:102:ARG:HH22	4:i:275:HIS:CD2	2.35	0.45
2:b:127:ALA:O	2:b:156:ASN:ND2	2.50	0.45
3:c:148:SER:OG	3:c:151:THR:O	2.30	0.45
4:g:64:ARG:NH2	4:g:102:ASN:OD1	2.49	0.45
2:B:148:CYS:HB2	4:I:184:ILE:HG13	1.99	0.44
4:D:41:ASP:OD1	4:D:41:ASP:N	2.48	0.44
4:d:332:LEU:HD23	4:d:333:ARG:HH11	1.81	0.44
4:e:310:GLN:NE2	4:e:312:LYS:O	2.50	0.44
4:g:291:PRO:HD3	4:g:321:LEU:HD23	1.99	0.44
4:h:285:THR:HA	4:h:300:ALA:HA	1.99	0.44
4:i:329:ASN:O	4:i:335:GLU:N	2.50	0.44
1:A:361:LEU:HD11	1:A:379:LEU:HA	1.99	0.44
2:B:198:GLU:O	2:B:202:THR:HG23	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:43:LEU:HD22	4:G:268:VAL:HG21	1.99	0.44
4:G:310:GLN:OE1	4:G:314:TYR:OH	2.32	0.44
2:b:128:ARG:NH2	4:i:186:GLN:OE1	2.46	0.44
3:c:10:ARG:NH2	3:c:81:ASP:O	2.50	0.44
4:e:98:VAL:HG13	4:e:263:LYS:HB3	1.98	0.44
4:f:289:TRP:CD1	4:f:340:GLU:HB2	2.52	0.44
4:E:123:GLY:HA3	4:E:141:VAL:HG11	1.99	0.44
4:F:36:LYS:HE3	4:F:122:ALA:HA	1.98	0.44
4:G:116:LEU:HD23	4:G:230:LEU:HD12	1.99	0.44
4:d:303:PRO:HG2	4:e:73:SER:HB2	2.00	0.44
4:e:246:PRO:HG2	4:e:265:LEU:HB3	2.00	0.44
4:h:301:VAL:HG21	4:h:347:ALA:HB1	1.99	0.44
2:B:194:GLN:NE2	2:B:197:LEU:HD23	2.32	0.44
4:H:278:LYS:NZ	6:M:16:C:OP1	2.41	0.44
2:b:247:TRP:N	2:b:288:GLU:OE1	2.48	0.44
4:H:303:PRO:HG2	4:I:73:SER:HB2	1.97	0.44
2:b:189:ARG:HD3	2:b:192:LEU:HD13	2.00	0.44
4:d:45:SER:HB3	4:d:111:LYS:HD3	1.99	0.44
4:d:287:ASP:HB2	4:d:301:VAL:HG22	1.98	0.44
4:i:116:LEU:HD23	4:i:230:LEU:HD13	1.99	0.44
1:A:189:LEU:HD13	2:B:277:LEU:HD12	1.99	0.44
4:G:169:ARG:NH1	6:M:23:G:OP1	2.50	0.44
5:K:140:LEU:HD13	5:K:177:THR:HG22	2.00	0.44
4:g:318:LYS:HE3	4:h:81:ARG:HB3	1.99	0.44
1:A:135:THR:O	1:A:156:ARG:NH2	2.51	0.44
4:E:179:VAL:HA	4:E:234:ALA:HA	1.98	0.44
4:F:76:LEU:HB3	4:F:80:ASP:HB2	1.99	0.44
4:H:204:ASP:HB3	4:H:206:LYS:HE2	1.99	0.44
4:I:42:ALA:HB1	4:I:112:VAL:HG13	1.99	0.44
4:E:289:TRP:CD1	4:E:340:GLU:HB3	2.53	0.44
4:I:337:PRO:HB2	4:I:341:GLN:HB2	2.00	0.44
1:a:274:ARG:CZ	2:b:65:ARG:HB2	2.48	0.44
2:b:10:LEU:HD22	2:b:111:LEU:HD12	2.00	0.44
4:E:110:LEU:HD13	4:E:244:VAL:HG11	2.00	0.44
4:f:340:GLU:HA	4:f:343:HIS:HD1	1.83	0.44
4:i:154:ALA:O	4:i:158:ALA:N	2.48	0.44
1:A:434:ASP:OXT	2:B:178:ARG:NH2	2.51	0.43
4:D:123:GLY:HA2	4:D:349:LEU:HD21	2.00	0.43
1:a:90:GLY:H	2:b:311:LYS:HE3	1.83	0.43
2:b:189:ARG:HB3	2:b:192:LEU:HB3	2.00	0.43
4:e:162:ALA:HB2	4:e:211:LEU:HD21	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:f:123:GLY:HA2	4:f:349:LEU:HD21	2.00	0.43
4:i:50:ALA:HA	4:i:52:ARG:HH21	1.83	0.43
2:b:161:MET:O	2:b:169:ARG:NH1	2.51	0.43
2:b:196:HIS:NE2	2:b:215:ASP:OD2	2.44	0.43
4:g:44:MET:HG2	4:g:112:VAL:HG22	1.99	0.43
4:I:256:ASP:OD1	4:I:256:ASP:N	2.51	0.43
4:e:66:LYS:HE3	4:e:100:VAL:HG11	2.01	0.43
4:f:106:ASP:OD1	4:f:106:ASP:N	2.51	0.43
4:D:139:GLN:O	4:D:143:THR:HG23	2.18	0.43
4:H:169:ARG:NH2	6:M:18:G:OP1	2.49	0.43
5:K:28:TRP:CD1	5:K:42:LEU:HB2	2.53	0.43
1:a:367:ARG:NH1	1:a:375:LEU:O	2.51	0.43
3:c:7:ILE:HG12	3:c:85:PHE:HD1	1.82	0.43
4:f:96:GLN:NE2	6:m:31:C:N3	2.66	0.43
4:g:285:THR:HA	4:g:300:ALA:HA	1.99	0.43
1:A:14:ARG:NH2	1:A:144:ALA:O	2.51	0.43
4:E:252:LEU:HB3	4:E:254:LYS:HE2	1.99	0.43
4:I:142:ALA:HA	4:I:145:VAL:HG22	2.00	0.43
4:i:287:ASP:OD2	4:i:315:ARG:NE	2.51	0.43
1:A:89:PRO:HD2	1:A:98:HIS:CD2	2.54	0.43
2:B:20:ALA:HB1	2:B:140:ALA:HB3	1.99	0.43
4:d:160:ASN:ND2	4:d:283:LEU:O	2.52	0.43
4:d:165:ARG:HH11	4:d:202:LEU:HD22	1.83	0.43
2:B:17:ILE:HG13	2:B:139:LEU:HD23	2.01	0.43
2:B:267:VAL:HG21	2:B:277:LEU:HD22	2.00	0.43
2:b:148:CYS:SG	4:i:115:THR:HG22	2.58	0.43
4:f:159:HIS:CE1	4:f:211:LEU:HD13	2.54	0.43
4:G:35:ARG:HB2	6:M:18:G:H5"	2.00	0.43
4:d:32:ALA:HB3	4:d:127:ALA:HB3	1.99	0.43
4:g:87:ASP:HA	4:g:90:ILE:HD12	2.00	0.43
2:b:43:ALA:HB1	2:b:137:MET:HE1	2.00	0.43
4:f:177:VAL:HG12	4:f:198:LEU:HG	2.01	0.43
4:g:153:LEU:HD11	4:g:346:ILE:HG23	2.01	0.43
4:g:304:TYR:HE2	4:h:76:LEU:HD13	1.84	0.43
4:h:317:PRO:HD2	4:i:86:LEU:HD22	2.00	0.43
4:I:181:ILE:HG12	4:I:232:VAL:HG13	2.00	0.43
5:K:154:HIS:CE1	5:K:226:ARG:HD3	2.53	0.43
4:e:40:SER:HB2	4:f:242:GLN:HE21	1.84	0.43
4:g:115:THR:O	4:h:242:GLN:NE2	2.52	0.43
5:K:198:TYR:OH	8:X:12:DC:OP2	2.33	0.42
1:a:94:LEU:HD12	2:b:283:LEU:HD22	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:287:ASP:HB3	4:d:299:ILE:HG13	2.01	0.42
4:h:155:ARG:HG2	4:h:159:HIS:HE1	1.83	0.42
4:i:285:THR:HG22	4:i:298:PRO:HB2	2.00	0.42
4:D:61:VAL:HG11	4:D:244:VAL:HG21	2.01	0.42
4:I:35:ARG:HB2	6:M:6:A:H5''	2.00	0.42
4:h:33:PHE:HB2	4:h:352:GLY:HA2	2.00	0.42
4:i:155:ARG:HG2	4:i:159:HIS:HE1	1.83	0.42
4:H:337:PRO:HB2	4:H:341:GLN:HB2	2.00	0.42
4:I:35:ARG:NH1	6:M:7:A:OP2	2.52	0.42
4:I:268:VAL:HG23	4:I:269:ARG:H	1.84	0.42
3:c:113:ARG:HG2	3:c:127:ALA:HB1	2.01	0.42
4:f:69:ARG:HD3	6:m:32:G:O2'	2.20	0.42
4:g:160:ASN:OD1	4:g:165:ARG:NE	2.51	0.42
3:C:68:ARG:HA	3:C:71:LEU:HG	2.02	0.42
4:E:24:ILE:HG12	5:J:122:PRO:HG2	2.00	0.42
4:E:313:ALA:HB3	4:E:316:GLN:NE2	2.34	0.42
4:F:313:ALA:HB3	4:F:316:GLN:HE21	1.83	0.42
5:K:28:TRP:HD1	5:K:42:LEU:HB2	1.84	0.42
4:d:52:ARG:HA	4:d:58:TRP:HH2	1.84	0.42
4:e:191:ARG:NH2	4:e:210:GLU:OE2	2.52	0.42
4:f:55:SER:HA	4:f:58:TRP:CD1	2.54	0.42
4:F:312:LYS:HE3	4:F:312:LYS:HB2	1.90	0.42
1:a:47:HIS:HA	1:a:52:TRP:HB2	2.01	0.42
2:b:243:ASP:OD1	2:b:243:ASP:N	2.52	0.42
4:d:167:LEU:HD23	4:d:170:ASN:HB2	2.00	0.42
4:i:42:ALA:HB3	4:i:274:ILE:HB	2.02	0.42
1:A:77:ALA:HB1	1:A:172:HIS:HB3	2.02	0.42
2:B:8:ALA:HB2	2:B:160:LEU:HD13	2.01	0.42
2:B:70:ILE:HD12	2:B:79:LYS:HD3	2.00	0.42
4:F:337:PRO:HB2	4:F:341:GLN:HB2	2.02	0.42
5:J:35:ARG:HH21	5:J:62:PHE:HE2	1.66	0.42
2:b:131:GLN:HG3	2:b:156:ASN:HD21	1.84	0.42
1:A:66:VAL:HG23	1:A:107:ASP:HB3	2.02	0.42
1:A:338:ALA:HB1	2:B:182:PRO:HG3	2.01	0.42
2:B:282:ASN:OD1	6:M:3:A:N6	2.42	0.42
4:E:69:ARG:N	6:M:39:U:OP2	2.52	0.42
4:H:208:ASP:O	4:H:212:ASP:N	2.50	0.42
4:I:69:ARG:NH1	6:M:15:G:N3	2.68	0.42
5:K:138:PRO:HG2	5:K:141:ALA:HB2	2.02	0.42
1:a:179:TYR:N	6:m:2:U:OP1	2.37	0.42
4:f:165:ARG:HG2	4:f:282:ALA:HB1	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:f:183:HIS:CE1	4:f:228:VAL:HG23	2.54	0.42
4:i:166:PHE:HB2	4:i:279:ILE:HG23	2.02	0.42
4:i:348:ASN:O	4:i:352:GLY:N	2.49	0.42
4:G:36:LYS:HG3	4:G:119:LEU:HB2	2.02	0.42
2:b:255:TYR:O	2:b:314:TYR:N	2.53	0.42
2:b:267:VAL:HG11	2:b:277:LEU:HD13	2.00	0.42
3:c:156:ARG:HG3	6:m:45:A:H5'	2.02	0.42
4:g:316:GLN:HG3	4:g:318:LYS:H	1.84	0.42
1:A:236:PRO:HB3	2:B:77:ARG:HH22	1.84	0.42
2:B:244:LYS:HB3	2:B:248:LEU:HD12	2.01	0.42
3:C:2:ASP:OD1	3:C:2:ASP:N	2.52	0.42
3:C:16:PRO:HG2	6:M:41:A:H4'	2.02	0.42
4:E:32:ALA:HB1	6:M:29:C:H1'	2.01	0.42
4:E:339:VAL:HA	4:E:342:GLN:HG2	2.01	0.42
6:M:40:G:H1'	6:M:41:A:C8	2.54	0.42
4:e:160:ASN:OD1	4:e:165:ARG:NH2	2.53	0.42
4:i:52:ARG:NH1	4:i:178:GLU:OE2	2.53	0.42
1:A:228:TRP:CG	1:A:229:PRO:HD2	2.54	0.42
2:B:84:THR:HG21	2:B:102:ARG:HH11	1.85	0.42
2:B:256:ASN:HB2	2:B:283:LEU:HD21	2.01	0.42
4:D:303:PRO:HG2	4:E:73:SER:HB2	2.01	0.42
5:K:25:HIS:CE1	5:K:43:PRO:HG3	2.55	0.42
4:d:117:ARG:HE	4:e:242:GLN:HE22	1.68	0.42
4:e:38:ASP:OD1	4:e:38:ASP:N	2.47	0.42
4:i:287:ASP:OD1	4:i:315:ARG:NH2	2.53	0.42
4:D:329:ASN:O	4:D:335:GLU:N	2.47	0.41
4:I:346:ILE:O	4:I:350:ILE:HG12	2.20	0.41
1:a:183:PRO:HD3	2:b:307:ALA:HB3	2.02	0.41
2:b:63:CYS:HA	2:b:107:VAL:HG22	2.01	0.41
4:e:52:ARG:NH1	4:e:178:GLU:OE1	2.52	0.41
4:f:287:ASP:HB3	4:f:299:ILE:HG13	2.02	0.41
4:h:304:TYR:HD1	4:h:317:PRO:HD3	1.85	0.41
4:E:44:MET:HG2	4:E:112:VAL:HG22	2.02	0.41
4:G:77:LYS:C	4:G:79:LYS:H	2.27	0.41
4:I:285:THR:HG22	4:I:298:PRO:HB2	2.02	0.41
2:b:248:LEU:N	2:b:288:GLU:OE1	2.50	0.41
4:f:208:ASP:OD1	4:f:209:ALA:N	2.53	0.41
4:g:316:GLN:HE22	4:h:86:LEU:HD12	1.86	0.41
2:B:85:ARG:NE	6:M:8:A:O2'	2.50	0.41
4:G:291:PRO:HB3	4:G:321:LEU:HD12	2.03	0.41
4:H:115:THR:HG21	4:I:240:ASP:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:344:TYR:O	4:H:348:ASN:ND2	2.43	0.41
6:M:51:G:N2	6:M:55:A:H62	2.19	0.41
2:b:177:THR:HG23	2:b:292:PRO:HB2	2.03	0.41
4:d:36:LYS:HB2	4:d:350:ILE:HG23	2.02	0.41
4:g:86:LEU:O	4:g:89:SER:OG	2.37	0.41
4:g:348:ASN:H	4:g:348:ASN:HD22	1.67	0.41
4:D:250:LEU:HB3	6:M:39:U:C5	2.55	0.41
4:I:161:LEU:HD22	4:I:232:VAL:HG21	2.02	0.41
1:a:390:ARG:HE	1:a:390:ARG:HB3	1.64	0.41
3:c:98:ARG:HD3	3:c:161:HIS:HD2	1.86	0.41
4:e:342:GLN:HA	4:e:345:VAL:HG12	2.03	0.41
4:f:301:VAL:HG11	4:f:347:ALA:HB3	2.02	0.41
4:i:160:ASN:HB3	4:i:283:LEU:HA	2.03	0.41
4:i:164:ALA:H	4:i:171:ARG:NH1	2.19	0.41
4:G:152:GLU:OE1	4:G:155:ARG:NH1	2.53	0.41
4:I:177:VAL:HB	4:I:197:ALA:HB3	2.02	0.41
2:b:257:ALA:HB2	2:b:312:GLY:HA3	2.02	0.41
4:D:281:ASN:ND2	6:M:38:C:O2	2.53	0.41
4:F:117:ARG:HH12	4:G:238:ILE:HG23	1.85	0.41
4:G:115:THR:HG21	4:H:240:ASP:HB2	2.01	0.41
4:H:318:LYS:HD3	4:H:318:LYS:HA	1.91	0.41
4:I:36:LYS:HG3	4:I:119:LEU:HB2	2.03	0.41
4:I:329:ASN:OD1	4:I:333:ARG:NH2	2.52	0.41
1:a:178:LEU:O	1:a:190:LEU:HB2	2.20	0.41
4:e:261:LYS:HD2	4:e:261:LYS:HA	1.87	0.41
4:e:324:TYR:OH	4:f:73:SER:O	2.37	0.41
4:e:357:GLU:HG3	4:e:358:ALA:H	1.85	0.41
4:f:35:ARG:HB3	6:m:24:A:H5"	2.02	0.41
4:g:49:TRP:HB2	4:g:237:ARG:HD3	2.03	0.41
4:D:112:VAL:HB	4:D:167:LEU:HD11	2.02	0.41
4:I:136:LYS:HD2	4:I:136:LYS:HA	1.89	0.41
3:c:10:ARG:HG2	4:d:203:ARG:NH1	2.35	0.41
3:c:12:ASP:HB2	3:c:20:LEU:HD11	2.03	0.41
4:i:35:ARG:HE	4:i:38:ASP:HB3	1.85	0.41
3:C:25:PHE:HA	3:C:28:LEU:HG	2.03	0.41
4:H:322:ASP:OD1	4:H:325:THR:OG1	2.30	0.41
4:I:144:TYR:OH	4:I:343:HIS:ND1	2.47	0.41
4:e:129:ASN:ND2	4:g:91:GLN:OE1	2.53	0.41
4:f:24:ILE:HD12	4:f:24:ILE:HA	1.99	0.41
1:A:234:GLU:OE2	2:B:77:ARG:NH2	2.53	0.41
2:B:189:ARG:HB2	2:B:286:LEU:HD23	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:289:TRP:CD1	4:D:340:GLU:HB3	2.56	0.41
4:F:69:ARG:NH1	6:M:33:U:O2'	2.54	0.41
4:H:326:LEU:HD13	4:H:341:GLN:HB3	2.03	0.41
5:J:94:LEU:HB3	5:J:98:LEU:HD12	2.02	0.41
5:K:18:LEU:HD12	4:i:95:LEU:HD12	2.02	0.41
5:K:42:LEU:HD11	5:K:54:GLU:HG2	2.02	0.41
2:b:181:LEU:HD23	2:b:181:LEU:HA	1.93	0.41
3:c:62:ALA:HB3	3:c:67:LEU:HG	2.01	0.41
4:e:29:SER:HB2	4:e:129:ASN:HD22	1.86	0.41
4:e:76:LEU:HD13	4:e:80:ASP:HB3	2.02	0.41
4:e:284:ARG:HD3	4:e:351:ARG:HB3	2.02	0.41
4:f:159:HIS:NE2	4:f:206:LYS:O	2.54	0.41
4:g:78:THR:HA	4:g:81:ARG:HH12	1.85	0.41
4:g:285:THR:HG22	4:g:298:PRO:HB2	2.02	0.41
4:i:160:ASN:OD1	4:i:165:ARG:NH2	2.46	0.41
3:C:116:LEU:HD11	3:C:127:ALA:HB2	2.03	0.41
4:d:160:ASN:HB3	4:d:283:LEU:HA	2.01	0.41
4:i:276:SER:O	4:i:280:GLY:N	2.45	0.41
4:i:326:LEU:HD23	4:i:326:LEU:HA	1.95	0.41
1:A:14:ARG:HA	1:A:17:ILE:HG12	2.03	0.40
3:C:45:PRO:HG3	3:C:59:ARG:HB2	2.02	0.40
4:E:87:ASP:O	4:E:91:GLN:HG2	2.21	0.40
4:F:25:LEU:HD21	4:F:136:LYS:HG2	2.04	0.40
4:F:144:TYR:CD2	4:F:346:ILE:HG13	2.56	0.40
4:F:160:ASN:ND2	4:F:286:ILE:HG22	2.37	0.40
4:F:208:ASP:HB3	4:F:211:LEU:HD23	2.04	0.40
1:a:265:LEU:HA	1:a:266:PRO:HD3	1.89	0.40
3:c:17:PRO:HA	3:c:20:LEU:HD12	2.03	0.40
4:g:159:HIS:CD2	4:g:205:PHE:HD1	2.38	0.40
4:i:61:VAL:HG11	4:i:244:VAL:HG21	2.01	0.40
2:B:245:PRO:HD2	2:B:248:LEU:HD11	2.03	0.40
4:D:160:ASN:OD1	4:D:165:ARG:NE	2.54	0.40
4:G:33:PHE:HZ	4:G:137:LEU:HD21	1.86	0.40
4:I:25:LEU:HD23	4:I:25:LEU:HA	1.89	0.40
5:K:93:ARG:HG3	5:K:135:LEU:HD22	2.02	0.40
4:d:45:SER:HB3	4:d:111:LYS:HB3	2.03	0.40
4:d:285:THR:HA	4:d:300:ALA:HA	2.04	0.40
4:h:164:ALA:HB1	4:h:167:LEU:HD12	2.03	0.40
4:E:337:PRO:HB2	4:E:341:GLN:HB2	2.03	0.40
4:G:168:TRP:CD1	4:G:278:LYS:HE3	2.56	0.40
4:f:49:TRP:HB2	4:f:237:ARG:HD3	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:LEU:HD13	2:B:283:LEU:HD22	2.02	0.40
2:B:247:TRP:HD1	2:B:249:VAL:HG13	1.87	0.40
4:D:277:GLN:HB2	6:M:37:C:H3'	2.03	0.40
4:I:137:LEU:O	4:I:141:VAL:HG23	2.22	0.40
5:J:98:LEU:HB3	5:J:119:LEU:HB3	2.03	0.40
1:a:242:LYS:N	2:b:99:GLU:OE1	2.53	0.40
2:b:290:LEU:HD12	2:b:321:PHE:HZ	1.85	0.40
4:d:116:LEU:HD13	4:d:161:LEU:HD12	2.04	0.40
1:A:99:GLU:HG2	2:B:208:THR:HB	2.04	0.40
2:B:248:LEU:HD22	2:B:286:LEU:HD21	2.02	0.40
4:E:208:ASP:HB3	4:E:211:LEU:HD12	2.04	0.40
5:K:110:TRP:CZ3	5:K:122:PRO:HG3	2.56	0.40
4:i:87:ASP:O	4:i:91:GLN:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	425/434 (98%)	401 (94%)	24 (6%)	0	100	100
1	a	425/434 (98%)	398 (94%)	27 (6%)	0	100	100
2	B	302/327 (92%)	284 (94%)	18 (6%)	0	100	100
2	b	302/327 (92%)	288 (95%)	14 (5%)	0	100	100
3	C	186/187 (100%)	181 (97%)	5 (3%)	0	100	100
3	c	186/187 (100%)	182 (98%)	4 (2%)	0	100	100
4	D	292/360 (81%)	276 (94%)	16 (6%)	0	100	100
4	E	333/360 (92%)	317 (95%)	16 (5%)	0	100	100
4	F	333/360 (92%)	317 (95%)	16 (5%)	0	100	100
4	G	333/360 (92%)	320 (96%)	13 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	H	333/360 (92%)	314 (94%)	19 (6%)	0	100	100
4	I	333/360 (92%)	316 (95%)	17 (5%)	0	100	100
4	d	292/360 (81%)	276 (94%)	16 (6%)	0	100	100
4	e	333/360 (92%)	318 (96%)	15 (4%)	0	100	100
4	f	333/360 (92%)	316 (95%)	17 (5%)	0	100	100
4	g	333/360 (92%)	324 (97%)	9 (3%)	0	100	100
4	h	333/360 (92%)	323 (97%)	10 (3%)	0	100	100
4	i	333/360 (92%)	320 (96%)	13 (4%)	0	100	100
5	J	226/228 (99%)	223 (99%)	3 (1%)	0	100	100
5	K	226/228 (99%)	219 (97%)	7 (3%)	0	100	100
All	All	6192/6672 (93%)	5913 (96%)	279 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	279/365 (76%)	279 (100%)	0	100	100
1	a	279/365 (76%)	279 (100%)	0	100	100
2	B	255/270 (94%)	255 (100%)	0	100	100
2	b	255/270 (94%)	253 (99%)	2 (1%)	73	88
3	C	146/160 (91%)	146 (100%)	0	100	100
3	c	146/160 (91%)	146 (100%)	0	100	100
4	D	234/290 (81%)	234 (100%)	0	100	100
4	E	266/290 (92%)	266 (100%)	0	100	100
4	F	266/290 (92%)	266 (100%)	0	100	100
4	G	266/290 (92%)	266 (100%)	0	100	100
4	H	266/290 (92%)	266 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	I	266/290 (92%)	266 (100%)	0	100	100
4	d	234/290 (81%)	234 (100%)	0	100	100
4	e	266/290 (92%)	266 (100%)	0	100	100
4	f	266/290 (92%)	266 (100%)	0	100	100
4	g	266/290 (92%)	265 (100%)	1 (0%)	84	93
4	h	266/290 (92%)	266 (100%)	0	100	100
4	i	266/290 (92%)	266 (100%)	0	100	100
5	J	182/182 (100%)	182 (100%)	0	100	100
5	K	182/182 (100%)	182 (100%)	0	100	100
All	All	4852/5434 (89%)	4849 (100%)	3 (0%)	87	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	180	LEU
2	b	218	ARG
4	g	348	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	111	ASN
1	A	124	GLN
1	A	255	ASN
1	A	289	HIS
1	A	320	GLN
1	A	393	ASN
2	B	18	GLN
2	B	86	ASN
2	B	240	GLN
2	B	306	HIS
3	C	165	GLN
4	E	163	ASN
4	E	281	ASN
4	E	348	ASN
4	F	182	ASN
4	F	183	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	F	242	GLN
4	G	56	GLN
4	G	163	ASN
4	G	182	ASN
4	H	51	GLN
5	J	154	HIS
5	J	206	ASN
5	K	25	HIS
5	K	206	ASN
1	a	11	GLN
1	a	22	GLN
1	a	87	GLN
1	a	124	GLN
1	a	393	ASN
2	b	18	GLN
2	b	19	ASN
2	b	306	HIS
3	c	153	GLN
4	d	56	GLN
4	d	102	ASN
4	d	182	ASN
4	d	281	ASN
4	e	91	GLN
4	e	146	ASN
4	e	148	GLN
4	e	227	HIS
4	e	242	GLN
4	e	329	ASN
4	f	91	GLN
4	f	146	ASN
4	f	183	HIS
4	f	242	GLN
4	g	74	ASN
4	g	159	HIS
4	g	348	ASN
4	h	102	ASN
4	h	170	ASN
4	h	260	GLN
4	h	319	GLN
4	h	342	GLN
4	i	51	GLN
4	i	310	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	i	329	ASN
4	i	341	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	M	59/61 (96%)	21 (35%)	1 (1%)
6	m	59/61 (96%)	21 (35%)	0
All	All	118/122 (96%)	42 (35%)	1 (0%)

All (42) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	M	3	A
6	M	9	U
6	M	10	U
6	M	15	G
6	M	16	C
6	M	17	G
6	M	20	C
6	M	21	U
6	M	22	U
6	M	23	G
6	M	27	U
6	M	28	C
6	M	33	U
6	M	38	C
6	M	39	U
6	M	40	G
6	M	41	A
6	M	42	U
6	M	43	U
6	M	54	U
6	M	55	A
6	m	3	A
6	m	9	U
6	m	10	U
6	m	11	C
6	m	15	G
6	m	16	C
6	m	17	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	m	20	C
6	m	21	U
6	m	22	U
6	m	23	G
6	m	27	U
6	m	28	C
6	m	33	U
6	m	37	C
6	m	38	C
6	m	39	U
6	m	40	G
6	m	42	U
6	m	43	U
6	m	54	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	M	16	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

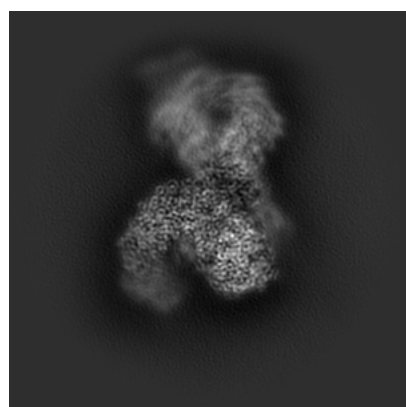
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25788. These allow visual inspection of the internal detail of the map and identification of artifacts.

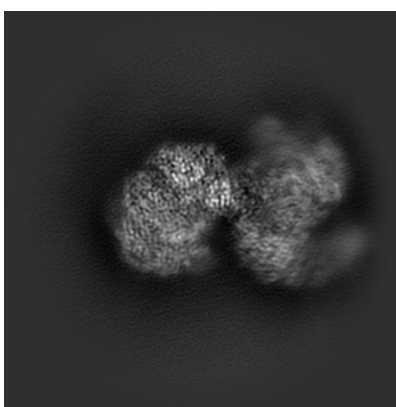
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

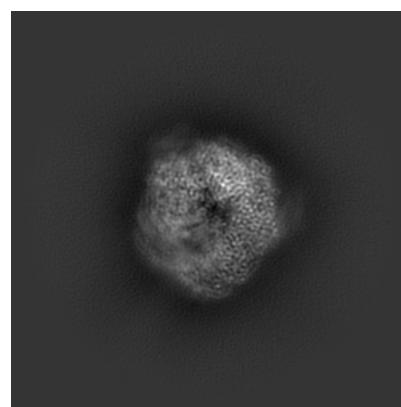
6.1.1 Primary map



X



Y

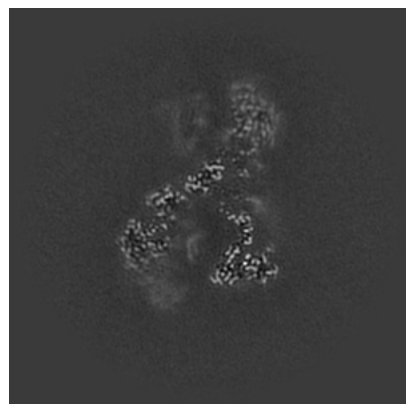


Z

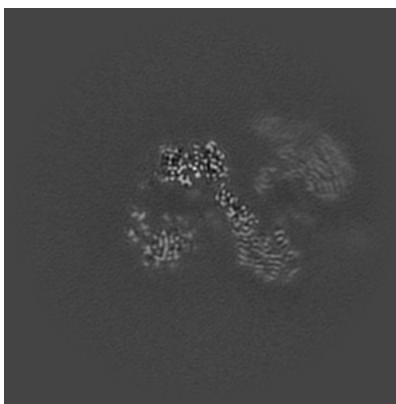
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

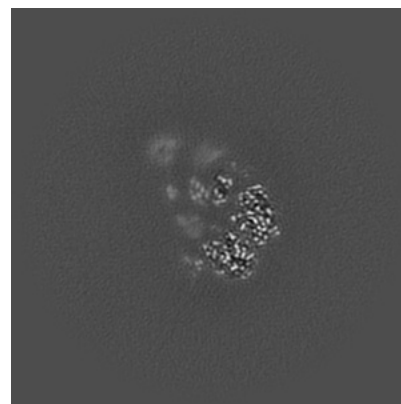
6.2.1 Primary map



X Index: 160



Y Index: 160

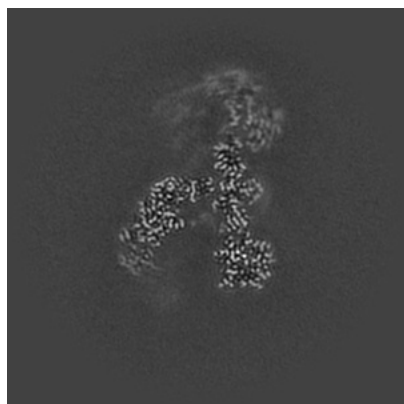


Z Index: 160

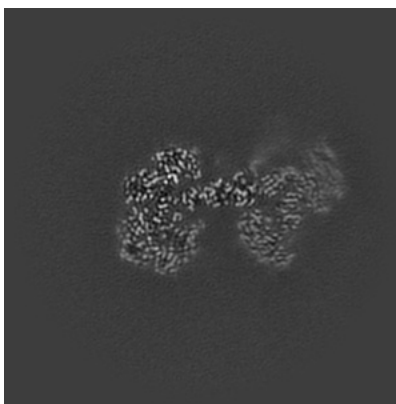
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

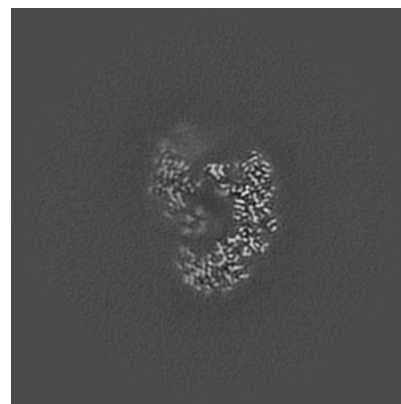
6.3.1 Primary map



X Index: 170



Y Index: 182

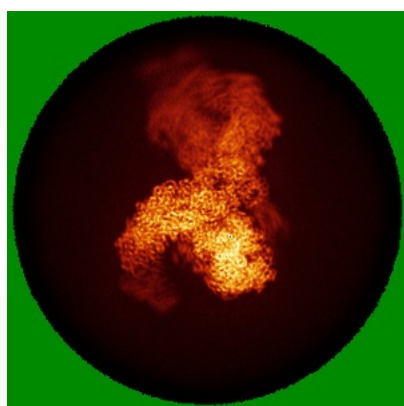


Z Index: 142

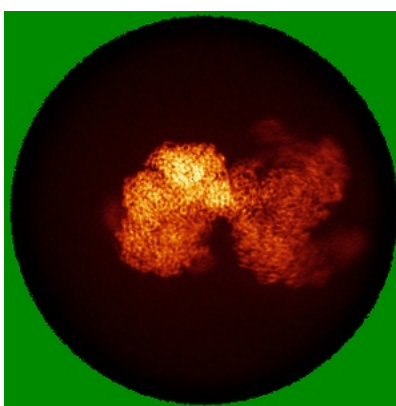
The images above show the largest variance slices of the map in three orthogonal directions.

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

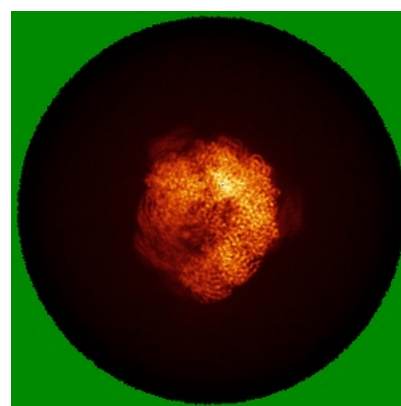
6.4.1 Primary map



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.

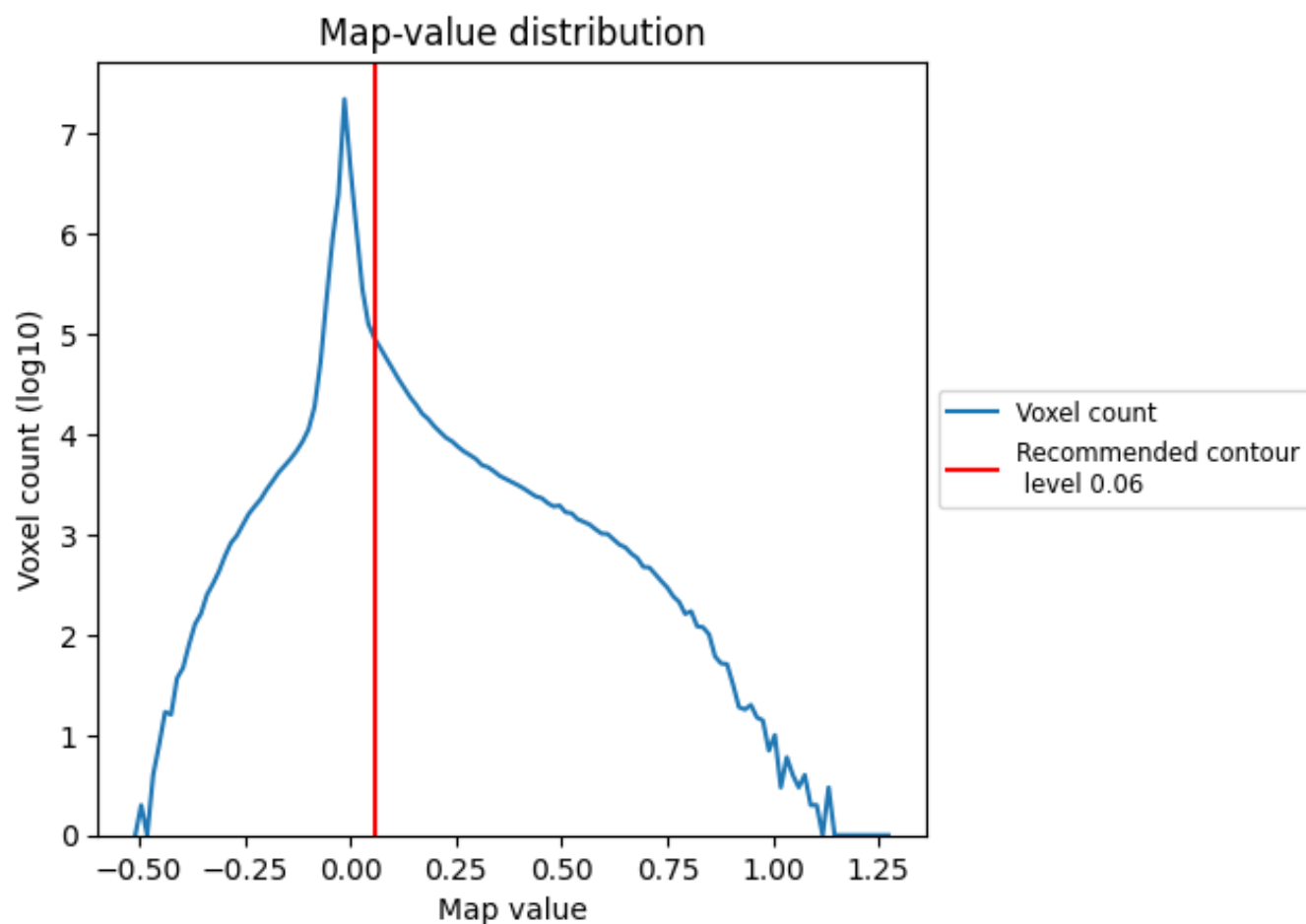
6.6 Mask visualisation

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

7 Map analysis [i](#)

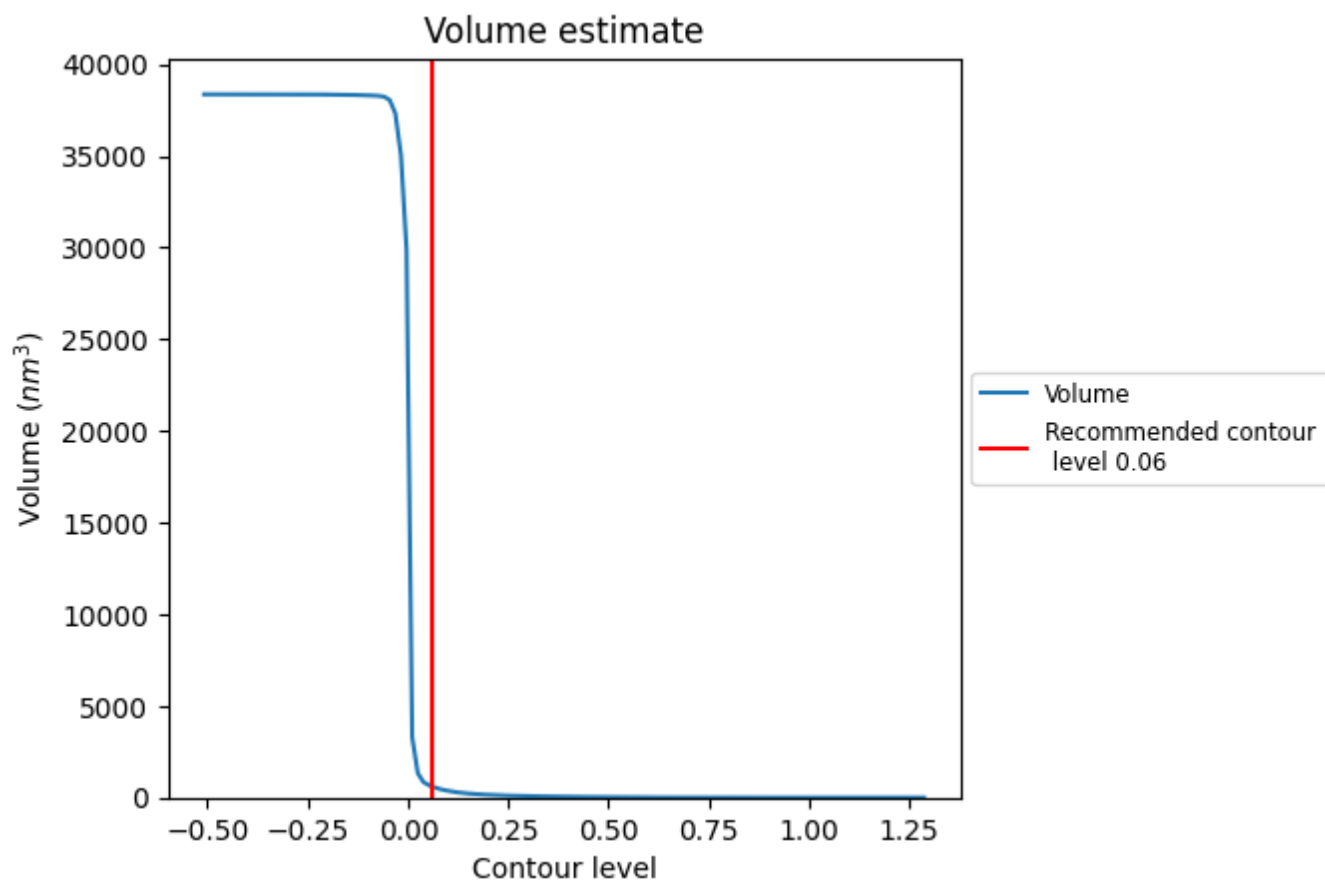
This section contains the results of statistical analysis of the map.

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.

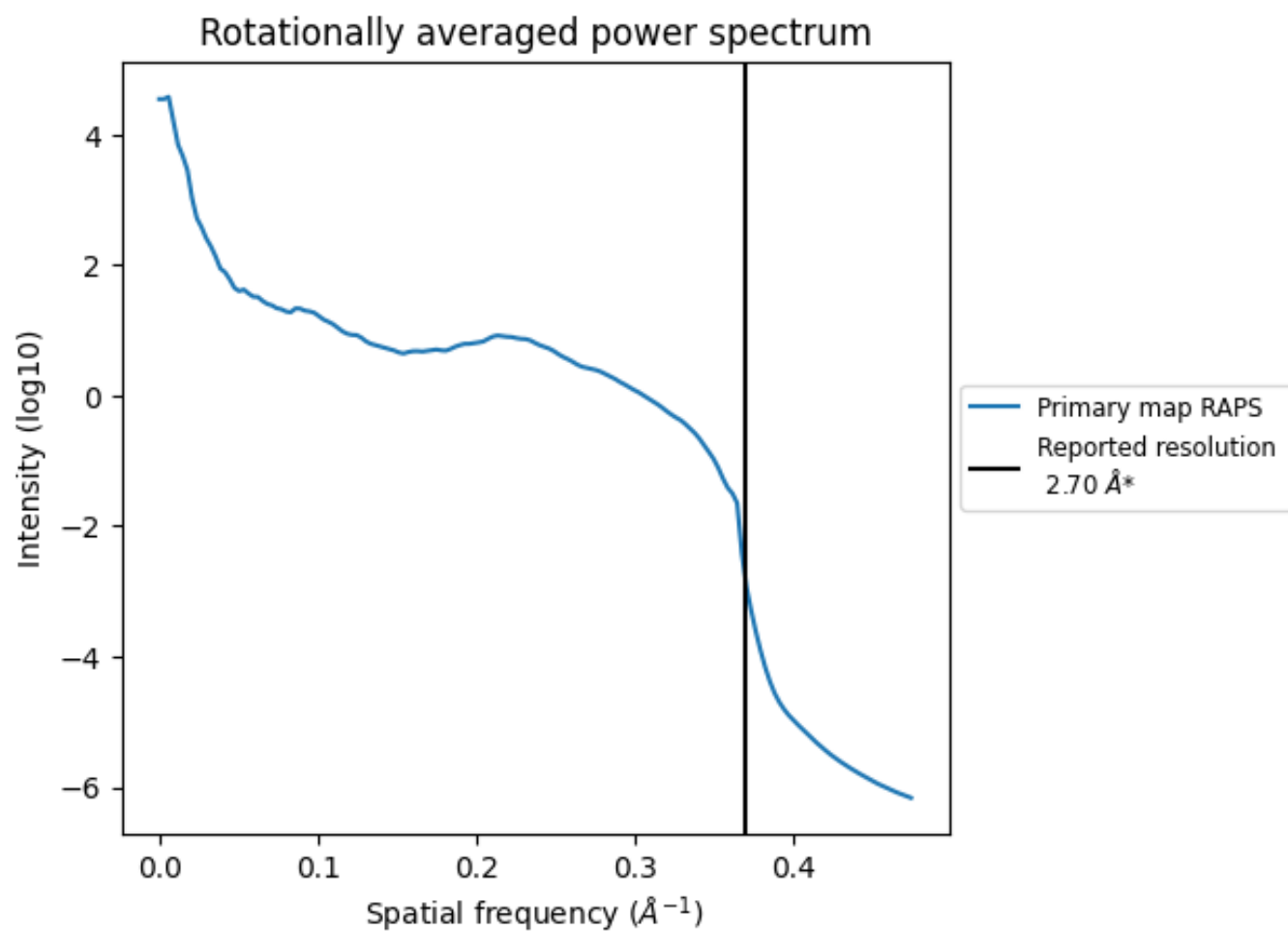
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 609 nm^3 ; this corresponds to an approximate mass of 550 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 0.370 Å⁻¹

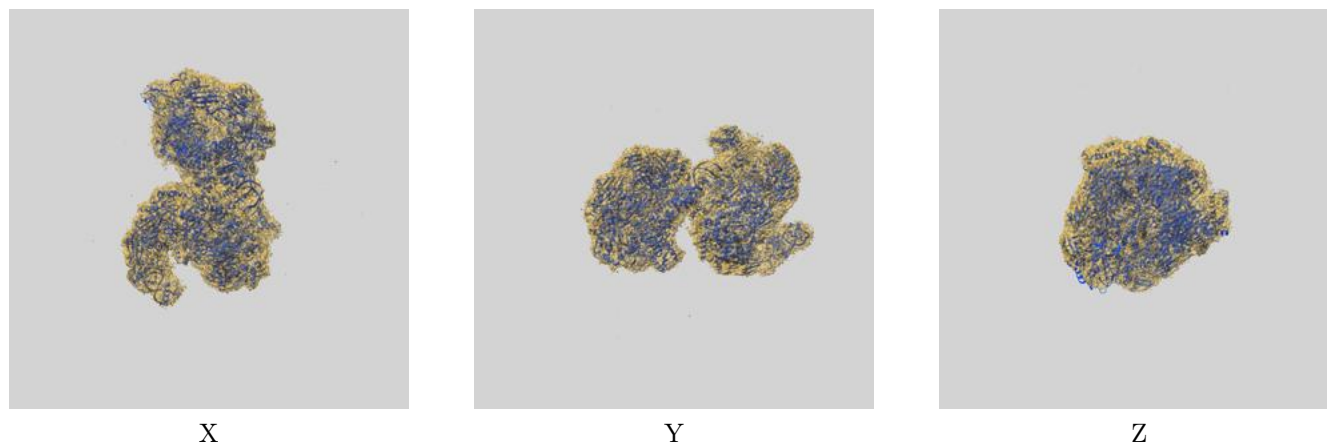
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

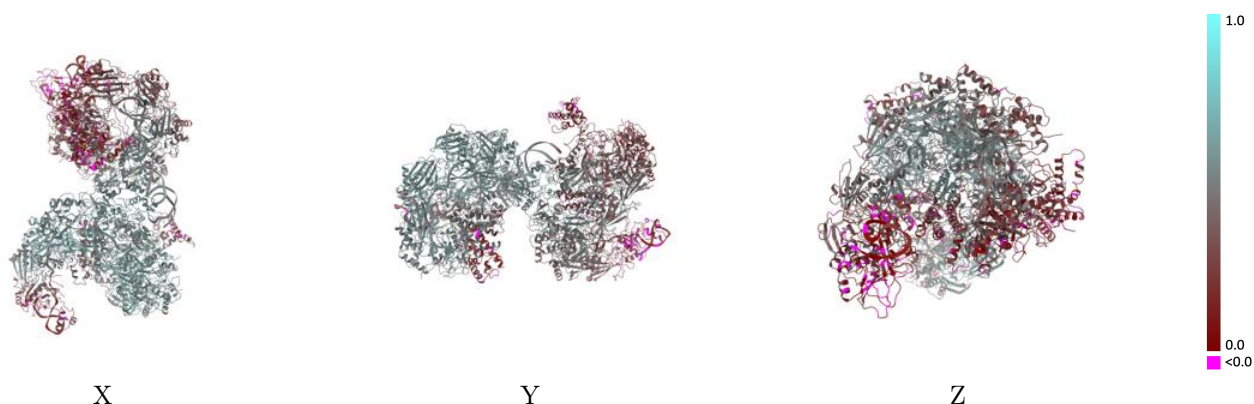
This section contains information regarding the fit between EMDB map EMD-25788 and PDB model 7TAW. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



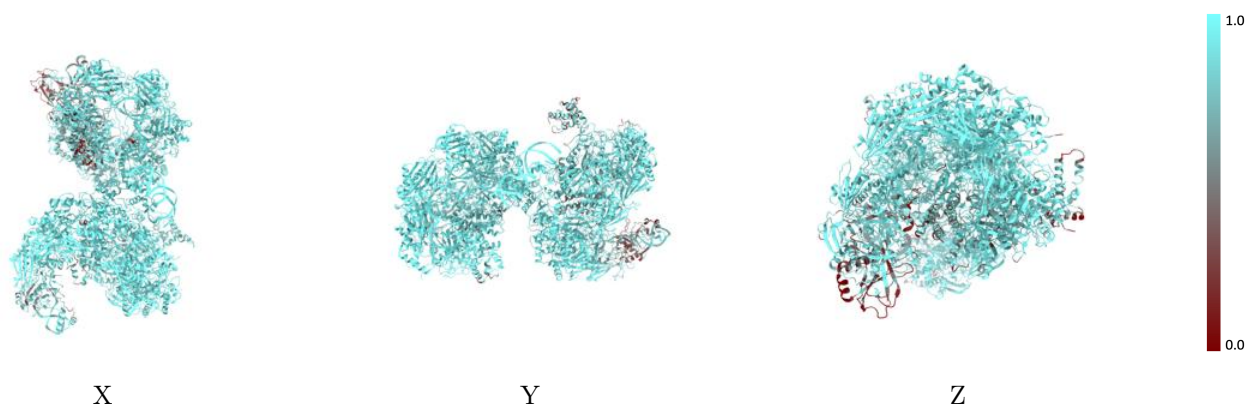
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



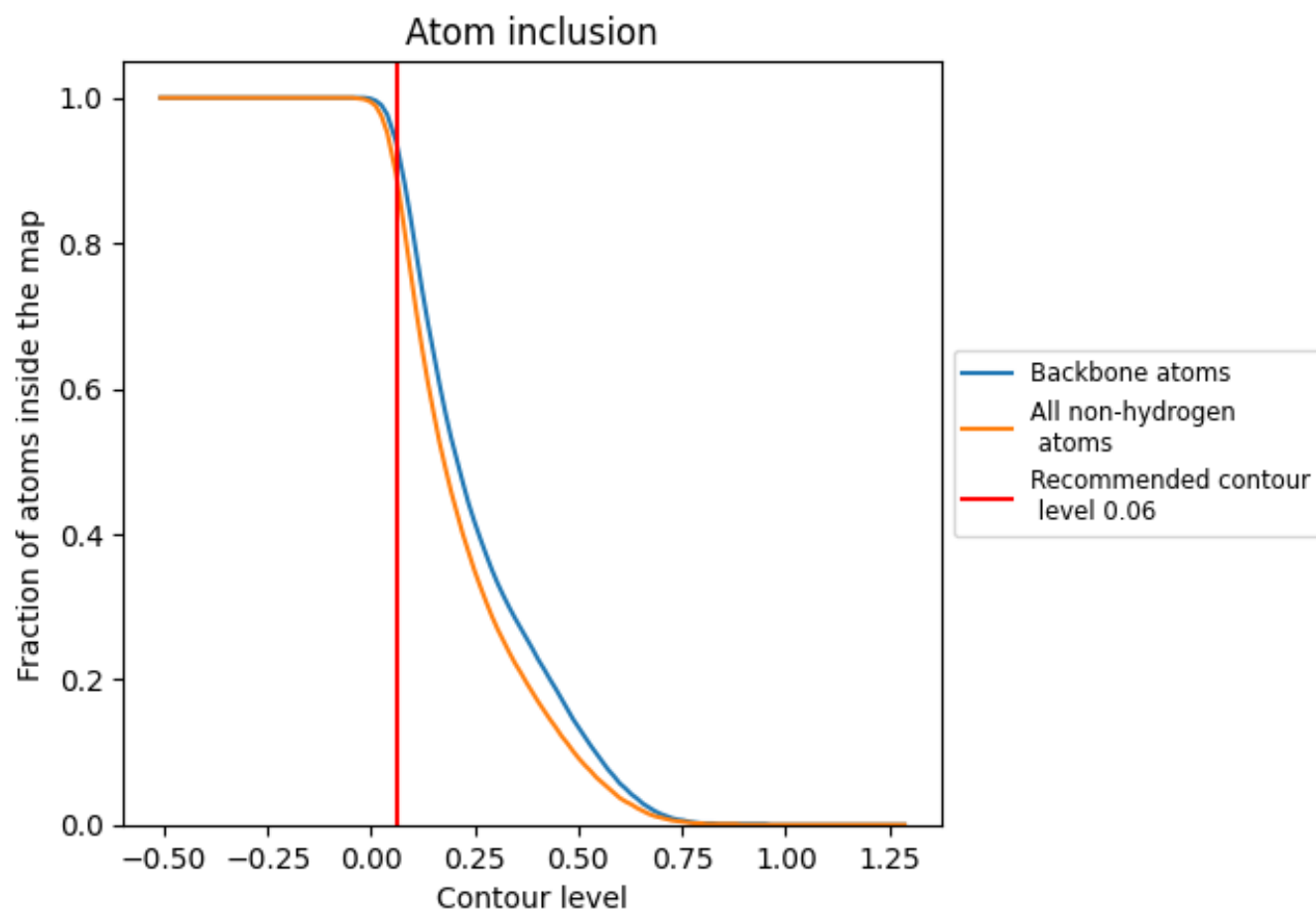
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

9.4 Atom inclusion ⓘ



At the recommended contour level, 94% of all backbone atoms, 90% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8950	 0.4250
A	 0.8930	 0.3830
B	 0.9600	 0.5150
C	 0.7560	 0.2330
D	 0.9390	 0.4910
E	 0.9530	 0.5490
F	 0.9740	 0.5670
G	 0.9640	 0.5590
H	 0.9760	 0.5680
I	 0.9780	 0.5480
J	 0.9730	 0.5710
K	 0.9620	 0.5400
M	 0.9430	 0.4330
X	 0.9920	 0.4840
Y	 0.9970	 0.4940
a	 0.7040	 0.2440
b	 0.7980	 0.2520
c	 0.4470	 0.0910
d	 0.8200	 0.2720
e	 0.8900	 0.3920
f	 0.9350	 0.4600
g	 0.9410	 0.4560
h	 0.9360	 0.4090
i	 0.8770	 0.3110
m	 0.8700	 0.3190

