



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 06:35 AM UTC

PDB ID : 7TBH / pdb_00007tbh
EMDB ID : EMD-25799
Title : cryo-EM structure of MBP-KIX-apoferritin complex with peptide 7
Authors : Zhang, K.; Horikoshi, N.; Li, S.; Powers, A.; Hameedi, M.; Pintilie, G.; Chae, H.; Khan, Y.; Suomivuori, C.; Dror, R.; Sakamoto, K.; Chiu, W.; Wakatsuki, S.
Deposited on : 2021-12-22
Resolution : 2.30 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

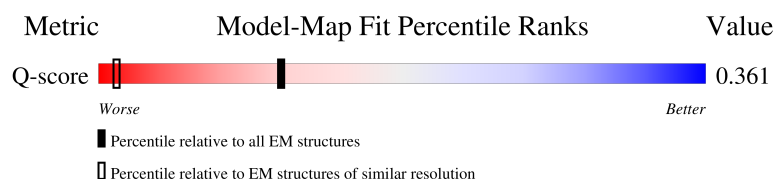
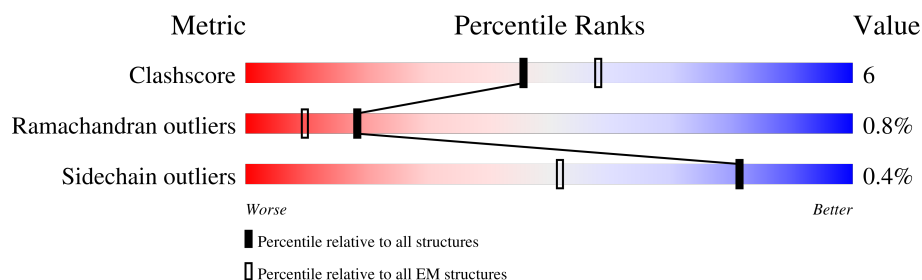
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4254 (1.80 - 2.80)

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	260	16% 80% 14% 7%
1	B	260	16% 79% 15% 7%
1	C	260	17% 78% 15% 7%
1	D	260	16% 78% 15% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	260	
1	F	260	
1	G	260	
1	H	260	
1	I	260	
1	J	260	
1	K	260	
1	L	260	
1	M	260	
1	N	260	
1	O	260	
1	P	260	
1	Q	260	
1	R	260	
1	S	260	
1	T	260	
1	U	260	
1	V	260	
1	W	260	
1	X	260	
2	a	19	
2	b	19	
2	c	19	
2	d	19	
2	e	19	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	f	19	95% 79% 21%
2	g	19	95% 79% 21%
2	h	19	95% 79% 21%
2	i	19	95% 79% 21%
2	j	19	95% 79% 21%
2	k	19	95% 79% 21%
2	l	19	95% 79% 21%
2	m	19	95% 79% 21%
2	n	19	95% 79% 21%
2	o	19	95% 79% 21%
2	p	19	95% 79% 21%
2	q	19	95% 79% 21%
2	r	19	95% 79% 21%
2	s	19	95% 79% 21%
2	t	19	95% 79% 21%
2	u	19	95% 79% 21%
2	v	19	95% 79% 21%
2	w	19	95% 79% 21%
2	x	19	95% 79% 21%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 51768 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 Isoform 2 of CREB-binding protein,Ferritin heavy chain, N-terminally processed.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	243	Total 2000	C 1257	N 352	O 378	S 13	1	0
1	B	243	Total 2000	C 1257	N 352	O 378	S 13	1	0
1	C	243	Total 2000	C 1257	N 352	O 378	S 13	1	0
1	D	243	Total 2000	C 1257	N 352	O 378	S 13	1	0
1	E	243	Total 2000	C 1257	N 352	O 378	S 13	1	0
1	F	243	Total 2000	C 1257	N 352	O 378	S 13	1	0
1	G	243	Total 2000	C 1257	N 352	O 378	S 13	1	0
1	H	243	Total 2000	C 1257	N 352	O 378	S 13	1	0
1	I	243	Total 2000	C 1257	N 352	O 378	S 13	1	0
1	J	243	Total 2000	C 1257	N 352	O 378	S 13	1	0
1	K	243	Total 2000	C 1257	N 352	O 378	S 13	1	0
1	L	243	Total 2000	C 1257	N 352	O 378	S 13	1	0
1	M	243	Total 2000	C 1257	N 352	O 378	S 13	1	0
1	N	243	Total 2000	C 1257	N 352	O 378	S 13	1	0
1	O	243	Total 2000	C 1257	N 352	O 378	S 13	1	0
1	P	243	Total 2000	C 1257	N 352	O 378	S 13	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Q	243	Total 2000	C 1257	N 352	O 378	S 13	1	0
1	R	243	Total 2000	C 1257	N 352	O 378	S 13	1	0
1	S	243	Total 2000	C 1257	N 352	O 378	S 13	1	0
1	T	243	Total 2000	C 1257	N 352	O 378	S 13	1	0
1	U	243	Total 2000	C 1257	N 352	O 378	S 13	1	0
1	V	243	Total 2000	C 1257	N 352	O 378	S 13	1	0
1	W	243	Total 2000	C 1257	N 352	O 378	S 13	1	0
1	X	243	Total 2000	C 1257	N 352	O 378	S 13	1	0

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	HIS	-	expression tag	UNP Q92793
A	-2	MET	-	expression tag	UNP Q92793
A	27	CYS	THR	conflict	UNP Q92793
A	31	CYS	ALA	conflict	UNP Q92793
A	169	CYS	GLU	conflict	UNP P09528
A	177	SER	CYS	conflict	UNP P09528
A	237	CYS	GLU	conflict	UNP P09528
B	-3	HIS	-	expression tag	UNP Q92793
B	-2	MET	-	expression tag	UNP Q92793
B	27	CYS	THR	conflict	UNP Q92793
B	31	CYS	ALA	conflict	UNP Q92793
B	169	CYS	GLU	conflict	UNP P09528
B	177	SER	CYS	conflict	UNP P09528
B	237	CYS	GLU	conflict	UNP P09528
C	-3	HIS	-	expression tag	UNP Q92793
C	-2	MET	-	expression tag	UNP Q92793
C	27	CYS	THR	conflict	UNP Q92793
C	31	CYS	ALA	conflict	UNP Q92793
C	169	CYS	GLU	conflict	UNP P09528
C	177	SER	CYS	conflict	UNP P09528
C	237	CYS	GLU	conflict	UNP P09528
D	-3	HIS	-	expression tag	UNP Q92793
D	-2	MET	-	expression tag	UNP Q92793

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	27	CYS	THR	conflict	UNP Q92793
D	31	CYS	ALA	conflict	UNP Q92793
D	169	CYS	GLU	conflict	UNP P09528
D	177	SER	CYS	conflict	UNP P09528
D	237	CYS	GLU	conflict	UNP P09528
E	-3	HIS	-	expression tag	UNP Q92793
E	-2	MET	-	expression tag	UNP Q92793
E	27	CYS	THR	conflict	UNP Q92793
E	31	CYS	ALA	conflict	UNP Q92793
E	169	CYS	GLU	conflict	UNP P09528
E	177	SER	CYS	conflict	UNP P09528
E	237	CYS	GLU	conflict	UNP P09528
F	-3	HIS	-	expression tag	UNP Q92793
F	-2	MET	-	expression tag	UNP Q92793
F	27	CYS	THR	conflict	UNP Q92793
F	31	CYS	ALA	conflict	UNP Q92793
F	169	CYS	GLU	conflict	UNP P09528
F	177	SER	CYS	conflict	UNP P09528
F	237	CYS	GLU	conflict	UNP P09528
G	-3	HIS	-	expression tag	UNP Q92793
G	-2	MET	-	expression tag	UNP Q92793
G	27	CYS	THR	conflict	UNP Q92793
G	31	CYS	ALA	conflict	UNP Q92793
G	169	CYS	GLU	conflict	UNP P09528
G	177	SER	CYS	conflict	UNP P09528
G	237	CYS	GLU	conflict	UNP P09528
H	-3	HIS	-	expression tag	UNP Q92793
H	-2	MET	-	expression tag	UNP Q92793
H	27	CYS	THR	conflict	UNP Q92793
H	31	CYS	ALA	conflict	UNP Q92793
H	169	CYS	GLU	conflict	UNP P09528
H	177	SER	CYS	conflict	UNP P09528
H	237	CYS	GLU	conflict	UNP P09528
I	-3	HIS	-	expression tag	UNP Q92793
I	-2	MET	-	expression tag	UNP Q92793
I	27	CYS	THR	conflict	UNP Q92793
I	31	CYS	ALA	conflict	UNP Q92793
I	169	CYS	GLU	conflict	UNP P09528
I	177	SER	CYS	conflict	UNP P09528
I	237	CYS	GLU	conflict	UNP P09528
J	-3	HIS	-	expression tag	UNP Q92793
J	-2	MET	-	expression tag	UNP Q92793

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	27	CYS	THR	conflict	UNP Q92793
J	31	CYS	ALA	conflict	UNP Q92793
J	169	CYS	GLU	conflict	UNP P09528
J	177	SER	CYS	conflict	UNP P09528
J	237	CYS	GLU	conflict	UNP P09528
K	-3	HIS	-	expression tag	UNP Q92793
K	-2	MET	-	expression tag	UNP Q92793
K	27	CYS	THR	conflict	UNP Q92793
K	31	CYS	ALA	conflict	UNP Q92793
K	169	CYS	GLU	conflict	UNP P09528
K	177	SER	CYS	conflict	UNP P09528
K	237	CYS	GLU	conflict	UNP P09528
L	-3	HIS	-	expression tag	UNP Q92793
L	-2	MET	-	expression tag	UNP Q92793
L	27	CYS	THR	conflict	UNP Q92793
L	31	CYS	ALA	conflict	UNP Q92793
L	169	CYS	GLU	conflict	UNP P09528
L	177	SER	CYS	conflict	UNP P09528
L	237	CYS	GLU	conflict	UNP P09528
M	-3	HIS	-	expression tag	UNP Q92793
M	-2	MET	-	expression tag	UNP Q92793
M	27	CYS	THR	conflict	UNP Q92793
M	31	CYS	ALA	conflict	UNP Q92793
M	169	CYS	GLU	conflict	UNP P09528
M	177	SER	CYS	conflict	UNP P09528
M	237	CYS	GLU	conflict	UNP P09528
N	-3	HIS	-	expression tag	UNP Q92793
N	-2	MET	-	expression tag	UNP Q92793
N	27	CYS	THR	conflict	UNP Q92793
N	31	CYS	ALA	conflict	UNP Q92793
N	169	CYS	GLU	conflict	UNP P09528
N	177	SER	CYS	conflict	UNP P09528
N	237	CYS	GLU	conflict	UNP P09528
O	-3	HIS	-	expression tag	UNP Q92793
O	-2	MET	-	expression tag	UNP Q92793
O	27	CYS	THR	conflict	UNP Q92793
O	31	CYS	ALA	conflict	UNP Q92793
O	169	CYS	GLU	conflict	UNP P09528
O	177	SER	CYS	conflict	UNP P09528
O	237	CYS	GLU	conflict	UNP P09528
P	-3	HIS	-	expression tag	UNP Q92793
P	-2	MET	-	expression tag	UNP Q92793

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
P	27	CYS	THR	conflict	UNP Q92793
P	31	CYS	ALA	conflict	UNP Q92793
P	169	CYS	GLU	conflict	UNP P09528
P	177	SER	CYS	conflict	UNP P09528
P	237	CYS	GLU	conflict	UNP P09528
Q	-3	HIS	-	expression tag	UNP Q92793
Q	-2	MET	-	expression tag	UNP Q92793
Q	27	CYS	THR	conflict	UNP Q92793
Q	31	CYS	ALA	conflict	UNP Q92793
Q	169	CYS	GLU	conflict	UNP P09528
Q	177	SER	CYS	conflict	UNP P09528
Q	237	CYS	GLU	conflict	UNP P09528
R	-3	HIS	-	expression tag	UNP Q92793
R	-2	MET	-	expression tag	UNP Q92793
R	27	CYS	THR	conflict	UNP Q92793
R	31	CYS	ALA	conflict	UNP Q92793
R	169	CYS	GLU	conflict	UNP P09528
R	177	SER	CYS	conflict	UNP P09528
R	237	CYS	GLU	conflict	UNP P09528
S	-3	HIS	-	expression tag	UNP Q92793
S	-2	MET	-	expression tag	UNP Q92793
S	27	CYS	THR	conflict	UNP Q92793
S	31	CYS	ALA	conflict	UNP Q92793
S	169	CYS	GLU	conflict	UNP P09528
S	177	SER	CYS	conflict	UNP P09528
S	237	CYS	GLU	conflict	UNP P09528
T	-3	HIS	-	expression tag	UNP Q92793
T	-2	MET	-	expression tag	UNP Q92793
T	27	CYS	THR	conflict	UNP Q92793
T	31	CYS	ALA	conflict	UNP Q92793
T	169	CYS	GLU	conflict	UNP P09528
T	177	SER	CYS	conflict	UNP P09528
T	237	CYS	GLU	conflict	UNP P09528
U	-3	HIS	-	expression tag	UNP Q92793
U	-2	MET	-	expression tag	UNP Q92793
U	27	CYS	THR	conflict	UNP Q92793
U	31	CYS	ALA	conflict	UNP Q92793
U	169	CYS	GLU	conflict	UNP P09528
U	177	SER	CYS	conflict	UNP P09528
U	237	CYS	GLU	conflict	UNP P09528
V	-3	HIS	-	expression tag	UNP Q92793
V	-2	MET	-	expression tag	UNP Q92793

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
V	27	CYS	THR	conflict	UNP Q92793
V	31	CYS	ALA	conflict	UNP Q92793
V	169	CYS	GLU	conflict	UNP P09528
V	177	SER	CYS	conflict	UNP P09528
V	237	CYS	GLU	conflict	UNP P09528
W	-3	HIS	-	expression tag	UNP Q92793
W	-2	MET	-	expression tag	UNP Q92793
W	27	CYS	THR	conflict	UNP Q92793
W	31	CYS	ALA	conflict	UNP Q92793
W	169	CYS	GLU	conflict	UNP P09528
W	177	SER	CYS	conflict	UNP P09528
W	237	CYS	GLU	conflict	UNP P09528
X	-3	HIS	-	expression tag	UNP Q92793
X	-2	MET	-	expression tag	UNP Q92793
X	27	CYS	THR	conflict	UNP Q92793
X	31	CYS	ALA	conflict	UNP Q92793
X	169	CYS	GLU	conflict	UNP P09528
X	177	SER	CYS	conflict	UNP P09528
X	237	CYS	GLU	conflict	UNP P09528

- Molecule 2 is a protein called LEU-SER-ARG-ARG-PRO-SEP-TYR-ARG-LYS-ILE-LEU-ASN-ASP-LEU-SER-SER-ASP-ALA-PRO.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	19	Total	C	N	O	P	0	0
			157	94	30	32	1		
2	b	19	Total	C	N	O	P	0	0
			157	94	30	32	1		
2	c	19	Total	C	N	O	P	0	0
			157	94	30	32	1		
2	d	19	Total	C	N	O	P	0	0
			157	94	30	32	1		
2	e	19	Total	C	N	O	P	0	0
			157	94	30	32	1		
2	f	19	Total	C	N	O	P	0	0
			157	94	30	32	1		
2	g	19	Total	C	N	O	P	0	0
			157	94	30	32	1		
2	h	19	Total	C	N	O	P	0	0
			157	94	30	32	1		
2	i	19	Total	C	N	O	P	0	0
			157	94	30	32	1		

Continued on next page...

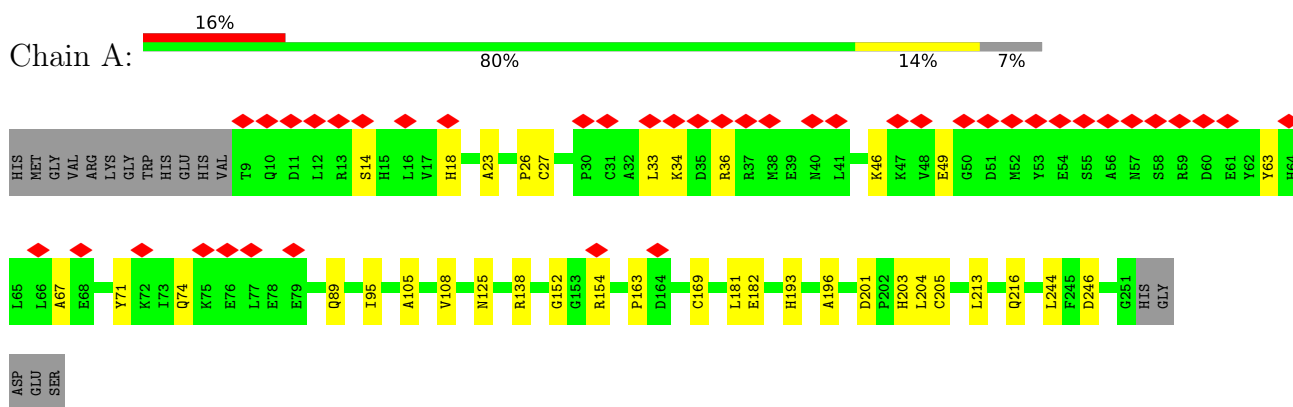
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	j	19	Total 157	C 94	N 30	O 32	P 1	0	0
2	k	19	Total 157	C 94	N 30	O 32	P 1	0	0
2	l	19	Total 157	C 94	N 30	O 32	P 1	0	0
2	m	19	Total 157	C 94	N 30	O 32	P 1	0	0
2	n	19	Total 157	C 94	N 30	O 32	P 1	0	0
2	o	19	Total 157	C 94	N 30	O 32	P 1	0	0
2	p	19	Total 157	C 94	N 30	O 32	P 1	0	0
2	q	19	Total 157	C 94	N 30	O 32	P 1	0	0
2	r	19	Total 157	C 94	N 30	O 32	P 1	0	0
2	s	19	Total 157	C 94	N 30	O 32	P 1	0	0
2	t	19	Total 157	C 94	N 30	O 32	P 1	0	0
2	u	19	Total 157	C 94	N 30	O 32	P 1	0	0
2	v	19	Total 157	C 94	N 30	O 32	P 1	0	0
2	w	19	Total 157	C 94	N 30	O 32	P 1	0	0
2	x	19	Total 157	C 94	N 30	O 32	P 1	0	0

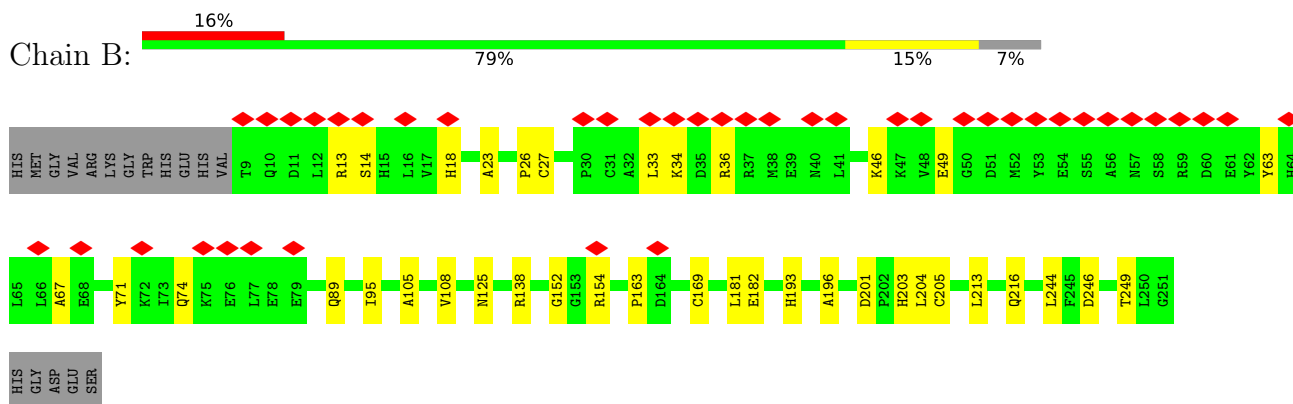
3 Residue-property plots

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

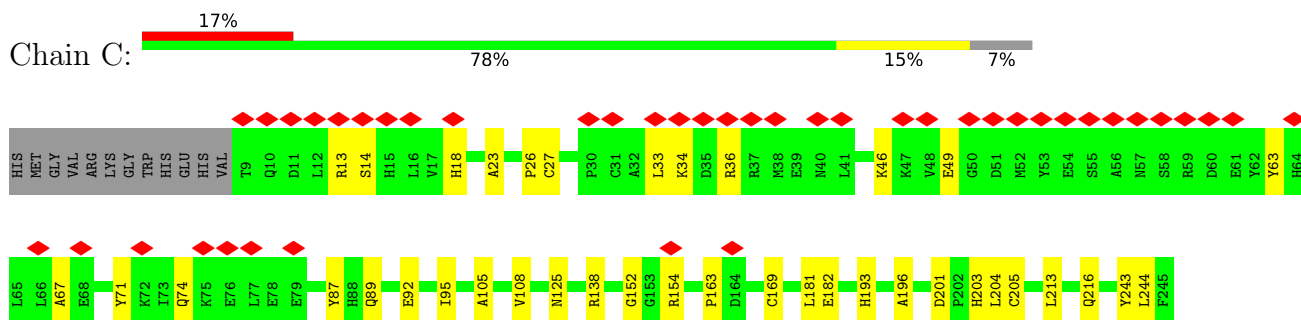
- Molecule 1: Isoform 2 of CREB-binding protein,Ferritin heavy chain, N-terminally processed



- Molecule 1: Isoform 2 of CREB-binding protein,Ferritin heavy chain, N-terminally processed

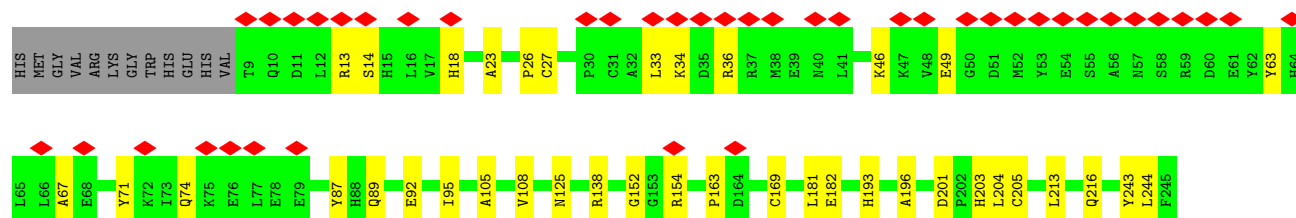
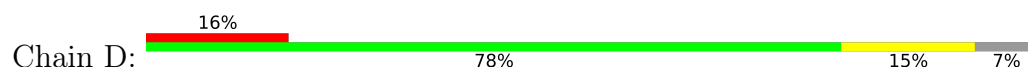


- Molecule 1: Isoform 2 of CREB-binding protein,Ferritin heavy chain, N-terminally processed

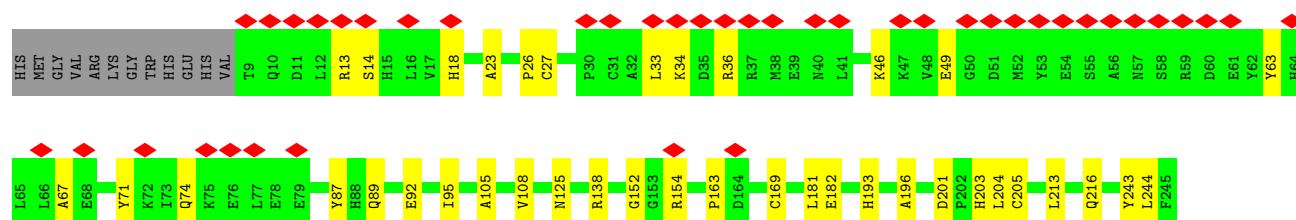
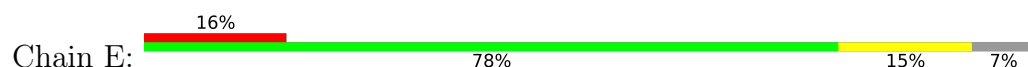




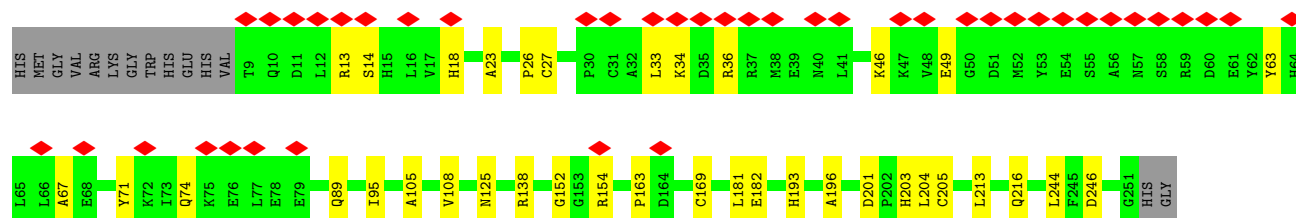
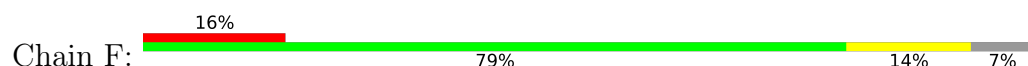
- Molecule 1: Isoform 2 of CREB-binding protein, Ferritin heavy chain, N-terminally processed



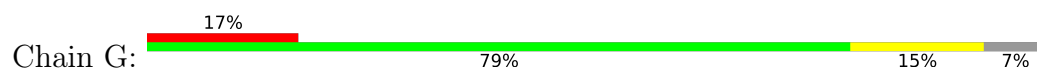
- Molecule 1: Isoform 2 of CREB-binding protein, Ferritin heavy chain, N-terminally processed

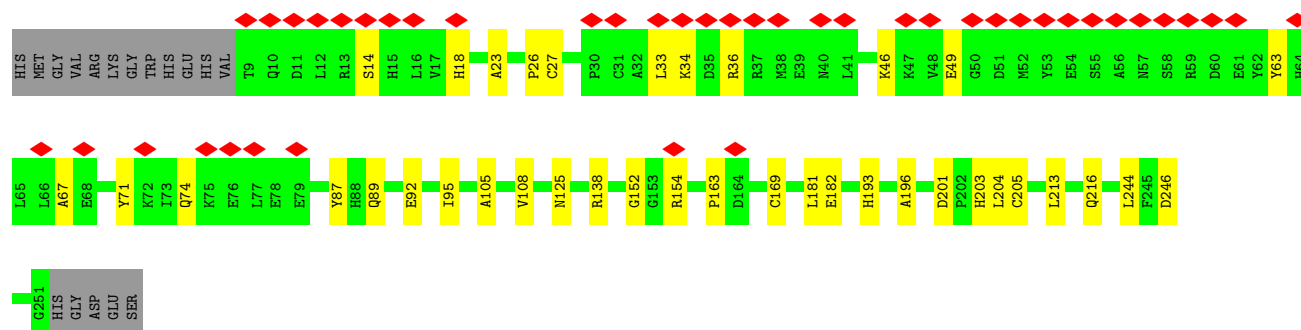


- Molecule 1: Isoform 2 of CREB-binding protein, Ferritin heavy chain, N-terminally processed



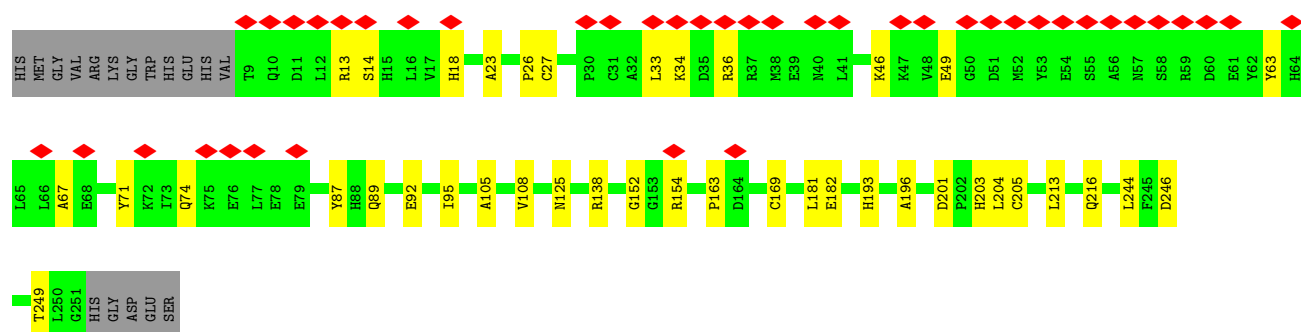
- Molecule 1: Isoform 2 of CREB-binding protein, Ferritin heavy chain, N-terminally processed





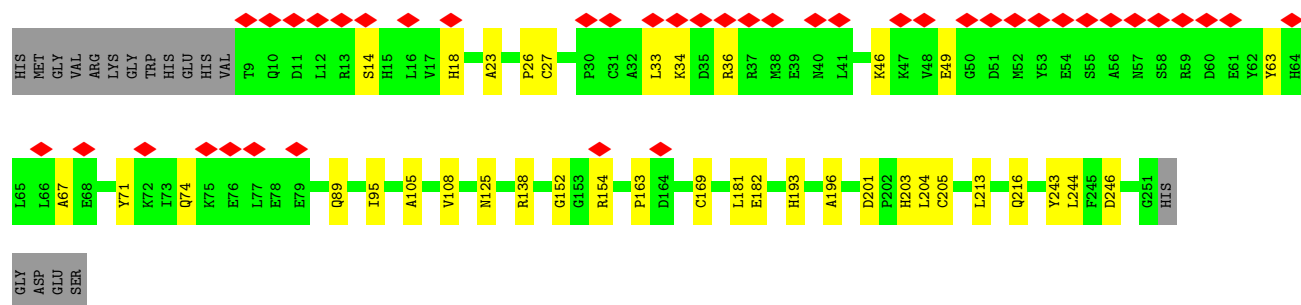
- Molecule 1: Isoform 2 of CREB-binding protein, Ferritin heavy chain, N-terminally processed

Chain H: 16% 78% 15% 7%



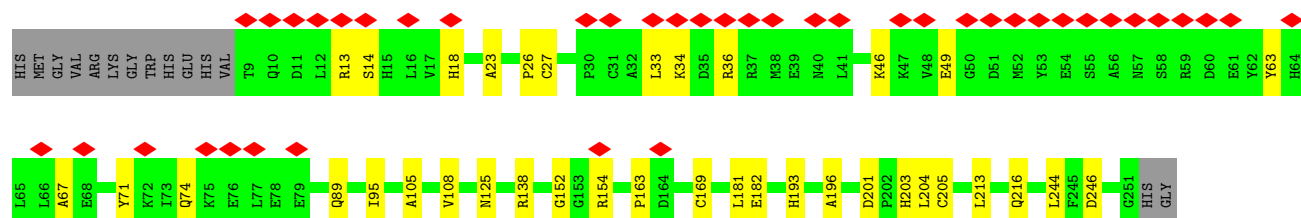
- Molecule 1: Isoform 2 of CREB-binding protein, Ferritin heavy chain, N-terminally processed

Chain I: 16% 79% 14% 7%



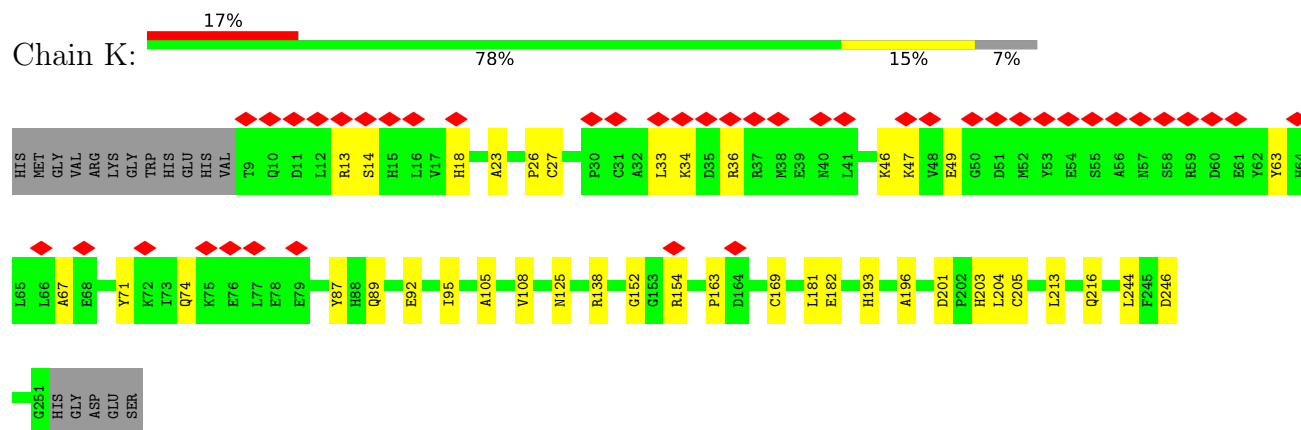
- Molecule 1: Isoform 2 of CREB-binding protein, Ferritin heavy chain, N-terminally processed

Chain J: 16% 79% 14% 7%

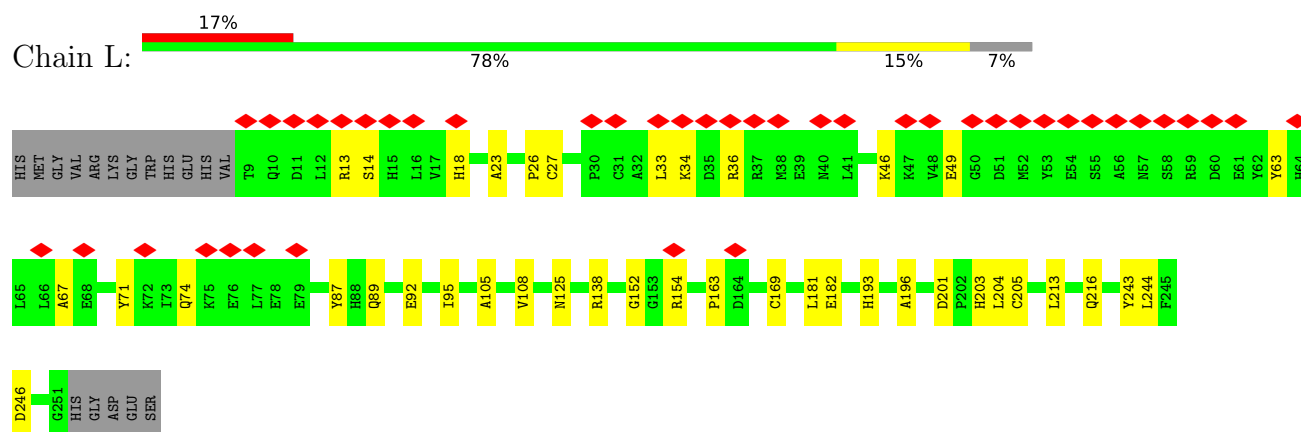


ASP
GLU
SER

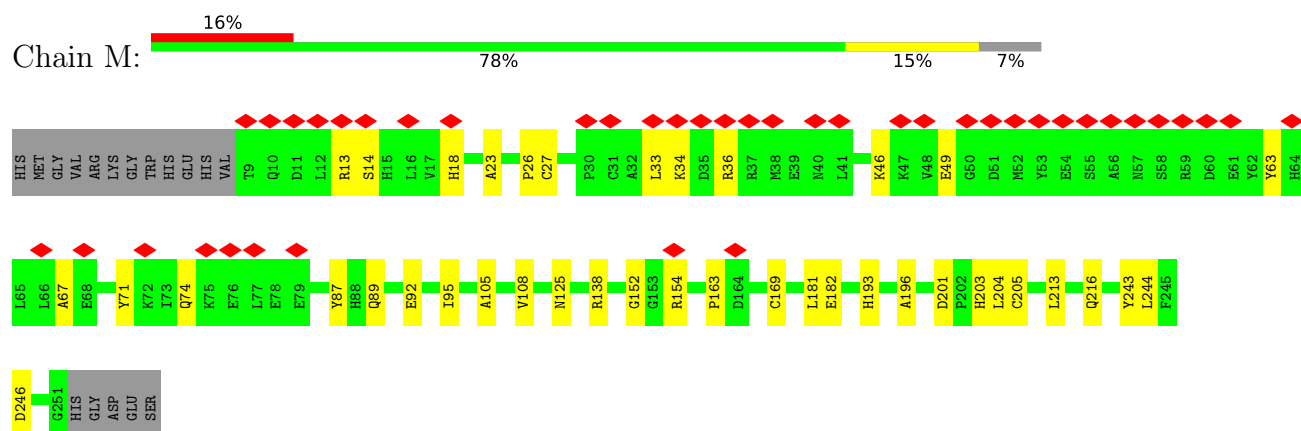
- Molecule 1: Isoform 2 of CREB-binding protein, Ferritin heavy chain, N-terminally processed



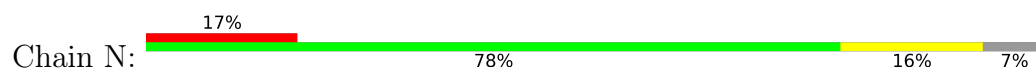
- Molecule 1: Isoform 2 of CREB-binding protein, Ferritin heavy chain, N-terminally processed

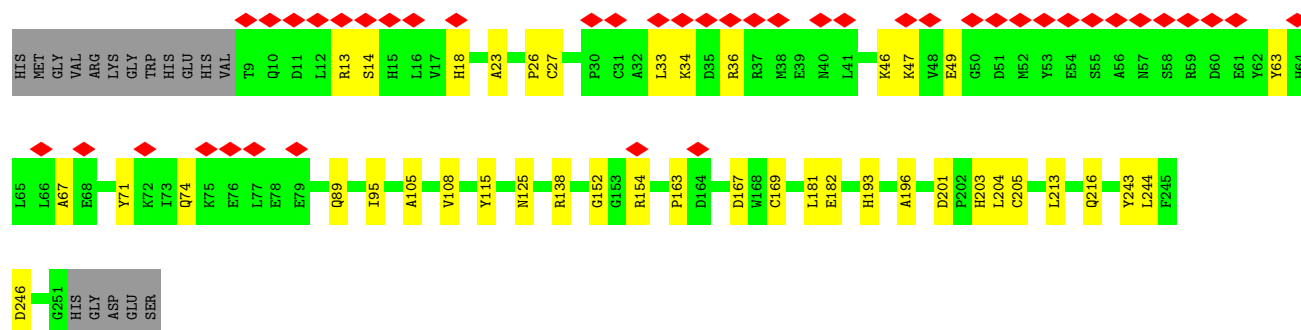


- Molecule 1: Isoform 2 of CREB-binding protein, Ferritin heavy chain, N-terminally processed



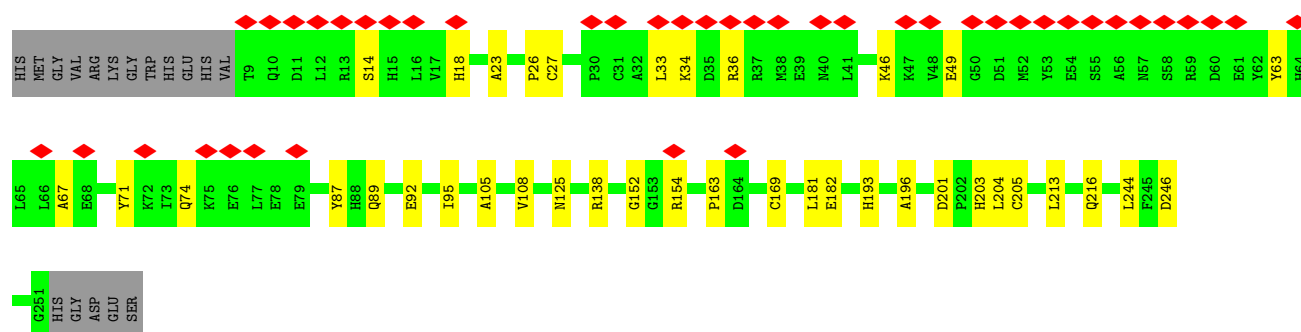
- Molecule 1: Isoform 2 of CREB-binding protein, Ferritin heavy chain, N-terminally processed





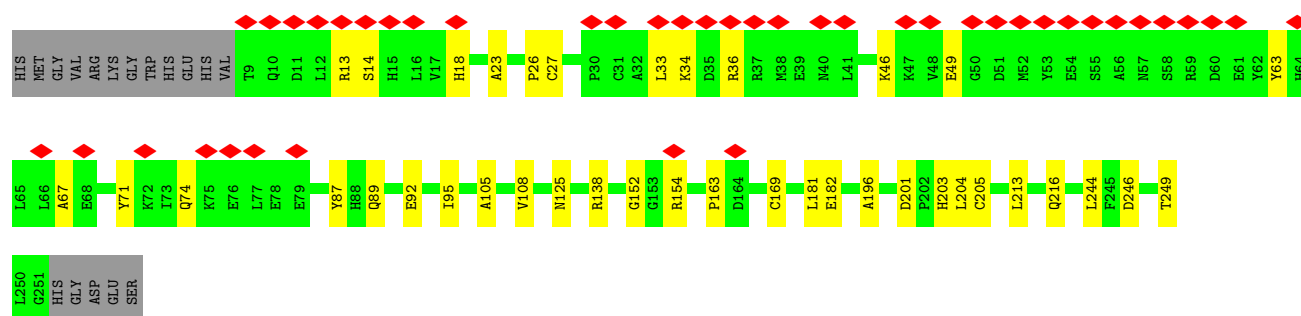
- Molecule 1: Isoform 2 of CREB-binding protein, Ferritin heavy chain, N-terminally processed

Chain O: 17% 79% 15% 7%



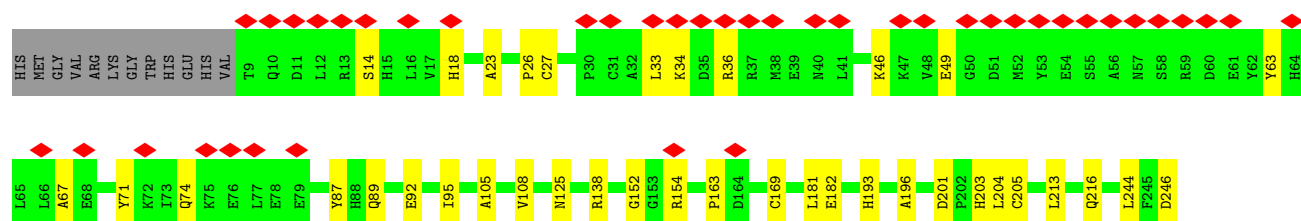
- Molecule 1: Isoform 2 of CREB-binding protein, Ferritin heavy chain, N-terminally processed

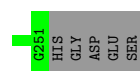
Chain P: 17% 78% 15% 7%



- Molecule 1: Isoform 2 of CREB-binding protein, Ferritin heavy chain, N-terminally processed

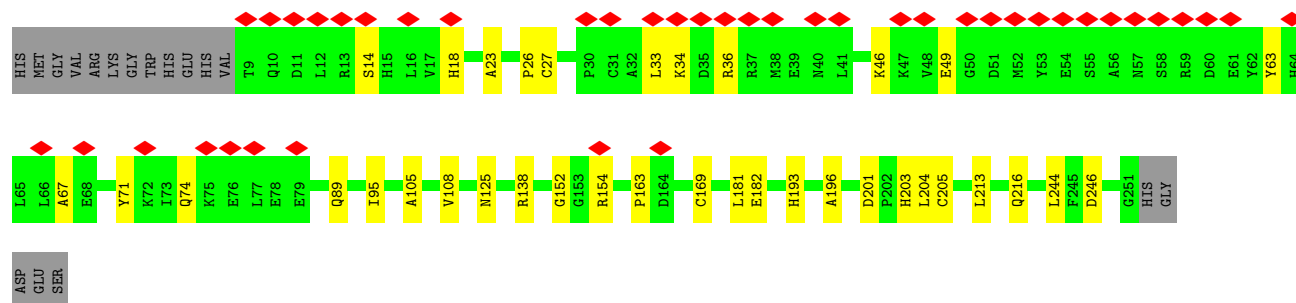
Chain Q: 16% 79% 15% 7%





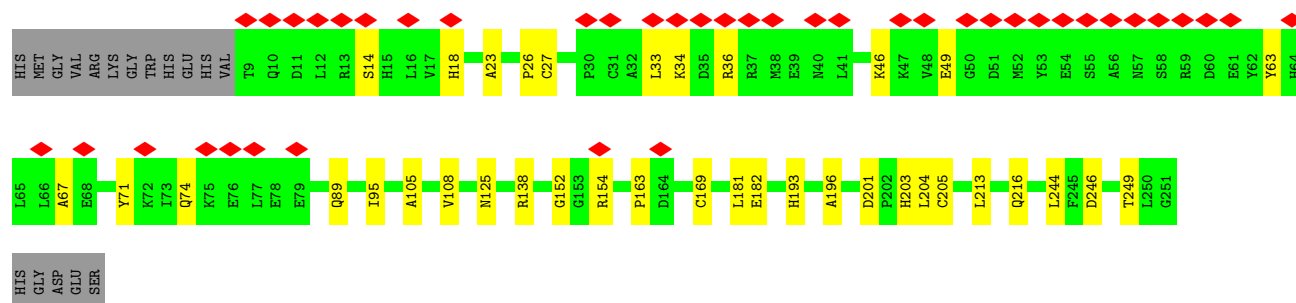
- Molecule 1: Isoform 2 of CREB-binding protein, Ferritin heavy chain, N-terminally processed

Chain R: 16% 80% 14% 7%



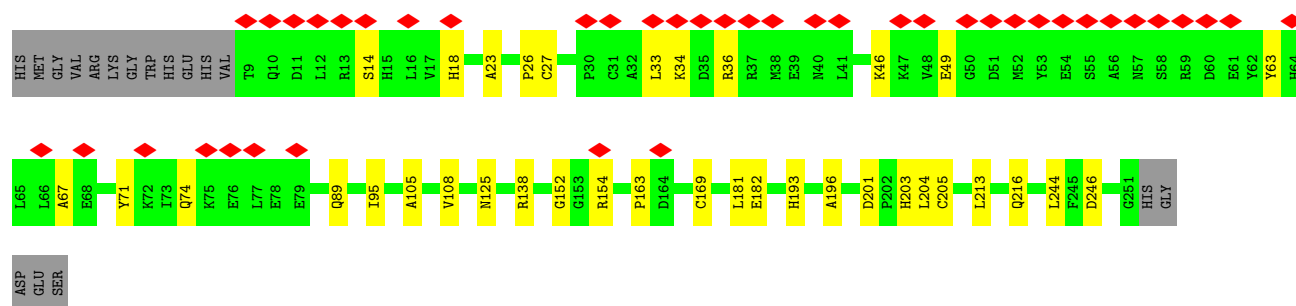
- Molecule 1: Isoform 2 of CREB-binding protein, Ferritin heavy chain, N-terminally processed

Chain S: 16% 79% 14% 7%



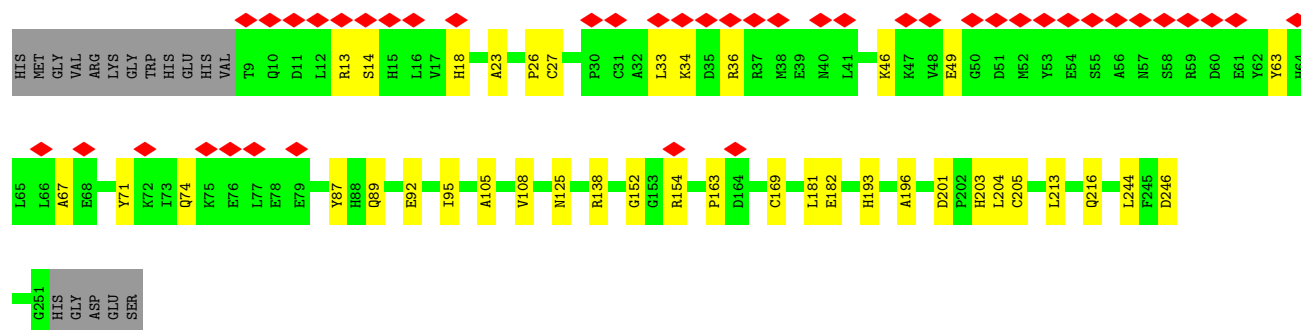
- Molecule 1: Isoform 2 of CREB-binding protein, Ferritin heavy chain, N-terminally processed

Chain T: 16% 80% 14% 7%

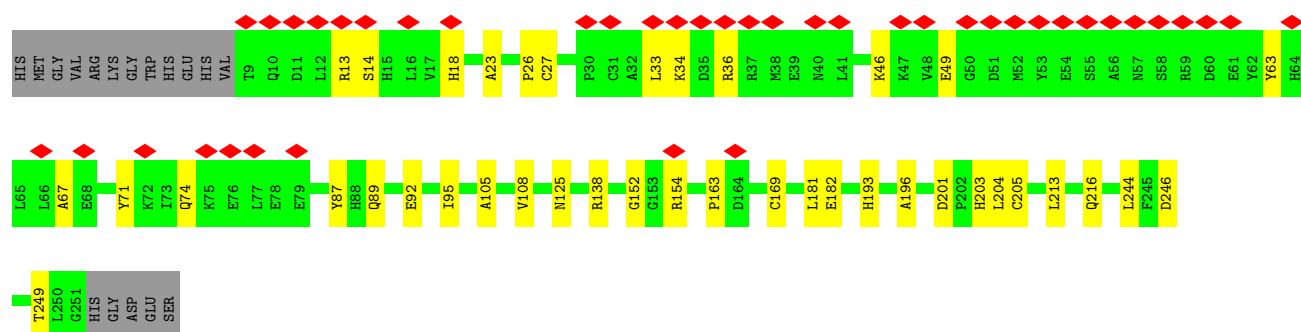
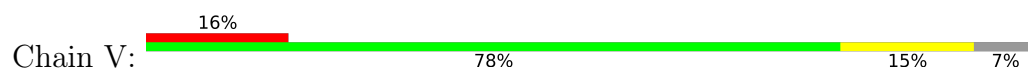


- Molecule 1: Isoform 2 of CREB-binding protein, Ferritin heavy chain, N-terminally processed

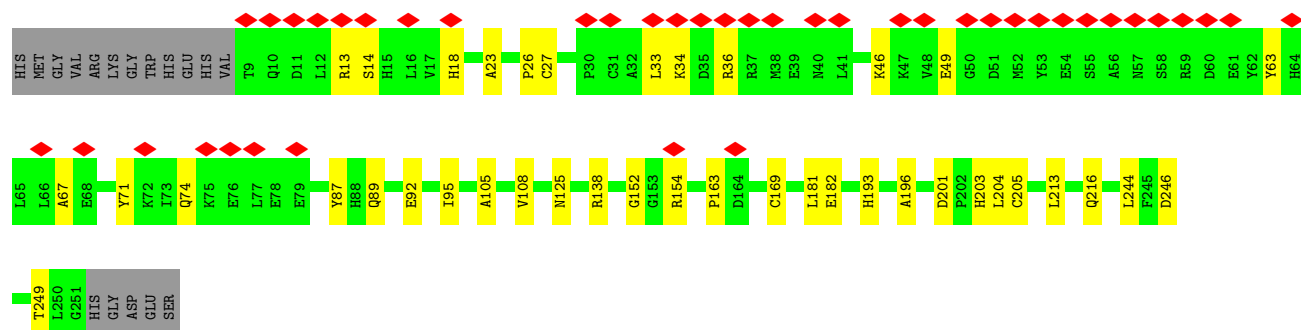
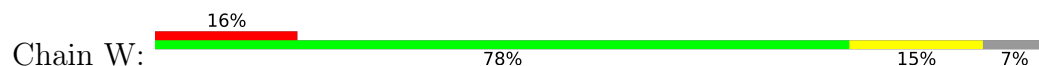
Chain U: 17% 78% 15% 7%



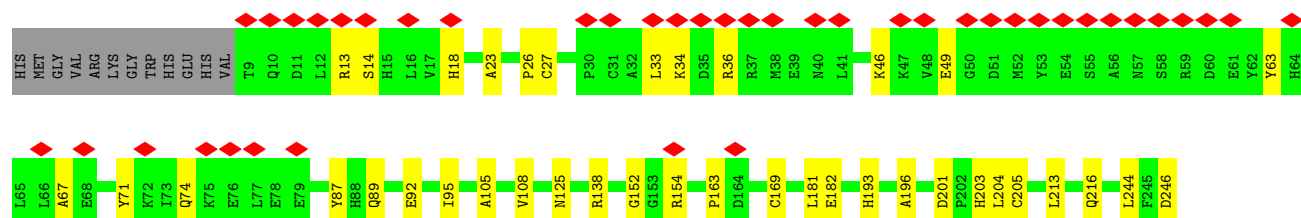
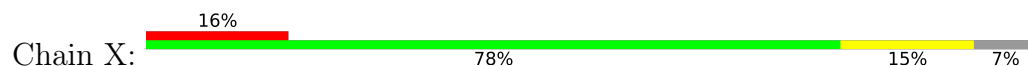
- Molecule 1: Isoform 2 of CREB-binding protein, Ferritin heavy chain, N-terminally processed

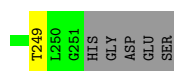


- Molecule 1: Isoform 2 of CREB-binding protein, Ferritin heavy chain, N-terminally processed

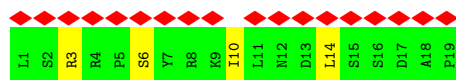
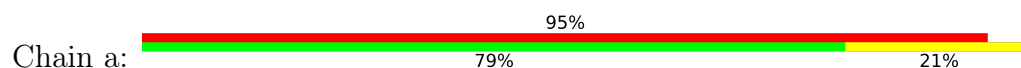


- Molecule 1: Isoform 2 of CREB-binding protein, Ferritin heavy chain, N-terminally processed

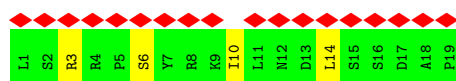
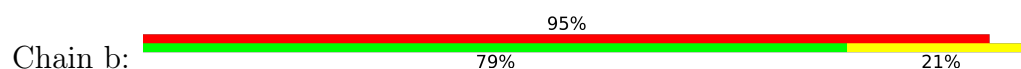




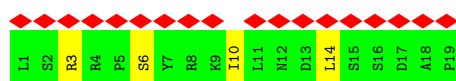
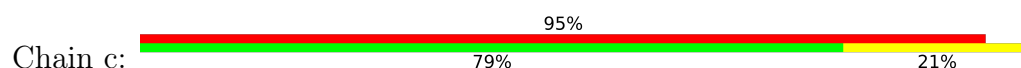
- Molecule 2: LEU-SER-ARG-ARG-PRO-SEP-TYR-ARG-LYS-ILE-LEU-ASN-ASP-LEU-SER-SER-ASP-ALA-PRO



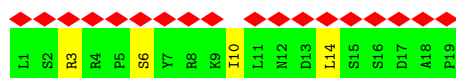
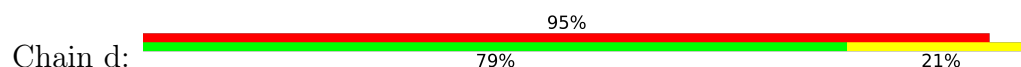
- Molecule 2: LEU-SER-ARG-ARG-PRO-SEP-TYR-ARG-LYS-ILE-LEU-ASN-ASP-LEU-SER-SER-ASP-ALA-PRO



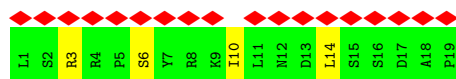
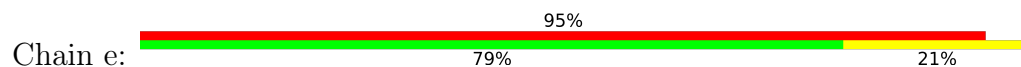
- Molecule 2: LEU-SER-ARG-ARG-PRO-SEP-TYR-ARG-LYS-ILE-LEU-ASN-ASP-LEU-SER-SER-ASP-ALA-PRO



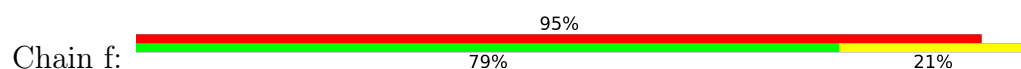
- Molecule 2: LEU-SER-ARG-ARG-PRO-SEP-TYR-ARG-LYS-ILE-LEU-ASN-ASP-LEU-SER-SER-ASP-ALA-PRO

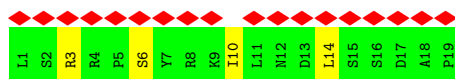


- Molecule 2: LEU-SER-ARG-ARG-PRO-SEP-TYR-ARG-LYS-ILE-LEU-ASN-ASP-LEU-SER-SER-ASP-ALA-PRO

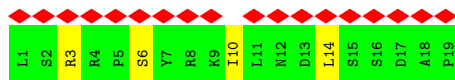
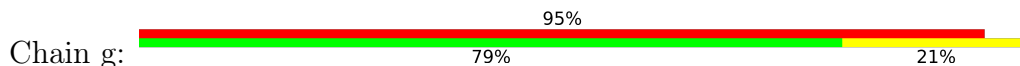


- Molecule 2: LEU-SER-ARG-ARG-PRO-SEP-TYR-ARG-LYS-ILE-LEU-ASN-ASP-LEU-SER-SER-ASP-ALA-PRO

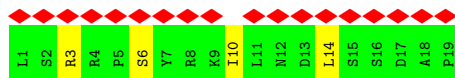




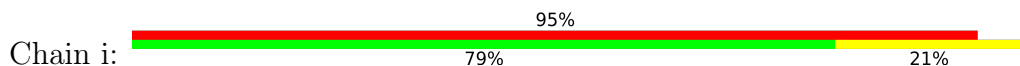
• Molecule 2: LEU-SER-ARG-ARG-PRO-SEP-TYR-ARG-LYS-ILE-LEU-ASN-ASP-LEU-SER-SER-ASP-ALA-PRO



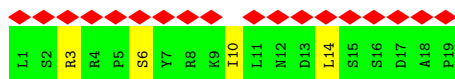
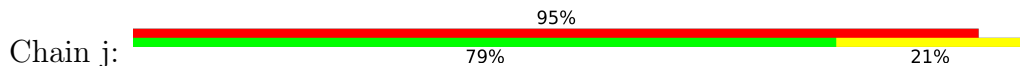
• Molecule 2: LEU-SER-ARG-ARG-PRO-SEP-TYR-ARG-LYS-ILE-LEU-ASN-ASP-LEU-SER-SER-ASP-ALA-PRO



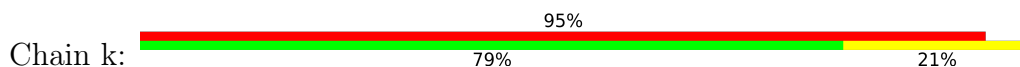
• Molecule 2: LEU-SER-ARG-ARG-PRO-SEP-TYR-ARG-LYS-ILE-LEU-ASN-ASP-LEU-SER-SER-ASP-ALA-PRO



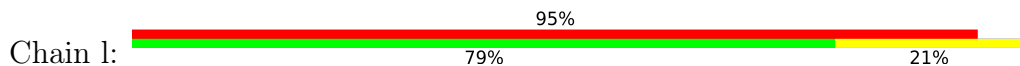
• Molecule 2: LEU-SER-ARG-ARG-PRO-SEP-TYR-ARG-LYS-ILE-LEU-ASN-ASP-LEU-SER-SER-ASP-ALA-PRO

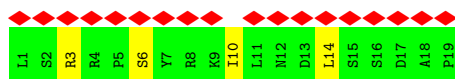


• Molecule 2: LEU-SER-ARG-ARG-PRO-SEP-TYR-ARG-LYS-ILE-LEU-ASN-ASP-LEU-SER-SER-ASP-ALA-PRO

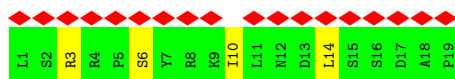
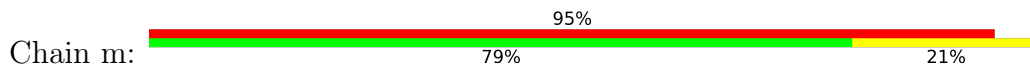


• Molecule 2: LEU-SER-ARG-ARG-PRO-SEP-TYR-ARG-LYS-ILE-LEU-ASN-ASP-LEU-SER-SER-ASP-ALA-PRO

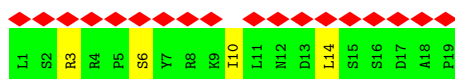
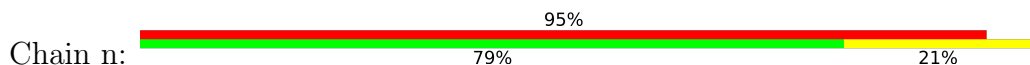




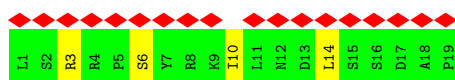
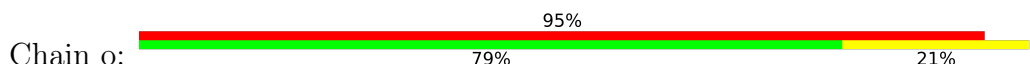
● Molecule 2: LEU-SER-ARG-ARG-PRO-SEP-TYR-ARG-LYS-ILE-LEU-ASN-ASP-LEU-SER-SER-ASP-ALA-PRO



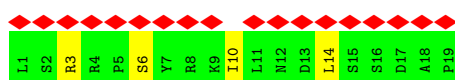
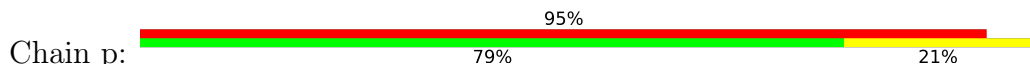
● Molecule 2: LEU-SER-ARG-ARG-PRO-SEP-TYR-ARG-LYS-ILE-LEU-ASN-ASP-LEU-SER-SER-ASP-ALA-PRO



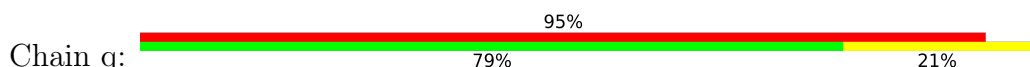
● Molecule 2: LEU-SER-ARG-ARG-PRO-SEP-TYR-ARG-LYS-ILE-LEU-ASN-ASP-LEU-SER-SER-ASP-ALA-PRO



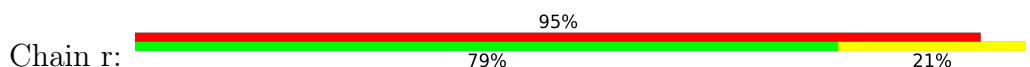
● Molecule 2: LEU-SER-ARG-ARG-PRO-SEP-TYR-ARG-LYS-ILE-LEU-ASN-ASP-LEU-SER-SER-ASP-ALA-PRO



● Molecule 2: LEU-SER-ARG-ARG-PRO-SEP-TYR-ARG-LYS-ILE-LEU-ASN-ASP-LEU-SER-SER-ASP-ALA-PRO

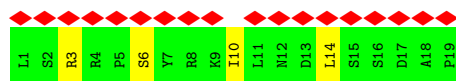
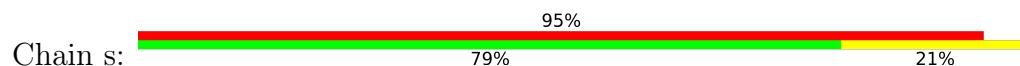


● Molecule 2: LEU-SER-ARG-ARG-PRO-SEP-TYR-ARG-LYS-ILE-LEU-ASN-ASP-LEU-SER-SER-ASP-ALA-PRO

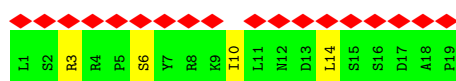
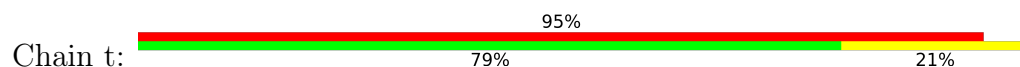




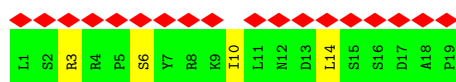
- Molecule 2: LEU-SER-ARG-ARG-PRO-SEP-TYR-ARG-LYS-ILE-LEU-ASN-ASP-LEU-SER-SER-ASP-ALA-PRO



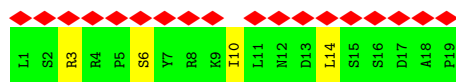
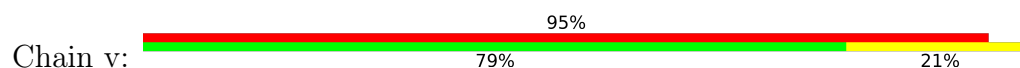
- Molecule 2: LEU-SER-ARG-ARG-PRO-SEP-TYR-ARG-LYS-ILE-LEU-ASN-ASP-LEU-SER-SER-ASP-ALA-PRO



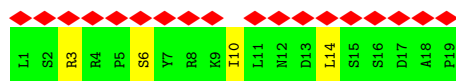
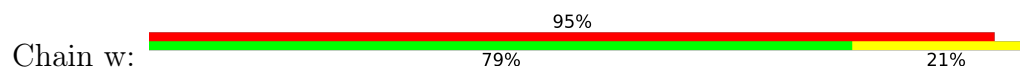
- Molecule 2: LEU-SER-ARG-ARG-PRO-SEP-TYR-ARG-LYS-ILE-LEU-ASN-ASP-LEU-SER-SER-ASP-ALA-PRO



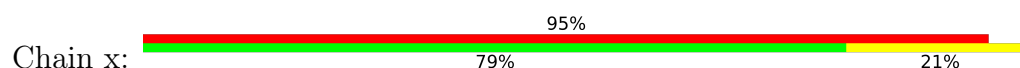
- Molecule 2: LEU-SER-ARG-ARG-PRO-SEP-TYR-ARG-LYS-ILE-LEU-ASN-ASP-LEU-SER-SER-ASP-ALA-PRO



- Molecule 2: LEU-SER-ARG-ARG-PRO-SEP-TYR-ARG-LYS-ILE-LEU-ASN-ASP-LEU-SER-SER-ASP-ALA-PRO



- Molecule 2: LEU-SER-ARG-ARG-PRO-SEP-TYR-ARG-LYS-ILE-LEU-ASN-ASP-LEU-SER-SER-ASP-ALA-PRO



L1	S2	R3	R4	P5	S6	Y7	R8	R9	I10	L11	N12	D13	L14	S15	S16	D17	A18	P19
----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35613	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 ($e^-/\text{\AA}^2$)	43.8	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	165000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.620	Depositor
Minimum map value	-0.172	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	314.88, 314.88, 314.88	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.09	0/2043	0.28	1/2747 (0.0%)
1	B	0.09	0/2043	0.28	1/2747 (0.0%)
1	C	0.09	0/2043	0.28	1/2747 (0.0%)
1	D	0.09	0/2043	0.28	1/2747 (0.0%)
1	E	0.09	0/2043	0.28	1/2747 (0.0%)
1	F	0.09	0/2043	0.28	1/2747 (0.0%)
1	G	0.09	0/2043	0.28	1/2747 (0.0%)
1	H	0.09	0/2043	0.28	1/2747 (0.0%)
1	I	0.09	0/2043	0.28	1/2747 (0.0%)
1	J	0.09	0/2043	0.28	1/2747 (0.0%)
1	K	0.09	0/2043	0.28	1/2747 (0.0%)
1	L	0.09	0/2043	0.28	1/2747 (0.0%)
1	M	0.09	0/2043	0.28	1/2747 (0.0%)
1	N	0.09	0/2043	0.28	1/2747 (0.0%)
1	O	0.09	0/2043	0.28	1/2747 (0.0%)
1	P	0.09	0/2043	0.28	1/2747 (0.0%)
1	Q	0.09	0/2043	0.28	1/2747 (0.0%)
1	R	0.09	0/2043	0.28	1/2747 (0.0%)
1	S	0.09	0/2043	0.28	1/2747 (0.0%)
1	T	0.09	0/2043	0.28	1/2747 (0.0%)
1	U	0.09	0/2043	0.28	1/2747 (0.0%)
1	V	0.09	0/2043	0.28	1/2747 (0.0%)
1	W	0.09	0/2043	0.28	1/2747 (0.0%)
1	X	0.09	0/2043	0.28	1/2747 (0.0%)
2	a	0.10	0/148	0.27	0/197
2	b	0.10	0/148	0.27	0/197
2	c	0.10	0/148	0.27	0/197
2	d	0.10	0/148	0.27	0/197
2	e	0.10	0/148	0.27	0/197
2	f	0.10	0/148	0.27	0/197
2	g	0.10	0/148	0.27	0/197
2	h	0.10	0/148	0.27	0/197

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	i	0.10	0/148	0.27	0/197
2	j	0.10	0/148	0.27	0/197
2	k	0.10	0/148	0.27	0/197
2	l	0.10	0/148	0.27	0/197
2	m	0.10	0/148	0.27	0/197
2	n	0.10	0/148	0.27	0/197
2	o	0.10	0/148	0.27	0/197
2	p	0.10	0/148	0.27	0/197
2	q	0.10	0/148	0.27	0/197
2	r	0.10	0/148	0.27	0/197
2	s	0.10	0/148	0.27	0/197
2	t	0.10	0/148	0.27	0/197
2	u	0.10	0/148	0.27	0/197
2	v	0.10	0/148	0.27	0/197
2	w	0.10	0/148	0.27	0/197
2	x	0.10	0/148	0.27	0/197
All	All	0.09	0/52584	0.28	24/70656 (0.0%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	LEU	CA-C-O	6.22	121.55	117.94
1	Q	33	LEU	CA-C-O	6.18	121.52	117.94
1	R	33	LEU	CA-C-O	6.18	121.52	117.94
1	B	33	LEU	CA-C-O	6.16	121.51	117.94
1	N	33	LEU	CA-C-O	6.16	121.51	117.94
1	S	33	LEU	CA-C-O	6.16	121.51	117.94
1	D	33	LEU	CA-C-O	6.16	121.51	117.94
1	I	33	LEU	CA-C-O	6.14	121.50	117.94
1	P	33	LEU	CA-C-O	6.14	121.50	117.94
1	W	33	LEU	CA-C-O	6.14	121.50	117.94
1	F	33	LEU	CA-C-O	6.14	121.50	117.94
1	G	33	LEU	CA-C-O	6.14	121.50	117.94
1	H	33	LEU	CA-C-O	6.14	121.50	117.94
1	C	33	LEU	CA-C-O	6.12	121.49	117.94
1	L	33	LEU	CA-C-O	6.12	121.49	117.94
1	O	33	LEU	CA-C-O	6.08	121.47	117.94
1	T	33	LEU	CA-C-O	6.08	121.47	117.94
1	K	33	LEU	CA-C-O	6.07	121.46	117.94
1	X	33	LEU	CA-C-O	6.07	121.46	117.94
1	E	33	LEU	CA-C-O	6.05	121.45	117.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	33	LEU	CA-C-O	6.05	121.45	117.94
1	M	33	LEU	CA-C-O	6.05	121.45	117.94
1	U	33	LEU	CA-C-O	6.05	121.45	117.94
1	V	33	LEU	CA-C-O	6.05	121.45	117.94

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	2000	0	1955	27	0
1	B	2000	0	1955	30	0
1	C	2000	0	1955	31	0
1	D	2000	0	1955	30	0
1	E	2000	0	1955	31	0
1	F	2000	0	1955	29	0
1	G	2000	0	1955	28	0
1	H	2000	0	1955	30	0
1	I	2000	0	1955	29	0
1	J	2000	0	1955	29	0
1	K	2000	0	1955	31	0
1	L	2000	0	1955	30	0
1	M	2000	0	1955	32	0
1	N	2000	0	1955	31	0
1	O	2000	0	1955	28	0
1	P	2000	0	1955	29	0
1	Q	2000	0	1955	28	0
1	R	2000	0	1955	27	0
1	S	2000	0	1955	28	0
1	T	2000	0	1955	27	0
1	U	2000	0	1955	29	0
1	V	2000	0	1955	32	0
1	W	2000	0	1955	31	0
1	X	2000	0	1955	31	0
2	a	157	0	159	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	b	157	0	159	6	0
2	c	157	0	159	6	0
2	d	157	0	159	6	0
2	e	157	0	159	6	0
2	f	157	0	159	6	0
2	g	157	0	159	6	0
2	h	157	0	159	6	0
2	i	157	0	159	6	0
2	j	157	0	159	6	0
2	k	157	0	159	6	0
2	l	157	0	159	6	0
2	m	157	0	159	6	0
2	n	157	0	159	6	0
2	o	157	0	159	6	0
2	p	157	0	159	6	0
2	q	157	0	159	6	0
2	r	157	0	159	6	0
2	s	157	0	159	6	0
2	t	157	0	159	6	0
2	u	157	0	159	6	0
2	v	157	0	159	6	0
2	w	157	0	159	6	0
2	x	157	0	159	6	0
All	All	51768	0	50736	640	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 6.

All (640) 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:M:71:TYR:OH	2:m:10:ILE:HB	1.40	1.22
1:E:71:TYR:OH	2:e:10:ILE:HB	1.40	1.22
1:R:71:TYR:OH	2:r:10:ILE:HB	1.40	1.21
1:U:71:TYR:OH	2:u:10:ILE:HB	1.40	1.21
1:T:71:TYR:OH	2:t:10:ILE:HB	1.40	1.21
1:W:71:TYR:OH	2:w:10:ILE:HB	1.40	1.21
1:I:71:TYR:OH	2:i:10:ILE:HB	1.40	1.20
1:V:71:TYR:OH	2:v:10:ILE:HB	1.40	1.20
1:X:71:TYR:OH	2:x:10:ILE:HB	1.40	1.20
1:A:71:TYR:OH	2:a:10:ILE:HB	1.40	1.19

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:71:TYR:OH	2:l:10:ILE:HB	1.40	1.19
1:P:71:TYR:OH	2:p:10:ILE:HB	1.40	1.19
1:B:71:TYR:OH	2:b:10:ILE:HB	1.40	1.19
1:H:71:TYR:OH	2:h:10:ILE:HB	1.40	1.19
1:F:71:TYR:OH	2:f:10:ILE:HB	1.40	1.19
1:D:71:TYR:OH	2:d:10:ILE:HB	1.40	1.18
1:K:71:TYR:OH	2:k:10:ILE:HB	1.40	1.18
1:J:71:TYR:OH	2:j:10:ILE:HB	1.40	1.18
1:N:71:TYR:OH	2:n:10:ILE:HB	1.41	1.18
1:C:71:TYR:OH	2:c:10:ILE:HB	1.40	1.17
1:Q:71:TYR:OH	2:q:10:ILE:HB	1.40	1.17
1:S:71:TYR:OH	2:s:10:ILE:HB	1.40	1.17
1:O:71:TYR:OH	2:o:10:ILE:HB	1.40	1.16
1:G:71:TYR:OH	2:g:10:ILE:HB	1.40	1.16
1:V:67:ALA:O	1:V:71:TYR:HD2	1.43	1.02
1:X:67:ALA:O	1:X:71:TYR:HD2	1.43	1.02
1:A:67:ALA:O	1:A:71:TYR:HD2	1.43	1.02
1:I:67:ALA:O	1:I:71:TYR:HD2	1.43	1.01
1:N:67:ALA:O	1:N:71:TYR:HD2	1.43	1.01
1:F:67:ALA:O	1:F:71:TYR:HD2	1.43	1.01
1:C:67:ALA:O	1:C:71:TYR:HD2	1.43	1.01
1:B:67:ALA:O	1:B:71:TYR:HD2	1.43	1.01
1:E:67:ALA:O	1:E:71:TYR:HD2	1.43	1.01
1:G:67:ALA:O	1:G:71:TYR:HD2	1.43	1.01
1:K:67:ALA:O	1:K:71:TYR:HD2	1.43	1.01
1:M:67:ALA:O	1:M:71:TYR:HD2	1.43	1.01
1:J:67:ALA:O	1:J:71:TYR:HD2	1.43	1.01
1:L:67:ALA:O	1:L:71:TYR:HD2	1.43	1.01
1:O:67:ALA:O	1:O:71:TYR:HD2	1.43	1.01
1:A:67:ALA:O	1:A:71:TYR:CD2	2.14	1.00
1:C:67:ALA:O	1:C:71:TYR:CD2	2.15	1.00
1:H:67:ALA:O	1:H:71:TYR:CD2	2.14	1.00
1:L:67:ALA:O	1:L:71:TYR:CD2	2.15	1.00
1:R:67:ALA:O	1:R:71:TYR:CD2	2.14	1.00
1:T:67:ALA:O	1:T:71:TYR:CD2	2.14	1.00
1:D:67:ALA:O	1:D:71:TYR:CD2	2.15	1.00
1:D:67:ALA:O	1:D:71:TYR:HD2	1.43	1.00
1:I:67:ALA:O	1:I:71:TYR:CD2	2.15	1.00
1:K:67:ALA:O	1:K:71:TYR:CD2	2.15	1.00
1:P:67:ALA:O	1:P:71:TYR:CD2	2.15	1.00
1:S:67:ALA:O	1:S:71:TYR:HD2	1.43	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:67:ALA:O	1:U:71:TYR:CD2	2.14	1.00
1:W:67:ALA:O	1:W:71:TYR:CD2	2.14	1.00
1:O:67:ALA:O	1:O:71:TYR:CD2	2.14	1.00
1:Q:67:ALA:O	1:Q:71:TYR:HD2	1.43	1.00
1:G:67:ALA:O	1:G:71:TYR:CD2	2.14	1.00
1:R:67:ALA:O	1:R:71:TYR:HD2	1.43	1.00
1:B:67:ALA:O	1:B:71:TYR:CD2	2.14	0.99
1:T:67:ALA:O	1:T:71:TYR:HD2	1.43	0.99
1:V:67:ALA:O	1:V:71:TYR:CD2	2.14	0.99
1:E:67:ALA:O	1:E:71:TYR:CD2	2.15	0.99
1:J:67:ALA:O	1:J:71:TYR:CD2	2.14	0.99
1:M:67:ALA:O	1:M:71:TYR:CD2	2.14	0.99
1:X:67:ALA:O	1:X:71:TYR:CD2	2.14	0.99
1:F:67:ALA:O	1:F:71:TYR:CD2	2.15	0.99
1:N:67:ALA:O	1:N:71:TYR:CD2	2.14	0.99
1:Q:67:ALA:O	1:Q:71:TYR:CD2	2.14	0.99
1:S:67:ALA:O	1:S:71:TYR:CD2	2.14	0.99
1:W:67:ALA:O	1:W:71:TYR:HD2	1.43	0.98
1:U:67:ALA:O	1:U:71:TYR:HD2	1.43	0.97
1:P:67:ALA:O	1:P:71:TYR:HD2	1.43	0.97
1:H:67:ALA:O	1:H:71:TYR:HD2	1.43	0.97
1:V:71:TYR:OH	2:v:10:ILE:CB	2.22	0.88
1:F:71:TYR:OH	2:f:10:ILE:CB	2.22	0.88
1:X:71:TYR:OH	2:x:10:ILE:CB	2.22	0.87
1:K:71:TYR:OH	2:k:10:ILE:CB	2.23	0.87
1:L:71:TYR:OH	2:l:10:ILE:CB	2.23	0.87
1:C:71:TYR:OH	2:c:10:ILE:CB	2.23	0.87
1:J:71:TYR:OH	2:j:10:ILE:CB	2.22	0.87
1:M:71:TYR:OH	2:m:10:ILE:CB	2.22	0.87
1:B:71:TYR:OH	2:b:10:ILE:CB	2.23	0.87
1:D:71:TYR:OH	2:d:10:ILE:CB	2.23	0.87
1:G:71:TYR:OH	2:g:10:ILE:CB	2.23	0.87
1:N:71:TYR:OH	2:n:10:ILE:CB	2.23	0.87
1:O:71:TYR:OH	2:o:10:ILE:CB	2.23	0.87
1:R:71:TYR:OH	2:r:10:ILE:CB	2.23	0.86
1:T:71:TYR:OH	2:t:10:ILE:CB	2.23	0.86
1:H:71:TYR:OH	2:h:10:ILE:CB	2.22	0.86
1:P:71:TYR:OH	2:p:10:ILE:CB	2.22	0.86
1:E:71:TYR:OH	2:e:10:ILE:CB	2.23	0.86
1:Q:71:TYR:OH	2:q:10:ILE:CB	2.23	0.86
1:I:71:TYR:OH	2:i:10:ILE:CB	2.22	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:71:TYR:OH	2:s:10:ILE:CB	2.23	0.85
1:U:71:TYR:OH	2:u:10:ILE:CB	2.22	0.85
1:W:71:TYR:OH	2:w:10:ILE:CB	2.22	0.85
1:A:71:TYR:OH	2:a:10:ILE:CB	2.23	0.84
1:W:71:TYR:CZ	2:w:10:ILE:HD12	2.29	0.68
1:J:71:TYR:CZ	2:j:10:ILE:HD12	2.28	0.68
1:P:71:TYR:CZ	2:p:10:ILE:HD12	2.29	0.68
1:M:71:TYR:CZ	2:m:10:ILE:HD12	2.28	0.68
1:U:71:TYR:CZ	2:u:10:ILE:HD12	2.29	0.68
1:V:71:TYR:CZ	2:v:10:ILE:HD12	2.28	0.68
1:H:71:TYR:CZ	2:h:10:ILE:HD12	2.29	0.68
1:K:71:TYR:CZ	2:k:10:ILE:HD12	2.29	0.68
1:X:71:TYR:CZ	2:x:10:ILE:HD12	2.29	0.68
1:B:71:TYR:CZ	2:b:10:ILE:HD12	2.29	0.67
1:C:71:TYR:CZ	2:c:10:ILE:HD12	2.30	0.67
1:I:71:TYR:CZ	2:i:10:ILE:HD12	2.29	0.67
1:Q:71:TYR:CZ	2:q:10:ILE:HD12	2.30	0.67
1:S:71:TYR:CZ	2:s:10:ILE:HD12	2.30	0.67
1:L:71:TYR:CZ	2:l:10:ILE:HD12	2.29	0.67
1:T:71:TYR:CZ	2:t:10:ILE:HD12	2.30	0.67
1:E:71:TYR:CZ	2:e:10:ILE:HD12	2.30	0.67
1:R:71:TYR:CZ	2:r:10:ILE:HD12	2.30	0.67
1:F:71:TYR:CZ	2:f:10:ILE:HD12	2.29	0.67
1:O:71:TYR:CZ	2:o:10:ILE:HD12	2.29	0.66
1:N:71:TYR:CZ	2:n:10:ILE:HD12	2.29	0.66
1:D:71:TYR:CZ	2:d:10:ILE:HD12	2.30	0.66
1:G:71:TYR:CZ	2:g:10:ILE:HD12	2.30	0.66
1:A:71:TYR:CZ	2:a:10:ILE:HD12	2.30	0.66
1:F:125:ASN:ND2	1:F:246:ASP:O	2.36	0.58
1:T:125:ASN:ND2	1:T:246:ASP:O	2.36	0.58
1:R:125:ASN:ND2	1:R:246:ASP:O	2.36	0.58
1:N:125:ASN:ND2	1:N:246:ASP:O	2.36	0.58
1:B:125:ASN:ND2	1:B:246:ASP:O	2.36	0.58
1:K:125:ASN:ND2	1:K:246:ASP:O	2.36	0.58
1:O:125:ASN:ND2	1:O:246:ASP:O	2.36	0.58
1:G:125:ASN:ND2	1:G:246:ASP:O	2.36	0.57
1:N:63:TYR:HB3	2:n:14:LEU:HD23	1.86	0.57
1:U:63:TYR:HB3	2:u:14:LEU:HD23	1.86	0.57
1:C:125:ASN:ND2	1:C:246:ASP:O	2.36	0.57
1:L:125:ASN:ND2	1:L:246:ASP:O	2.36	0.57
1:P:63:TYR:HB3	2:p:14:LEU:HD23	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:125:ASN:ND2	1:P:246:ASP:O	2.36	0.57
1:D:125:ASN:ND2	1:D:246:ASP:O	2.36	0.57
1:H:125:ASN:ND2	1:H:246:ASP:O	2.36	0.57
1:W:63:TYR:HB3	2:w:14:LEU:HD23	1.86	0.57
1:H:63:TYR:HB3	2:h:14:LEU:HD23	1.87	0.57
1:J:14:SER:O	1:J:18:HIS:ND1	2.35	0.57
1:J:63:TYR:HB3	2:j:14:LEU:HD23	1.86	0.57
1:Q:63:TYR:HB3	2:q:14:LEU:HD23	1.87	0.57
1:S:63:TYR:HB3	2:s:14:LEU:HD23	1.86	0.57
1:T:63:TYR:HB3	2:t:14:LEU:HD23	1.86	0.57
1:F:63:TYR:HB3	2:f:14:LEU:HD23	1.87	0.57
1:R:63:TYR:HB3	2:r:14:LEU:HD23	1.87	0.57
1:B:14:SER:O	1:B:18:HIS:ND1	2.35	0.57
1:U:125:ASN:ND2	1:U:246:ASP:O	2.36	0.57
1:W:125:ASN:ND2	1:W:246:ASP:O	2.36	0.57
1:B:63:TYR:HB3	2:b:14:LEU:HD23	1.87	0.57
1:X:63:TYR:HB3	2:x:14:LEU:HD23	1.86	0.57
1:K:63:TYR:HB3	2:k:14:LEU:HD23	1.86	0.57
1:L:63:TYR:HB3	2:l:14:LEU:HD23	1.86	0.57
1:H:244:LEU:HD13	1:L:244:LEU:HD21	1.87	0.56
1:I:125:ASN:ND2	1:I:246:ASP:O	2.36	0.56
1:V:63:TYR:HB3	2:v:14:LEU:HD23	1.86	0.56
1:A:125:ASN:ND2	1:A:246:ASP:O	2.36	0.56
1:G:63:TYR:HB3	2:g:14:LEU:HD23	1.86	0.56
1:O:63:TYR:HB3	2:o:14:LEU:HD23	1.86	0.56
1:C:63:TYR:HB3	2:c:14:LEU:HD23	1.86	0.56
1:O:244:LEU:HD21	1:R:244:LEU:HD13	1.88	0.56
1:O:244:LEU:HD13	1:X:244:LEU:HD21	1.88	0.56
1:D:63:TYR:HB3	2:d:14:LEU:HD23	1.86	0.56
1:D:244:LEU:HD21	1:P:244:LEU:HD13	1.88	0.56
1:G:244:LEU:HD13	1:V:244:LEU:HD21	1.88	0.56
1:F:244:LEU:HD21	1:J:244:LEU:HD13	1.88	0.56
1:M:63:TYR:HB3	2:m:14:LEU:HD23	1.86	0.56
1:G:244:LEU:HD21	1:T:244:LEU:HD13	1.88	0.56
1:I:63:TYR:HB3	2:i:14:LEU:HD23	1.86	0.56
1:K:244:LEU:HD21	1:Q:244:LEU:HD13	1.88	0.56
1:K:14:SER:O	1:K:18:HIS:ND1	2.35	0.56
1:R:14:SER:O	1:R:18:HIS:ND1	2.35	0.56
1:C:244:LEU:HD21	1:S:244:LEU:HD13	1.88	0.56
1:B:244:LEU:HD13	1:N:244:LEU:HD21	1.88	0.56
1:C:14:SER:O	1:C:18:HIS:ND1	2.35	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:14:SER:O	1:U:18:HIS:ND1	2.35	0.56
1:W:14:SER:O	1:W:18:HIS:ND1	2.35	0.56
1:E:63:TYR:HB3	2:e:14:LEU:HD23	1.87	0.55
1:T:14:SER:O	1:T:18:HIS:ND1	2.35	0.55
1:L:244:LEU:HD13	1:P:244:LEU:HD21	1.88	0.55
1:A:63:TYR:HB3	2:a:14:LEU:HD23	1.87	0.55
1:M:244:LEU:HD13	1:T:244:LEU:HD21	1.88	0.55
1:M:244:LEU:HD21	1:V:244:LEU:HD13	1.87	0.55
1:Q:125:ASN:ND2	1:Q:246:ASP:O	2.36	0.55
1:S:125:ASN:ND2	1:S:246:ASP:O	2.36	0.55
1:X:67:ALA:HB1	1:X:71:TYR:HE2	1.72	0.55
1:D:244:LEU:HD13	1:H:244:LEU:HD21	1.88	0.55
1:I:244:LEU:HD21	1:W:244:LEU:HD13	1.87	0.55
1:V:67:ALA:HB1	1:V:71:TYR:HE2	1.72	0.55
1:E:244:LEU:HD21	1:X:244:LEU:HD13	1.88	0.55
1:G:67:ALA:HB1	1:G:71:TYR:HE2	1.72	0.55
1:H:67:ALA:HB1	1:H:71:TYR:HE2	1.72	0.55
1:W:67:ALA:HB1	1:W:71:TYR:HE2	1.72	0.55
1:A:244:LEU:HD21	1:U:244:LEU:HD13	1.88	0.55
1:I:244:LEU:HD13	1:S:244:LEU:HD21	1.88	0.55
1:K:67:ALA:HB1	1:K:71:TYR:HE2	1.72	0.55
1:M:67:ALA:HB1	1:M:71:TYR:HE2	1.72	0.55
1:O:67:ALA:HB1	1:O:71:TYR:HE2	1.72	0.55
1:U:67:ALA:HB1	1:U:71:TYR:HE2	1.72	0.55
1:C:67:ALA:HB1	1:C:71:TYR:HE2	1.72	0.55
1:C:182:GLU:OE1	1:C:216:GLN:NE2	2.40	0.55
1:K:244:LEU:HD13	1:U:244:LEU:HD21	1.88	0.55
1:L:14:SER:O	1:L:18:HIS:ND1	2.35	0.55
1:N:182:GLU:OE1	1:N:216:GLN:NE2	2.40	0.55
1:R:182:GLU:OE1	1:R:216:GLN:NE2	2.40	0.55
1:T:182:GLU:OE1	1:T:216:GLN:NE2	2.40	0.55
1:F:182:GLU:OE1	1:F:216:GLN:NE2	2.40	0.55
1:H:182:GLU:OE1	1:H:216:GLN:NE2	2.40	0.55
1:K:182:GLU:OE1	1:K:216:GLN:NE2	2.40	0.55
1:P:67:ALA:HB1	1:P:71:TYR:HE2	1.72	0.55
1:P:182:GLU:OE1	1:P:216:GLN:NE2	2.40	0.55
1:B:67:ALA:HB1	1:B:71:TYR:HE2	1.72	0.55
1:C:244:LEU:HD13	1:W:244:LEU:HD21	1.88	0.55
1:G:182:GLU:OE1	1:G:216:GLN:NE2	2.40	0.55
1:I:182:GLU:OE1	1:I:216:GLN:NE2	2.40	0.55
1:O:182:GLU:OE1	1:O:216:GLN:NE2	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:67:ALA:HB1	1:Q:71:TYR:HE2	1.72	0.55
1:U:182:GLU:OE1	1:U:216:GLN:NE2	2.40	0.55
1:X:182:GLU:OE1	1:X:216:GLN:NE2	2.40	0.55
1:A:67:ALA:HB1	1:A:71:TYR:HE2	1.72	0.54
1:A:182:GLU:OE1	1:A:216:GLN:NE2	2.40	0.54
1:B:182:GLU:OE1	1:B:216:GLN:NE2	2.40	0.54
1:E:67:ALA:HB1	1:E:71:TYR:HE2	1.72	0.54
1:J:182:GLU:OE1	1:J:216:GLN:NE2	2.40	0.54
1:V:182:GLU:OE1	1:V:216:GLN:NE2	2.40	0.54
1:W:182:GLU:OE1	1:W:216:GLN:NE2	2.40	0.54
1:E:244:LEU:HD13	1:R:244:LEU:HD21	1.88	0.54
1:J:67:ALA:HB1	1:J:71:TYR:HE2	1.72	0.54
1:Q:182:GLU:OE1	1:Q:216:GLN:NE2	2.40	0.54
1:S:182:GLU:OE1	1:S:216:GLN:NE2	2.40	0.54
1:D:14:SER:O	1:D:18:HIS:ND1	2.35	0.54
1:J:244:LEU:HD21	1:N:244:LEU:HD13	1.88	0.54
1:B:244:LEU:HD21	1:F:244:LEU:HD13	1.88	0.54
1:D:182:GLU:OE1	1:D:216:GLN:NE2	2.40	0.54
1:L:67:ALA:HB1	1:L:71:TYR:HE2	1.72	0.54
1:D:67:ALA:HB1	1:D:71:TYR:HE2	1.72	0.54
1:I:67:ALA:HB1	1:I:71:TYR:HE2	1.72	0.54
1:J:125:ASN:ND2	1:J:246:ASP:O	2.36	0.54
1:L:182:GLU:OE1	1:L:216:GLN:NE2	2.40	0.54
1:S:67:ALA:HB1	1:S:71:TYR:HE2	1.72	0.54
1:E:125:ASN:ND2	1:E:246:ASP:O	2.36	0.54
1:M:125:ASN:ND2	1:M:246:ASP:O	2.36	0.54
1:A:244:LEU:HD13	1:Q:244:LEU:HD21	1.89	0.54
1:E:182:GLU:OE1	1:E:216:GLN:NE2	2.40	0.53
1:H:14:SER:O	1:H:18:HIS:ND1	2.35	0.53
1:N:67:ALA:HB1	1:N:71:TYR:HE2	1.72	0.53
1:M:182:GLU:OE1	1:M:216:GLN:NE2	2.40	0.53
1:P:14:SER:O	1:P:18:HIS:ND1	2.35	0.53
1:T:67:ALA:HB1	1:T:71:TYR:HE2	1.72	0.53
1:X:125:ASN:ND2	1:X:246:ASP:O	2.36	0.53
1:O:14:SER:O	1:O:18:HIS:ND1	2.35	0.53
1:R:67:ALA:HB1	1:R:71:TYR:HE2	1.72	0.53
1:I:14:SER:O	1:I:18:HIS:ND1	2.35	0.53
1:V:125:ASN:ND2	1:V:246:ASP:O	2.36	0.53
1:F:67:ALA:HB1	1:F:71:TYR:HE2	1.72	0.53
1:G:14:SER:O	1:G:18:HIS:ND1	2.35	0.53
1:A:14:SER:O	1:A:18:HIS:ND1	2.35	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:138[A]:ARG:HE	1:P:138[A]:ARG:HE	1.58	0.52
1:H:138[A]:ARG:HE	1:O:138[A]:ARG:HE	1.58	0.52
1:B:138[A]:ARG:HE	1:I:138[A]:ARG:HE	1.58	0.52
1:A:138[A]:ARG:HE	1:J:138[A]:ARG:HE	1.58	0.52
1:S:138[A]:ARG:HE	1:V:138[A]:ARG:HE	1.58	0.51
1:Q:138[A]:ARG:HE	1:X:138[A]:ARG:HE	1.58	0.51
1:R:138[A]:ARG:HE	1:W:138[A]:ARG:HE	1.58	0.51
1:T:138[A]:ARG:HE	1:U:138[A]:ARG:HE	1.58	0.51
1:E:14:SER:O	1:E:18:HIS:ND1	2.35	0.51
1:F:14:SER:O	1:F:18:HIS:ND1	2.35	0.51
1:N:14:SER:O	1:N:18:HIS:ND1	2.35	0.51
1:T:23:ALA:O	1:T:74:GLN:NE2	2.44	0.51
1:M:14:SER:O	1:M:18:HIS:ND1	2.35	0.51
1:R:23:ALA:O	1:R:74:GLN:NE2	2.44	0.51
1:F:138[A]:ARG:HE	1:M:138[A]:ARG:HE	1.58	0.50
1:Q:14:SER:O	1:Q:18:HIS:ND1	2.35	0.50
1:S:14:SER:O	1:S:18:HIS:ND1	2.35	0.50
1:E:138[A]:ARG:HE	1:N:138[A]:ARG:HE	1.58	0.50
1:E:243:TYR:HH	1:X:249:THR:HG1	1.60	0.50
1:V:23:ALA:O	1:V:74:GLN:NE2	2.44	0.50
1:X:23:ALA:O	1:X:74:GLN:NE2	2.44	0.50
1:W:23:ALA:O	1:W:74:GLN:NE2	2.44	0.50
1:C:138[A]:ARG:HE	1:L:138[A]:ARG:HE	1.58	0.50
1:D:138[A]:ARG:HE	1:K:138[A]:ARG:HE	1.58	0.50
1:P:23:ALA:O	1:P:74:GLN:NE2	2.44	0.50
1:U:23:ALA:O	1:U:74:GLN:NE2	2.44	0.50
1:H:23:ALA:O	1:H:74:GLN:NE2	2.44	0.50
1:O:71:TYR:OH	2:o:10:ILE:CG1	2.60	0.50
1:V:71:TYR:OH	2:v:10:ILE:CG1	2.60	0.50
1:E:23:ALA:O	1:E:74:GLN:NE2	2.44	0.50
1:M:23:ALA:O	1:M:74:GLN:NE2	2.44	0.50
1:P:71:TYR:OH	2:p:10:ILE:CG1	2.60	0.50
1:A:23:ALA:O	1:A:74:GLN:NE2	2.44	0.49
1:I:23:ALA:O	1:I:74:GLN:NE2	2.44	0.49
1:J:71:TYR:OH	2:j:10:ILE:CG1	2.60	0.49
1:W:71:TYR:OH	2:w:10:ILE:CG1	2.60	0.49
1:X:71:TYR:OH	2:x:10:ILE:CG1	2.60	0.49
1:U:71:TYR:OH	2:u:10:ILE:CG1	2.60	0.49
1:C:23:ALA:O	1:C:74:GLN:NE2	2.44	0.49
1:D:23:ALA:O	1:D:74:GLN:NE2	2.44	0.49
1:G:23:ALA:O	1:G:74:GLN:NE2	2.44	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:71:TYR:OH	2:g:10:ILE:CG1	2.61	0.49
1:H:71:TYR:OH	2:h:10:ILE:CG1	2.61	0.49
1:L:23:ALA:O	1:L:74:GLN:NE2	2.44	0.49
1:R:71:TYR:OH	2:r:10:ILE:CG1	2.61	0.49
1:T:71:TYR:OH	2:t:10:ILE:CG1	2.61	0.49
1:F:71:TYR:OH	2:f:10:ILE:CG1	2.60	0.49
1:K:23:ALA:O	1:K:74:GLN:NE2	2.44	0.49
1:O:23:ALA:O	1:O:74:GLN:NE2	2.44	0.49
1:Q:71:TYR:OH	2:q:10:ILE:CG1	2.61	0.49
1:M:71:TYR:OH	2:m:10:ILE:CG1	2.60	0.49
1:S:71:TYR:OH	2:s:10:ILE:CG1	2.61	0.49
1:B:71:TYR:OH	2:b:10:ILE:CG1	2.61	0.48
1:I:71:TYR:OH	2:i:10:ILE:CG1	2.60	0.48
1:L:71:TYR:OH	2:l:10:ILE:CG1	2.60	0.48
1:X:14:SER:O	1:X:18:HIS:ND1	2.35	0.48
1:K:71:TYR:OH	2:k:10:ILE:CG1	2.60	0.48
1:I:105:ALA:HA	1:I:181:LEU:HD21	1.96	0.48
1:K:152:GLY:O	1:K:154:ARG:NH1	2.47	0.48
1:A:105:ALA:HA	1:A:181:LEU:HD21	1.96	0.48
1:C:152:GLY:O	1:C:154:ARG:NH1	2.47	0.48
1:N:71:TYR:OH	2:n:10:ILE:CG1	2.61	0.48
1:B:105:ALA:HA	1:B:181:LEU:HD21	1.96	0.48
1:J:105:ALA:HA	1:J:181:LEU:HD21	1.96	0.48
1:J:152:GLY:O	1:J:154:ARG:NH1	2.47	0.48
1:S:105:ALA:HA	1:S:181:LEU:HD21	1.96	0.48
1:S:152:GLY:O	1:S:154:ARG:NH1	2.47	0.48
1:B:152:GLY:O	1:B:154:ARG:NH1	2.47	0.48
1:Q:105:ALA:HA	1:Q:181:LEU:HD21	1.96	0.48
1:Q:152:GLY:O	1:Q:154:ARG:NH1	2.47	0.48
1:U:34:LYS:HB2	1:U:36:ARG:HH11	1.79	0.48
1:U:152:GLY:O	1:U:154:ARG:NH1	2.47	0.48
1:V:14:SER:O	1:V:18:HIS:ND1	2.35	0.48
1:V:152:GLY:O	1:V:154:ARG:NH1	2.47	0.48
1:X:152:GLY:O	1:X:154:ARG:NH1	2.47	0.48
1:D:71:TYR:OH	2:d:10:ILE:CG1	2.61	0.48
1:D:152:GLY:O	1:D:154:ARG:NH1	2.47	0.48
1:P:34:LYS:HB2	1:P:36:ARG:HH11	1.79	0.48
1:Q:34:LYS:HB2	1:Q:36:ARG:HH11	1.79	0.48
1:R:105:ALA:HA	1:R:181:LEU:HD21	1.96	0.48
1:S:34:LYS:HB2	1:S:36:ARG:HH11	1.79	0.48
1:T:105:ALA:HA	1:T:181:LEU:HD21	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:152:GLY:O	1:W:154:ARG:NH1	2.47	0.48
1:D:34:LYS:HB2	1:D:36:ARG:HH11	1.79	0.48
1:D:105:ALA:HA	1:D:181:LEU:HD21	1.96	0.48
1:H:34:LYS:HB2	1:H:36:ARG:HH11	1.79	0.48
1:L:34:LYS:HB2	1:L:36:ARG:HH11	1.79	0.48
1:L:152:GLY:O	1:L:154:ARG:NH1	2.47	0.48
1:U:105:ALA:HA	1:U:181:LEU:HD21	1.96	0.48
1:V:196:ALA:HB1	1:V:201:ASP:HB3	1.96	0.48
1:W:34:LYS:HB2	1:W:36:ARG:HH11	1.79	0.48
1:W:196:ALA:HB1	1:W:201:ASP:HB3	1.96	0.48
1:X:196:ALA:HB1	1:X:201:ASP:HB3	1.96	0.48
1:A:196:ALA:HB1	1:A:201:ASP:HB3	1.96	0.48
1:C:71:TYR:OH	2:c:10:ILE:CG1	2.61	0.48
1:I:152:GLY:O	1:I:154:ARG:NH1	2.47	0.48
1:U:196:ALA:HB1	1:U:201:ASP:HB3	1.96	0.48
1:W:105:ALA:HA	1:W:181:LEU:HD21	1.96	0.48
1:A:152:GLY:O	1:A:154:ARG:NH1	2.47	0.47
1:G:196:ALA:HB1	1:G:201:ASP:HB3	1.96	0.47
1:I:196:ALA:HB1	1:I:201:ASP:HB3	1.96	0.47
1:O:196:ALA:HB1	1:O:201:ASP:HB3	1.96	0.47
1:P:152:GLY:O	1:P:154:ARG:NH1	2.47	0.47
1:C:105:ALA:HA	1:C:181:LEU:HD21	1.96	0.47
1:E:71:TYR:OH	2:e:10:ILE:CG1	2.61	0.47
1:G:105:ALA:HA	1:G:181:LEU:HD21	1.96	0.47
1:H:152:GLY:O	1:H:154:ARG:NH1	2.47	0.47
1:K:105:ALA:HA	1:K:181:LEU:HD21	1.96	0.47
1:L:105:ALA:HA	1:L:181:LEU:HD21	1.96	0.47
1:O:105:ALA:HA	1:O:181:LEU:HD21	1.96	0.47
1:Q:23:ALA:O	1:Q:74:GLN:NE2	2.44	0.47
1:R:152:GLY:O	1:R:154:ARG:NH1	2.47	0.47
1:T:152:GLY:O	1:T:154:ARG:NH1	2.47	0.47
1:E:152:GLY:O	1:E:154:ARG:NH1	2.47	0.47
1:F:34:LYS:HB2	1:F:36:ARG:HH11	1.79	0.47
1:M:152:GLY:O	1:M:154:ARG:NH1	2.47	0.47
1:N:34:LYS:HB2	1:N:36:ARG:HH11	1.79	0.47
1:B:23:ALA:O	1:B:74:GLN:NE2	2.44	0.47
1:B:196:ALA:HB1	1:B:201:ASP:HB3	1.96	0.47
1:J:196:ALA:HB1	1:J:201:ASP:HB3	1.96	0.47
1:S:23:ALA:O	1:S:74:GLN:NE2	2.44	0.47
1:A:71:TYR:OH	2:a:10:ILE:CG1	2.61	0.47
1:F:152:GLY:O	1:F:154:ARG:NH1	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:105:ALA:HA	1:H:181:LEU:HD21	1.96	0.47
1:J:23:ALA:O	1:J:74:GLN:NE2	2.44	0.47
1:K:34:LYS:HB2	1:K:36:ARG:HH11	1.79	0.47
1:L:196:ALA:HB1	1:L:201:ASP:HB3	1.96	0.47
1:N:152:GLY:O	1:N:154:ARG:NH1	2.47	0.47
1:P:105:ALA:HA	1:P:181:LEU:HD21	1.96	0.47
1:C:34:LYS:HB2	1:C:36:ARG:HH11	1.79	0.47
1:C:196:ALA:HB1	1:C:201:ASP:HB3	1.96	0.47
1:D:196:ALA:HB1	1:D:201:ASP:HB3	1.96	0.47
1:D:243:TYR:OH	1:P:249:THR:OG1	2.32	0.47
1:G:34:LYS:HB2	1:G:36:ARG:HH11	1.79	0.47
1:G:152:GLY:O	1:G:154:ARG:NH1	2.47	0.47
1:I:34:LYS:HB2	1:I:36:ARG:HH11	1.79	0.47
1:K:196:ALA:HB1	1:K:201:ASP:HB3	1.96	0.47
1:M:243:TYR:OH	1:V:249:THR:OG1	2.33	0.47
1:N:23:ALA:O	1:N:74:GLN:NE2	2.44	0.47
1:A:34:LYS:HB2	1:A:36:ARG:HH11	1.79	0.47
1:E:105:ALA:HA	1:E:181:LEU:HD21	1.96	0.47
1:F:23:ALA:O	1:F:74:GLN:NE2	2.44	0.47
1:N:105:ALA:HA	1:N:181:LEU:HD21	1.96	0.47
1:O:34:LYS:HB2	1:O:36:ARG:HH11	1.79	0.47
1:M:105:ALA:HA	1:M:181:LEU:HD21	1.96	0.47
1:O:152:GLY:O	1:O:154:ARG:NH1	2.47	0.47
1:R:196:ALA:HB1	1:R:201:ASP:HB3	1.96	0.47
1:X:34:LYS:HB2	1:X:36:ARG:HH11	1.79	0.47
1:C:243:TYR:OH	1:S:249:THR:OG1	2.32	0.47
1:F:105:ALA:HA	1:F:181:LEU:HD21	1.96	0.47
1:T:196:ALA:HB1	1:T:201:ASP:HB3	1.96	0.47
1:V:34:LYS:HB2	1:V:36:ARG:HH11	1.79	0.47
1:X:105:ALA:HA	1:X:181:LEU:HD21	1.96	0.47
1:F:196:ALA:HB1	1:F:201:ASP:HB3	1.96	0.46
1:H:95:ILE:HD11	1:H:204:LEU:HD21	1.98	0.46
1:J:34:LYS:HB2	1:J:36:ARG:HH11	1.79	0.46
1:P:95:ILE:HD11	1:P:204:LEU:HD21	1.98	0.46
1:V:105:ALA:HA	1:V:181:LEU:HD21	1.96	0.46
1:N:196:ALA:HB1	1:N:201:ASP:HB3	1.96	0.46
1:Q:95:ILE:HD11	1:Q:204:LEU:HD21	1.98	0.46
1:B:34:LYS:HB2	1:B:36:ARG:HH11	1.79	0.46
1:H:196:ALA:HB1	1:H:201:ASP:HB3	1.96	0.46
1:Q:196:ALA:HB1	1:Q:201:ASP:HB3	1.96	0.46
1:S:95:ILE:HD11	1:S:204:LEU:HD21	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:196:ALA:HB1	1:S:201:ASP:HB3	1.96	0.46
1:E:34:LYS:HB2	1:E:36:ARG:HH11	1.79	0.46
1:E:196:ALA:HB1	1:E:201:ASP:HB3	1.96	0.46
1:M:34:LYS:HB2	1:M:36:ARG:HH11	1.79	0.46
1:O:95:ILE:HD11	1:O:204:LEU:HD21	1.98	0.46
1:P:196:ALA:HB1	1:P:201:ASP:HB3	1.96	0.46
1:G:95:ILE:HD11	1:G:204:LEU:HD21	1.98	0.46
1:M:196:ALA:HB1	1:M:201:ASP:HB3	1.96	0.46
1:R:34:LYS:HB2	1:R:36:ARG:HH11	1.79	0.46
1:U:95:ILE:HD11	1:U:204:LEU:HD21	1.98	0.46
1:K:95:ILE:HD11	1:K:204:LEU:HD21	1.98	0.46
1:R:89:GLN:HE22	2:r:3:ARG:HB3	1.81	0.46
1:W:95:ILE:HD11	1:W:204:LEU:HD21	1.98	0.46
1:A:95:ILE:HD11	1:A:204:LEU:HD21	1.98	0.46
1:C:95:ILE:HD11	1:C:204:LEU:HD21	1.98	0.46
1:I:95:ILE:HD11	1:I:204:LEU:HD21	1.98	0.46
1:T:34:LYS:HB2	1:T:36:ARG:HH11	1.79	0.46
1:H:249:THR:OG1	1:L:243:TYR:OH	2.33	0.45
1:T:89:GLN:HE22	2:t:3:ARG:HB3	1.82	0.45
1:V:95:ILE:HD11	1:V:204:LEU:HD21	1.98	0.45
1:X:95:ILE:HD11	1:X:204:LEU:HD21	1.98	0.45
1:B:95:ILE:HD11	1:B:204:LEU:HD21	1.98	0.45
1:J:95:ILE:HD11	1:J:204:LEU:HD21	1.98	0.45
1:Q:46:LYS:O	1:Q:49:GLU:HG3	2.17	0.45
1:S:46:LYS:O	1:S:49:GLU:HG3	2.17	0.45
1:E:46:LYS:O	1:E:49:GLU:HG3	2.17	0.45
1:F:95:ILE:HD11	1:F:204:LEU:HD21	1.98	0.45
1:P:46:LYS:O	1:P:49:GLU:HG3	2.17	0.45
1:R:108:VAL:HG22	1:R:163:PRO:HG3	1.99	0.45
1:D:95:ILE:HD11	1:D:204:LEU:HD21	1.98	0.45
1:H:46:LYS:O	1:H:49:GLU:HG3	2.17	0.45
1:L:95:ILE:HD11	1:L:204:LEU:HD21	1.98	0.45
1:M:46:LYS:O	1:M:49:GLU:HG3	2.17	0.45
1:N:46:LYS:O	1:N:49:GLU:HG3	2.17	0.45
1:N:95:ILE:HD11	1:N:204:LEU:HD21	1.98	0.45
1:T:108:VAL:HG22	1:T:163:PRO:HG3	1.99	0.45
1:D:89:GLN:HE22	2:d:3:ARG:HB3	1.82	0.45
1:F:46:LYS:O	1:F:49:GLU:HG3	2.17	0.45
1:G:108:VAL:HG22	1:G:163:PRO:HG3	1.99	0.45
1:X:108:VAL:HG22	1:X:163:PRO:HG3	1.99	0.45
1:B:46:LYS:O	1:B:49:GLU:HG3	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:46:LYS:O	1:J:49:GLU:HG3	2.17	0.45
1:M:95:ILE:HD11	1:M:204:LEU:HD21	1.98	0.45
1:O:108:VAL:HG22	1:O:163:PRO:HG3	1.99	0.45
1:V:108:VAL:HG22	1:V:163:PRO:HG3	1.99	0.45
1:E:95:ILE:HD11	1:E:204:LEU:HD21	1.98	0.45
1:U:46:LYS:O	1:U:49:GLU:HG3	2.17	0.45
1:W:46:LYS:O	1:W:49:GLU:HG3	2.17	0.45
1:X:46:LYS:O	1:X:49:GLU:HG3	2.17	0.45
1:U:108:VAL:HG22	1:U:163:PRO:HG3	1.99	0.45
1:V:46:LYS:O	1:V:49:GLU:HG3	2.17	0.45
1:W:108:VAL:HG22	1:W:163:PRO:HG3	1.99	0.45
1:D:46:LYS:O	1:D:49:GLU:HG3	2.17	0.45
1:L:46:LYS:O	1:L:49:GLU:HG3	2.17	0.45
1:G:46:LYS:O	1:G:49:GLU:HG3	2.17	0.44
1:I:67:ALA:C	1:I:71:TYR:HD2	2.22	0.44
1:J:108:VAL:HG22	1:J:163:PRO:HG3	1.99	0.44
1:P:108:VAL:HG22	1:P:163:PRO:HG3	1.99	0.44
1:R:46:LYS:O	1:R:49:GLU:HG3	2.17	0.44
1:V:89:GLN:HE22	2:v:3:ARG:HB3	1.82	0.44
1:B:249:THR:HG1	1:N:243:TYR:HH	1.64	0.44
1:M:67:ALA:C	1:M:71:TYR:HD2	2.22	0.44
1:M:89:GLN:HE22	2:m:3:ARG:HB3	1.82	0.44
1:O:46:LYS:O	1:O:49:GLU:HG3	2.17	0.44
1:T:46:LYS:O	1:T:49:GLU:HG3	2.17	0.44
1:T:95:ILE:HD11	1:T:204:LEU:HD21	1.98	0.44
1:A:89:GLN:HE22	2:a:3:ARG:HB3	1.82	0.44
1:B:108:VAL:HG22	1:B:163:PRO:HG3	1.99	0.44
1:C:46:LYS:O	1:C:49:GLU:HG3	2.17	0.44
1:E:89:GLN:HE22	2:e:3:ARG:HB3	1.82	0.44
1:F:89:GLN:HE22	2:f:3:ARG:HB3	1.81	0.44
1:H:108:VAL:HG22	1:H:163:PRO:HG3	1.99	0.44
1:I:108:VAL:HG22	1:I:163:PRO:HG3	1.99	0.44
1:L:89:GLN:HE22	2:l:3:ARG:HB3	1.83	0.44
1:M:108:VAL:HG22	1:M:163:PRO:HG3	1.99	0.44
1:R:95:ILE:HD11	1:R:204:LEU:HD21	1.98	0.44
1:E:67:ALA:C	1:E:71:TYR:HD2	2.22	0.44
1:E:108:VAL:HG22	1:E:163:PRO:HG3	1.99	0.44
1:K:46:LYS:O	1:K:49:GLU:HG3	2.17	0.44
1:S:108:VAL:HG22	1:S:163:PRO:HG3	1.99	0.44
1:V:67:ALA:C	1:V:71:TYR:HD2	2.22	0.44
1:X:89:GLN:HE22	2:x:3:ARG:HB3	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:VAL:HG22	1:A:163:PRO:HG3	1.99	0.44
1:B:89:GLN:HE22	2:b:3:ARG:HB3	1.82	0.44
1:C:89:GLN:HE22	2:c:3:ARG:HB3	1.82	0.44
1:C:108:VAL:HG22	1:C:163:PRO:HG3	1.99	0.44
1:I:89:GLN:HE22	2:i:3:ARG:HB3	1.82	0.44
1:U:89:GLN:HE22	2:u:3:ARG:HB3	1.82	0.44
1:K:108:VAL:HG22	1:K:163:PRO:HG3	1.99	0.44
1:X:67:ALA:C	1:X:71:TYR:HD2	2.22	0.44
1:Q:108:VAL:HG22	1:Q:163:PRO:HG3	1.99	0.44
1:A:46:LYS:O	1:A:49:GLU:HG3	2.17	0.44
1:F:108:VAL:HG22	1:F:163:PRO:HG3	1.99	0.44
1:N:13:ARG:NH2	1:N:49:GLU:OE1	2.50	0.44
1:W:89:GLN:HE22	2:w:3:ARG:HB3	1.82	0.44
1:G:89:GLN:HE22	2:g:3:ARG:HB3	1.82	0.44
1:J:89:GLN:HE22	2:j:3:ARG:HB3	1.82	0.44
1:F:13:ARG:NH2	1:F:49:GLU:OE1	2.50	0.43
1:H:89:GLN:HE22	2:h:3:ARG:HB3	1.82	0.43
1:D:108:VAL:HG22	1:D:163:PRO:HG3	1.99	0.43
1:I:46:LYS:O	1:I:49:GLU:HG3	2.17	0.43
1:K:89:GLN:HE22	2:k:3:ARG:HB3	1.83	0.43
1:N:108:VAL:HG22	1:N:163:PRO:HG3	1.99	0.43
1:B:67:ALA:C	1:B:71:TYR:HD2	2.22	0.43
1:N:89:GLN:HE22	2:n:3:ARG:HB3	1.83	0.43
1:F:67:ALA:C	1:F:71:TYR:HD2	2.22	0.43
1:L:108:VAL:HG22	1:L:163:PRO:HG3	1.99	0.43
1:P:89:GLN:HE22	2:p:3:ARG:HB3	1.82	0.43
1:S:89:GLN:HE22	2:s:3:ARG:HB3	1.82	0.43
1:A:213:LEU:HD13	1:X:203:HIS:HB2	2.01	0.43
1:I:213:LEU:HD13	1:V:203:HIS:HB2	2.01	0.43
1:K:213:LEU:HD13	1:T:203:HIS:HB2	2.01	0.43
1:O:89:GLN:HE22	2:o:3:ARG:HB3	1.82	0.43
1:Q:89:GLN:HE22	2:q:3:ARG:HB3	1.82	0.43
1:C:213:LEU:HD13	1:R:203:HIS:HB2	2.01	0.43
1:J:67:ALA:C	1:J:71:TYR:HD2	2.22	0.43
1:N:47:LYS:HE2	1:N:47:LYS:HB3	1.88	0.43
1:D:203:HIS:HB2	1:Q:213:LEU:HD13	2.01	0.42
1:H:13:ARG:NH2	1:H:49:GLU:OE1	2.50	0.42
1:J:203:HIS:HB2	1:U:213:LEU:HD13	2.01	0.42
1:L:203:HIS:HB2	1:S:213:LEU:HD13	2.01	0.42
1:P:13:ARG:NH2	1:P:49:GLU:OE1	2.50	0.42
1:B:203:HIS:HB2	1:W:213:LEU:HD13	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:ARG:NH2	1:C:49:GLU:OE1	2.50	0.42
1:G:213:LEU:HD13	1:S:203:HIS:HB2	2.01	0.42
1:K:13:ARG:NH2	1:K:49:GLU:OE1	2.50	0.42
1:P:203:HIS:HB2	1:T:213:LEU:HD13	2.01	0.42
1:O:213:LEU:HD13	1:Q:203:HIS:HB2	2.01	0.42
1:B:196:ALA:HB3	1:B:205:CYS:HB3	2.02	0.42
1:C:196:ALA:HB3	1:C:205:CYS:HB3	2.02	0.42
1:F:196:ALA:HB3	1:F:205:CYS:HB3	2.02	0.42
1:J:196:ALA:HB3	1:J:205:CYS:HB3	2.02	0.42
1:N:196:ALA:HB3	1:N:205:CYS:HB3	2.02	0.42
1:C:67:ALA:C	1:C:71:TYR:HD2	2.22	0.42
1:H:203:HIS:HB2	1:R:213:LEU:HD13	2.01	0.42
1:M:13:ARG:NH2	1:M:49:GLU:OE1	2.50	0.42
1:X:196:ALA:HB3	1:X:205:CYS:HB3	2.02	0.42
1:H:196:ALA:HB3	1:H:205:CYS:HB3	2.02	0.42
1:I:243:TYR:OH	1:W:249:THR:OG1	2.33	0.42
1:K:196:ALA:HB3	1:K:205:CYS:HB3	2.02	0.42
1:K:203:HIS:HB2	1:P:213:LEU:HD13	2.01	0.42
1:P:196:ALA:HB3	1:P:205:CYS:HB3	2.02	0.42
1:S:196:ALA:HB3	1:S:205:CYS:HB3	2.02	0.42
1:V:196:ALA:HB3	1:V:205:CYS:HB3	2.02	0.42
1:D:213:LEU:HD13	1:O:203:HIS:HB2	2.01	0.41
1:G:203:HIS:HB2	1:L:213:LEU:HD13	2.01	0.41
1:N:203:HIS:HB2	1:X:213:LEU:HD13	2.01	0.41
1:Q:196:ALA:HB3	1:Q:205:CYS:HB3	2.02	0.41
1:C:193:HIS:CD2	1:C:205:CYS:HB2	2.55	0.41
1:C:203:HIS:HB2	1:H:213:LEU:HD13	2.01	0.41
1:D:193:HIS:CD2	1:D:205:CYS:HB2	2.56	0.41
1:E:13:ARG:NH2	1:E:49:GLU:OE1	2.50	0.41
1:E:193:HIS:CD2	1:E:205:CYS:HB2	2.55	0.41
1:G:193:HIS:CD2	1:G:205:CYS:HB2	2.55	0.41
1:M:213:LEU:HD13	1:U:203:HIS:HB2	2.01	0.41
1:O:193:HIS:CD2	1:O:205:CYS:HB2	2.56	0.41
1:E:213:LEU:HD13	1:W:203:HIS:HB2	2.01	0.41
1:K:47:LYS:HE2	1:K:47:LYS:HB3	1.88	0.41
1:K:67:ALA:C	1:K:71:TYR:HD2	2.22	0.41
1:K:193:HIS:CD2	1:K:205:CYS:HB2	2.56	0.41
1:L:193:HIS:CD2	1:L:205:CYS:HB2	2.56	0.41
1:L:196:ALA:HB3	1:L:205:CYS:HB3	2.02	0.41
1:Q:193:HIS:CD2	1:Q:205:CYS:HB2	2.55	0.41
1:U:196:ALA:HB3	1:U:205:CYS:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:196:ALA:HB3	1:W:205:CYS:HB3	2.02	0.41
1:F:213:LEU:HD13	1:I:203:HIS:HB2	2.01	0.41
1:M:193:HIS:CD2	1:M:205:CYS:HB2	2.56	0.41
1:S:193:HIS:CD2	1:S:205:CYS:HB2	2.55	0.41
1:T:193:HIS:CD2	1:T:205:CYS:HB2	2.55	0.41
1:A:196:ALA:HB3	1:A:205:CYS:HB3	2.02	0.41
1:D:196:ALA:HB3	1:D:205:CYS:HB3	2.02	0.41
1:R:193:HIS:CD2	1:R:205:CYS:HB2	2.56	0.41
1:B:213:LEU:HD13	1:E:203:HIS:HB2	2.01	0.41
1:E:87:TYR:HE2	1:E:92:GLU:HB2	1.86	0.41
1:E:196:ALA:HB3	1:E:205:CYS:HB3	2.02	0.41
1:I:196:ALA:HB3	1:I:205:CYS:HB3	2.02	0.41
1:J:213:LEU:HD13	1:M:203:HIS:HB2	2.01	0.41
1:L:87:TYR:HE2	1:L:92:GLU:HB2	1.86	0.41
1:M:87:TYR:HE2	1:M:92:GLU:HB2	1.86	0.41
1:A:203:HIS:HB2	1:N:213:LEU:HD13	2.01	0.41
1:B:193:HIS:CD2	1:B:205:CYS:HB2	2.56	0.41
1:D:87:TYR:HE2	1:D:92:GLU:HB2	1.86	0.41
1:J:193:HIS:CD2	1:J:205:CYS:HB2	2.56	0.41
1:V:193:HIS:CD2	1:V:205:CYS:HB2	2.55	0.41
1:W:87:TYR:HE2	1:W:92:GLU:HB2	1.86	0.41
1:F:203:HIS:HB2	1:V:213:LEU:HD13	2.02	0.41
1:G:196:ALA:HB3	1:G:205:CYS:HB3	2.02	0.41
1:O:196:ALA:HB3	1:O:205:CYS:HB3	2.02	0.41
1:V:13:ARG:NH2	1:V:49:GLU:OE1	2.50	0.41
1:H:87:TYR:HE2	1:H:92:GLU:HB2	1.86	0.41
1:L:13:ARG:NH2	1:L:49:GLU:OE1	2.50	0.41
1:M:196:ALA:HB3	1:M:205:CYS:HB3	2.02	0.41
1:N:115:TYR:OH	1:N:167:ASP:OD1	2.32	0.41
1:P:87:TYR:HE2	1:P:92:GLU:HB2	1.86	0.41
1:R:196:ALA:HB3	1:R:205:CYS:HB3	2.02	0.41
1:T:196:ALA:HB3	1:T:205:CYS:HB3	2.02	0.41
1:U:87:TYR:HE2	1:U:92:GLU:HB2	1.86	0.41
1:W:13:ARG:NH2	1:W:49:GLU:OE1	2.50	0.41
1:X:193:HIS:CD2	1:X:205:CYS:HB2	2.56	0.41
1:D:13:ARG:NH2	1:D:49:GLU:OE1	2.50	0.41
1:G:87:TYR:HE2	1:G:92:GLU:HB2	1.86	0.41
1:J:13:ARG:NH2	1:J:49:GLU:OE1	2.50	0.41
1:V:87:TYR:HE2	1:V:92:GLU:HB2	1.86	0.41
1:X:13:ARG:NH2	1:X:49:GLU:OE1	2.50	0.41
1:X:87:TYR:HE2	1:X:92:GLU:HB2	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:193:HIS:CD2	1:F:205:CYS:HB2	2.55	0.40
1:K:87:TYR:HE2	1:K:92:GLU:HB2	1.86	0.40
1:O:87:TYR:HE2	1:O:92:GLU:HB2	1.86	0.40
1:W:193:HIS:CD2	1:W:205:CYS:HB2	2.55	0.40
1:A:193:HIS:CD2	1:A:205:CYS:HB2	2.55	0.40
1:U:13:ARG:NH2	1:U:49:GLU:OE1	2.50	0.40
1:B:13:ARG:NH2	1:B:49:GLU:OE1	2.50	0.40
1:C:87:TYR:HE2	1:C:92:GLU:HB2	1.86	0.40
1:N:193:HIS:CD2	1:N:205:CYS:HB2	2.56	0.40
1:U:193:HIS:CD2	1:U:205:CYS:HB2	2.56	0.40
1:M:243:TYR:HH	1:V:249:THR:HG1	1.64	0.40
1:Q:87:TYR:HE2	1:Q:92:GLU:HB2	1.86	0.40
1:W:67:ALA:C	1:W:71:TYR:HD2	2.22	0.40
1:H:193:HIS:CD2	1:H:205:CYS:HB2	2.55	0.40
1:I:193:HIS:CD2	1:I:205:CYS:HB2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	242/260 (93%)	220 (91%)	20 (8%)	2 (1%)	16	20
1	B	242/260 (93%)	220 (91%)	20 (8%)	2 (1%)	16	20
1	C	242/260 (93%)	220 (91%)	20 (8%)	2 (1%)	16	20
1	D	242/260 (93%)	220 (91%)	20 (8%)	2 (1%)	16	20
1	E	242/260 (93%)	220 (91%)	20 (8%)	2 (1%)	16	20
1	F	242/260 (93%)	220 (91%)	20 (8%)	2 (1%)	16	20
1	G	242/260 (93%)	220 (91%)	20 (8%)	2 (1%)	16	20
1	H	242/260 (93%)	220 (91%)	20 (8%)	2 (1%)	16	20

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	242/260 (93%)	220 (91%)	20 (8%)	2 (1%)	16	20
1	J	242/260 (93%)	220 (91%)	20 (8%)	2 (1%)	16	20
1	K	242/260 (93%)	220 (91%)	20 (8%)	2 (1%)	16	20
1	L	242/260 (93%)	220 (91%)	20 (8%)	2 (1%)	16	20
1	M	242/260 (93%)	220 (91%)	20 (8%)	2 (1%)	16	20
1	N	242/260 (93%)	220 (91%)	20 (8%)	2 (1%)	16	20
1	O	242/260 (93%)	220 (91%)	20 (8%)	2 (1%)	16	20
1	P	242/260 (93%)	220 (91%)	20 (8%)	2 (1%)	16	20
1	Q	242/260 (93%)	220 (91%)	20 (8%)	2 (1%)	16	20
1	R	242/260 (93%)	220 (91%)	20 (8%)	2 (1%)	16	20
1	S	242/260 (93%)	220 (91%)	20 (8%)	2 (1%)	16	20
1	T	242/260 (93%)	220 (91%)	20 (8%)	2 (1%)	16	20
1	U	242/260 (93%)	220 (91%)	20 (8%)	2 (1%)	16	20
1	V	242/260 (93%)	220 (91%)	20 (8%)	2 (1%)	16	20
1	W	242/260 (93%)	220 (91%)	20 (8%)	2 (1%)	16	20
1	X	242/260 (93%)	220 (91%)	20 (8%)	2 (1%)	16	20
2	a	16/19 (84%)	16 (100%)	0	0	100	100
2	b	16/19 (84%)	16 (100%)	0	0	100	100
2	c	16/19 (84%)	16 (100%)	0	0	100	100
2	d	16/19 (84%)	16 (100%)	0	0	100	100
2	e	16/19 (84%)	16 (100%)	0	0	100	100
2	f	16/19 (84%)	16 (100%)	0	0	100	100
2	g	16/19 (84%)	16 (100%)	0	0	100	100
2	h	16/19 (84%)	16 (100%)	0	0	100	100
2	i	16/19 (84%)	16 (100%)	0	0	100	100
2	j	16/19 (84%)	16 (100%)	0	0	100	100
2	k	16/19 (84%)	16 (100%)	0	0	100	100
2	l	16/19 (84%)	16 (100%)	0	0	100	100
2	m	16/19 (84%)	16 (100%)	0	0	100	100
2	n	16/19 (84%)	16 (100%)	0	0	100	100
2	o	16/19 (84%)	16 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	p	16/19 (84%)	16 (100%)	0	0	100	100
2	q	16/19 (84%)	16 (100%)	0	0	100	100
2	r	16/19 (84%)	16 (100%)	0	0	100	100
2	s	16/19 (84%)	16 (100%)	0	0	100	100
2	t	16/19 (84%)	16 (100%)	0	0	100	100
2	u	16/19 (84%)	16 (100%)	0	0	100	100
2	v	16/19 (84%)	16 (100%)	0	0	100	100
2	w	16/19 (84%)	16 (100%)	0	0	100	100
2	x	16/19 (84%)	16 (100%)	0	0	100	100
All	All	6192/6696 (92%)	5664 (92%)	480 (8%)	48 (1%)	18	20

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	PRO
1	B	26	PRO
1	C	26	PRO
1	D	26	PRO
1	E	26	PRO
1	F	26	PRO
1	G	26	PRO
1	H	26	PRO
1	I	26	PRO
1	J	26	PRO
1	K	26	PRO
1	L	26	PRO
1	M	26	PRO
1	N	26	PRO
1	O	26	PRO
1	P	26	PRO
1	Q	26	PRO
1	R	26	PRO
1	S	26	PRO
1	T	26	PRO
1	U	26	PRO
1	V	26	PRO
1	W	26	PRO
1	X	26	PRO
1	A	169	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	169	CYS
1	C	169	CYS
1	D	169	CYS
1	E	169	CYS
1	F	169	CYS
1	G	169	CYS
1	H	169	CYS
1	I	169	CYS
1	J	169	CYS
1	K	169	CYS
1	L	169	CYS
1	M	169	CYS
1	N	169	CYS
1	O	169	CYS
1	P	169	CYS
1	Q	169	CYS
1	R	169	CYS
1	S	169	CYS
1	T	169	CYS
1	U	169	CYS
1	V	169	CYS
1	W	169	CYS
1	X	169	CYS

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	217/230 (94%)	216 (100%)	1 (0%)	81	90
1	B	217/230 (94%)	216 (100%)	1 (0%)	81	90
1	C	217/230 (94%)	216 (100%)	1 (0%)	81	90
1	D	217/230 (94%)	216 (100%)	1 (0%)	81	90
1	E	217/230 (94%)	216 (100%)	1 (0%)	81	90
1	F	217/230 (94%)	216 (100%)	1 (0%)	81	90

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	217/230 (94%)	216 (100%)	1 (0%)	81	90
1	H	217/230 (94%)	216 (100%)	1 (0%)	81	90
1	I	217/230 (94%)	216 (100%)	1 (0%)	81	90
1	J	217/230 (94%)	216 (100%)	1 (0%)	81	90
1	K	217/230 (94%)	216 (100%)	1 (0%)	81	90
1	L	217/230 (94%)	216 (100%)	1 (0%)	81	90
1	M	217/230 (94%)	216 (100%)	1 (0%)	81	90
1	N	217/230 (94%)	216 (100%)	1 (0%)	81	90
1	O	217/230 (94%)	216 (100%)	1 (0%)	81	90
1	P	217/230 (94%)	216 (100%)	1 (0%)	81	90
1	Q	217/230 (94%)	216 (100%)	1 (0%)	81	90
1	R	217/230 (94%)	216 (100%)	1 (0%)	81	90
1	S	217/230 (94%)	216 (100%)	1 (0%)	81	90
1	T	217/230 (94%)	216 (100%)	1 (0%)	81	90
1	U	217/230 (94%)	216 (100%)	1 (0%)	81	90
1	V	217/230 (94%)	216 (100%)	1 (0%)	81	90
1	W	217/230 (94%)	216 (100%)	1 (0%)	81	90
1	X	217/230 (94%)	216 (100%)	1 (0%)	81	90
2	a	17/17 (100%)	17 (100%)	0	100	100
2	b	17/17 (100%)	17 (100%)	0	100	100
2	c	17/17 (100%)	17 (100%)	0	100	100
2	d	17/17 (100%)	17 (100%)	0	100	100
2	e	17/17 (100%)	17 (100%)	0	100	100
2	f	17/17 (100%)	17 (100%)	0	100	100
2	g	17/17 (100%)	17 (100%)	0	100	100
2	h	17/17 (100%)	17 (100%)	0	100	100
2	i	17/17 (100%)	17 (100%)	0	100	100
2	j	17/17 (100%)	17 (100%)	0	100	100
2	k	17/17 (100%)	17 (100%)	0	100	100
2	l	17/17 (100%)	17 (100%)	0	100	100
2	m	17/17 (100%)	17 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	n	17/17 (100%)	17 (100%)	0	100	100
2	o	17/17 (100%)	17 (100%)	0	100	100
2	p	17/17 (100%)	17 (100%)	0	100	100
2	q	17/17 (100%)	17 (100%)	0	100	100
2	r	17/17 (100%)	17 (100%)	0	100	100
2	s	17/17 (100%)	17 (100%)	0	100	100
2	t	17/17 (100%)	17 (100%)	0	100	100
2	u	17/17 (100%)	17 (100%)	0	100	100
2	v	17/17 (100%)	17 (100%)	0	100	100
2	w	17/17 (100%)	17 (100%)	0	100	100
2	x	17/17 (100%)	17 (100%)	0	100	100
All	All	5616/5928 (95%)	5592 (100%)	24 (0%)	81	92

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	CYS
1	B	27	CYS
1	C	27	CYS
1	D	27	CYS
1	E	27	CYS
1	F	27	CYS
1	G	27	CYS
1	H	27	CYS
1	I	27	CYS
1	J	27	CYS
1	K	27	CYS
1	L	27	CYS
1	M	27	CYS
1	N	27	CYS
1	O	27	CYS
1	P	27	CYS
1	Q	27	CYS
1	R	27	CYS
1	S	27	CYS
1	T	27	CYS
1	U	27	CYS
1	V	27	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	W	27	CYS
1	X	27	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (128) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	89	GLN
1	A	186	ASN
1	A	187	GLN
1	A	216	GLN
1	A	248	HIS
1	B	89	GLN
1	B	186	ASN
1	B	187	GLN
1	B	216	GLN
1	B	248	HIS
1	C	89	GLN
1	C	186	ASN
1	C	187	GLN
1	C	216	GLN
1	C	248	HIS
1	D	82	GLN
1	D	89	GLN
1	D	187	GLN
1	D	216	GLN
1	D	248	HIS
1	E	89	GLN
1	E	186	ASN
1	E	187	GLN
1	E	216	GLN
1	E	248	HIS
1	F	89	GLN
1	F	187	GLN
1	F	216	GLN
1	F	248	HIS
1	G	82	GLN
1	G	89	GLN
1	G	187	GLN
1	G	216	GLN
1	G	248	HIS
1	H	89	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	187	GLN
1	H	216	GLN
1	H	248	HIS
1	I	82	GLN
1	I	89	GLN
1	I	186	ASN
1	I	187	GLN
1	I	216	GLN
1	I	248	HIS
1	J	89	GLN
1	J	186	ASN
1	J	187	GLN
1	J	216	GLN
1	J	248	HIS
1	K	82	GLN
1	K	89	GLN
1	K	186	ASN
1	K	187	GLN
1	K	216	GLN
1	K	248	HIS
1	L	82	GLN
1	L	89	GLN
1	L	187	GLN
1	L	216	GLN
1	L	248	HIS
1	M	89	GLN
1	M	186	ASN
1	M	187	GLN
1	M	216	GLN
1	M	248	HIS
1	N	82	GLN
1	N	89	GLN
1	N	187	GLN
1	N	216	GLN
1	N	248	HIS
1	O	82	GLN
1	O	89	GLN
1	O	186	ASN
1	O	187	GLN
1	O	216	GLN
1	O	248	HIS
1	P	89	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	P	187	GLN
1	P	216	GLN
1	P	248	HIS
1	Q	82	GLN
1	Q	89	GLN
1	Q	186	ASN
1	Q	187	GLN
1	Q	216	GLN
1	Q	248	HIS
1	R	89	GLN
1	R	186	ASN
1	R	187	GLN
1	R	216	GLN
1	R	248	HIS
1	S	89	GLN
1	S	186	ASN
1	S	187	GLN
1	S	216	GLN
1	S	248	HIS
1	T	89	GLN
1	T	186	ASN
1	T	187	GLN
1	T	203	HIS
1	T	216	GLN
1	T	248	HIS
1	U	82	GLN
1	U	89	GLN
1	U	187	GLN
1	U	216	GLN
1	U	248	HIS
1	V	89	GLN
1	V	186	ASN
1	V	187	GLN
1	V	216	GLN
1	V	248	HIS
1	W	82	GLN
1	W	89	GLN
1	W	187	GLN
1	W	216	GLN
1	W	248	HIS
1	X	89	GLN
1	X	186	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	187	GLN
1	X	216	GLN
1	X	248	HIS
2	g	12	ASN
2	m	12	ASN
2	o	12	ASN
2	q	12	ASN
2	s	12	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

24 non-standard protein/DNA/RNA residues 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	SEP	c	6	2	8,9,10	1.62	1 (12%)	7,12,14	1.54	1 (14%)
2	SEP	p	6	2	8,9,10	1.62	1 (12%)	7,12,14	1.54	1 (14%)
2	SEP	i	6	2	8,9,10	1.61	1 (12%)	7,12,14	1.54	1 (14%)
2	SEP	x	6	2	8,9,10	1.61	1 (12%)	7,12,14	1.54	1 (14%)
2	SEP	f	6	2	8,9,10	1.62	1 (12%)	7,12,14	1.54	1 (14%)
2	SEP	d	6	2	8,9,10	1.62	1 (12%)	7,12,14	1.54	1 (14%)
2	SEP	q	6	2	8,9,10	1.62	1 (12%)	7,12,14	1.54	1 (14%)
2	SEP	a	6	2	8,9,10	1.62	1 (12%)	7,12,14	1.54	1 (14%)
2	SEP	t	6	2	8,9,10	1.62	1 (12%)	7,12,14	1.54	1 (14%)
2	SEP	b	6	2	8,9,10	1.62	1 (12%)	7,12,14	1.54	1 (14%)
2	SEP	g	6	2	8,9,10	1.62	1 (12%)	7,12,14	1.54	1 (14%)
2	SEP	s	6	2	8,9,10	1.62	1 (12%)	7,12,14	1.54	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SEP	u	6	2	8,9,10	1.62	1 (12%)	7,12,14	1.54	1 (14%)
2	SEP	v	6	2	8,9,10	1.62	1 (12%)	7,12,14	1.54	1 (14%)
2	SEP	e	6	2	8,9,10	1.61	1 (12%)	7,12,14	1.54	1 (14%)
2	SEP	m	6	2	8,9,10	1.62	1 (12%)	7,12,14	1.54	1 (14%)
2	SEP	k	6	2	8,9,10	1.61	1 (12%)	7,12,14	1.54	1 (14%)
2	SEP	l	6	2	8,9,10	1.61	1 (12%)	7,12,14	1.54	1 (14%)
2	SEP	r	6	2	8,9,10	1.61	1 (12%)	7,12,14	1.54	1 (14%)
2	SEP	o	6	2	8,9,10	1.61	1 (12%)	7,12,14	1.54	1 (14%)
2	SEP	n	6	2	8,9,10	1.62	1 (12%)	7,12,14	1.54	1 (14%)
2	SEP	w	6	2	8,9,10	1.62	1 (12%)	7,12,14	1.54	1 (14%)
2	SEP	h	6	2	8,9,10	1.62	1 (12%)	7,12,14	1.54	1 (14%)
2	SEP	j	6	2	8,9,10	1.61	1 (12%)	7,12,14	1.54	1 (14%)

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	SEP	c	6	2	-	4/6/8/10	-
2	SEP	p	6	2	-	5/6/8/10	-
2	SEP	i	6	2	-	5/6/8/10	-
2	SEP	x	6	2	-	5/6/8/10	-
2	SEP	f	6	2	-	5/6/8/10	-
2	SEP	d	6	2	-	4/6/8/10	-
2	SEP	q	6	2	-	4/6/8/10	-
2	SEP	a	6	2	-	4/6/8/10	-
2	SEP	t	6	2	-	5/6/8/10	-
2	SEP	b	6	2	-	4/6/8/10	-
2	SEP	g	6	2	-	5/6/8/10	-
2	SEP	s	6	2	-	5/6/8/10	-
2	SEP	u	6	2	-	5/6/8/10	-
2	SEP	v	6	2	-	5/6/8/10	-
2	SEP	e	6	2	-	5/6/8/10	-
2	SEP	m	6	2	-	5/6/8/10	-
2	SEP	k	6	2	-	5/6/8/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SEP	l	6	2	-	5/6/8/10	-
2	SEP	r	6	2	-	5/6/8/10	-
2	SEP	o	6	2	-	5/6/8/10	-
2	SEP	n	6	2	-	4/6/8/10	-
2	SEP	w	6	2	-	4/6/8/10	-
2	SEP	h	6	2	-	4/6/8/10	-
2	SEP	j	6	2	-	5/6/8/10	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	f	6	SEP	P-O1P	3.55	1.61	1.50
2	g	6	SEP	P-O1P	3.55	1.61	1.50
2	m	6	SEP	P-O1P	3.55	1.61	1.50
2	p	6	SEP	P-O1P	3.55	1.61	1.50
2	s	6	SEP	P-O1P	3.55	1.61	1.50
2	t	6	SEP	P-O1P	3.55	1.61	1.50
2	u	6	SEP	P-O1P	3.55	1.61	1.50
2	v	6	SEP	P-O1P	3.55	1.61	1.50
2	a	6	SEP	P-O1P	3.54	1.61	1.50
2	b	6	SEP	P-O1P	3.54	1.61	1.50
2	c	6	SEP	P-O1P	3.54	1.61	1.50
2	d	6	SEP	P-O1P	3.54	1.61	1.50
2	h	6	SEP	P-O1P	3.54	1.61	1.50
2	n	6	SEP	P-O1P	3.54	1.61	1.50
2	q	6	SEP	P-O1P	3.54	1.61	1.50
2	w	6	SEP	P-O1P	3.54	1.61	1.50
2	e	6	SEP	P-O1P	3.51	1.61	1.50
2	i	6	SEP	P-O1P	3.51	1.61	1.50
2	j	6	SEP	P-O1P	3.51	1.61	1.50
2	k	6	SEP	P-O1P	3.51	1.61	1.50
2	l	6	SEP	P-O1P	3.51	1.61	1.50
2	o	6	SEP	P-O1P	3.51	1.61	1.50
2	r	6	SEP	P-O1P	3.51	1.61	1.50
2	x	6	SEP	P-O1P	3.51	1.61	1.50

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	a	6	SEP	OG-CB-CA	3.53	111.58	108.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	6	SEP	OG-CB-CA	3.53	111.58	108.14
2	c	6	SEP	OG-CB-CA	3.53	111.58	108.14
2	d	6	SEP	OG-CB-CA	3.53	111.58	108.14
2	e	6	SEP	OG-CB-CA	3.53	111.58	108.14
2	f	6	SEP	OG-CB-CA	3.53	111.58	108.14
2	g	6	SEP	OG-CB-CA	3.53	111.58	108.14
2	h	6	SEP	OG-CB-CA	3.53	111.58	108.14
2	i	6	SEP	OG-CB-CA	3.53	111.58	108.14
2	j	6	SEP	OG-CB-CA	3.53	111.58	108.14
2	k	6	SEP	OG-CB-CA	3.53	111.58	108.14
2	l	6	SEP	OG-CB-CA	3.53	111.58	108.14
2	m	6	SEP	OG-CB-CA	3.53	111.58	108.14
2	n	6	SEP	OG-CB-CA	3.53	111.58	108.14
2	o	6	SEP	OG-CB-CA	3.53	111.58	108.14
2	p	6	SEP	OG-CB-CA	3.53	111.58	108.14
2	q	6	SEP	OG-CB-CA	3.53	111.58	108.14
2	r	6	SEP	OG-CB-CA	3.53	111.58	108.14
2	s	6	SEP	OG-CB-CA	3.53	111.58	108.14
2	t	6	SEP	OG-CB-CA	3.53	111.58	108.14
2	u	6	SEP	OG-CB-CA	3.53	111.58	108.14
2	v	6	SEP	OG-CB-CA	3.53	111.58	108.14
2	w	6	SEP	OG-CB-CA	3.53	111.58	108.14
2	x	6	SEP	OG-CB-CA	3.53	111.58	108.14

There are no chirality outliers.

All (112) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	a	6	SEP	N-CA-CB-OG
2	a	6	SEP	C-CA-CB-OG
2	a	6	SEP	CB-OG-P-O2P
2	a	6	SEP	CB-OG-P-O3P
2	b	6	SEP	N-CA-CB-OG
2	b	6	SEP	C-CA-CB-OG
2	b	6	SEP	CB-OG-P-O2P
2	b	6	SEP	CB-OG-P-O3P
2	c	6	SEP	N-CA-CB-OG
2	c	6	SEP	C-CA-CB-OG
2	c	6	SEP	CB-OG-P-O2P
2	c	6	SEP	CB-OG-P-O3P
2	d	6	SEP	N-CA-CB-OG
2	d	6	SEP	C-CA-CB-OG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	d	6	SEP	CB-OG-P-O2P
2	d	6	SEP	CB-OG-P-O3P
2	e	6	SEP	N-CA-CB-OG
2	e	6	SEP	C-CA-CB-OG
2	e	6	SEP	CB-OG-P-O2P
2	f	6	SEP	N-CA-CB-OG
2	f	6	SEP	C-CA-CB-OG
2	f	6	SEP	CB-OG-P-O1P
2	f	6	SEP	CB-OG-P-O2P
2	g	6	SEP	N-CA-CB-OG
2	g	6	SEP	C-CA-CB-OG
2	g	6	SEP	CB-OG-P-O1P
2	g	6	SEP	CB-OG-P-O2P
2	h	6	SEP	N-CA-CB-OG
2	h	6	SEP	C-CA-CB-OG
2	h	6	SEP	CB-OG-P-O2P
2	h	6	SEP	CB-OG-P-O3P
2	i	6	SEP	N-CA-CB-OG
2	i	6	SEP	C-CA-CB-OG
2	i	6	SEP	CB-OG-P-O2P
2	j	6	SEP	N-CA-CB-OG
2	j	6	SEP	C-CA-CB-OG
2	j	6	SEP	CB-OG-P-O2P
2	k	6	SEP	N-CA-CB-OG
2	k	6	SEP	C-CA-CB-OG
2	k	6	SEP	CB-OG-P-O2P
2	l	6	SEP	N-CA-CB-OG
2	l	6	SEP	C-CA-CB-OG
2	l	6	SEP	CB-OG-P-O2P
2	m	6	SEP	N-CA-CB-OG
2	m	6	SEP	C-CA-CB-OG
2	m	6	SEP	CB-OG-P-O1P
2	m	6	SEP	CB-OG-P-O2P
2	n	6	SEP	N-CA-CB-OG
2	n	6	SEP	C-CA-CB-OG
2	n	6	SEP	CB-OG-P-O2P
2	n	6	SEP	CB-OG-P-O3P
2	o	6	SEP	N-CA-CB-OG
2	o	6	SEP	C-CA-CB-OG
2	o	6	SEP	CB-OG-P-O2P
2	p	6	SEP	N-CA-CB-OG
2	p	6	SEP	C-CA-CB-OG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	p	6	SEP	CB-OG-P-O1P
2	p	6	SEP	CB-OG-P-O2P
2	q	6	SEP	N-CA-CB-OG
2	q	6	SEP	C-CA-CB-OG
2	q	6	SEP	CB-OG-P-O2P
2	q	6	SEP	CB-OG-P-O3P
2	r	6	SEP	N-CA-CB-OG
2	r	6	SEP	C-CA-CB-OG
2	r	6	SEP	CB-OG-P-O2P
2	s	6	SEP	N-CA-CB-OG
2	s	6	SEP	C-CA-CB-OG
2	s	6	SEP	CB-OG-P-O1P
2	s	6	SEP	CB-OG-P-O2P
2	t	6	SEP	N-CA-CB-OG
2	t	6	SEP	C-CA-CB-OG
2	t	6	SEP	CB-OG-P-O1P
2	t	6	SEP	CB-OG-P-O2P
2	u	6	SEP	N-CA-CB-OG
2	u	6	SEP	C-CA-CB-OG
2	u	6	SEP	CB-OG-P-O1P
2	u	6	SEP	CB-OG-P-O2P
2	v	6	SEP	N-CA-CB-OG
2	v	6	SEP	C-CA-CB-OG
2	v	6	SEP	CB-OG-P-O1P
2	v	6	SEP	CB-OG-P-O2P
2	w	6	SEP	N-CA-CB-OG
2	w	6	SEP	C-CA-CB-OG
2	w	6	SEP	CB-OG-P-O2P
2	w	6	SEP	CB-OG-P-O3P
2	x	6	SEP	N-CA-CB-OG
2	x	6	SEP	C-CA-CB-OG
2	x	6	SEP	CB-OG-P-O2P
2	e	6	SEP	CB-OG-P-O1P
2	i	6	SEP	CB-OG-P-O1P
2	j	6	SEP	CB-OG-P-O1P
2	k	6	SEP	CB-OG-P-O1P
2	l	6	SEP	CB-OG-P-O1P
2	o	6	SEP	CB-OG-P-O1P
2	r	6	SEP	CB-OG-P-O1P
2	x	6	SEP	CB-OG-P-O1P
2	e	6	SEP	CB-OG-P-O3P
2	f	6	SEP	CB-OG-P-O3P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	g	6	SEP	CB-OG-P-O3P
2	i	6	SEP	CB-OG-P-O3P
2	j	6	SEP	CB-OG-P-O3P
2	k	6	SEP	CB-OG-P-O3P
2	l	6	SEP	CB-OG-P-O3P
2	m	6	SEP	CB-OG-P-O3P
2	o	6	SEP	CB-OG-P-O3P
2	p	6	SEP	CB-OG-P-O3P
2	r	6	SEP	CB-OG-P-O3P
2	s	6	SEP	CB-OG-P-O3P
2	t	6	SEP	CB-OG-P-O3P
2	u	6	SEP	CB-OG-P-O3P
2	v	6	SEP	CB-OG-P-O3P
2	x	6	SEP	CB-OG-P-O3P

There are no ring outliers.

No monomer is involved in short contacts.

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.

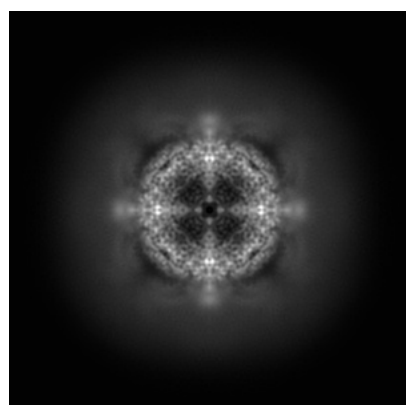
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25799. These allow visual inspection of the internal detail of the map and identification of artifacts.

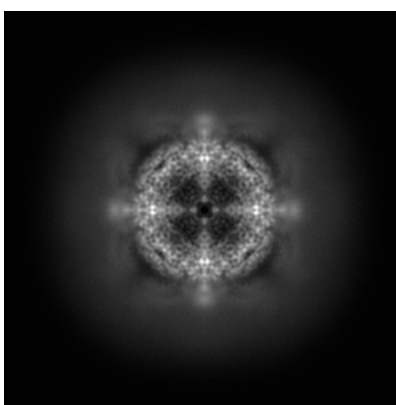
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

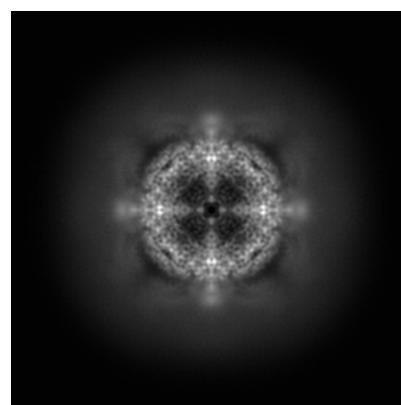
6.1.1 Primary map



X



Y

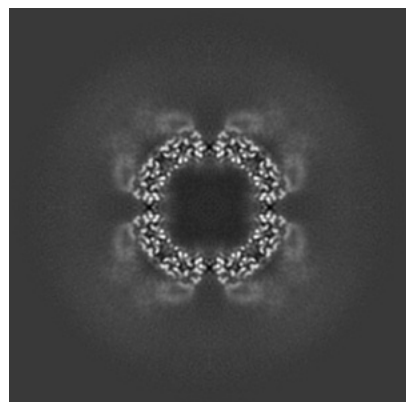


Z

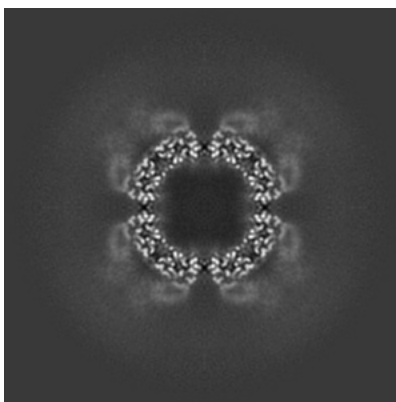
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

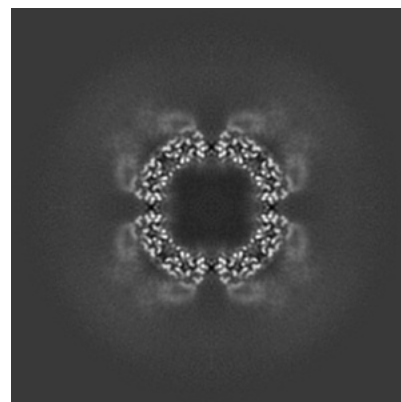
6.2.1 Primary map



X Index: 192



Y Index: 192

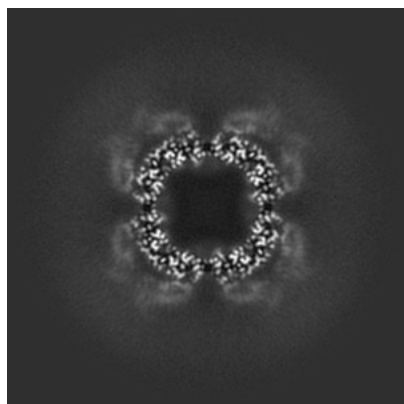


Z Index: 192

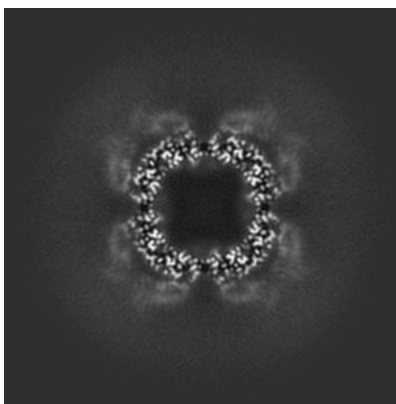
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

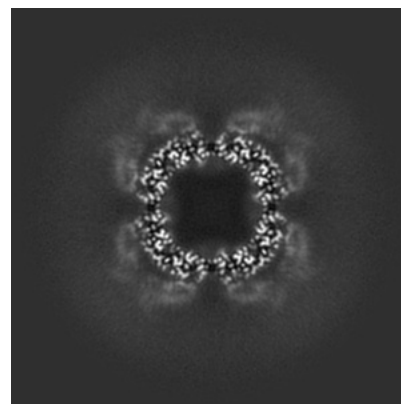
6.3.1 Primary map



X Index: 194



Y Index: 194

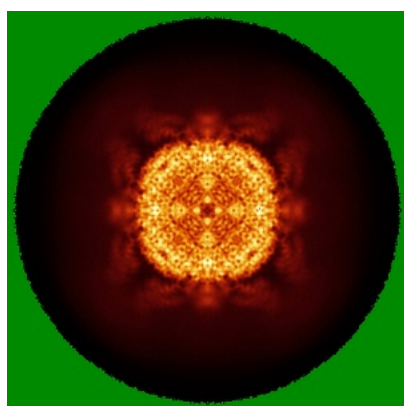


Z Index: 194

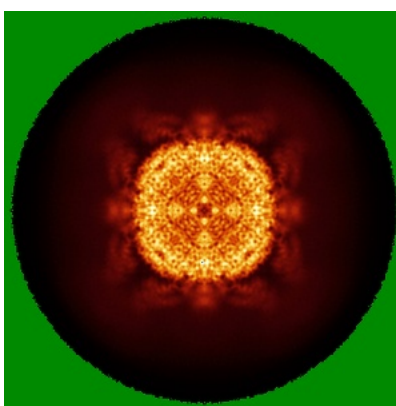
The images above show the largest variance slices of the map in three orthogonal directions.

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

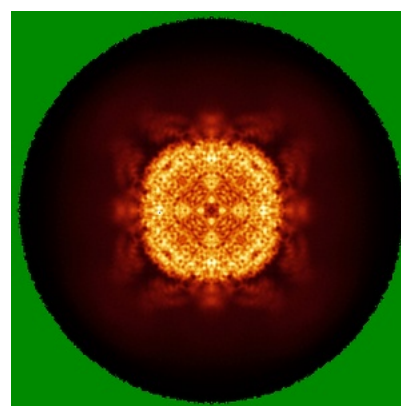
6.4.1 Primary map



X



Y

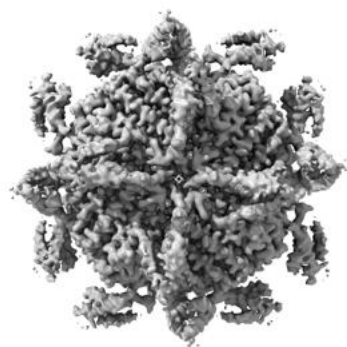


Z

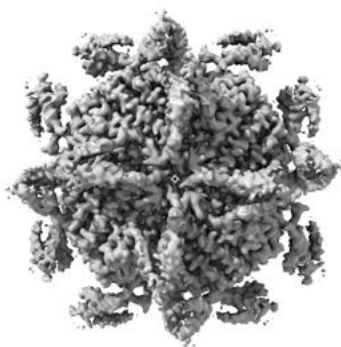
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

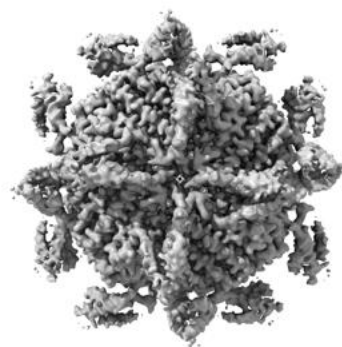
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

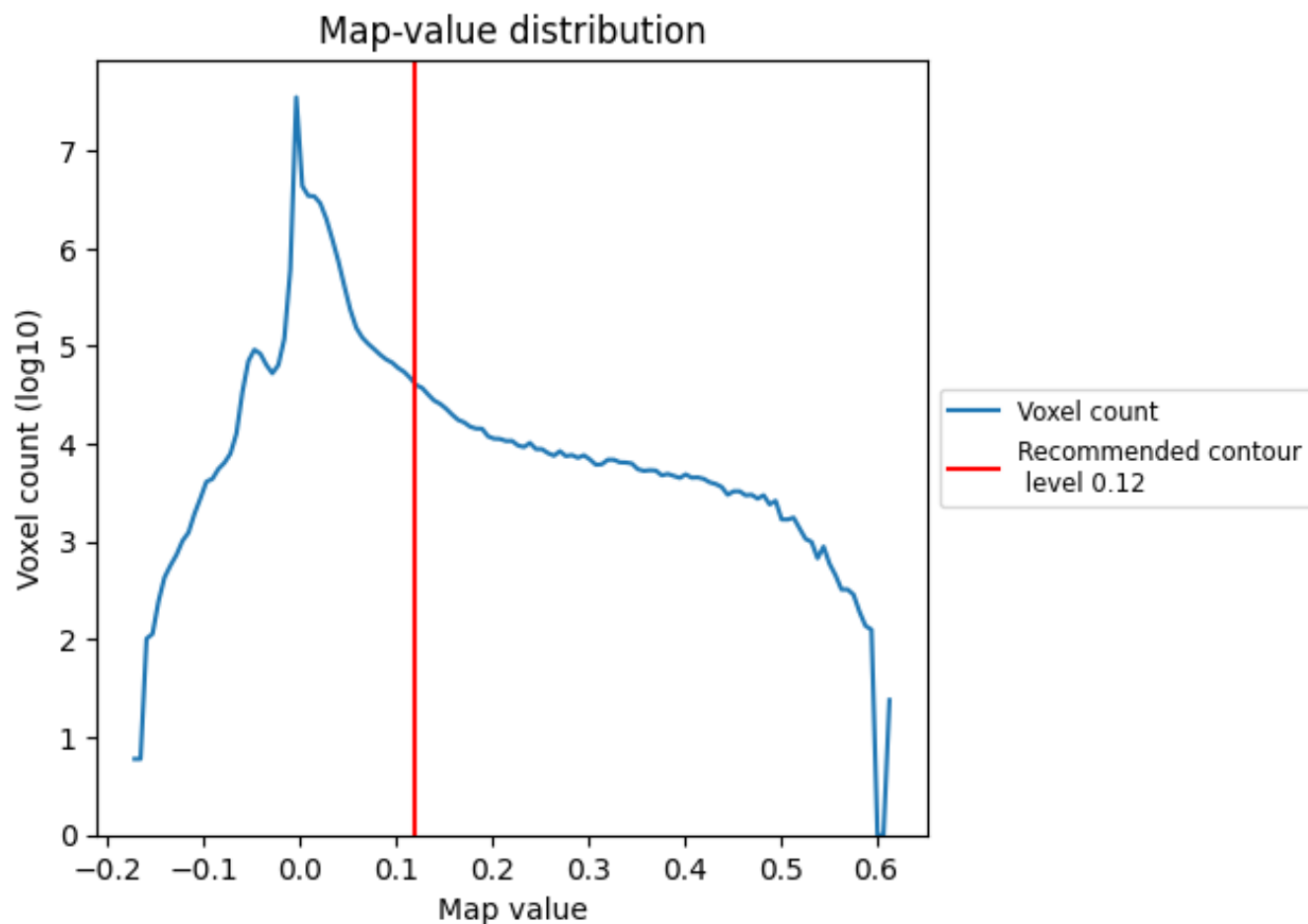
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

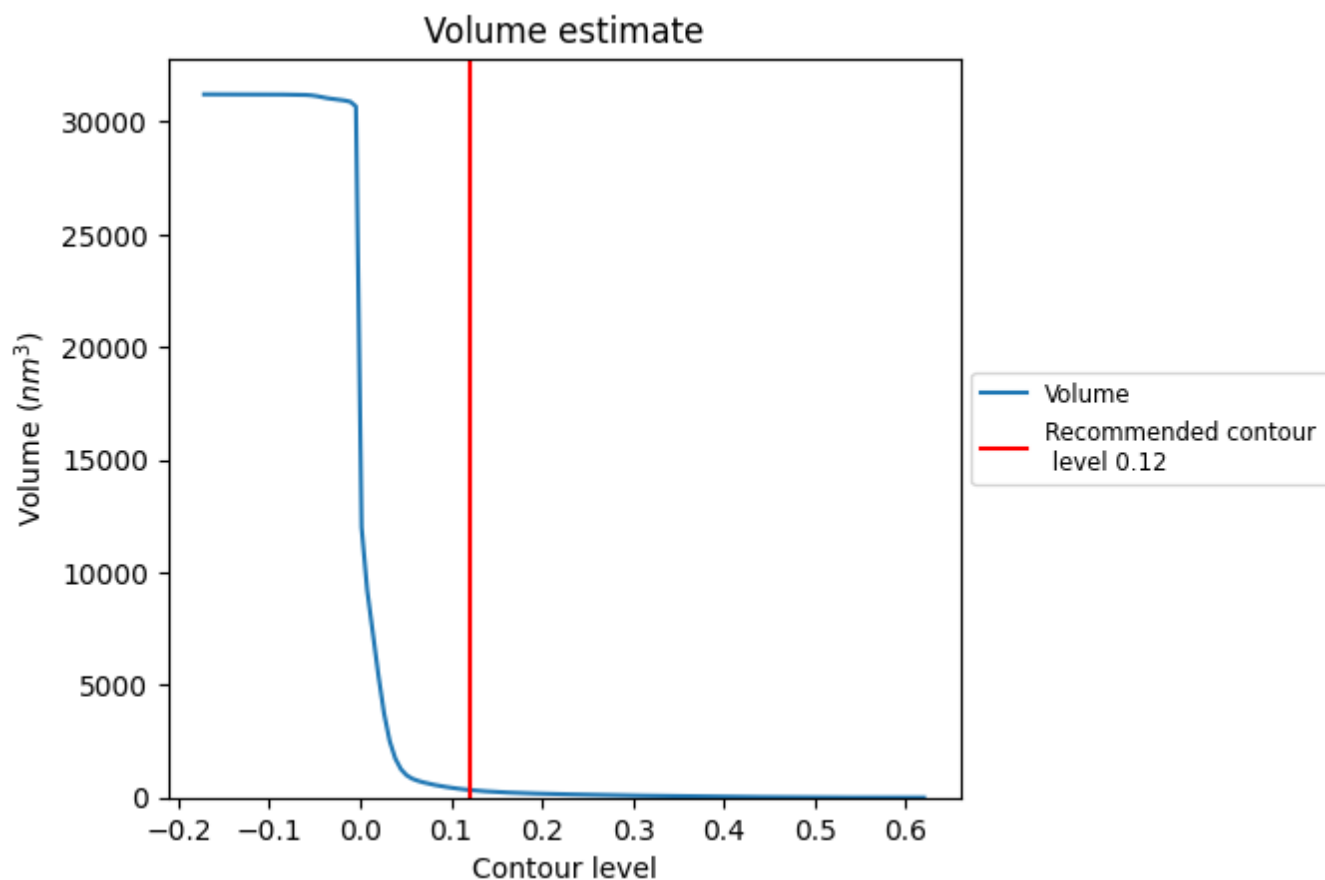
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

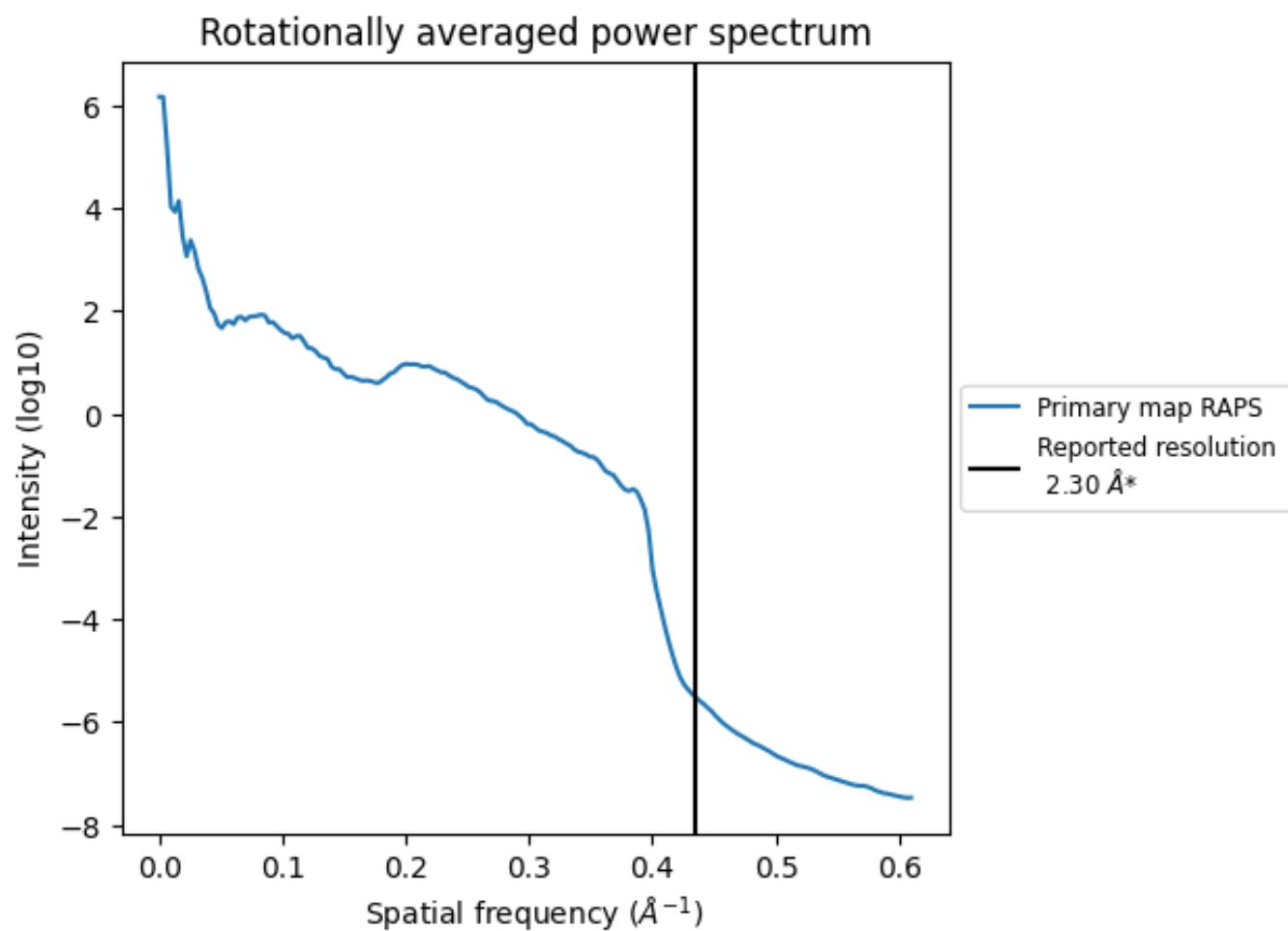
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 338 nm³; this corresponds to an approximate mass of 305 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 0.435 Å⁻¹

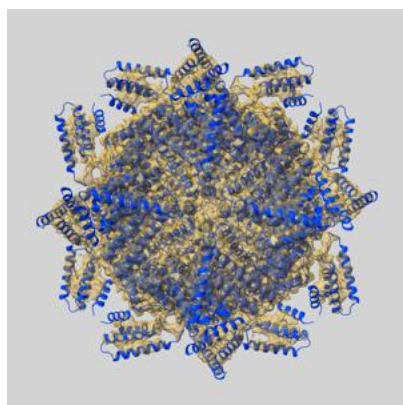
8 Fourier-Shell correlation

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

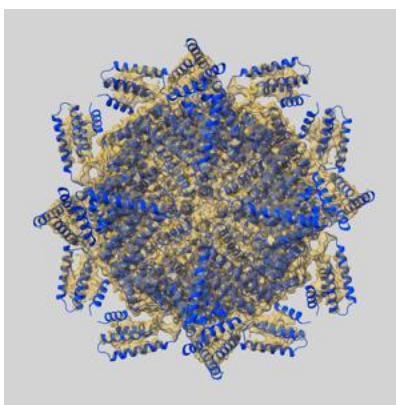
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25799 and PDB model 7TBH. Per-residue inclusion information can be found in section 3 on page 12.

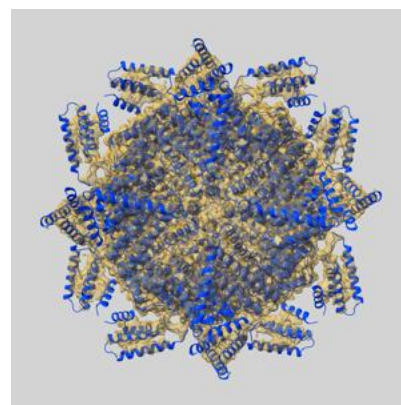
9.1 Map-model overlay [i](#)



X



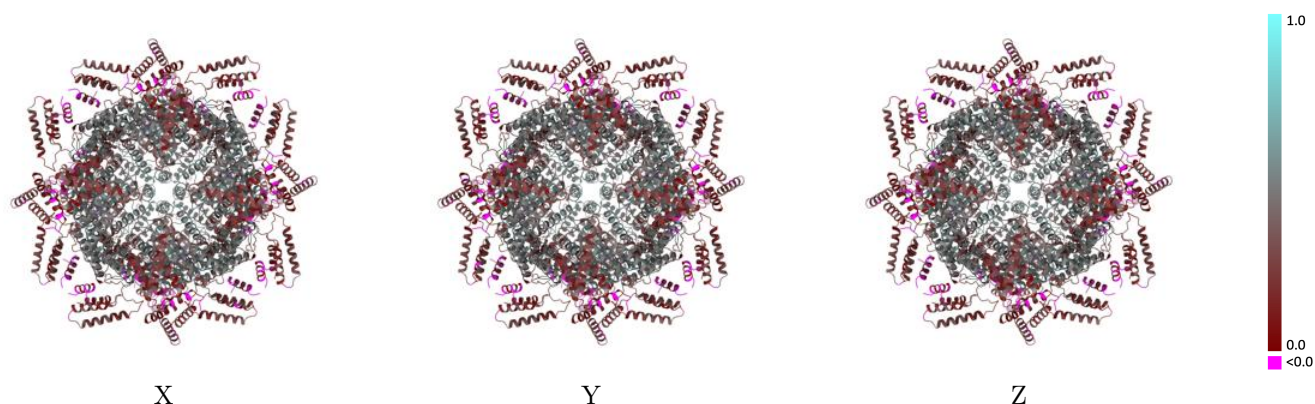
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12 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](#)

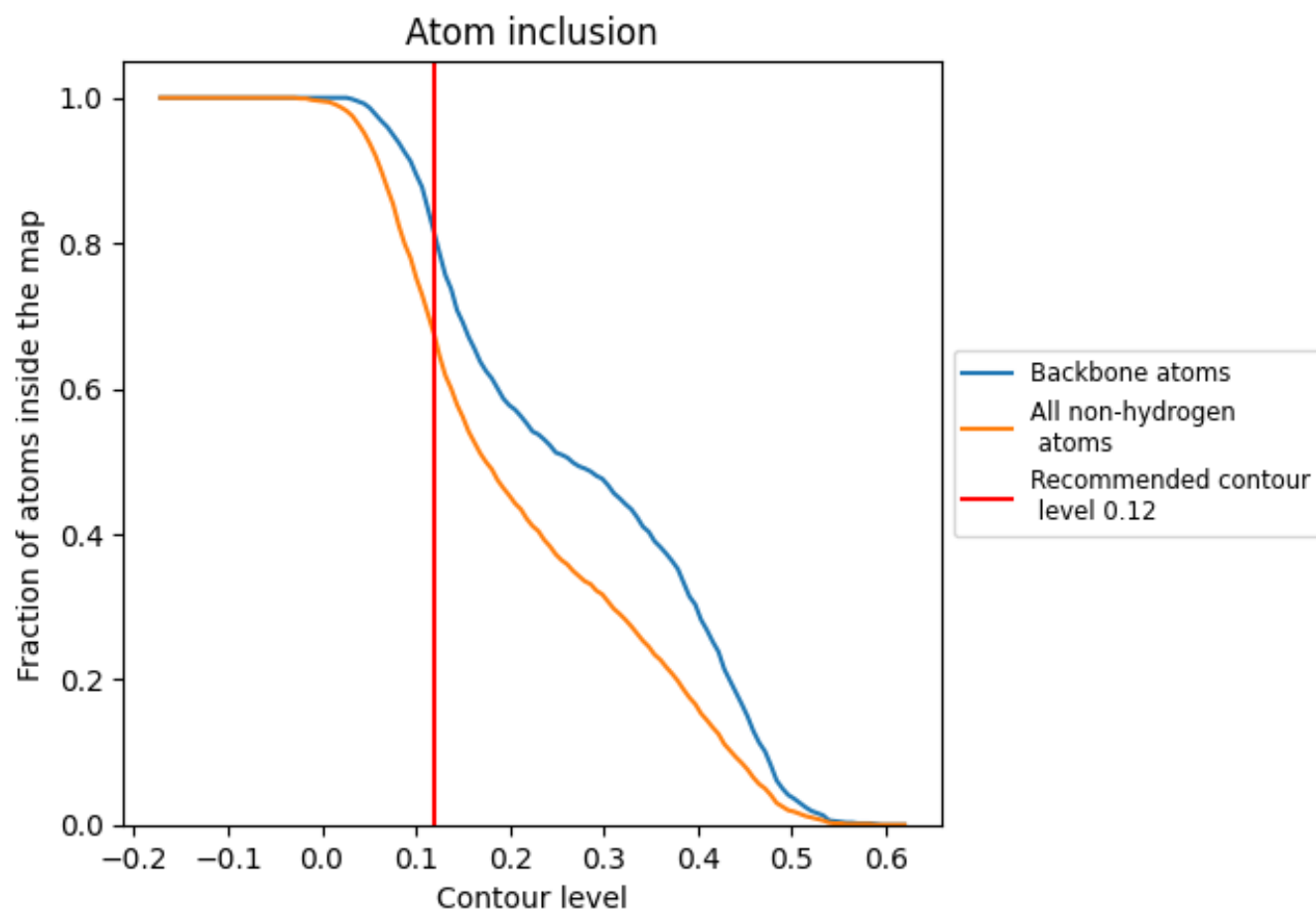


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 67% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6720	 0.3610
A	 0.7160	 0.3890
B	 0.7150	 0.3910
C	 0.7150	 0.3880
D	 0.7150	 0.3870
E	 0.7160	 0.3900
F	 0.7160	 0.3870
G	 0.7150	 0.3850
H	 0.7160	 0.3870
I	 0.7170	 0.3900
J	 0.7170	 0.3870
K	 0.7170	 0.3870
L	 0.7170	 0.3890
M	 0.7170	 0.3850
N	 0.7150	 0.3900
O	 0.7160	 0.3860
P	 0.7160	 0.3870
Q	 0.7150	 0.3890
R	 0.7160	 0.3850
S	 0.7150	 0.3860
T	 0.7160	 0.3850
U	 0.7160	 0.3870
V	 0.7170	 0.3860
W	 0.7170	 0.3890
X	 0.7170	 0.3890
a	 0.0930	 0.0280
b	 0.0930	 0.0260
c	 0.0930	 0.0260
d	 0.0930	 0.0310
e	 0.0930	 0.0210
f	 0.0930	 0.0420
g	 0.0930	 0.0250
h	 0.0930	 0.0240
i	 0.0930	 0.0180
j	 0.0930	 0.0290



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
k	 0.0930	 0.0280
l	 0.0930	 0.0220
m	 0.0930	 0.0180
n	 0.0930	 0.0280
o	 0.0930	 0.0360
p	 0.0930	 0.0310
q	 0.0930	 0.0160
r	 0.0930	 0.0270
s	 0.0930	 0.0400
t	 0.0930	 0.0190
u	 0.0930	 0.0400
v	 0.0930	 0.0230
w	 0.0930	 0.0240
x	 0.0930	 0.0270