



Full wwPDB EM Validation Report ⓘ

Jun 3, 2025 – 06:21 PM JST

PDB ID : 8ZUJ / pdb_00008zuj
EMDB ID : EMD-60485
Title : Pentagonal cluster of BAFF-BAFFR ectodomain complex
Authors : Lim, C.S.; Lee, J.O.
Deposited on : 2024-06-09
Resolution : 2.58 Å(reported)
Based on initial model : 4V46

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.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

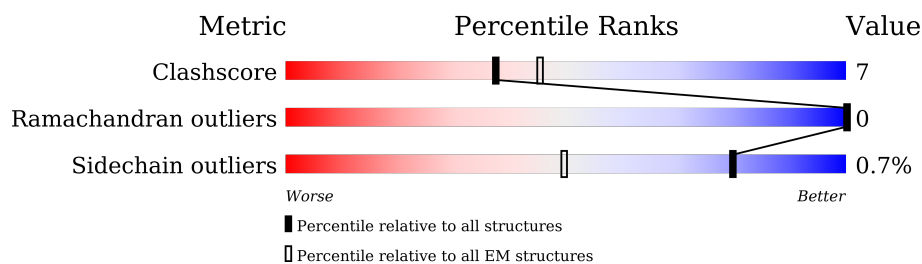
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.58 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	101	
1	B	101	
1	C	101	
1	G	101	
1	H	101	
1	I	101	
1	M	101	
1	N	101	

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Mol	Chain	Length	Quality of chain
1	O	101	
1	S	101	
1	T	101	
1	U	101	
1	Y	101	
1	Z	101	
1	a	101	
2	D	157	
2	E	157	
2	F	157	
2	J	157	
2	K	157	
2	L	157	
2	P	157	
2	Q	157	
2	R	157	
2	V	157	
2	W	157	
2	X	157	
2	b	157	
2	c	157	
2	d	157	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19830 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 Tumor necrosis factor receptor superfamily member 13C.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	24	Total	C	N	O	S	0	0
			179	114	32	29	4		
1	B	24	Total	C	N	O	S	0	0
			179	114	32	29	4		
1	C	24	Total	C	N	O	S	0	0
			179	114	32	29	4		
1	G	24	Total	C	N	O	S	0	0
			179	114	32	29	4		
1	H	24	Total	C	N	O	S	0	0
			179	114	32	29	4		
1	I	24	Total	C	N	O	S	0	0
			179	114	32	29	4		
1	M	24	Total	C	N	O	S	0	0
			179	114	32	29	4		
1	N	24	Total	C	N	O	S	0	0
			179	114	32	29	4		
1	O	24	Total	C	N	O	S	0	0
			179	114	32	29	4		
1	S	24	Total	C	N	O	S	0	0
			179	114	32	29	4		
1	T	24	Total	C	N	O	S	0	0
			179	114	32	29	4		
1	U	24	Total	C	N	O	S	0	0
			179	114	32	29	4		
1	Y	24	Total	C	N	O	S	0	0
			179	114	32	29	4		
1	Z	24	Total	C	N	O	S	0	0
			179	114	32	29	4		
1	a	24	Total	C	N	O	S	0	0
			179	114	32	29	4		

There are 360 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	ALA	-	expression tag	UNP Q96RJ3
A	-8	ASP	-	expression tag	UNP Q96RJ3
A	-7	PRO	-	expression tag	UNP Q96RJ3
A	-6	ASP	-	expression tag	UNP Q96RJ3
A	-5	TYR	-	expression tag	UNP Q96RJ3
A	-4	LYS	-	expression tag	UNP Q96RJ3
A	-3	ASP	-	expression tag	UNP Q96RJ3
A	-2	ASP	-	expression tag	UNP Q96RJ3
A	-1	ASP	-	expression tag	UNP Q96RJ3
A	0	ASP	-	expression tag	UNP Q96RJ3
A	1	LYS	-	expression tag	UNP Q96RJ3
A	79	GLY	-	expression tag	UNP Q96RJ3
A	80	GLY	-	expression tag	UNP Q96RJ3
A	81	GLY	-	expression tag	UNP Q96RJ3
A	82	GLY	-	expression tag	UNP Q96RJ3
A	83	SER	-	expression tag	UNP Q96RJ3
A	84	HIS	-	expression tag	UNP Q96RJ3
A	85	HIS	-	expression tag	UNP Q96RJ3
A	86	HIS	-	expression tag	UNP Q96RJ3
A	87	HIS	-	expression tag	UNP Q96RJ3
A	88	HIS	-	expression tag	UNP Q96RJ3
A	89	HIS	-	expression tag	UNP Q96RJ3
A	90	HIS	-	expression tag	UNP Q96RJ3
A	91	HIS	-	expression tag	UNP Q96RJ3
B	-9	ALA	-	expression tag	UNP Q96RJ3
B	-8	ASP	-	expression tag	UNP Q96RJ3
B	-7	PRO	-	expression tag	UNP Q96RJ3
B	-6	ASP	-	expression tag	UNP Q96RJ3
B	-5	TYR	-	expression tag	UNP Q96RJ3
B	-4	LYS	-	expression tag	UNP Q96RJ3
B	-3	ASP	-	expression tag	UNP Q96RJ3
B	-2	ASP	-	expression tag	UNP Q96RJ3
B	-1	ASP	-	expression tag	UNP Q96RJ3
B	0	ASP	-	expression tag	UNP Q96RJ3
B	1	LYS	-	expression tag	UNP Q96RJ3
B	79	GLY	-	expression tag	UNP Q96RJ3
B	80	GLY	-	expression tag	UNP Q96RJ3
B	81	GLY	-	expression tag	UNP Q96RJ3
B	82	GLY	-	expression tag	UNP Q96RJ3
B	83	SER	-	expression tag	UNP Q96RJ3
B	84	HIS	-	expression tag	UNP Q96RJ3
B	85	HIS	-	expression tag	UNP Q96RJ3
B	86	HIS	-	expression tag	UNP Q96RJ3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	87	HIS	-	expression tag	UNP Q96RJ3
B	88	HIS	-	expression tag	UNP Q96RJ3
B	89	HIS	-	expression tag	UNP Q96RJ3
B	90	HIS	-	expression tag	UNP Q96RJ3
B	91	HIS	-	expression tag	UNP Q96RJ3
C	-9	ALA	-	expression tag	UNP Q96RJ3
C	-8	ASP	-	expression tag	UNP Q96RJ3
C	-7	PRO	-	expression tag	UNP Q96RJ3
C	-6	ASP	-	expression tag	UNP Q96RJ3
C	-5	TYR	-	expression tag	UNP Q96RJ3
C	-4	LYS	-	expression tag	UNP Q96RJ3
C	-3	ASP	-	expression tag	UNP Q96RJ3
C	-2	ASP	-	expression tag	UNP Q96RJ3
C	-1	ASP	-	expression tag	UNP Q96RJ3
C	0	ASP	-	expression tag	UNP Q96RJ3
C	1	LYS	-	expression tag	UNP Q96RJ3
C	79	GLY	-	expression tag	UNP Q96RJ3
C	80	GLY	-	expression tag	UNP Q96RJ3
C	81	GLY	-	expression tag	UNP Q96RJ3
C	82	GLY	-	expression tag	UNP Q96RJ3
C	83	SER	-	expression tag	UNP Q96RJ3
C	84	HIS	-	expression tag	UNP Q96RJ3
C	85	HIS	-	expression tag	UNP Q96RJ3
C	86	HIS	-	expression tag	UNP Q96RJ3
C	87	HIS	-	expression tag	UNP Q96RJ3
C	88	HIS	-	expression tag	UNP Q96RJ3
C	89	HIS	-	expression tag	UNP Q96RJ3
C	90	HIS	-	expression tag	UNP Q96RJ3
C	91	HIS	-	expression tag	UNP Q96RJ3
G	-9	ALA	-	expression tag	UNP Q96RJ3
G	-8	ASP	-	expression tag	UNP Q96RJ3
G	-7	PRO	-	expression tag	UNP Q96RJ3
G	-6	ASP	-	expression tag	UNP Q96RJ3
G	-5	TYR	-	expression tag	UNP Q96RJ3
G	-4	LYS	-	expression tag	UNP Q96RJ3
G	-3	ASP	-	expression tag	UNP Q96RJ3
G	-2	ASP	-	expression tag	UNP Q96RJ3
G	-1	ASP	-	expression tag	UNP Q96RJ3
G	0	ASP	-	expression tag	UNP Q96RJ3
G	1	LYS	-	expression tag	UNP Q96RJ3
G	79	GLY	-	expression tag	UNP Q96RJ3
G	80	GLY	-	expression tag	UNP Q96RJ3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	81	GLY	-	expression tag	UNP Q96RJ3
G	82	GLY	-	expression tag	UNP Q96RJ3
G	83	SER	-	expression tag	UNP Q96RJ3
G	84	HIS	-	expression tag	UNP Q96RJ3
G	85	HIS	-	expression tag	UNP Q96RJ3
G	86	HIS	-	expression tag	UNP Q96RJ3
G	87	HIS	-	expression tag	UNP Q96RJ3
G	88	HIS	-	expression tag	UNP Q96RJ3
G	89	HIS	-	expression tag	UNP Q96RJ3
G	90	HIS	-	expression tag	UNP Q96RJ3
G	91	HIS	-	expression tag	UNP Q96RJ3
H	-9	ALA	-	expression tag	UNP Q96RJ3
H	-8	ASP	-	expression tag	UNP Q96RJ3
H	-7	PRO	-	expression tag	UNP Q96RJ3
H	-6	ASP	-	expression tag	UNP Q96RJ3
H	-5	TYR	-	expression tag	UNP Q96RJ3
H	-4	LYS	-	expression tag	UNP Q96RJ3
H	-3	ASP	-	expression tag	UNP Q96RJ3
H	-2	ASP	-	expression tag	UNP Q96RJ3
H	-1	ASP	-	expression tag	UNP Q96RJ3
H	0	ASP	-	expression tag	UNP Q96RJ3
H	1	LYS	-	expression tag	UNP Q96RJ3
H	79	GLY	-	expression tag	UNP Q96RJ3
H	80	GLY	-	expression tag	UNP Q96RJ3
H	81	GLY	-	expression tag	UNP Q96RJ3
H	82	GLY	-	expression tag	UNP Q96RJ3
H	83	SER	-	expression tag	UNP Q96RJ3
H	84	HIS	-	expression tag	UNP Q96RJ3
H	85	HIS	-	expression tag	UNP Q96RJ3
H	86	HIS	-	expression tag	UNP Q96RJ3
H	87	HIS	-	expression tag	UNP Q96RJ3
H	88	HIS	-	expression tag	UNP Q96RJ3
H	89	HIS	-	expression tag	UNP Q96RJ3
H	90	HIS	-	expression tag	UNP Q96RJ3
H	91	HIS	-	expression tag	UNP Q96RJ3
I	-9	ALA	-	expression tag	UNP Q96RJ3
I	-8	ASP	-	expression tag	UNP Q96RJ3
I	-7	PRO	-	expression tag	UNP Q96RJ3
I	-6	ASP	-	expression tag	UNP Q96RJ3
I	-5	TYR	-	expression tag	UNP Q96RJ3
I	-4	LYS	-	expression tag	UNP Q96RJ3
I	-3	ASP	-	expression tag	UNP Q96RJ3

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-2	ASP	-	expression tag	UNP Q96RJ3
I	-1	ASP	-	expression tag	UNP Q96RJ3
I	0	ASP	-	expression tag	UNP Q96RJ3
I	1	LYS	-	expression tag	UNP Q96RJ3
I	79	GLY	-	expression tag	UNP Q96RJ3
I	80	GLY	-	expression tag	UNP Q96RJ3
I	81	GLY	-	expression tag	UNP Q96RJ3
I	82	GLY	-	expression tag	UNP Q96RJ3
I	83	SER	-	expression tag	UNP Q96RJ3
I	84	HIS	-	expression tag	UNP Q96RJ3
I	85	HIS	-	expression tag	UNP Q96RJ3
I	86	HIS	-	expression tag	UNP Q96RJ3
I	87	HIS	-	expression tag	UNP Q96RJ3
I	88	HIS	-	expression tag	UNP Q96RJ3
I	89	HIS	-	expression tag	UNP Q96RJ3
I	90	HIS	-	expression tag	UNP Q96RJ3
I	91	HIS	-	expression tag	UNP Q96RJ3
M	-9	ALA	-	expression tag	UNP Q96RJ3
M	-8	ASP	-	expression tag	UNP Q96RJ3
M	-7	PRO	-	expression tag	UNP Q96RJ3
M	-6	ASP	-	expression tag	UNP Q96RJ3
M	-5	TYR	-	expression tag	UNP Q96RJ3
M	-4	LYS	-	expression tag	UNP Q96RJ3
M	-3	ASP	-	expression tag	UNP Q96RJ3
M	-2	ASP	-	expression tag	UNP Q96RJ3
M	-1	ASP	-	expression tag	UNP Q96RJ3
M	0	ASP	-	expression tag	UNP Q96RJ3
M	1	LYS	-	expression tag	UNP Q96RJ3
M	79	GLY	-	expression tag	UNP Q96RJ3
M	80	GLY	-	expression tag	UNP Q96RJ3
M	81	GLY	-	expression tag	UNP Q96RJ3
M	82	GLY	-	expression tag	UNP Q96RJ3
M	83	SER	-	expression tag	UNP Q96RJ3
M	84	HIS	-	expression tag	UNP Q96RJ3
M	85	HIS	-	expression tag	UNP Q96RJ3
M	86	HIS	-	expression tag	UNP Q96RJ3
M	87	HIS	-	expression tag	UNP Q96RJ3
M	88	HIS	-	expression tag	UNP Q96RJ3
M	89	HIS	-	expression tag	UNP Q96RJ3
M	90	HIS	-	expression tag	UNP Q96RJ3
M	91	HIS	-	expression tag	UNP Q96RJ3
N	-9	ALA	-	expression tag	UNP Q96RJ3

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-8	ASP	-	expression tag	UNP Q96RJ3
N	-7	PRO	-	expression tag	UNP Q96RJ3
N	-6	ASP	-	expression tag	UNP Q96RJ3
N	-5	TYR	-	expression tag	UNP Q96RJ3
N	-4	LYS	-	expression tag	UNP Q96RJ3
N	-3	ASP	-	expression tag	UNP Q96RJ3
N	-2	ASP	-	expression tag	UNP Q96RJ3
N	-1	ASP	-	expression tag	UNP Q96RJ3
N	0	ASP	-	expression tag	UNP Q96RJ3
N	1	LYS	-	expression tag	UNP Q96RJ3
N	79	GLY	-	expression tag	UNP Q96RJ3
N	80	GLY	-	expression tag	UNP Q96RJ3
N	81	GLY	-	expression tag	UNP Q96RJ3
N	82	GLY	-	expression tag	UNP Q96RJ3
N	83	SER	-	expression tag	UNP Q96RJ3
N	84	HIS	-	expression tag	UNP Q96RJ3
N	85	HIS	-	expression tag	UNP Q96RJ3
N	86	HIS	-	expression tag	UNP Q96RJ3
N	87	HIS	-	expression tag	UNP Q96RJ3
N	88	HIS	-	expression tag	UNP Q96RJ3
N	89	HIS	-	expression tag	UNP Q96RJ3
N	90	HIS	-	expression tag	UNP Q96RJ3
N	91	HIS	-	expression tag	UNP Q96RJ3
O	-9	ALA	-	expression tag	UNP Q96RJ3
O	-8	ASP	-	expression tag	UNP Q96RJ3
O	-7	PRO	-	expression tag	UNP Q96RJ3
O	-6	ASP	-	expression tag	UNP Q96RJ3
O	-5	TYR	-	expression tag	UNP Q96RJ3
O	-4	LYS	-	expression tag	UNP Q96RJ3
O	-3	ASP	-	expression tag	UNP Q96RJ3
O	-2	ASP	-	expression tag	UNP Q96RJ3
O	-1	ASP	-	expression tag	UNP Q96RJ3
O	0	ASP	-	expression tag	UNP Q96RJ3
O	1	LYS	-	expression tag	UNP Q96RJ3
O	79	GLY	-	expression tag	UNP Q96RJ3
O	80	GLY	-	expression tag	UNP Q96RJ3
O	81	GLY	-	expression tag	UNP Q96RJ3
O	82	GLY	-	expression tag	UNP Q96RJ3
O	83	SER	-	expression tag	UNP Q96RJ3
O	84	HIS	-	expression tag	UNP Q96RJ3
O	85	HIS	-	expression tag	UNP Q96RJ3
O	86	HIS	-	expression tag	UNP Q96RJ3

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Chain	Residue	Modelled	Actual	Comment	Reference
O	87	HIS	-	expression tag	UNP Q96RJ3
O	88	HIS	-	expression tag	UNP Q96RJ3
O	89	HIS	-	expression tag	UNP Q96RJ3
O	90	HIS	-	expression tag	UNP Q96RJ3
O	91	HIS	-	expression tag	UNP Q96RJ3
S	-9	ALA	-	expression tag	UNP Q96RJ3
S	-8	ASP	-	expression tag	UNP Q96RJ3
S	-7	PRO	-	expression tag	UNP Q96RJ3
S	-6	ASP	-	expression tag	UNP Q96RJ3
S	-5	TYR	-	expression tag	UNP Q96RJ3
S	-4	LYS	-	expression tag	UNP Q96RJ3
S	-3	ASP	-	expression tag	UNP Q96RJ3
S	-2	ASP	-	expression tag	UNP Q96RJ3
S	-1	ASP	-	expression tag	UNP Q96RJ3
S	0	ASP	-	expression tag	UNP Q96RJ3
S	1	LYS	-	expression tag	UNP Q96RJ3
S	79	GLY	-	expression tag	UNP Q96RJ3
S	80	GLY	-	expression tag	UNP Q96RJ3
S	81	GLY	-	expression tag	UNP Q96RJ3
S	82	GLY	-	expression tag	UNP Q96RJ3
S	83	SER	-	expression tag	UNP Q96RJ3
S	84	HIS	-	expression tag	UNP Q96RJ3
S	85	HIS	-	expression tag	UNP Q96RJ3
S	86	HIS	-	expression tag	UNP Q96RJ3
S	87	HIS	-	expression tag	UNP Q96RJ3
S	88	HIS	-	expression tag	UNP Q96RJ3
S	89	HIS	-	expression tag	UNP Q96RJ3
S	90	HIS	-	expression tag	UNP Q96RJ3
S	91	HIS	-	expression tag	UNP Q96RJ3
T	-9	ALA	-	expression tag	UNP Q96RJ3
T	-8	ASP	-	expression tag	UNP Q96RJ3
T	-7	PRO	-	expression tag	UNP Q96RJ3
T	-6	ASP	-	expression tag	UNP Q96RJ3
T	-5	TYR	-	expression tag	UNP Q96RJ3
T	-4	LYS	-	expression tag	UNP Q96RJ3
T	-3	ASP	-	expression tag	UNP Q96RJ3
T	-2	ASP	-	expression tag	UNP Q96RJ3
T	-1	ASP	-	expression tag	UNP Q96RJ3
T	0	ASP	-	expression tag	UNP Q96RJ3
T	1	LYS	-	expression tag	UNP Q96RJ3
T	79	GLY	-	expression tag	UNP Q96RJ3
T	80	GLY	-	expression tag	UNP Q96RJ3

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Chain	Residue	Modelled	Actual	Comment	Reference
T	81	GLY	-	expression tag	UNP Q96RJ3
T	82	GLY	-	expression tag	UNP Q96RJ3
T	83	SER	-	expression tag	UNP Q96RJ3
T	84	HIS	-	expression tag	UNP Q96RJ3
T	85	HIS	-	expression tag	UNP Q96RJ3
T	86	HIS	-	expression tag	UNP Q96RJ3
T	87	HIS	-	expression tag	UNP Q96RJ3
T	88	HIS	-	expression tag	UNP Q96RJ3
T	89	HIS	-	expression tag	UNP Q96RJ3
T	90	HIS	-	expression tag	UNP Q96RJ3
T	91	HIS	-	expression tag	UNP Q96RJ3
U	-9	ALA	-	expression tag	UNP Q96RJ3
U	-8	ASP	-	expression tag	UNP Q96RJ3
U	-7	PRO	-	expression tag	UNP Q96RJ3
U	-6	ASP	-	expression tag	UNP Q96RJ3
U	-5	TYR	-	expression tag	UNP Q96RJ3
U	-4	LYS	-	expression tag	UNP Q96RJ3
U	-3	ASP	-	expression tag	UNP Q96RJ3
U	-2	ASP	-	expression tag	UNP Q96RJ3
U	-1	ASP	-	expression tag	UNP Q96RJ3
U	0	ASP	-	expression tag	UNP Q96RJ3
U	1	LYS	-	expression tag	UNP Q96RJ3
U	79	GLY	-	expression tag	UNP Q96RJ3
U	80	GLY	-	expression tag	UNP Q96RJ3
U	81	GLY	-	expression tag	UNP Q96RJ3
U	82	GLY	-	expression tag	UNP Q96RJ3
U	83	SER	-	expression tag	UNP Q96RJ3
U	84	HIS	-	expression tag	UNP Q96RJ3
U	85	HIS	-	expression tag	UNP Q96RJ3
U	86	HIS	-	expression tag	UNP Q96RJ3
U	87	HIS	-	expression tag	UNP Q96RJ3
U	88	HIS	-	expression tag	UNP Q96RJ3
U	89	HIS	-	expression tag	UNP Q96RJ3
U	90	HIS	-	expression tag	UNP Q96RJ3
U	91	HIS	-	expression tag	UNP Q96RJ3
Y	-9	ALA	-	expression tag	UNP Q96RJ3
Y	-8	ASP	-	expression tag	UNP Q96RJ3
Y	-7	PRO	-	expression tag	UNP Q96RJ3
Y	-6	ASP	-	expression tag	UNP Q96RJ3
Y	-5	TYR	-	expression tag	UNP Q96RJ3
Y	-4	LYS	-	expression tag	UNP Q96RJ3
Y	-3	ASP	-	expression tag	UNP Q96RJ3

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	-2	ASP	-	expression tag	UNP Q96RJ3
Y	-1	ASP	-	expression tag	UNP Q96RJ3
Y	0	ASP	-	expression tag	UNP Q96RJ3
Y	1	LYS	-	expression tag	UNP Q96RJ3
Y	79	GLY	-	expression tag	UNP Q96RJ3
Y	80	GLY	-	expression tag	UNP Q96RJ3
Y	81	GLY	-	expression tag	UNP Q96RJ3
Y	82	GLY	-	expression tag	UNP Q96RJ3
Y	83	SER	-	expression tag	UNP Q96RJ3
Y	84	HIS	-	expression tag	UNP Q96RJ3
Y	85	HIS	-	expression tag	UNP Q96RJ3
Y	86	HIS	-	expression tag	UNP Q96RJ3
Y	87	HIS	-	expression tag	UNP Q96RJ3
Y	88	HIS	-	expression tag	UNP Q96RJ3
Y	89	HIS	-	expression tag	UNP Q96RJ3
Y	90	HIS	-	expression tag	UNP Q96RJ3
Y	91	HIS	-	expression tag	UNP Q96RJ3
Z	-9	ALA	-	expression tag	UNP Q96RJ3
Z	-8	ASP	-	expression tag	UNP Q96RJ3
Z	-7	PRO	-	expression tag	UNP Q96RJ3
Z	-6	ASP	-	expression tag	UNP Q96RJ3
Z	-5	TYR	-	expression tag	UNP Q96RJ3
Z	-4	LYS	-	expression tag	UNP Q96RJ3
Z	-3	ASP	-	expression tag	UNP Q96RJ3
Z	-2	ASP	-	expression tag	UNP Q96RJ3
Z	-1	ASP	-	expression tag	UNP Q96RJ3
Z	0	ASP	-	expression tag	UNP Q96RJ3
Z	1	LYS	-	expression tag	UNP Q96RJ3
Z	79	GLY	-	expression tag	UNP Q96RJ3
Z	80	GLY	-	expression tag	UNP Q96RJ3
Z	81	GLY	-	expression tag	UNP Q96RJ3
Z	82	GLY	-	expression tag	UNP Q96RJ3
Z	83	SER	-	expression tag	UNP Q96RJ3
Z	84	HIS	-	expression tag	UNP Q96RJ3
Z	85	HIS	-	expression tag	UNP Q96RJ3
Z	86	HIS	-	expression tag	UNP Q96RJ3
Z	87	HIS	-	expression tag	UNP Q96RJ3
Z	88	HIS	-	expression tag	UNP Q96RJ3
Z	89	HIS	-	expression tag	UNP Q96RJ3
Z	90	HIS	-	expression tag	UNP Q96RJ3
Z	91	HIS	-	expression tag	UNP Q96RJ3
a	-9	ALA	-	expression tag	UNP Q96RJ3

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Chain	Residue	Modelled	Actual	Comment	Reference
a	-8	ASP	-	expression tag	UNP Q96RJ3
a	-7	PRO	-	expression tag	UNP Q96RJ3
a	-6	ASP	-	expression tag	UNP Q96RJ3
a	-5	TYR	-	expression tag	UNP Q96RJ3
a	-4	LYS	-	expression tag	UNP Q96RJ3
a	-3	ASP	-	expression tag	UNP Q96RJ3
a	-2	ASP	-	expression tag	UNP Q96RJ3
a	-1	ASP	-	expression tag	UNP Q96RJ3
a	0	ASP	-	expression tag	UNP Q96RJ3
a	1	LYS	-	expression tag	UNP Q96RJ3
a	79	GLY	-	expression tag	UNP Q96RJ3
a	80	GLY	-	expression tag	UNP Q96RJ3
a	81	GLY	-	expression tag	UNP Q96RJ3
a	82	GLY	-	expression tag	UNP Q96RJ3
a	83	SER	-	expression tag	UNP Q96RJ3
a	84	HIS	-	expression tag	UNP Q96RJ3
a	85	HIS	-	expression tag	UNP Q96RJ3
a	86	HIS	-	expression tag	UNP Q96RJ3
a	87	HIS	-	expression tag	UNP Q96RJ3
a	88	HIS	-	expression tag	UNP Q96RJ3
a	89	HIS	-	expression tag	UNP Q96RJ3
a	90	HIS	-	expression tag	UNP Q96RJ3
a	91	HIS	-	expression tag	UNP Q96RJ3

- Molecule 2 is a protein called Tumor necrosis factor ligand superfamily member 13b, soluble form.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	144	Total	C	N	O	S	0	0
			1143	736	184	218	5		
2	E	144	Total	C	N	O	S	0	0
			1143	736	184	218	5		
2	F	144	Total	C	N	O	S	0	0
			1143	736	184	218	5		
2	J	144	Total	C	N	O	S	0	0
			1143	736	184	218	5		
2	K	144	Total	C	N	O	S	0	0
			1143	736	184	218	5		
2	L	144	Total	C	N	O	S	0	0
			1143	736	184	218	5		
2	P	144	Total	C	N	O	S	0	0
			1143	736	184	218	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Q	144	Total	C	N	O	S	0	0
			1143	736	184	218	5		
2	R	144	Total	C	N	O	S	0	0
			1143	736	184	218	5		
2	V	144	Total	C	N	O	S	0	0
			1143	736	184	218	5		
2	W	144	Total	C	N	O	S	0	0
			1143	736	184	218	5		
2	X	144	Total	C	N	O	S	0	0
			1143	736	184	218	5		
2	b	144	Total	C	N	O	S	0	0
			1143	736	184	218	5		
2	c	144	Total	C	N	O	S	0	0
			1143	736	184	218	5		
2	d	144	Total	C	N	O	S	0	0
			1143	736	184	218	5		

There are 75 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	129	GLY	-	expression tag	UNP Q9Y275
D	130	SER	-	expression tag	UNP Q9Y275
D	131	GLY	-	expression tag	UNP Q9Y275
D	132	GLY	-	expression tag	UNP Q9Y275
D	133	SER	-	expression tag	UNP Q9Y275
E	129	GLY	-	expression tag	UNP Q9Y275
E	130	SER	-	expression tag	UNP Q9Y275
E	131	GLY	-	expression tag	UNP Q9Y275
E	132	GLY	-	expression tag	UNP Q9Y275
E	133	SER	-	expression tag	UNP Q9Y275
F	129	GLY	-	expression tag	UNP Q9Y275
F	130	SER	-	expression tag	UNP Q9Y275
F	131	GLY	-	expression tag	UNP Q9Y275
F	132	GLY	-	expression tag	UNP Q9Y275
F	133	SER	-	expression tag	UNP Q9Y275
J	129	GLY	-	expression tag	UNP Q9Y275
J	130	SER	-	expression tag	UNP Q9Y275
J	131	GLY	-	expression tag	UNP Q9Y275
J	132	GLY	-	expression tag	UNP Q9Y275
J	133	SER	-	expression tag	UNP Q9Y275
K	129	GLY	-	expression tag	UNP Q9Y275
K	130	SER	-	expression tag	UNP Q9Y275
K	131	GLY	-	expression tag	UNP Q9Y275

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Chain	Residue	Modelled	Actual	Comment	Reference
K	132	GLY	-	expression tag	UNP Q9Y275
K	133	SER	-	expression tag	UNP Q9Y275
L	129	GLY	-	expression tag	UNP Q9Y275
L	130	SER	-	expression tag	UNP Q9Y275
L	131	GLY	-	expression tag	UNP Q9Y275
L	132	GLY	-	expression tag	UNP Q9Y275
L	133	SER	-	expression tag	UNP Q9Y275
P	129	GLY	-	expression tag	UNP Q9Y275
P	130	SER	-	expression tag	UNP Q9Y275
P	131	GLY	-	expression tag	UNP Q9Y275
P	132	GLY	-	expression tag	UNP Q9Y275
P	133	SER	-	expression tag	UNP Q9Y275
Q	129	GLY	-	expression tag	UNP Q9Y275
Q	130	SER	-	expression tag	UNP Q9Y275
Q	131	GLY	-	expression tag	UNP Q9Y275
Q	132	GLY	-	expression tag	UNP Q9Y275
Q	133	SER	-	expression tag	UNP Q9Y275
R	129	GLY	-	expression tag	UNP Q9Y275
R	130	SER	-	expression tag	UNP Q9Y275
R	131	GLY	-	expression tag	UNP Q9Y275
R	132	GLY	-	expression tag	UNP Q9Y275
R	133	SER	-	expression tag	UNP Q9Y275
V	129	GLY	-	expression tag	UNP Q9Y275
V	130	SER	-	expression tag	UNP Q9Y275
V	131	GLY	-	expression tag	UNP Q9Y275
V	132	GLY	-	expression tag	UNP Q9Y275
V	133	SER	-	expression tag	UNP Q9Y275
W	129	GLY	-	expression tag	UNP Q9Y275
W	130	SER	-	expression tag	UNP Q9Y275
W	131	GLY	-	expression tag	UNP Q9Y275
W	132	GLY	-	expression tag	UNP Q9Y275
W	133	SER	-	expression tag	UNP Q9Y275
X	129	GLY	-	expression tag	UNP Q9Y275
X	130	SER	-	expression tag	UNP Q9Y275
X	131	GLY	-	expression tag	UNP Q9Y275
X	132	GLY	-	expression tag	UNP Q9Y275
X	133	SER	-	expression tag	UNP Q9Y275
b	129	GLY	-	expression tag	UNP Q9Y275
b	130	SER	-	expression tag	UNP Q9Y275
b	131	GLY	-	expression tag	UNP Q9Y275
b	132	GLY	-	expression tag	UNP Q9Y275
b	133	SER	-	expression tag	UNP Q9Y275

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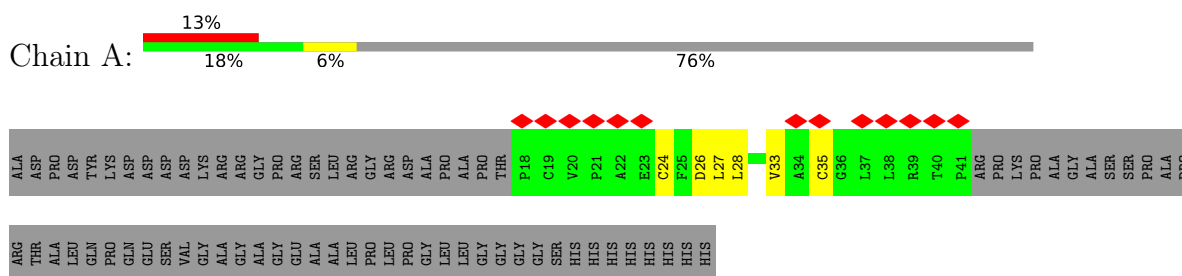
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Chain	Residue	Modelled	Actual	Comment	Reference
c	129	GLY	-	expression tag	UNP Q9Y275
c	130	SER	-	expression tag	UNP Q9Y275
c	131	GLY	-	expression tag	UNP Q9Y275
c	132	GLY	-	expression tag	UNP Q9Y275
c	133	SER	-	expression tag	UNP Q9Y275
d	129	GLY	-	expression tag	UNP Q9Y275
d	130	SER	-	expression tag	UNP Q9Y275
d	131	GLY	-	expression tag	UNP Q9Y275
d	132	GLY	-	expression tag	UNP Q9Y275
d	133	SER	-	expression tag	UNP Q9Y275

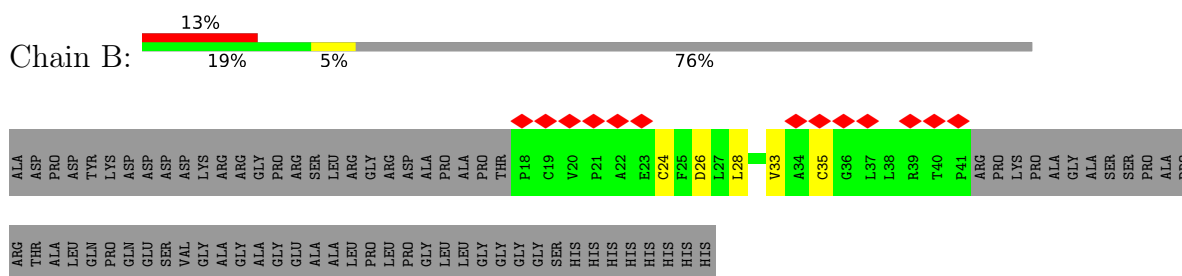
3 Residue-property plots [i](#)

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.

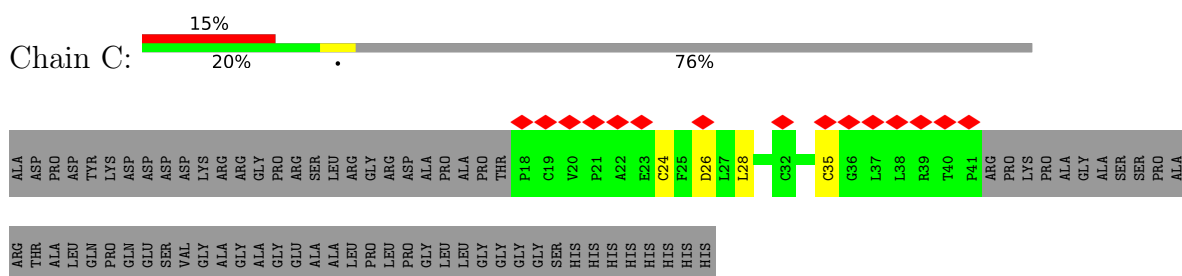
- Molecule 1: Tumor necrosis factor receptor superfamily member 13C



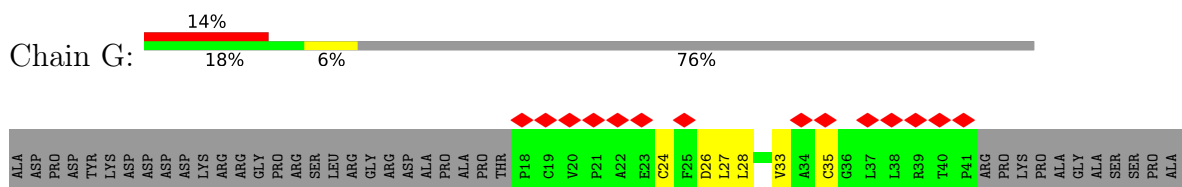
- Molecule 1: Tumor necrosis factor receptor superfamily member 13C



- Molecule 1: Tumor necrosis factor receptor superfamily member 13C



- Molecule 1: Tumor necrosis factor receptor superfamily member 13C



ARG THR ALA ASP PRO GLN GLN GLU VAL ASP SER GLY ALA ARG GLY ALA GLY GLU GLU ALA ALA LEU PRO PRO LEU PRO PRO GLY GLY GLY GLY SER HIS HIS HIS HIS HIS HIS HIS

- Molecule 1: Tumor necrosis factor receptor superfamily member 13C



ALA ASP PRO TYR LYS ASP ASP ASP VAL ASP LYS ARG ARG GLY PRO ARG SER LEU ARG GLY PRO ARG ASP PRO ALA ALA PRO THR P18 C19 V20 P21 A22 E23 C24 F25 D26 L27 L28 V33 A34 C35 G36 L37 L38 R39 T40 P41 ARG PRO LYS PRO PRO GLY ALA ALA SER PRO ALA PRO

ARG THR ALA ASP PRO GLN GLN GLU VAL ASP SER GLY ALA ARG GLY ALA GLY GLU GLU ALA ALA LEU PRO PRO LEU PRO PRO GLY GLY GLY GLY SER HIS HIS HIS HIS HIS HIS HIS

- Molecule 1: Tumor necrosis factor receptor superfamily member 13C



ALA ASP PRO TYR LYS ASP ASP ASP VAL ASP LYS ARG ARG GLY PRO ARG SER LEU ARG GLY PRO ARG ASP PRO ALA ALA PRO THR P18 C19 V20 P21 A22 E23 C24 F25 D26 L27 L28 V33 A34 C35 G36 L37 L38 R39 T40 P41 ARG PRO LYS PRO PRO GLY ALA ALA SER PRO ALA PRO

PRO ARG THR ALA ASP PRO GLN GLN GLU VAL ASP SER GLY ALA ARG GLY ALA GLY GLU GLU ALA ALA LEU PRO PRO LEU PRO PRO GLY GLY GLY GLY SER HIS HIS HIS HIS HIS HIS HIS

- Molecule 1: Tumor necrosis factor receptor superfamily member 13C



ALA ASP PRO TYR LYS ASP ASP ASP VAL ASP LYS ARG ARG GLY PRO ARG SER LEU ARG GLY PRO ARG ASP PRO ALA ALA PRO THR P18 C19 V20 P21 A22 E23 C24 F25 D26 L27 L28 V33 A34 C35 G36 L37 L38 R39 T40 P41 ARG PRO LYS PRO PRO GLY ALA ALA SER PRO ALA PRO

THR ALA ASP PRO GLN GLN GLU VAL ASP SER GLY ALA ARG GLY ALA GLY GLU GLU ALA ALA LEU PRO PRO LEU PRO PRO GLY GLY GLY GLY SER HIS HIS HIS HIS HIS HIS HIS

- Molecule 1: Tumor necrosis factor receptor superfamily member 13C



ALA ASP PRO TYR LYS ASP ASP ASP VAL ASP LYS ARG ARG GLY PRO ARG SER LEU ARG GLY PRO ARG ASP PRO ALA ALA PRO THR P18 C19 V20 P21 A22 E23 C24 F25 D26 L27 L28 V33 A34 C35 G36 L37 L38 R39 T40 P41 ARG PRO LYS PRO PRO GLY ALA ALA SER PRO ALA PRO

ARG THR ALA ASP PRO GLN GLN GLU VAL ASP SER GLY ALA ARG GLY ALA GLY GLU GLU ALA ALA LEU PRO PRO LEU PRO PRO GLY GLY GLY GLY SER HIS HIS HIS HIS HIS HIS HIS

- Molecule 1: Tumor necrosis factor receptor superfamily member 13C



ALA ASP PRO TYR LYS ASP ASP ASP VAL ASP LYS ARG ARG GLY PRO ARG SER LEU ARG GLY PRO ARG ASP PRO ALA ALA PRO THR P18 C19 V20 P21 A22 E23 C24 F25 D26 L27 L28 V33 A34 C35 G36 L37 L38 R39 T40 P41 ARG PRO LYS PRO PRO GLY ALA ALA SER PRO ALA PRO

PRO ARG ASP THR ALA ASP THR LEU GLN LYS PRO GLN GLU SER VAL GLY ARG ALA GLY ALA GLY ALA GLU ALA LEU ALA LEU PRO PRO LEU PRO PRO PRO GLY LEU LEU GLY THR GLY GLY GLY SER HIS HIS HIS HIS HIS HIS HIS

- Molecule 1: Tumor necrosis factor receptor superfamily member 13C

Chain S: 

ALA ASP THR ALA ASP THR LEU GLN LYS PRO GLN GLU SER VAL GLY ARG ALA GLY ALA GLY ALA GLU ALA LEU ALA LEU PRO PRO THR P18 C19 V20 F21 A22 E23 C24 F25 D26 L27 L28 V33 A34 C35 G36 L37 L38 R39 T40 P41 ARG PRO LYS PRO PRO GLY ALA ALA SER SER PRO PRO ALA PRO

- Molecule 1: Tumor necrosis factor receptor superfamily member 13C

Chain T: 

ALA ASP THR ALA ASP THR LEU GLN LYS PRO GLN GLU SER VAL GLY ARG ALA GLY ALA GLY ALA GLU ALA LEU ALA LEU PRO PRO THR P18 C19 V20 F21 A22 E23 C24 F25 D26 L27 L28 V33 A34 C35 G36 L37 L38 R39 T40 P41 ARG PRO LYS PRO PRO GLY ALA ALA SER SER PRO PRO ALA PRO

- Molecule 1: Tumor necrosis factor receptor superfamily member 13C

Chain U: 

ALA ASP THR ALA ASP THR LEU GLN LYS PRO GLN GLU SER VAL GLY ARG ALA GLY ALA GLY ALA GLU ALA LEU ALA LEU PRO PRO THR P18 C19 V20 F21 A22 E23 C24 F25 D26 L27 L28 V33 A34 C35 G36 L37 L38 R39 T40 P41 ARG PRO LYS PRO PRO GLY ALA ALA SER SER PRO PRO ALA PRO

- Molecule 1: Tumor necrosis factor receptor superfamily member 13C

Chain Y: 

ALA ASP THR ALA ASP THR LEU GLN LYS PRO GLN GLU SER VAL GLY ARG ALA GLY ALA GLY ALA GLU ALA LEU ALA LEU PRO PRO THR P18 C19 V20 F21 A22 E23 C24 F25 D26 L27 L28 V33 A34 C35 G36 L37 L38 R39 T40 P41 ARG PRO LYS PRO PRO GLY ALA ALA SER SER PRO PRO ALA PRO

- Molecule 1: Tumor necrosis factor receptor superfamily member 13C

Chain Z: 

ALA ASP THR ALA ASP THR LEU GLN LYS PRO GLN GLU SER VAL GLY ARG ALA GLY ALA GLY ALA GLU ALA LEU ALA LEU PRO PRO THR P18 C19 V20 F21 A22 E23 C24 F25 D26 L27 L28 V33 A34 C35 G36 L37 L38 R39 T40 P41 ARG PRO LYS PRO PRO GLY ALA ALA SER SER PRO PRO ALA PRO

ARG THR
ALA
LEU
GLN
PRO
GLN
GLU
SER
VAL
GLY
ALA
ALA
GLY
GLU
GLY
ALA
ALA
LEU
PRO
LEU
PRO
PRO
GLY
GLY
LEU
LEU
GLY
GLY
GLY
GLY
SER
HIS
HIS
HIS
HIS
HIS
HIS

- Molecule 1: Tumor necrosis factor receptor superfamily member 13C

Chain a: 


ALA ASP PRO THR TYR LYS ASP ASP LYS ARG ARG GLY PRO ARG SER LEU ALA ARG LEU PRO THR P18 C19 V20 P21 A22 E23 C24 F25 D26 L27 L28 C32 V33 A34 C35 G36 L37 L38 R39 T40 P41 ARG PRO LYS PRO PRO ALA GLY ALA SER SER PRO ALA

- Molecule 2: Tumor necrosis factor ligand superfamily member 13b, soluble form

Chain D: 

GLY SER GLY GLY SER ALA VAL GLN GLY PRO GLU GLU THR V142 T143 I150 A151 D152 S153 E154 T155 P156 T157 I158 Y163 T164 F165 S171 F172 K173 R174 G175 S176 K181 E182 I185 L186 V187 K188 E189 T190 G191 Q198 V199 L200 D203 G209 R214 K215 V216 V217 H218 V219 F220 G221 D222 E223 L224 L229 F230 R231 C232 I233 E238 C245 Y246 K252 L253 E254 E255 G256 D257 E258 L259 T263 P264 D269 V276 L285

- Molecule 2: Tumor necrosis factor ligand superfamily member 13b, soluble form

Chain E: 

GLY SER GLY GLY SER ALA VAL GLN GLY PRO GLU GLU THR V142 D145 I150 S153 E154 I158 T164 F165 S171 F172 K173 R174 G175 S176 E179 E180 E182 I185 L186 E189 Q198 V199 L200 G209 K215 K216 E223 L226 V227 C232 I233 E238 C245 Y246 E254 E258 L259 I263 P264 A268 D275 V276 K283 L284 L285

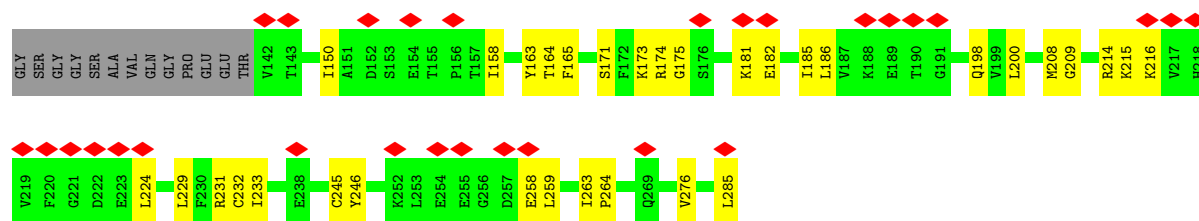
- Molecule 2: Tumor necrosis factor ligand superfamily member 13b, soluble form

Chain F: 

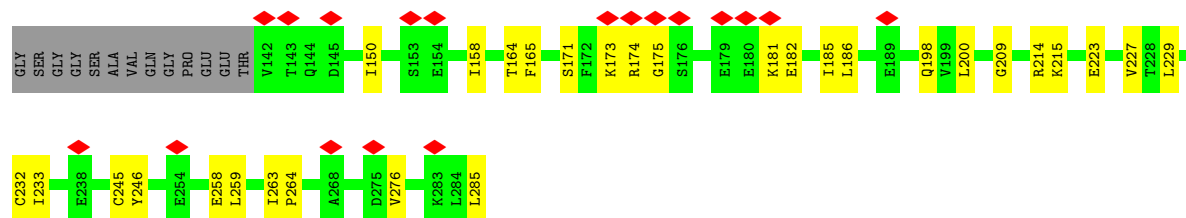
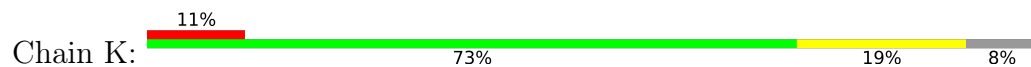
GLY SER GLY GLY SER ALA VAL GLN GLY PRO GLU GLU THR V142 I150 E154 T157 I158 Q159 K160 G161 S162 Y163 T164 F165 S171 F172 K173 R174 G175 S176 K181 E182 I185 L186 Q198 V199 L200 K204 T205 Y206 A207 M208 G209 R214 K215 E223 L224 S225 L226 V227 T228 L229 F230 R231 C232 I233 E238 T239 L240 C245 Y246 E258 L259 I263 E266 N267 V276 L285

- Molecule 2: Tumor necrosis factor ligand superfamily member 13b, soluble form

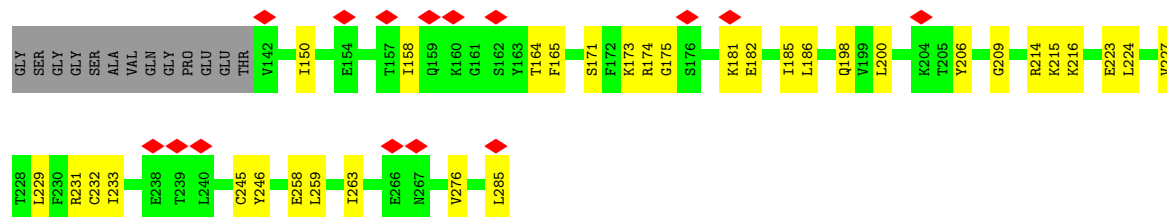
Chain J: 



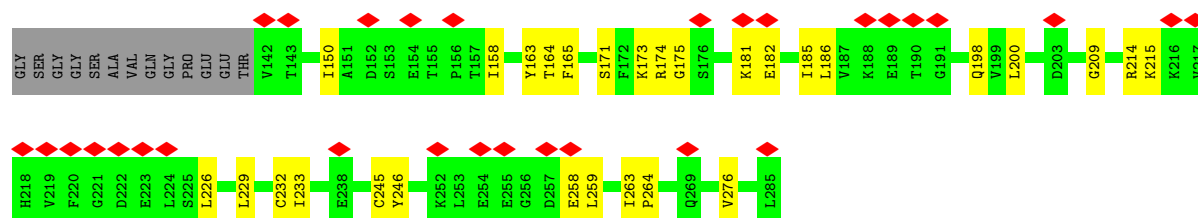
- Molecule 2: Tumor necrosis factor ligand superfamily member 13b, soluble form



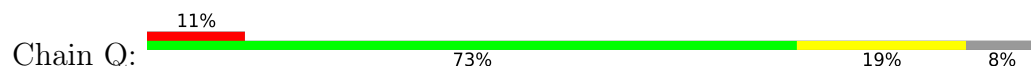
- Molecule 2: Tumor necrosis factor ligand superfamily member 13b, soluble form

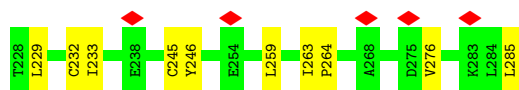


- Molecule 2: Tumor necrosis factor ligand superfamily member 13b, soluble form

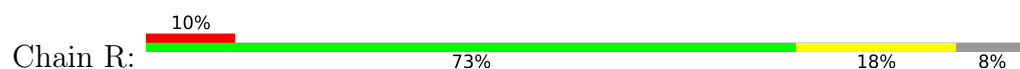


- Molecule 2: Tumor necrosis factor ligand superfamily member 13b, soluble form

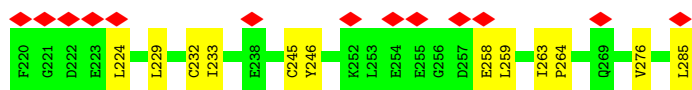
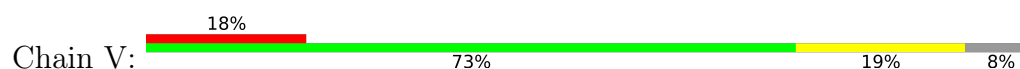




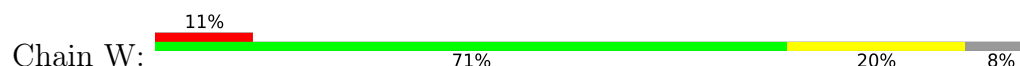
- Molecule 2: Tumor necrosis factor ligand superfamily member 13b, soluble form



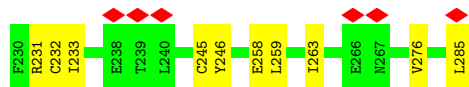
- Molecule 2: Tumor necrosis factor ligand superfamily member 13b, soluble form



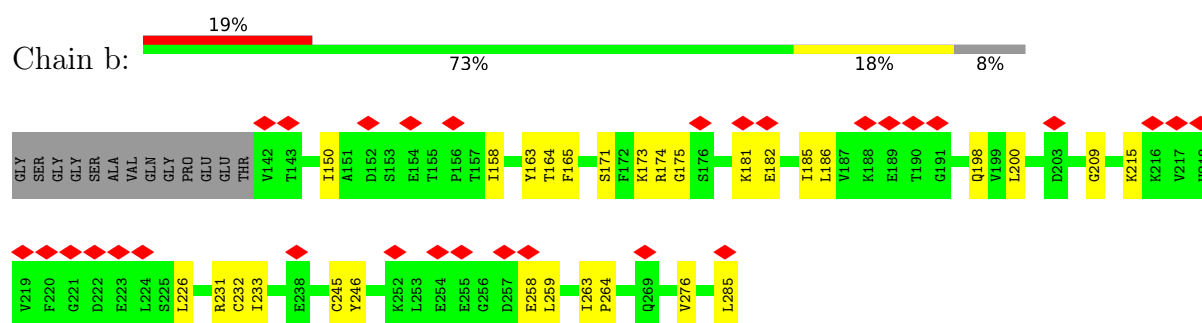
- Molecule 2: Tumor necrosis factor ligand superfamily member 13b, soluble form



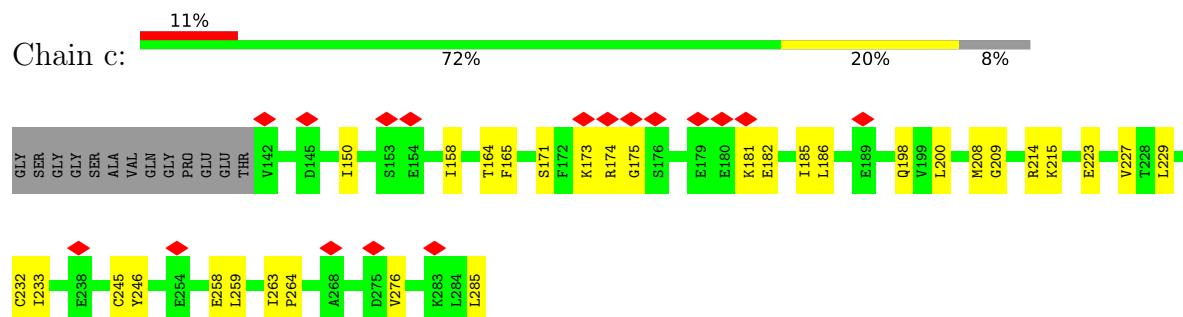
- Molecule 2: Tumor necrosis factor ligand superfamily member 13b, soluble form



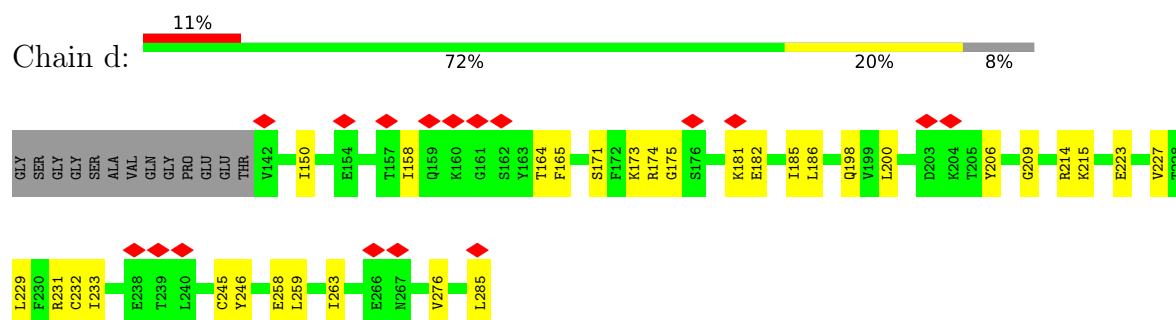
- Molecule 2: Tumor necrosis factor ligand superfamily member 13b, soluble form



- Molecule 2: Tumor necrosis factor ligand superfamily member 13b, soluble form



- Molecule 2: Tumor necrosis factor ligand superfamily member 13b, soluble form



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	220800	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	100500	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.429	Depositor
Minimum map value	-2.346	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.062	Depositor
Recommended contour level	0.38	Depositor
Map size (Å)	328.80002, 328.80002, 328.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	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	0.20	0/183	0.49	0/249
1	B	0.19	0/183	0.48	0/249
1	C	0.20	0/183	0.49	0/249
1	G	0.19	0/183	0.49	0/249
1	H	0.20	0/183	0.48	0/249
1	I	0.19	0/183	0.49	0/249
1	M	0.20	0/183	0.49	0/249
1	N	0.20	0/183	0.48	0/249
1	O	0.19	0/183	0.48	0/249
1	S	0.19	0/183	0.48	0/249
1	T	0.20	0/183	0.48	0/249
1	U	0.19	0/183	0.49	0/249
1	Y	0.19	0/183	0.48	0/249
1	Z	0.20	0/183	0.48	0/249
1	a	0.19	0/183	0.49	0/249
2	D	0.12	0/1165	0.35	0/1574
2	E	0.12	0/1165	0.35	0/1574
2	F	0.12	0/1165	0.35	0/1574
2	J	0.12	0/1165	0.35	0/1574
2	K	0.12	0/1165	0.35	0/1574
2	L	0.12	0/1165	0.35	0/1574
2	P	0.12	0/1165	0.35	0/1574
2	Q	0.12	0/1165	0.35	0/1574
2	R	0.12	0/1165	0.35	0/1574
2	V	0.12	0/1165	0.35	0/1574
2	W	0.12	0/1165	0.35	0/1574
2	X	0.12	0/1165	0.35	0/1574
2	b	0.12	0/1165	0.35	0/1574
2	c	0.12	0/1165	0.35	0/1574
2	d	0.12	0/1165	0.35	0/1574
All	All	0.13	0/20220	0.37	0/27345

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	179	0	180	5	0
1	B	179	0	180	3	0
1	C	179	0	180	3	0
1	G	179	0	180	5	0
1	H	179	0	180	3	0
1	I	179	0	180	4	0
1	M	179	0	180	3	0
1	N	179	0	180	4	0
1	O	179	0	180	4	0
1	S	179	0	180	4	0
1	T	179	0	180	3	0
1	U	179	0	180	4	0
1	Y	179	0	180	4	0
1	Z	179	0	180	3	0
1	a	179	0	180	4	0
2	D	1143	0	1145	19	0
2	E	1143	0	1145	19	0
2	F	1143	0	1145	20	0
2	J	1143	0	1145	21	0
2	K	1143	0	1145	18	0
2	L	1143	0	1145	21	0
2	P	1143	0	1145	18	0
2	Q	1143	0	1145	20	0
2	R	1143	0	1145	18	0
2	V	1143	0	1145	18	0
2	W	1143	0	1145	20	0
2	X	1143	0	1145	20	0
2	b	1143	0	1145	18	0
2	c	1143	0	1145	19	0
2	d	1143	0	1145	19	0
All	All	19830	0	19875	291	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 (291) 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:O:28:LEU:O	2:R:231:ARG:NH1	2.31	0.64
1:I:28:LEU:O	2:L:231:ARG:NH1	2.31	0.64
1:U:28:LEU:O	2:X:231:ARG:NH1	2.31	0.64
1:C:28:LEU:O	2:F:231:ARG:NH1	2.31	0.63
1:a:28:LEU:O	2:d:231:ARG:NH1	2.31	0.63
2:J:198:GLN:HB2	2:J:246:TYR:HD1	1.67	0.60
2:D:198:GLN:HB2	2:D:246:TYR:HD1	1.67	0.60
2:P:198:GLN:HB2	2:P:246:TYR:HD1	1.67	0.60
2:E:198:GLN:HB2	2:E:246:TYR:HD1	1.67	0.59
2:F:198:GLN:HB2	2:F:246:TYR:HD1	1.67	0.59
2:R:198:GLN:HB2	2:R:246:TYR:HD1	1.67	0.59
2:V:198:GLN:HB2	2:V:246:TYR:HD1	1.67	0.59
2:K:198:GLN:HB2	2:K:246:TYR:HD1	1.67	0.59
2:X:198:GLN:HB2	2:X:246:TYR:HD1	1.67	0.59
2:b:198:GLN:HB2	2:b:246:TYR:HD1	1.67	0.59
2:d:198:GLN:HB2	2:d:246:TYR:HD1	1.67	0.59
2:Q:198:GLN:HB2	2:Q:246:TYR:HD1	1.67	0.58
2:c:198:GLN:HB2	2:c:246:TYR:HD1	1.67	0.58
2:L:198:GLN:HB2	2:L:246:TYR:HD1	1.67	0.58
2:F:223:GLU:HG3	2:K:227:VAL:HG21	1.86	0.58
2:W:198:GLN:HB2	2:W:246:TYR:HD1	1.67	0.58
2:X:164:THR:HB	2:X:263:ILE:HB	1.87	0.57
2:L:164:THR:HB	2:L:263:ILE:HB	1.87	0.57
2:Q:164:THR:HB	2:Q:263:ILE:HB	1.87	0.57
2:d:164:THR:HB	2:d:263:ILE:HB	1.87	0.57
2:E:164:THR:HB	2:E:263:ILE:HB	1.87	0.57
2:F:164:THR:HB	2:F:263:ILE:HB	1.87	0.57
2:K:164:THR:HB	2:K:263:ILE:HB	1.87	0.56
2:V:164:THR:HB	2:V:263:ILE:HB	1.87	0.56
2:b:164:THR:HB	2:b:263:ILE:HB	1.87	0.56
2:c:164:THR:HB	2:c:263:ILE:HB	1.87	0.56
2:R:164:THR:HB	2:R:263:ILE:HB	1.87	0.56
2:W:164:THR:HB	2:W:263:ILE:HB	1.87	0.56
2:D:164:THR:HB	2:D:263:ILE:HB	1.87	0.56
2:L:223:GLU:HG3	2:Q:227:VAL:HG21	1.87	0.56
2:R:223:GLU:HG3	2:W:227:VAL:HG21	1.88	0.56
2:E:227:VAL:HG21	2:d:223:GLU:HG3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:164:THR:HB	2:J:263:ILE:HB	1.87	0.55
2:P:164:THR:HB	2:P:263:ILE:HB	1.87	0.55
2:F:181:LYS:HD2	2:F:186:LEU:HD22	1.90	0.54
2:Q:181:LYS:HD2	2:Q:186:LEU:HD22	1.90	0.54
2:X:223:GLU:HG3	2:c:227:VAL:HG21	1.87	0.54
2:b:181:LYS:HD2	2:b:186:LEU:HD22	1.90	0.54
2:J:185:ILE:HB	2:J:259:LEU:HB2	1.90	0.54
2:E:181:LYS:HD2	2:E:186:LEU:HD22	1.90	0.54
2:L:185:ILE:HB	2:L:259:LEU:HB2	1.90	0.54
2:D:185:ILE:HB	2:D:259:LEU:HB2	1.90	0.54
2:E:185:ILE:HB	2:E:259:LEU:HB2	1.90	0.54
2:c:181:LYS:HD2	2:c:186:LEU:HD22	1.90	0.54
2:R:185:ILE:HB	2:R:259:LEU:HB2	1.90	0.53
2:b:185:ILE:HB	2:b:259:LEU:HB2	1.90	0.53
2:K:185:ILE:HB	2:K:259:LEU:HB2	1.90	0.53
2:W:185:ILE:HB	2:W:259:LEU:HB2	1.90	0.53
2:c:185:ILE:HB	2:c:259:LEU:HB2	1.90	0.53
2:P:185:ILE:HB	2:P:259:LEU:HB2	1.90	0.53
2:W:181:LYS:HD2	2:W:186:LEU:HD22	1.90	0.53
2:d:181:LYS:HD2	2:d:186:LEU:HD22	1.90	0.53
2:L:181:LYS:HD2	2:L:186:LEU:HD22	1.90	0.53
2:V:185:ILE:HB	2:V:259:LEU:HB2	1.90	0.53
2:Q:185:ILE:HB	2:Q:259:LEU:HB2	1.90	0.53
1:U:26:ASP:OD2	2:X:206:TYR:OH	2.25	0.53
2:K:181:LYS:HD2	2:K:186:LEU:HD22	1.90	0.53
2:J:181:LYS:HD2	2:J:186:LEU:HD22	1.90	0.53
2:X:185:ILE:HB	2:X:259:LEU:HB2	1.90	0.53
2:F:185:ILE:HB	2:F:259:LEU:HB2	1.90	0.53
2:D:181:LYS:HD2	2:D:186:LEU:HD22	1.90	0.52
2:V:181:LYS:HD2	2:V:186:LEU:HD22	1.90	0.52
2:d:185:ILE:HB	2:d:259:LEU:HB2	1.90	0.52
1:O:26:ASP:OD2	2:R:206:TYR:OH	2.25	0.52
2:P:181:LYS:HD2	2:P:186:LEU:HD22	1.90	0.52
2:X:181:LYS:HD2	2:X:186:LEU:HD22	1.90	0.52
2:R:181:LYS:HD2	2:R:186:LEU:HD22	1.90	0.52
2:E:285:LEU:OXT	2:F:174:ARG:NH1	2.43	0.52
2:c:285:LEU:OXT	2:d:174:ARG:NH1	2.43	0.51
2:Q:285:LEU:OXT	2:R:174:ARG:NH1	2.43	0.51
2:W:285:LEU:OXT	2:X:174:ARG:NH1	2.43	0.51
1:a:26:ASP:OD2	2:d:206:TYR:OH	2.25	0.50
2:K:285:LEU:OXT	2:L:174:ARG:NH1	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:181:LYS:HG2	2:E:182:GLU:HG3	1.96	0.48
2:W:173:LYS:NZ	2:W:175:GLY:O	2.47	0.48
2:d:181:LYS:HG2	2:d:182:GLU:HG3	1.96	0.48
2:J:150:ILE:HG23	2:J:171:SER:HB2	1.96	0.48
2:L:150:ILE:HG23	2:L:171:SER:HB2	1.96	0.48
2:Q:173:LYS:NZ	2:Q:175:GLY:O	2.47	0.48
2:E:150:ILE:HG23	2:E:171:SER:HB2	1.96	0.48
2:P:150:ILE:HG23	2:P:171:SER:HB2	1.96	0.48
2:Q:150:ILE:HG23	2:Q:171:SER:HB2	1.96	0.48
2:R:173:LYS:NZ	2:R:175:GLY:O	2.47	0.48
2:X:150:ILE:HG23	2:X:171:SER:HB2	1.96	0.48
2:b:150:ILE:HG23	2:b:171:SER:HB2	1.96	0.48
2:d:150:ILE:HG23	2:d:171:SER:HB2	1.96	0.48
2:F:150:ILE:HG23	2:F:171:SER:HB2	1.96	0.48
2:V:150:ILE:HG23	2:V:171:SER:HB2	1.96	0.48
2:D:150:ILE:HG23	2:D:171:SER:HB2	1.96	0.48
2:F:181:LYS:HG2	2:F:182:GLU:HG3	1.96	0.48
2:K:150:ILE:HG23	2:K:171:SER:HB2	1.96	0.48
2:L:173:LYS:NZ	2:L:175:GLY:O	2.47	0.48
2:R:150:ILE:HG23	2:R:171:SER:HB2	1.96	0.48
2:b:181:LYS:HG2	2:b:182:GLU:HG3	1.96	0.48
2:J:173:LYS:NZ	2:J:175:GLY:O	2.47	0.48
2:P:181:LYS:HG2	2:P:182:GLU:HG3	1.96	0.47
1:H:28:LEU:HB2	2:K:264:PRO:HG2	1.96	0.47
2:W:150:ILE:HG23	2:W:171:SER:HB2	1.96	0.47
2:P:174:ARG:NH1	2:R:285:LEU:OXT	2.48	0.47
2:X:173:LYS:NZ	2:X:175:GLY:O	2.47	0.47
2:D:181:LYS:HG2	2:D:182:GLU:HG3	1.96	0.47
2:R:181:LYS:HG2	2:R:182:GLU:HG3	1.96	0.47
2:b:173:LYS:NZ	2:b:175:GLY:O	2.47	0.47
1:C:26:ASP:OD2	2:F:206:TYR:OH	2.26	0.47
1:G:24:CYS:N	1:G:35:CYS:SG	2.88	0.47
1:H:24:CYS:N	1:H:35:CYS:SG	2.88	0.47
1:I:24:CYS:N	1:I:35:CYS:SG	2.88	0.47
2:J:174:ARG:NH1	2:L:285:LEU:OXT	2.48	0.47
2:K:173:LYS:NZ	2:K:175:GLY:O	2.47	0.47
2:L:181:LYS:HG2	2:L:182:GLU:HG3	1.96	0.47
1:N:24:CYS:N	1:N:35:CYS:SG	2.88	0.47
1:O:24:CYS:N	1:O:35:CYS:SG	2.88	0.47
2:Q:181:LYS:HG2	2:Q:182:GLU:HG3	1.96	0.47
1:T:24:CYS:N	1:T:35:CYS:SG	2.88	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:LEU:HB2	2:E:264:PRO:HG2	1.97	0.47
2:F:173:LYS:NZ	2:F:175:GLY:O	2.47	0.47
2:V:181:LYS:HG2	2:V:182:GLU:HG3	1.96	0.47
2:X:181:LYS:HG2	2:X:182:GLU:HG3	1.96	0.47
2:c:150:ILE:HG23	2:c:171:SER:HB2	1.96	0.47
2:D:173:LYS:NZ	2:D:175:GLY:O	2.47	0.47
2:K:181:LYS:HG2	2:K:182:GLU:HG3	1.96	0.47
2:L:198:GLN:HA	2:L:245:CYS:O	2.15	0.47
1:M:24:CYS:N	1:M:35:CYS:SG	2.88	0.47
2:R:198:GLN:HA	2:R:245:CYS:O	2.15	0.47
1:Z:24:CYS:N	1:Z:35:CYS:SG	2.88	0.47
2:d:173:LYS:NZ	2:d:175:GLY:O	2.47	0.47
2:K:198:GLN:HA	2:K:245:CYS:O	2.15	0.47
1:Y:24:CYS:N	1:Y:35:CYS:SG	2.88	0.47
2:V:198:GLN:HA	2:V:245:CYS:O	2.15	0.46
2:W:181:LYS:HG2	2:W:182:GLU:HG3	1.96	0.46
2:X:198:GLN:HA	2:X:245:CYS:O	2.15	0.46
2:J:198:GLN:HA	2:J:245:CYS:O	2.15	0.46
1:N:28:LEU:HB2	2:Q:264:PRO:HG2	1.96	0.46
1:C:24:CYS:N	1:C:35:CYS:SG	2.88	0.46
2:Q:198:GLN:HA	2:Q:245:CYS:O	2.15	0.46
1:T:28:LEU:HB2	2:W:264:PRO:HG2	1.96	0.46
1:U:24:CYS:N	1:U:35:CYS:SG	2.88	0.46
2:c:181:LYS:HG2	2:c:182:GLU:HG3	1.96	0.46
2:d:198:GLN:HA	2:d:245:CYS:O	2.15	0.46
1:B:24:CYS:N	1:B:35:CYS:SG	2.88	0.46
2:V:174:ARG:NH1	2:X:285:LEU:OXT	2.48	0.46
2:F:198:GLN:HA	2:F:245:CYS:O	2.15	0.46
2:P:198:GLN:HA	2:P:245:CYS:O	2.15	0.46
2:J:181:LYS:HG2	2:J:182:GLU:HG3	1.96	0.46
2:P:173:LYS:NZ	2:P:175:GLY:O	2.47	0.46
1:S:24:CYS:N	1:S:35:CYS:SG	2.88	0.46
1:a:24:CYS:N	1:a:35:CYS:SG	2.88	0.46
2:b:174:ARG:NH1	2:d:285:LEU:OXT	2.48	0.46
1:A:24:CYS:N	1:A:35:CYS:SG	2.88	0.46
2:b:198:GLN:HA	2:b:245:CYS:O	2.15	0.46
2:D:198:GLN:HA	2:D:245:CYS:O	2.15	0.46
2:V:173:LYS:NZ	2:V:175:GLY:O	2.47	0.45
1:Z:28:LEU:HB2	2:c:264:PRO:HG2	1.96	0.45
2:E:198:GLN:HA	2:E:245:CYS:O	2.15	0.45
2:W:198:GLN:HA	2:W:245:CYS:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:173:LYS:NZ	2:E:175:GLY:O	2.47	0.45
2:c:158:ILE:HB	2:c:165:PHE:HB2	1.99	0.45
2:c:173:LYS:NZ	2:c:175:GLY:O	2.47	0.45
2:F:158:ILE:HB	2:F:165:PHE:HB2	1.99	0.45
2:V:158:ILE:HB	2:V:165:PHE:HB2	1.99	0.45
2:Q:158:ILE:HB	2:Q:165:PHE:HB2	1.99	0.45
2:X:158:ILE:HB	2:X:165:PHE:HB2	1.99	0.45
2:D:174:ARG:NH1	2:F:285:LEU:OXT	2.48	0.45
2:E:158:ILE:HB	2:E:165:PHE:HB2	1.99	0.44
2:c:198:GLN:HA	2:c:245:CYS:O	2.15	0.44
1:G:27:LEU:HD13	2:J:163:TYR:HE1	1.82	0.44
2:K:158:ILE:HB	2:K:165:PHE:HB2	1.99	0.44
2:D:158:ILE:HB	2:D:165:PHE:HB2	1.99	0.44
1:S:27:LEU:HD13	2:V:163:TYR:HE1	1.82	0.44
1:Y:27:LEU:HD13	2:b:163:TYR:HE1	1.82	0.44
2:J:158:ILE:HB	2:J:165:PHE:HB2	1.99	0.43
2:K:200:LEU:HD22	2:K:276:VAL:HG21	2.00	0.43
2:L:200:LEU:HD22	2:L:276:VAL:HG21	2.00	0.43
2:b:158:ILE:HB	2:b:165:PHE:HB2	1.99	0.43
2:F:227:VAL:HG21	2:K:223:GLU:HG3	2.00	0.43
1:M:27:LEU:HD13	2:P:163:TYR:HE1	1.82	0.43
2:V:200:LEU:HD22	2:V:276:VAL:HG21	2.00	0.43
2:c:200:LEU:HD22	2:c:276:VAL:HG21	2.00	0.43
2:d:158:ILE:HB	2:d:165:PHE:HB2	1.99	0.43
2:J:200:LEU:HD22	2:J:276:VAL:HG21	2.00	0.43
2:P:200:LEU:HD22	2:P:276:VAL:HG21	2.00	0.43
2:J:224:LEU:HD23	2:J:224:LEU:HA	1.88	0.43
2:R:200:LEU:HD22	2:R:276:VAL:HG21	2.00	0.43
2:R:209:GLY:HA3	2:R:232:CYS:O	2.19	0.43
2:P:158:ILE:HB	2:P:165:PHE:HB2	1.99	0.43
2:Q:200:LEU:HD22	2:Q:276:VAL:HG21	2.00	0.43
2:J:209:GLY:HA3	2:J:232:CYS:O	2.19	0.43
2:X:200:LEU:HD22	2:X:276:VAL:HG21	2.00	0.43
2:d:209:GLY:HA3	2:d:232:CYS:O	2.19	0.43
2:E:223:GLU:HG3	2:d:227:VAL:HG21	2.00	0.43
1:I:26:ASP:OD2	2:L:206:TYR:OH	2.26	0.43
2:K:209:GLY:HA3	2:K:232:CYS:O	2.19	0.43
2:L:158:ILE:HB	2:L:165:PHE:HB2	1.99	0.43
2:Q:209:GLY:HA3	2:Q:232:CYS:O	2.19	0.43
2:Q:224:LEU:HD23	2:Q:224:LEU:HA	1.88	0.43
2:V:209:GLY:HA3	2:V:232:CYS:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:209:GLY:HA3	2:W:232:CYS:O	2.19	0.43
2:b:209:GLY:HA3	2:b:232:CYS:O	2.19	0.43
2:P:209:GLY:HA3	2:P:232:CYS:O	2.19	0.43
2:W:158:ILE:HB	2:W:165:PHE:HB2	1.99	0.43
2:c:209:GLY:HA3	2:c:232:CYS:O	2.19	0.43
1:A:27:LEU:HD13	2:D:163:TYR:HE1	1.82	0.43
2:F:200:LEU:HD22	2:F:276:VAL:HG21	2.00	0.43
2:R:158:ILE:HB	2:R:165:PHE:HB2	1.99	0.43
2:d:200:LEU:HD22	2:d:276:VAL:HG21	2.00	0.43
2:L:209:GLY:HA3	2:L:232:CYS:O	2.19	0.42
2:W:200:LEU:HD22	2:W:276:VAL:HG21	2.00	0.42
2:b:200:LEU:HD22	2:b:276:VAL:HG21	2.00	0.42
2:D:209:GLY:HA3	2:D:232:CYS:O	2.19	0.42
2:W:208:MET:HE3	2:W:208:MET:HB3	1.95	0.42
2:E:200:LEU:HD22	2:E:276:VAL:HG21	2.00	0.42
2:L:224:LEU:HD23	2:L:224:LEU:HA	1.88	0.42
2:X:227:VAL:HG21	2:c:223:GLU:HG3	2.02	0.42
2:L:227:VAL:HG21	2:Q:223:GLU:HG3	2.01	0.42
2:X:209:GLY:HA3	2:X:232:CYS:O	2.19	0.42
2:E:209:GLY:HA3	2:E:232:CYS:O	2.19	0.42
1:Y:28:LEU:HB2	2:b:264:PRO:HG2	2.02	0.42
1:A:28:LEU:HB2	2:D:264:PRO:HG2	2.02	0.42
1:M:28:LEU:HB2	2:P:264:PRO:HG2	2.02	0.42
1:S:28:LEU:HB2	2:V:264:PRO:HG2	2.02	0.42
2:c:208:MET:HE3	2:c:208:MET:HB3	1.95	0.42
2:F:209:GLY:HA3	2:F:232:CYS:O	2.19	0.42
1:G:28:LEU:HB2	2:J:264:PRO:HG2	2.02	0.42
2:L:214:ARG:HB2	2:L:229:LEU:HD11	2.02	0.42
2:V:214:ARG:HB2	2:V:229:LEU:HD11	2.02	0.42
2:D:200:LEU:HD22	2:D:276:VAL:HG21	2.00	0.41
2:J:214:ARG:HB2	2:J:229:LEU:HD11	2.02	0.41
2:J:285:LEU:OXT	2:K:174:ARG:NH1	2.53	0.41
2:X:224:LEU:HD23	2:X:224:LEU:HA	1.88	0.41
2:b:226:LEU:HD12	2:b:226:LEU:HA	1.91	0.41
2:d:214:ARG:HB2	2:d:229:LEU:HD11	2.02	0.41
2:E:215:LYS:HB3	2:E:258:GLU:HB2	2.03	0.41
2:W:214:ARG:HB2	2:W:229:LEU:HD11	2.02	0.41
2:b:285:LEU:OXT	2:c:174:ARG:NH1	2.53	0.41
2:D:214:ARG:HB2	2:D:229:LEU:HD11	2.02	0.41
2:F:215:LYS:HB3	2:F:258:GLU:HB2	2.03	0.41
2:X:215:LYS:HB3	2:X:258:GLU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:214:ARG:HB2	2:c:229:LEU:HD11	2.02	0.41
2:D:224:LEU:HD23	2:D:224:LEU:HA	1.88	0.41
2:D:285:LEU:OXT	2:E:174:ARG:NH1	2.53	0.41
2:L:215:LYS:HB3	2:L:258:GLU:HB2	2.03	0.41
2:V:215:LYS:HB3	2:V:258:GLU:HB2	2.03	0.41
2:c:215:LYS:HB3	2:c:258:GLU:HB2	2.03	0.41
1:G:26:ASP:HB2	1:G:33:VAL:HG22	2.03	0.41
2:J:216:LYS:HB3	2:J:216:LYS:HE3	1.86	0.41
2:P:214:ARG:HB2	2:P:229:LEU:HD11	2.02	0.41
2:P:215:LYS:HB3	2:P:258:GLU:HB2	2.03	0.41
2:b:215:LYS:HB3	2:b:258:GLU:HB2	2.03	0.41
1:I:26:ASP:HB2	1:I:33:VAL:HG22	2.03	0.41
2:J:215:LYS:HB3	2:J:258:GLU:HB2	2.03	0.41
1:O:26:ASP:HB2	1:O:33:VAL:HG22	2.03	0.41
2:P:226:LEU:HD12	2:P:226:LEU:HA	1.91	0.41
2:R:215:LYS:HB3	2:R:258:GLU:HB2	2.03	0.41
2:R:227:VAL:HG21	2:W:223:GLU:HG3	2.02	0.41
2:V:285:LEU:OXT	2:W:174:ARG:NH1	2.53	0.41
2:W:226:LEU:HD12	2:W:226:LEU:HA	1.91	0.41
2:E:226:LEU:HD12	2:E:226:LEU:HA	1.91	0.41
1:H:26:ASP:HB2	1:H:33:VAL:HG22	2.03	0.41
2:J:208:MET:HE3	2:J:208:MET:HB3	1.95	0.41
1:S:26:ASP:HB2	1:S:33:VAL:HG22	2.03	0.41
1:U:26:ASP:HB2	1:U:33:VAL:HG22	2.03	0.41
2:V:224:LEU:HD23	2:V:224:LEU:HA	1.88	0.41
2:d:215:LYS:HB3	2:d:258:GLU:HB2	2.03	0.41
1:B:26:ASP:HB2	1:B:33:VAL:HG22	2.03	0.40
2:D:215:LYS:HB3	2:D:258:GLU:HB2	2.03	0.40
2:F:208:MET:HE3	2:F:208:MET:HB3	1.95	0.40
2:F:214:ARG:HB2	2:F:229:LEU:HD11	2.02	0.40
2:K:215:LYS:HB3	2:K:258:GLU:HB2	2.03	0.40
2:W:215:LYS:HB3	2:W:258:GLU:HB2	2.03	0.40
1:A:28:LEU:O	2:D:231:ARG:NH1	2.54	0.40
2:L:216:LYS:HE3	2:L:216:LYS:HB3	1.86	0.40
2:Q:214:ARG:HB2	2:Q:229:LEU:HD11	2.02	0.40
2:Q:226:LEU:HD12	2:Q:226:LEU:HA	1.91	0.40
1:Y:28:LEU:O	2:b:231:ARG:NH1	2.54	0.40
1:Z:26:ASP:HB2	1:Z:33:VAL:HG22	2.03	0.40
1:a:26:ASP:HB2	1:a:33:VAL:HG22	2.03	0.40
2:K:214:ARG:HB2	2:K:229:LEU:HD11	2.02	0.40
2:P:198:GLN:HB2	2:P:246:TYR:CD1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:198:GLN:HB2	2:Q:246:TYR:CD1	2.53	0.40
2:X:214:ARG:HB2	2:X:229:LEU:HD11	2.02	0.40
2:E:216:LYS:HE3	2:E:216:LYS:HB3	1.86	0.40
1:G:28:LEU:O	2:J:231:ARG:NH1	2.54	0.40
1:N:33:VAL:HG11	2:Q:206:TYR:OH	2.21	0.40
1:A:26:ASP:HB2	1:A:33:VAL:HG22	2.03	0.40
1:N:26:ASP:HB2	1:N:33:VAL:HG22	2.03	0.40
1:T:26:ASP:HB2	1:T:33:VAL:HG22	2.03	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	22/101 (22%)	21 (96%)	1 (4%)	0	100	100
1	B	22/101 (22%)	21 (96%)	1 (4%)	0	100	100
1	C	22/101 (22%)	21 (96%)	1 (4%)	0	100	100
1	G	22/101 (22%)	21 (96%)	1 (4%)	0	100	100
1	H	22/101 (22%)	21 (96%)	1 (4%)	0	100	100
1	I	22/101 (22%)	21 (96%)	1 (4%)	0	100	100
1	M	22/101 (22%)	21 (96%)	1 (4%)	0	100	100
1	N	22/101 (22%)	21 (96%)	1 (4%)	0	100	100
1	O	22/101 (22%)	21 (96%)	1 (4%)	0	100	100
1	S	22/101 (22%)	21 (96%)	1 (4%)	0	100	100
1	T	22/101 (22%)	21 (96%)	1 (4%)	0	100	100
1	U	22/101 (22%)	21 (96%)	1 (4%)	0	100	100
1	Y	22/101 (22%)	21 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Z	22/101 (22%)	21 (96%)	1 (4%)	0	100	100
1	a	22/101 (22%)	21 (96%)	1 (4%)	0	100	100
2	D	142/157 (90%)	139 (98%)	3 (2%)	0	100	100
2	E	142/157 (90%)	139 (98%)	3 (2%)	0	100	100
2	F	142/157 (90%)	139 (98%)	3 (2%)	0	100	100
2	J	142/157 (90%)	139 (98%)	3 (2%)	0	100	100
2	K	142/157 (90%)	139 (98%)	3 (2%)	0	100	100
2	L	142/157 (90%)	139 (98%)	3 (2%)	0	100	100
2	P	142/157 (90%)	139 (98%)	3 (2%)	0	100	100
2	Q	142/157 (90%)	139 (98%)	3 (2%)	0	100	100
2	R	142/157 (90%)	139 (98%)	3 (2%)	0	100	100
2	V	142/157 (90%)	139 (98%)	3 (2%)	0	100	100
2	W	142/157 (90%)	139 (98%)	3 (2%)	0	100	100
2	X	142/157 (90%)	139 (98%)	3 (2%)	0	100	100
2	b	142/157 (90%)	139 (98%)	3 (2%)	0	100	100
2	c	142/157 (90%)	139 (98%)	3 (2%)	0	100	100
2	d	142/157 (90%)	139 (98%)	3 (2%)	0	100	100
All	All	2460/3870 (64%)	2400 (98%)	60 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	21/76 (28%)	21 (100%)	0	100	100
1	B	21/76 (28%)	21 (100%)	0	100	100
1	C	21/76 (28%)	21 (100%)	0	100	100
1	G	21/76 (28%)	21 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	21/76 (28%)	21 (100%)	0	100	100
1	I	21/76 (28%)	21 (100%)	0	100	100
1	M	21/76 (28%)	21 (100%)	0	100	100
1	N	21/76 (28%)	21 (100%)	0	100	100
1	O	21/76 (28%)	21 (100%)	0	100	100
1	S	21/76 (28%)	21 (100%)	0	100	100
1	T	21/76 (28%)	21 (100%)	0	100	100
1	U	21/76 (28%)	21 (100%)	0	100	100
1	Y	21/76 (28%)	21 (100%)	0	100	100
1	Z	21/76 (28%)	21 (100%)	0	100	100
1	a	21/76 (28%)	21 (100%)	0	100	100
2	D	126/134 (94%)	125 (99%)	1 (1%)	79	91
2	E	126/134 (94%)	125 (99%)	1 (1%)	79	91
2	F	126/134 (94%)	125 (99%)	1 (1%)	79	91
2	J	126/134 (94%)	125 (99%)	1 (1%)	79	91
2	K	126/134 (94%)	125 (99%)	1 (1%)	79	91
2	L	126/134 (94%)	125 (99%)	1 (1%)	79	91
2	P	126/134 (94%)	125 (99%)	1 (1%)	79	91
2	Q	126/134 (94%)	125 (99%)	1 (1%)	79	91
2	R	126/134 (94%)	125 (99%)	1 (1%)	79	91
2	V	126/134 (94%)	125 (99%)	1 (1%)	79	91
2	W	126/134 (94%)	125 (99%)	1 (1%)	79	91
2	X	126/134 (94%)	125 (99%)	1 (1%)	79	91
2	b	126/134 (94%)	125 (99%)	1 (1%)	79	91
2	c	126/134 (94%)	125 (99%)	1 (1%)	79	91
2	d	126/134 (94%)	125 (99%)	1 (1%)	79	91
All	All	2205/3150 (70%)	2190 (99%)	15 (1%)	80	92

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	233	ILE
2	E	233	ILE

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Mol	Chain	Res	Type
2	F	233	ILE
2	J	233	ILE
2	K	233	ILE
2	L	233	ILE
2	P	233	ILE
2	Q	233	ILE
2	R	233	ILE
2	V	233	ILE
2	W	233	ILE
2	X	233	ILE
2	b	233	ILE
2	c	233	ILE
2	d	233	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	242	ASN
2	F	218	HIS
2	J	242	ASN
2	L	218	HIS
2	L	242	ASN
2	P	242	ASN
2	R	218	HIS
2	R	242	ASN
2	V	242	ASN
2	X	218	HIS
2	X	242	ASN
2	b	242	ASN
2	d	218	HIS
2	d	242	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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.

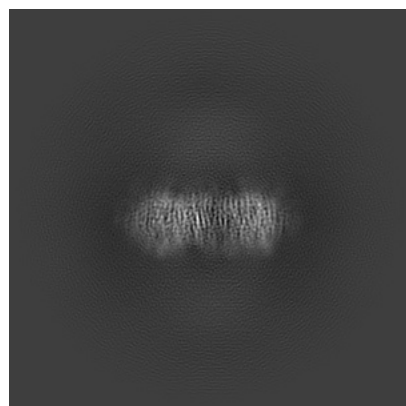
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60485. These allow visual inspection of the internal detail of the map and identification of artifacts.

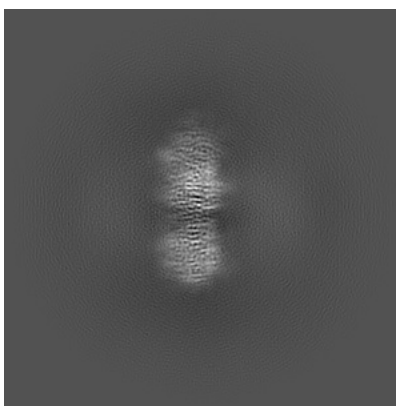
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

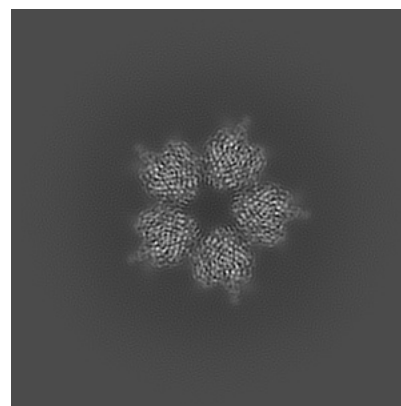
6.1.1 Primary map



X

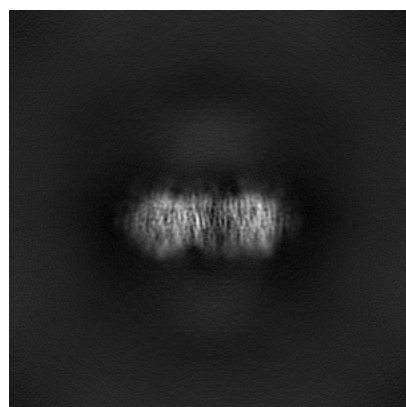


Y

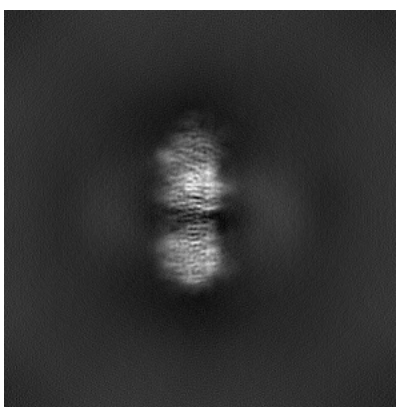


Z

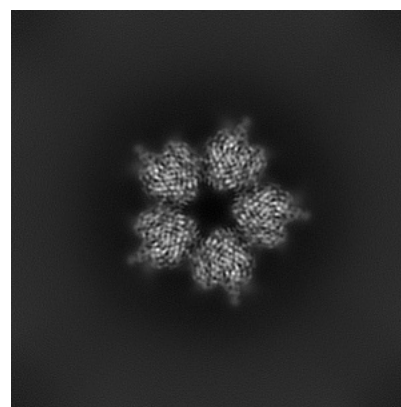
6.1.2 Raw map



X



Y

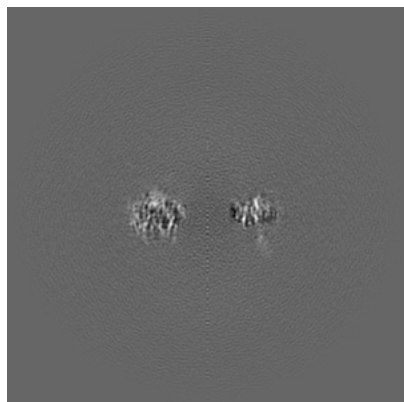


Z

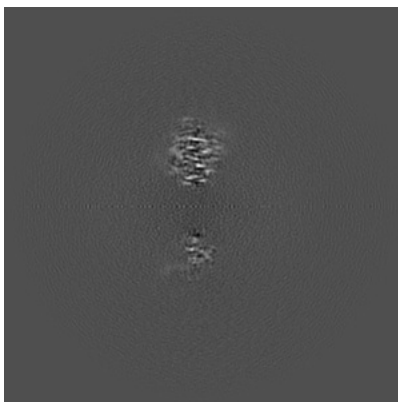
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

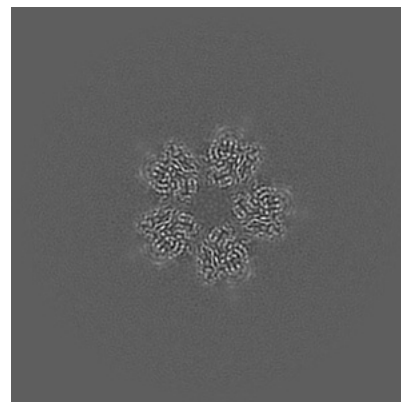
6.2.1 Primary map



X Index: 200

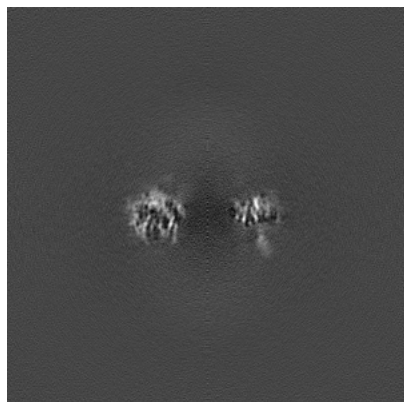


Y Index: 200

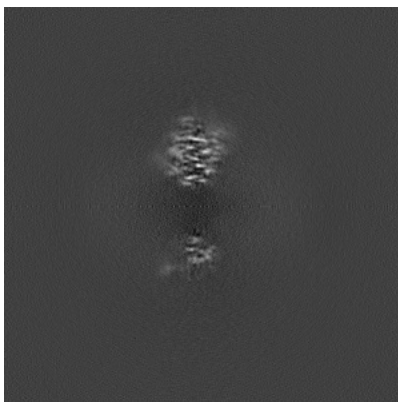


Z Index: 200

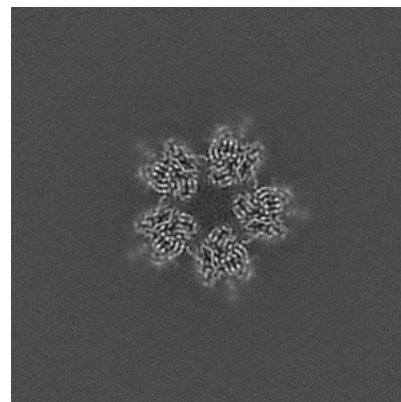
6.2.2 Raw map



X Index: 200



Y Index: 200

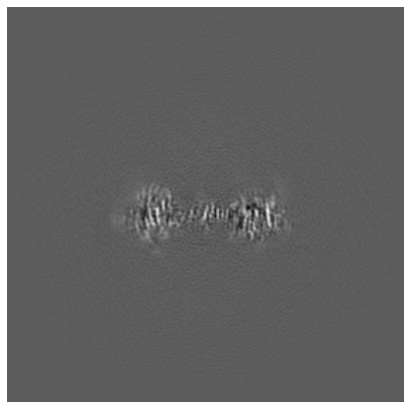


Z Index: 200

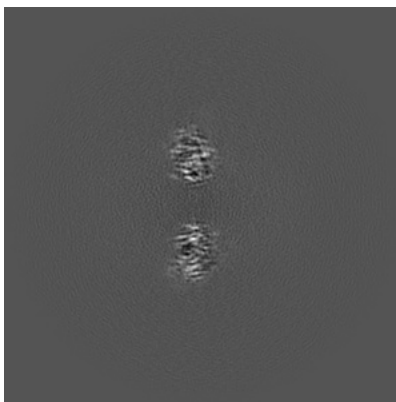
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

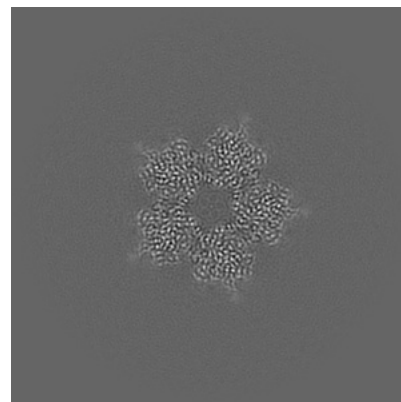
6.3.1 Primary map



X Index: 225

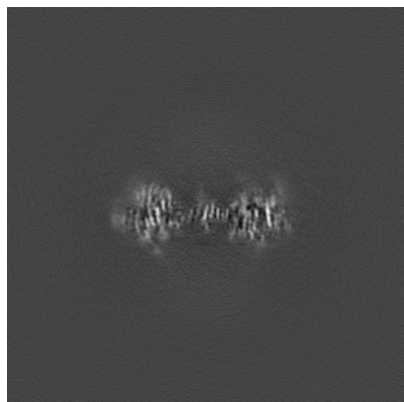


Y Index: 188

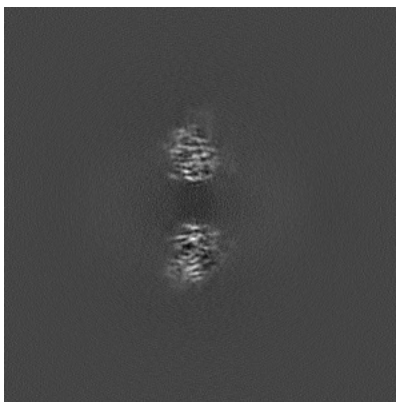


Z Index: 191

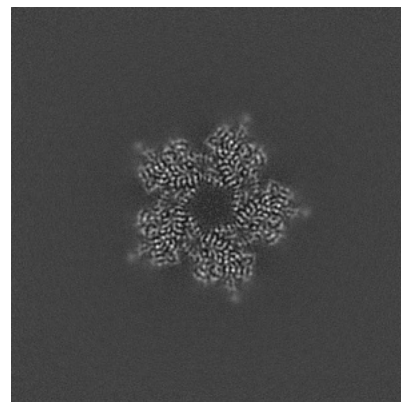
6.3.2 Raw map



X Index: 225



Y Index: 188

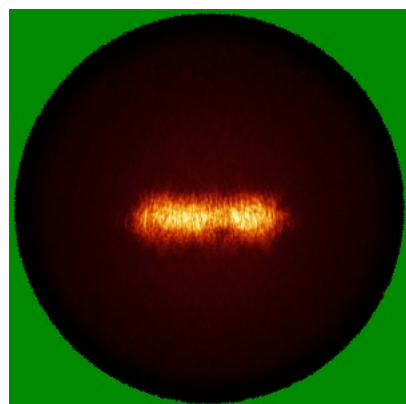


Z Index: 192

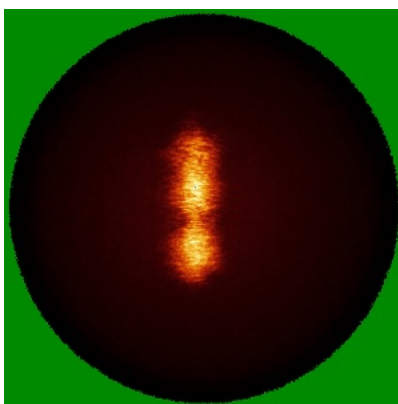
The images above show the largest variance slices of the map in three orthogonal directions.

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

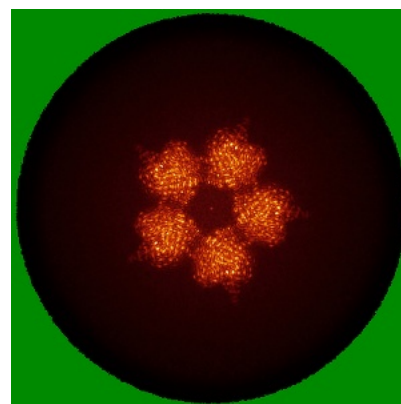
6.4.1 Primary map



X

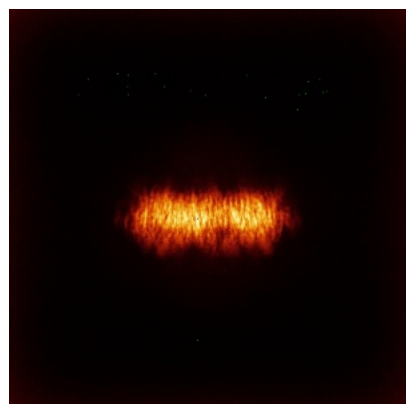


Y

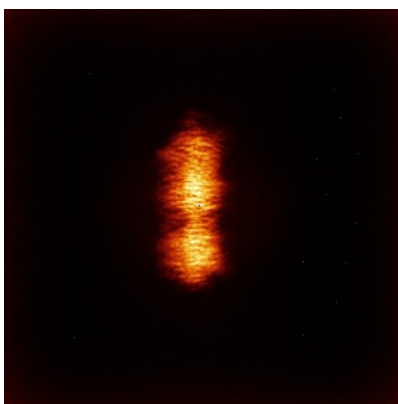


Z

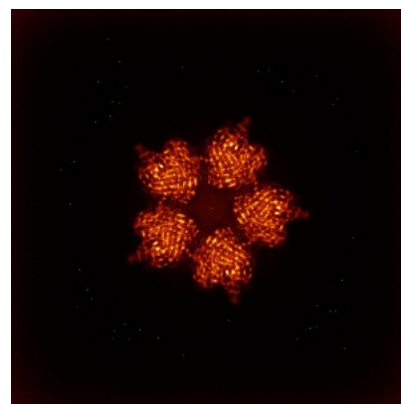
6.4.2 Raw map



X



Y

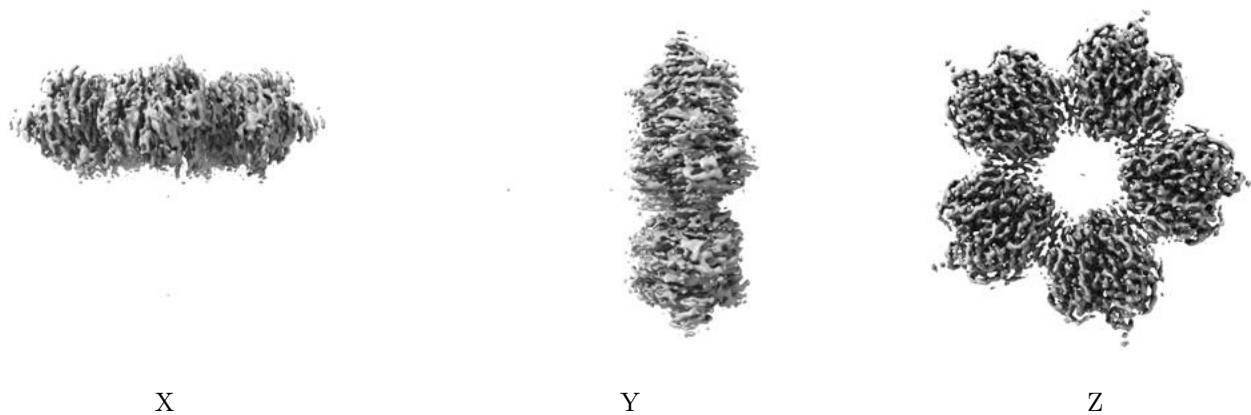


Z

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

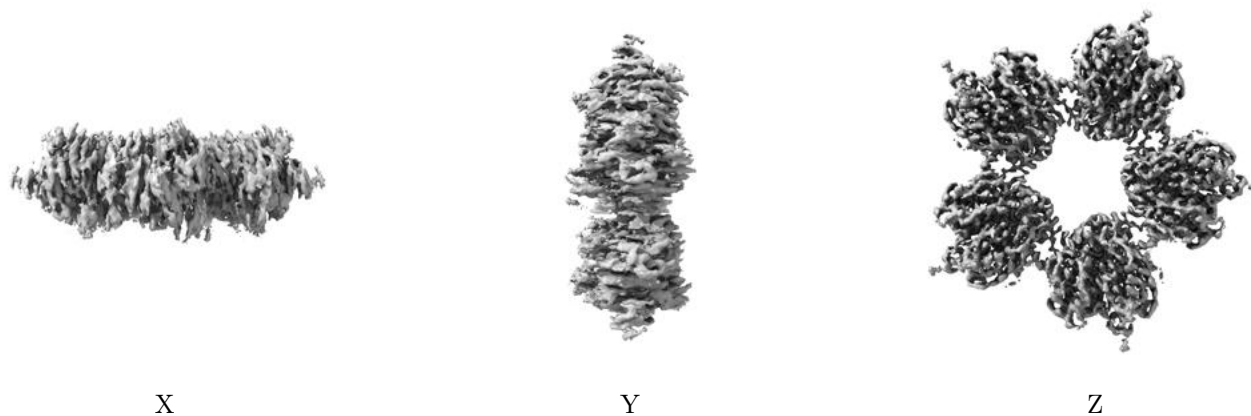
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.38. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

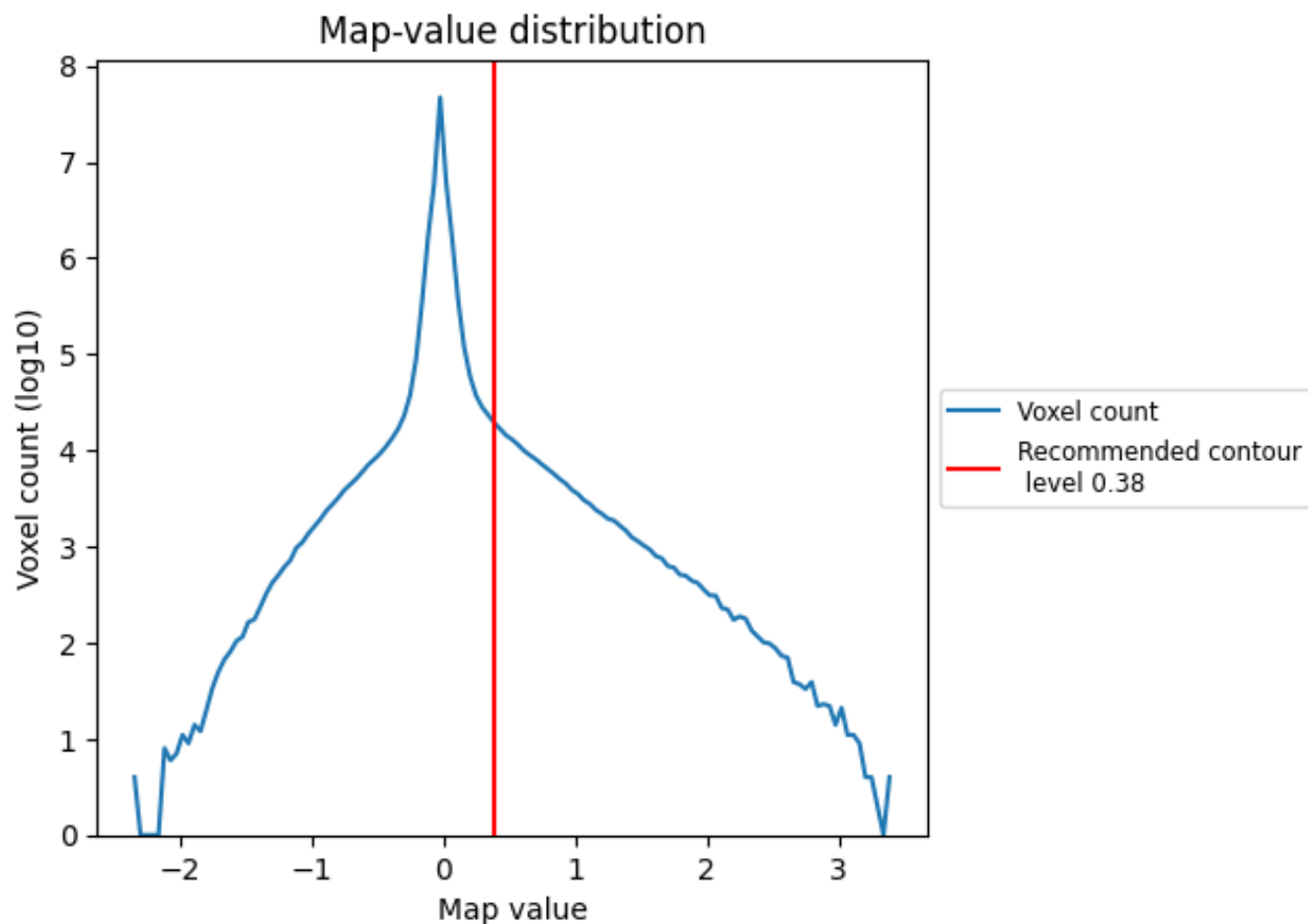
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

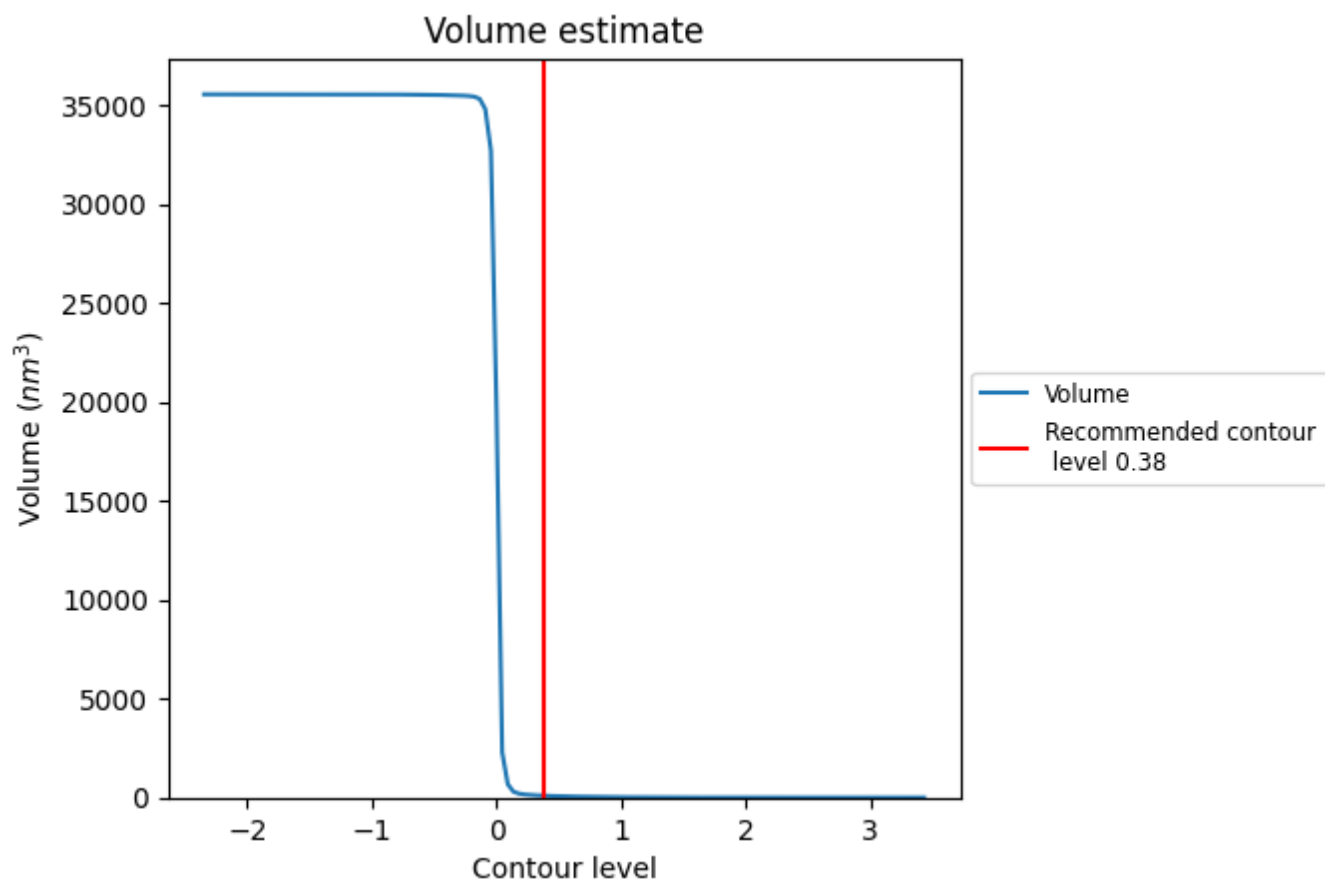
This section contains the results of statistical analysis of the map.

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.

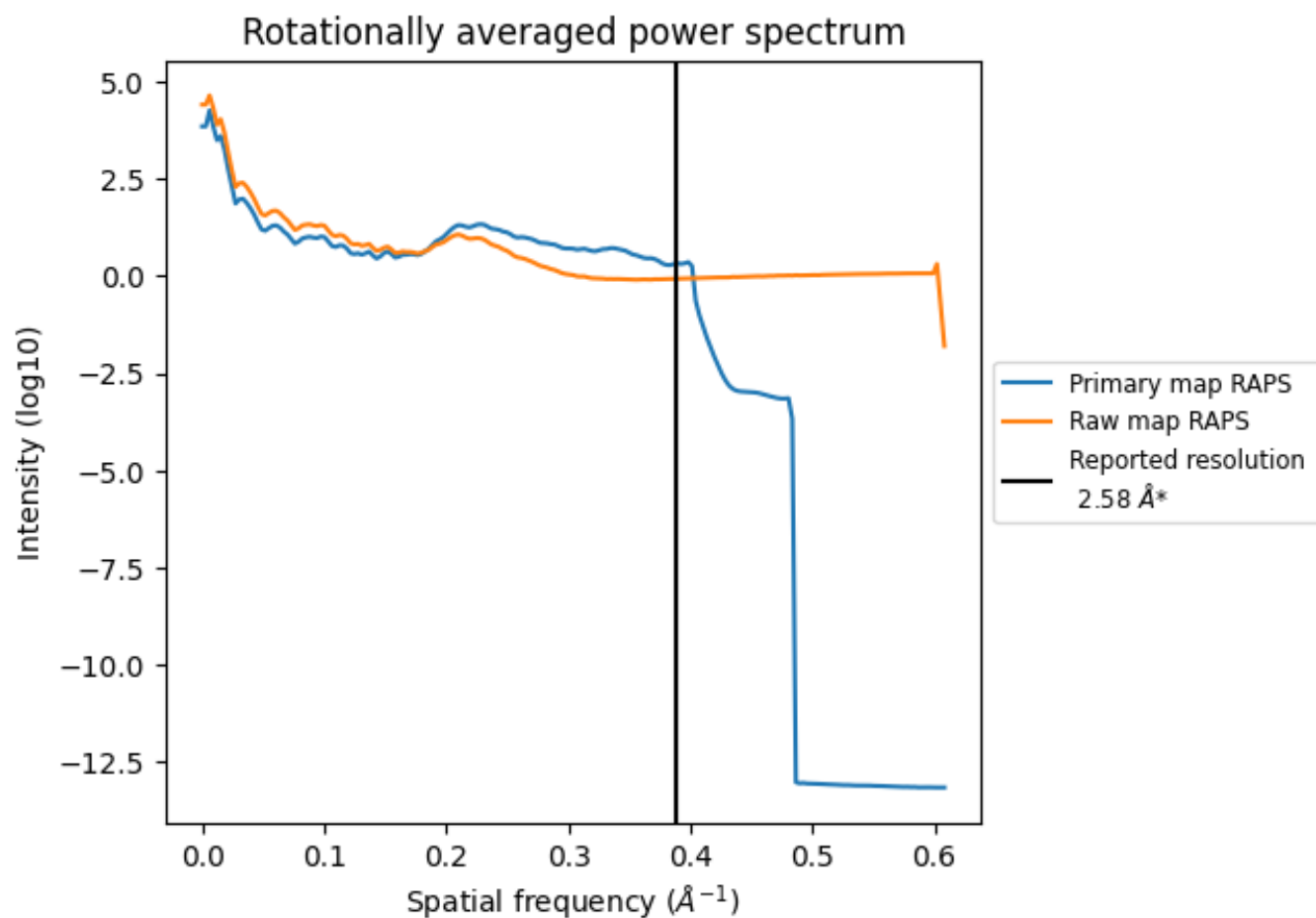
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 94 nm³; this corresponds to an approximate mass of 85 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 ⓘ

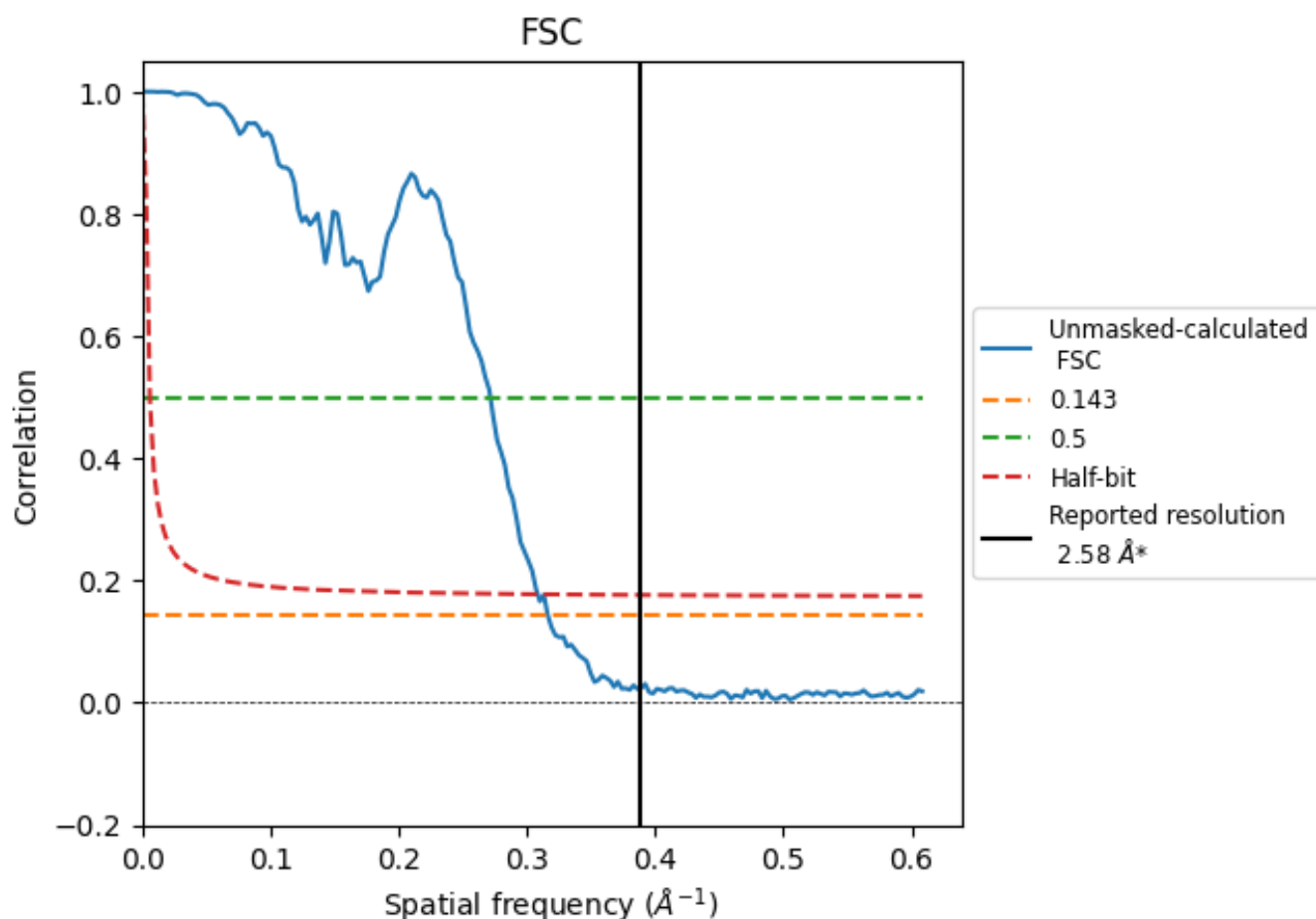


*Reported resolution corresponds to spatial frequency of 0.388 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.388 \AA^{-1}

8.2 Resolution estimates [i](#)

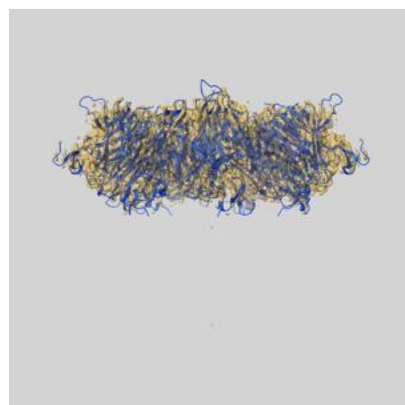
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.58	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.16	3.68	3.24

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.16 differs from the reported value 2.58 by more than 10 %

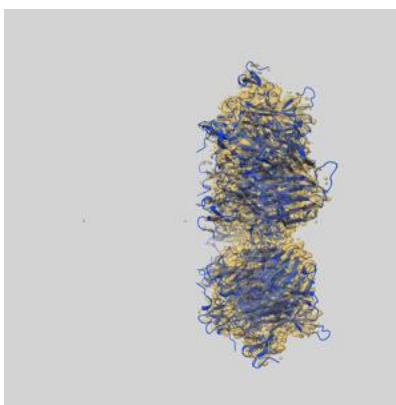
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60485 and PDB model 8ZUJ. Per-residue inclusion information can be found in section 3 on page 17.

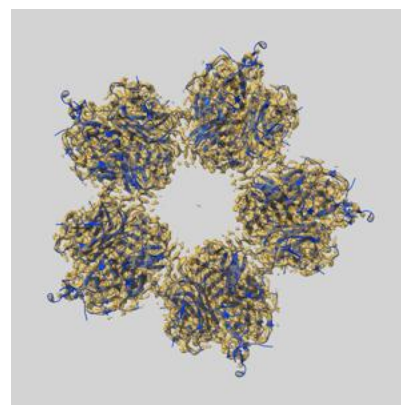
9.1 Map-model overlay [i](#)



X



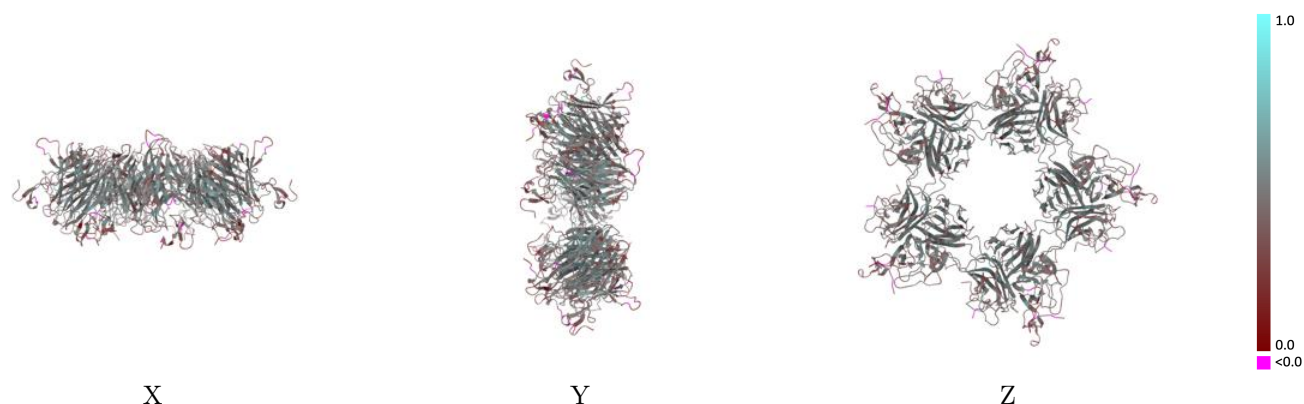
Y



Z

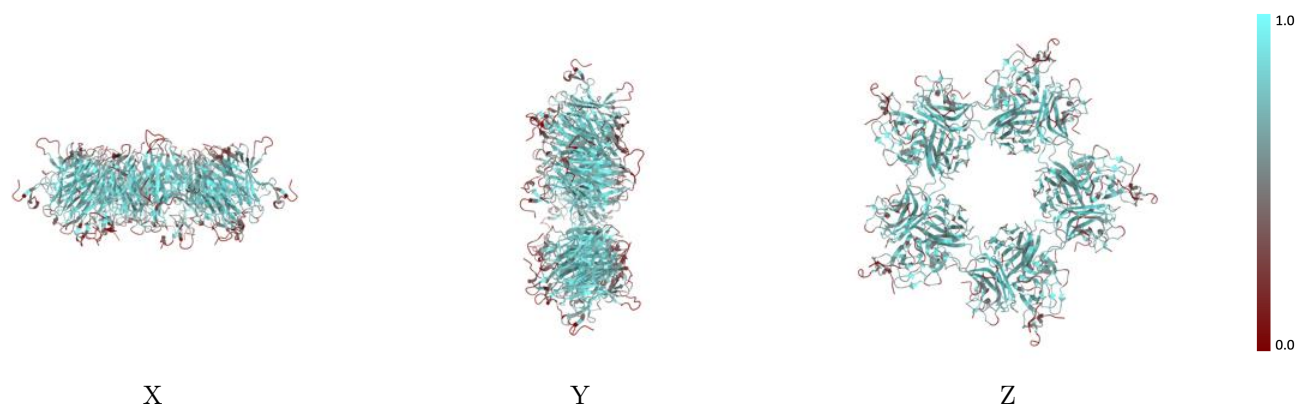
The images above show the 3D surface view of the map at the recommended contour level 0.38 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



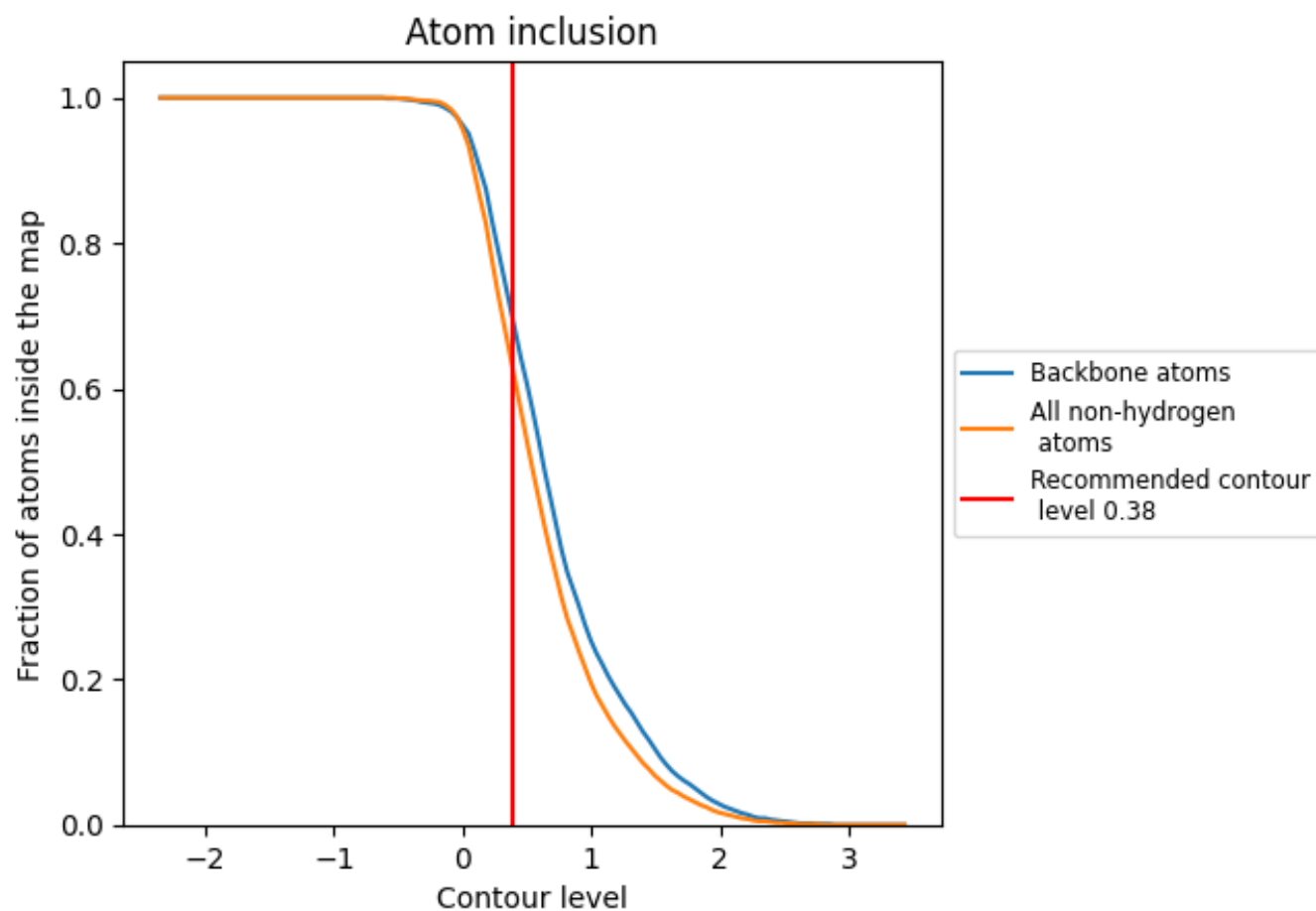
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.38).































































9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 63% 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 (0.38) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6340	 0.4240
A	 0.3490	 0.3160
B	 0.3770	 0.3310
C	 0.3660	 0.2880
D	 0.6270	 0.4180
E	 0.6890	 0.4390
F	 0.7080	 0.4630
G	 0.3540	 0.3200
H	 0.3710	 0.3370
I	 0.3770	 0.2840
J	 0.6270	 0.4170
K	 0.6890	 0.4410
L	 0.7080	 0.4650
M	 0.3540	 0.3160
N	 0.3710	 0.3430
O	 0.3830	 0.2900
P	 0.6290	 0.4200
Q	 0.6880	 0.4400
R	 0.7090	 0.4660
S	 0.3370	 0.3140
T	 0.3710	 0.3380
U	 0.3770	 0.2990
V	 0.6340	 0.4190
W	 0.6900	 0.4410
X	 0.7060	 0.4640
Y	 0.3370	 0.3170
Z	 0.3660	 0.3340
a	 0.3660	 0.2920
b	 0.6310	 0.4200
c	 0.6890	 0.4400
d	 0.7140	 0.4620

