



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 03:15 PM UTC

PDB ID : 8Z6U / pdb_00008z6u
EMDB ID : EMD-39805
Title : SARS-CoV-2 EG.5.1 Spike in complex with CYFN1006-2(S-CYFN1006-2 dimer trimer).
Authors : Wang, Y.J.; Sun, L.
Deposited on : 2024-04-19
Resolution : 3.83 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
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

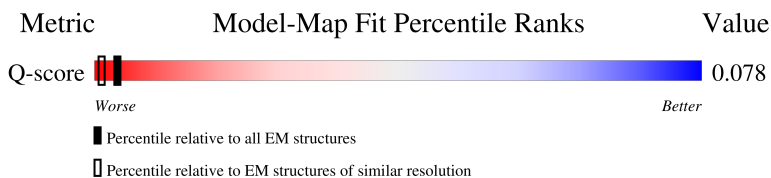
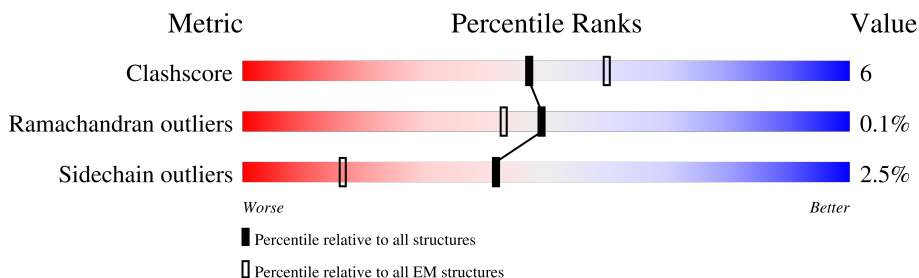
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.83 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.



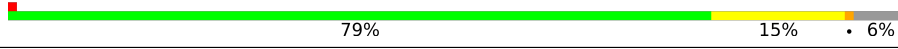
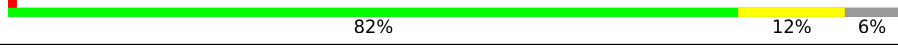
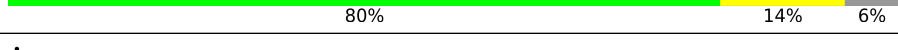
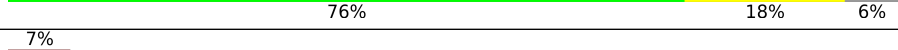
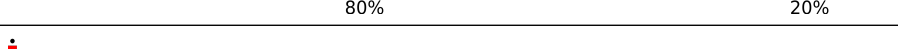
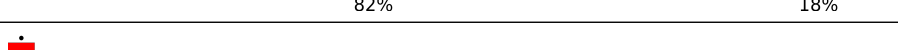
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	9087 (3.33 - 4.33)

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	1295	
1	B	1295	
1	C	1295	
1	D	1295	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	1295	
1	F	1295	
2	J	215	
2	K	215	
2	L	215	
2	P	215	
2	Q	215	
2	R	215	
3	G	218	
3	H	218	
3	I	218	
3	M	218	
3	N	218	
3	O	218	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 69900 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 Spike glycoprotein,Fibritin,Expression Tag.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1087	Total	C	N	O	S	0	0
			8502	5432	1416	1616	38		
1	A	1087	Total	C	N	O	S	0	0
			8502	5432	1416	1616	38		
1	C	1087	Total	C	N	O	S	0	0
			8502	5432	1416	1616	38		
1	E	1087	Total	C	N	O	S	0	0
			8502	5432	1416	1616	38		
1	D	1087	Total	C	N	O	S	0	0
			8502	5432	1416	1616	38		
1	F	1087	Total	C	N	O	S	0	0
			8502	5432	1416	1616	38		

There are 474 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	MET	-	initiating methionine	UNP P0DTC2
B	-5	PRO	-	expression tag	UNP P0DTC2
B	-4	MET	-	expression tag	UNP P0DTC2
B	-3	GLY	-	expression tag	UNP P0DTC2
B	-2	SER	-	expression tag	UNP P0DTC2
B	-1	LEU	-	expression tag	UNP P0DTC2
B	0	GLN	-	expression tag	UNP P0DTC2
B	1	PRO	-	expression tag	UNP P0DTC2
B	2	LEU	-	expression tag	UNP P0DTC2
B	3	ALA	-	expression tag	UNP P0DTC2
B	4	THR	-	expression tag	UNP P0DTC2
B	5	LEU	-	expression tag	UNP P0DTC2
B	6	TYR	-	expression tag	UNP P0DTC2
B	7	LEU	-	expression tag	UNP P0DTC2
B	8	LEU	-	expression tag	UNP P0DTC2
B	9	GLY	-	expression tag	UNP P0DTC2
B	10	MET	-	expression tag	UNP P0DTC2
B	11	LEU	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	12	VAL	-	expression tag	UNP P0DTC2
B	13	ALA	-	expression tag	UNP P0DTC2
B	14	SER	-	expression tag	UNP P0DTC2
B	15	VAL	-	expression tag	UNP P0DTC2
B	16	LEU	-	expression tag	UNP P0DTC2
B	17	ALA	-	expression tag	UNP P0DTC2
B	23	ILE	THR	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	28	SER	ALA	variant	UNP P0DTC2
B	53	HIS	GLN	conflict	UNP P0DTC2
B	84	ALA	VAL	conflict	UNP P0DTC2
B	143	ASP	GLY	variant	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	146	GLN	HIS	conflict	UNP P0DTC2
B	183	GLU	GLN	conflict	UNP P0DTC2
B	213	GLU	VAL	variant	UNP P0DTC2
B	252	VAL	GLY	variant	UNP P0DTC2
B	339	HIS	GLY	variant	UNP P0DTC2
B	346	THR	ARG	variant	UNP P0DTC2
B	368	ILE	LEU	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	445	PRO	VAL	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	456	LEU	PHE	variant	UNP P0DTC2
B	460	LYS	ASN	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	conflict	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	486	PRO	PHE	variant	UNP P0DTC2
B	490	SER	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	conflict	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	UNP P0DTC2
B	1209	GLY	-	linker	UNP P0DTC2
B	1210	SER	-	linker	UNP P0DTC2
A	-6	MET	-	initiating methionine	UNP P0DTC2
A	-5	PRO	-	expression tag	UNP P0DTC2
A	-4	MET	-	expression tag	UNP P0DTC2
A	-3	GLY	-	expression tag	UNP P0DTC2
A	-2	SER	-	expression tag	UNP P0DTC2
A	-1	LEU	-	expression tag	UNP P0DTC2
A	0	GLN	-	expression tag	UNP P0DTC2
A	1	PRO	-	expression tag	UNP P0DTC2
A	2	LEU	-	expression tag	UNP P0DTC2
A	3	ALA	-	expression tag	UNP P0DTC2
A	4	THR	-	expression tag	UNP P0DTC2
A	5	LEU	-	expression tag	UNP P0DTC2
A	6	TYR	-	expression tag	UNP P0DTC2
A	7	LEU	-	expression tag	UNP P0DTC2
A	8	LEU	-	expression tag	UNP P0DTC2
A	9	GLY	-	expression tag	UNP P0DTC2
A	10	MET	-	expression tag	UNP P0DTC2
A	11	LEU	-	expression tag	UNP P0DTC2
A	12	VAL	-	expression tag	UNP P0DTC2
A	13	ALA	-	expression tag	UNP P0DTC2
A	14	SER	-	expression tag	UNP P0DTC2
A	15	VAL	-	expression tag	UNP P0DTC2
A	16	LEU	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	ALA	-	expression tag	UNP P0DTC2
A	23	ILE	THR	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	28	SER	ALA	variant	UNP P0DTC2
A	53	HIS	GLN	conflict	UNP P0DTC2
A	84	ALA	VAL	conflict	UNP P0DTC2
A	143	ASP	GLY	variant	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	146	GLN	HIS	conflict	UNP P0DTC2
A	183	GLU	GLN	conflict	UNP P0DTC2
A	213	GLU	VAL	variant	UNP P0DTC2
A	252	VAL	GLY	variant	UNP P0DTC2
A	339	HIS	GLY	variant	UNP P0DTC2
A	346	THR	ARG	variant	UNP P0DTC2
A	368	ILE	LEU	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	445	PRO	VAL	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	456	LEU	PHE	variant	UNP P0DTC2
A	460	LYS	ASN	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	conflict	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	486	PRO	PHE	variant	UNP P0DTC2
A	490	SER	PHE	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	conflict	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	682	GLY	ARG	conflict	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
A	1209	GLY	-	linker	UNP P0DTC2
A	1210	SER	-	linker	UNP P0DTC2
C	-6	MET	-	initiating methionine	UNP P0DTC2
C	-5	PRO	-	expression tag	UNP P0DTC2
C	-4	MET	-	expression tag	UNP P0DTC2
C	-3	GLY	-	expression tag	UNP P0DTC2
C	-2	SER	-	expression tag	UNP P0DTC2
C	-1	LEU	-	expression tag	UNP P0DTC2
C	0	GLN	-	expression tag	UNP P0DTC2
C	1	PRO	-	expression tag	UNP P0DTC2
C	2	LEU	-	expression tag	UNP P0DTC2
C	3	ALA	-	expression tag	UNP P0DTC2
C	4	THR	-	expression tag	UNP P0DTC2
C	5	LEU	-	expression tag	UNP P0DTC2
C	6	TYR	-	expression tag	UNP P0DTC2
C	7	LEU	-	expression tag	UNP P0DTC2
C	8	LEU	-	expression tag	UNP P0DTC2
C	9	GLY	-	expression tag	UNP P0DTC2
C	10	MET	-	expression tag	UNP P0DTC2
C	11	LEU	-	expression tag	UNP P0DTC2
C	12	VAL	-	expression tag	UNP P0DTC2
C	13	ALA	-	expression tag	UNP P0DTC2
C	14	SER	-	expression tag	UNP P0DTC2
C	15	VAL	-	expression tag	UNP P0DTC2
C	16	LEU	-	expression tag	UNP P0DTC2
C	17	ALA	-	expression tag	UNP P0DTC2
C	23	ILE	THR	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	28	SER	ALA	variant	UNP P0DTC2
C	53	HIS	GLN	conflict	UNP P0DTC2
C	84	ALA	VAL	conflict	UNP P0DTC2
C	143	ASP	GLY	variant	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	146	GLN	HIS	conflict	UNP P0DTC2
C	183	GLU	GLN	conflict	UNP P0DTC2
C	213	GLU	VAL	variant	UNP P0DTC2
C	252	VAL	GLY	variant	UNP P0DTC2
C	339	HIS	GLY	variant	UNP P0DTC2
C	346	THR	ARG	variant	UNP P0DTC2
C	368	ILE	LEU	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	445	PRO	VAL	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	456	LEU	PHE	variant	UNP P0DTC2
C	460	LYS	ASN	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	conflict	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	486	PRO	PHE	variant	UNP P0DTC2
C	490	SER	PHE	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	conflict	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2
C	1209	GLY	-	linker	UNP P0DTC2
C	1210	SER	-	linker	UNP P0DTC2
E	-6	MET	-	initiating methionine	UNP P0DTC2
E	-5	PRO	-	expression tag	UNP P0DTC2
E	-4	MET	-	expression tag	UNP P0DTC2
E	-3	GLY	-	expression tag	UNP P0DTC2
E	-2	SER	-	expression tag	UNP P0DTC2
E	-1	LEU	-	expression tag	UNP P0DTC2
E	0	GLN	-	expression tag	UNP P0DTC2
E	1	PRO	-	expression tag	UNP P0DTC2
E	2	LEU	-	expression tag	UNP P0DTC2
E	3	ALA	-	expression tag	UNP P0DTC2
E	4	THR	-	expression tag	UNP P0DTC2
E	5	LEU	-	expression tag	UNP P0DTC2
E	6	TYR	-	expression tag	UNP P0DTC2
E	7	LEU	-	expression tag	UNP P0DTC2
E	8	LEU	-	expression tag	UNP P0DTC2
E	9	GLY	-	expression tag	UNP P0DTC2
E	10	MET	-	expression tag	UNP P0DTC2
E	11	LEU	-	expression tag	UNP P0DTC2
E	12	VAL	-	expression tag	UNP P0DTC2
E	13	ALA	-	expression tag	UNP P0DTC2
E	14	SER	-	expression tag	UNP P0DTC2
E	15	VAL	-	expression tag	UNP P0DTC2
E	16	LEU	-	expression tag	UNP P0DTC2
E	17	ALA	-	expression tag	UNP P0DTC2
E	23	ILE	THR	variant	UNP P0DTC2
E	?	-	LEU	deletion	UNP P0DTC2
E	?	-	PRO	deletion	UNP P0DTC2
E	?	-	PRO	deletion	UNP P0DTC2
E	28	SER	ALA	variant	UNP P0DTC2
E	53	HIS	GLN	conflict	UNP P0DTC2
E	84	ALA	VAL	conflict	UNP P0DTC2
E	143	ASP	GLY	variant	UNP P0DTC2
E	?	-	TYR	deletion	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	146	GLN	HIS	conflict	UNP P0DTC2
E	183	GLU	GLN	conflict	UNP P0DTC2
E	213	GLU	VAL	variant	UNP P0DTC2
E	252	VAL	GLY	variant	UNP P0DTC2
E	339	HIS	GLY	variant	UNP P0DTC2
E	346	THR	ARG	variant	UNP P0DTC2
E	368	ILE	LEU	variant	UNP P0DTC2
E	371	PHE	SER	variant	UNP P0DTC2
E	373	PRO	SER	variant	UNP P0DTC2
E	375	PHE	SER	variant	UNP P0DTC2
E	376	ALA	THR	variant	UNP P0DTC2
E	405	ASN	ASP	variant	UNP P0DTC2
E	408	SER	ARG	variant	UNP P0DTC2
E	417	ASN	LYS	variant	UNP P0DTC2
E	440	LYS	ASN	variant	UNP P0DTC2
E	445	PRO	VAL	variant	UNP P0DTC2
E	446	SER	GLY	variant	UNP P0DTC2
E	456	LEU	PHE	variant	UNP P0DTC2
E	460	LYS	ASN	variant	UNP P0DTC2
E	477	ASN	SER	variant	UNP P0DTC2
E	478	LYS	THR	conflict	UNP P0DTC2
E	484	ALA	GLU	variant	UNP P0DTC2
E	486	PRO	PHE	variant	UNP P0DTC2
E	490	SER	PHE	variant	UNP P0DTC2
E	498	ARG	GLN	variant	UNP P0DTC2
E	501	TYR	ASN	variant	UNP P0DTC2
E	505	HIS	TYR	conflict	UNP P0DTC2
E	614	GLY	ASP	variant	UNP P0DTC2
E	655	TYR	HIS	variant	UNP P0DTC2
E	679	LYS	ASN	variant	UNP P0DTC2
E	681	HIS	PRO	variant	UNP P0DTC2
E	682	GLY	ARG	conflict	UNP P0DTC2
E	683	SER	ARG	conflict	UNP P0DTC2
E	685	SER	ARG	conflict	UNP P0DTC2
E	764	LYS	ASN	variant	UNP P0DTC2
E	796	TYR	ASP	variant	UNP P0DTC2
E	817	PRO	PHE	conflict	UNP P0DTC2
E	892	PRO	ALA	conflict	UNP P0DTC2
E	899	PRO	ALA	conflict	UNP P0DTC2
E	942	PRO	ALA	conflict	UNP P0DTC2
E	954	HIS	GLN	variant	UNP P0DTC2
E	969	LYS	ASN	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	986	PRO	LYS	variant	UNP P0DTC2
E	987	PRO	VAL	variant	UNP P0DTC2
E	1209	GLY	-	linker	UNP P0DTC2
E	1210	SER	-	linker	UNP P0DTC2
D	-6	MET	-	initiating methionine	UNP P0DTC2
D	-5	PRO	-	expression tag	UNP P0DTC2
D	-4	MET	-	expression tag	UNP P0DTC2
D	-3	GLY	-	expression tag	UNP P0DTC2
D	-2	SER	-	expression tag	UNP P0DTC2
D	-1	LEU	-	expression tag	UNP P0DTC2
D	0	GLN	-	expression tag	UNP P0DTC2
D	1	PRO	-	expression tag	UNP P0DTC2
D	2	LEU	-	expression tag	UNP P0DTC2
D	3	ALA	-	expression tag	UNP P0DTC2
D	4	THR	-	expression tag	UNP P0DTC2
D	5	LEU	-	expression tag	UNP P0DTC2
D	6	TYR	-	expression tag	UNP P0DTC2
D	7	LEU	-	expression tag	UNP P0DTC2
D	8	LEU	-	expression tag	UNP P0DTC2
D	9	GLY	-	expression tag	UNP P0DTC2
D	10	MET	-	expression tag	UNP P0DTC2
D	11	LEU	-	expression tag	UNP P0DTC2
D	12	VAL	-	expression tag	UNP P0DTC2
D	13	ALA	-	expression tag	UNP P0DTC2
D	14	SER	-	expression tag	UNP P0DTC2
D	15	VAL	-	expression tag	UNP P0DTC2
D	16	LEU	-	expression tag	UNP P0DTC2
D	17	ALA	-	expression tag	UNP P0DTC2
D	23	ILE	THR	variant	UNP P0DTC2
D	?	-	LEU	deletion	UNP P0DTC2
D	?	-	PRO	deletion	UNP P0DTC2
D	?	-	PRO	deletion	UNP P0DTC2
D	28	SER	ALA	variant	UNP P0DTC2
D	53	HIS	GLN	conflict	UNP P0DTC2
D	84	ALA	VAL	conflict	UNP P0DTC2
D	143	ASP	GLY	variant	UNP P0DTC2
D	?	-	TYR	deletion	UNP P0DTC2
D	146	GLN	HIS	conflict	UNP P0DTC2
D	183	GLU	GLN	conflict	UNP P0DTC2
D	213	GLU	VAL	variant	UNP P0DTC2
D	252	VAL	GLY	variant	UNP P0DTC2
D	339	HIS	GLY	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	346	THR	ARG	variant	UNP P0DTC2
D	368	ILE	LEU	variant	UNP P0DTC2
D	371	PHE	SER	variant	UNP P0DTC2
D	373	PRO	SER	variant	UNP P0DTC2
D	375	PHE	SER	variant	UNP P0DTC2
D	376	ALA	THR	variant	UNP P0DTC2
D	405	ASN	ASP	variant	UNP P0DTC2
D	408	SER	ARG	variant	UNP P0DTC2
D	417	ASN	LYS	variant	UNP P0DTC2
D	440	LYS	ASN	variant	UNP P0DTC2
D	445	PRO	VAL	variant	UNP P0DTC2
D	446	SER	GLY	variant	UNP P0DTC2
D	456	LEU	PHE	variant	UNP P0DTC2
D	460	LYS	ASN	variant	UNP P0DTC2
D	477	ASN	SER	variant	UNP P0DTC2
D	478	LYS	THR	conflict	UNP P0DTC2
D	484	ALA	GLU	variant	UNP P0DTC2
D	486	PRO	PHE	variant	UNP P0DTC2
D	490	SER	PHE	variant	UNP P0DTC2
D	498	ARG	GLN	variant	UNP P0DTC2
D	501	TYR	ASN	variant	UNP P0DTC2
D	505	HIS	TYR	conflict	UNP P0DTC2
D	614	GLY	ASP	variant	UNP P0DTC2
D	655	TYR	HIS	variant	UNP P0DTC2
D	679	LYS	ASN	variant	UNP P0DTC2
D	681	HIS	PRO	variant	UNP P0DTC2
D	682	GLY	ARG	conflict	UNP P0DTC2
D	683	SER	ARG	conflict	UNP P0DTC2
D	685	SER	ARG	conflict	UNP P0DTC2
D	764	LYS	ASN	variant	UNP P0DTC2
D	796	TYR	ASP	variant	UNP P0DTC2
D	817	PRO	PHE	conflict	UNP P0DTC2
D	892	PRO	ALA	conflict	UNP P0DTC2
D	899	PRO	ALA	conflict	UNP P0DTC2
D	942	PRO	ALA	conflict	UNP P0DTC2
D	954	HIS	GLN	variant	UNP P0DTC2
D	969	LYS	ASN	variant	UNP P0DTC2
D	986	PRO	LYS	variant	UNP P0DTC2
D	987	PRO	VAL	variant	UNP P0DTC2
D	1209	GLY	-	linker	UNP P0DTC2
D	1210	SER	-	linker	UNP P0DTC2
F	-6	MET	-	initiating methionine	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	-5	PRO	-	expression tag	UNP P0DTC2
F	-4	MET	-	expression tag	UNP P0DTC2
F	-3	GLY	-	expression tag	UNP P0DTC2
F	-2	SER	-	expression tag	UNP P0DTC2
F	-1	LEU	-	expression tag	UNP P0DTC2
F	0	GLN	-	expression tag	UNP P0DTC2
F	1	PRO	-	expression tag	UNP P0DTC2
F	2	LEU	-	expression tag	UNP P0DTC2
F	3	ALA	-	expression tag	UNP P0DTC2
F	4	THR	-	expression tag	UNP P0DTC2
F	5	LEU	-	expression tag	UNP P0DTC2
F	6	TYR	-	expression tag	UNP P0DTC2
F	7	LEU	-	expression tag	UNP P0DTC2
F	8	LEU	-	expression tag	UNP P0DTC2
F	9	GLY	-	expression tag	UNP P0DTC2
F	10	MET	-	expression tag	UNP P0DTC2
F	11	LEU	-	expression tag	UNP P0DTC2
F	12	VAL	-	expression tag	UNP P0DTC2
F	13	ALA	-	expression tag	UNP P0DTC2
F	14	SER	-	expression tag	UNP P0DTC2
F	15	VAL	-	expression tag	UNP P0DTC2
F	16	LEU	-	expression tag	UNP P0DTC2
F	17	ALA	-	expression tag	UNP P0DTC2
F	23	ILE	THR	variant	UNP P0DTC2
F	?	-	LEU	deletion	UNP P0DTC2
F	?	-	PRO	deletion	UNP P0DTC2
F	?	-	PRO	deletion	UNP P0DTC2
F	28	SER	ALA	variant	UNP P0DTC2
F	53	HIS	GLN	conflict	UNP P0DTC2
F	84	ALA	VAL	conflict	UNP P0DTC2
F	143	ASP	GLY	variant	UNP P0DTC2
F	?	-	TYR	deletion	UNP P0DTC2
F	146	GLN	HIS	conflict	UNP P0DTC2
F	183	GLU	GLN	conflict	UNP P0DTC2
F	213	GLU	VAL	variant	UNP P0DTC2
F	252	VAL	GLY	variant	UNP P0DTC2
F	339	HIS	GLY	variant	UNP P0DTC2
F	346	THR	ARG	variant	UNP P0DTC2
F	368	ILE	LEU	variant	UNP P0DTC2
F	371	PHE	SER	variant	UNP P0DTC2
F	373	PRO	SER	variant	UNP P0DTC2
F	375	PHE	SER	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	376	ALA	THR	variant	UNP P0DTC2
F	405	ASN	ASP	variant	UNP P0DTC2
F	408	SER	ARG	variant	UNP P0DTC2
F	417	ASN	LYS	variant	UNP P0DTC2
F	440	LYS	ASN	variant	UNP P0DTC2
F	445	PRO	VAL	variant	UNP P0DTC2
F	446	SER	GLY	variant	UNP P0DTC2
F	456	LEU	PHE	variant	UNP P0DTC2
F	460	LYS	ASN	variant	UNP P0DTC2
F	477	ASN	SER	variant	UNP P0DTC2
F	478	LYS	THR	conflict	UNP P0DTC2
F	484	ALA	GLU	variant	UNP P0DTC2
F	486	PRO	PHE	variant	UNP P0DTC2
F	490	SER	PHE	variant	UNP P0DTC2
F	498	ARG	GLN	variant	UNP P0DTC2
F	501	TYR	ASN	variant	UNP P0DTC2
F	505	HIS	TYR	conflict	UNP P0DTC2
F	614	GLY	ASP	variant	UNP P0DTC2
F	655	TYR	HIS	variant	UNP P0DTC2
F	679	LYS	ASN	variant	UNP P0DTC2
F	681	HIS	PRO	variant	UNP P0DTC2
F	682	GLY	ARG	conflict	UNP P0DTC2
F	683	SER	ARG	conflict	UNP P0DTC2
F	685	SER	ARG	conflict	UNP P0DTC2
F	764	LYS	ASN	variant	UNP P0DTC2
F	796	TYR	ASP	variant	UNP P0DTC2
F	817	PRO	PHE	conflict	UNP P0DTC2
F	892	PRO	ALA	conflict	UNP P0DTC2
F	899	PRO	ALA	conflict	UNP P0DTC2
F	942	PRO	ALA	conflict	UNP P0DTC2
F	954	HIS	GLN	variant	UNP P0DTC2
F	969	LYS	ASN	variant	UNP P0DTC2
F	986	PRO	LYS	variant	UNP P0DTC2
F	987	PRO	VAL	variant	UNP P0DTC2
F	1209	GLY	-	linker	UNP P0DTC2
F	1210	SER	-	linker	UNP P0DTC2

- Molecule 2 is a protein called CYFN1006-2 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	203	Total	C	N	O	S	0	0
			1502	938	251	306	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	203	Total	C	N	O	S	0	0
			1502	938	251	306	7		
2	L	203	Total	C	N	O	S	0	0
			1502	938	251	306	7		
2	P	203	Total	C	N	O	S	0	0
			1502	938	251	306	7		
2	Q	203	Total	C	N	O	S	0	0
			1502	938	251	306	7		
2	R	203	Total	C	N	O	S	0	0
			1502	938	251	306	7		

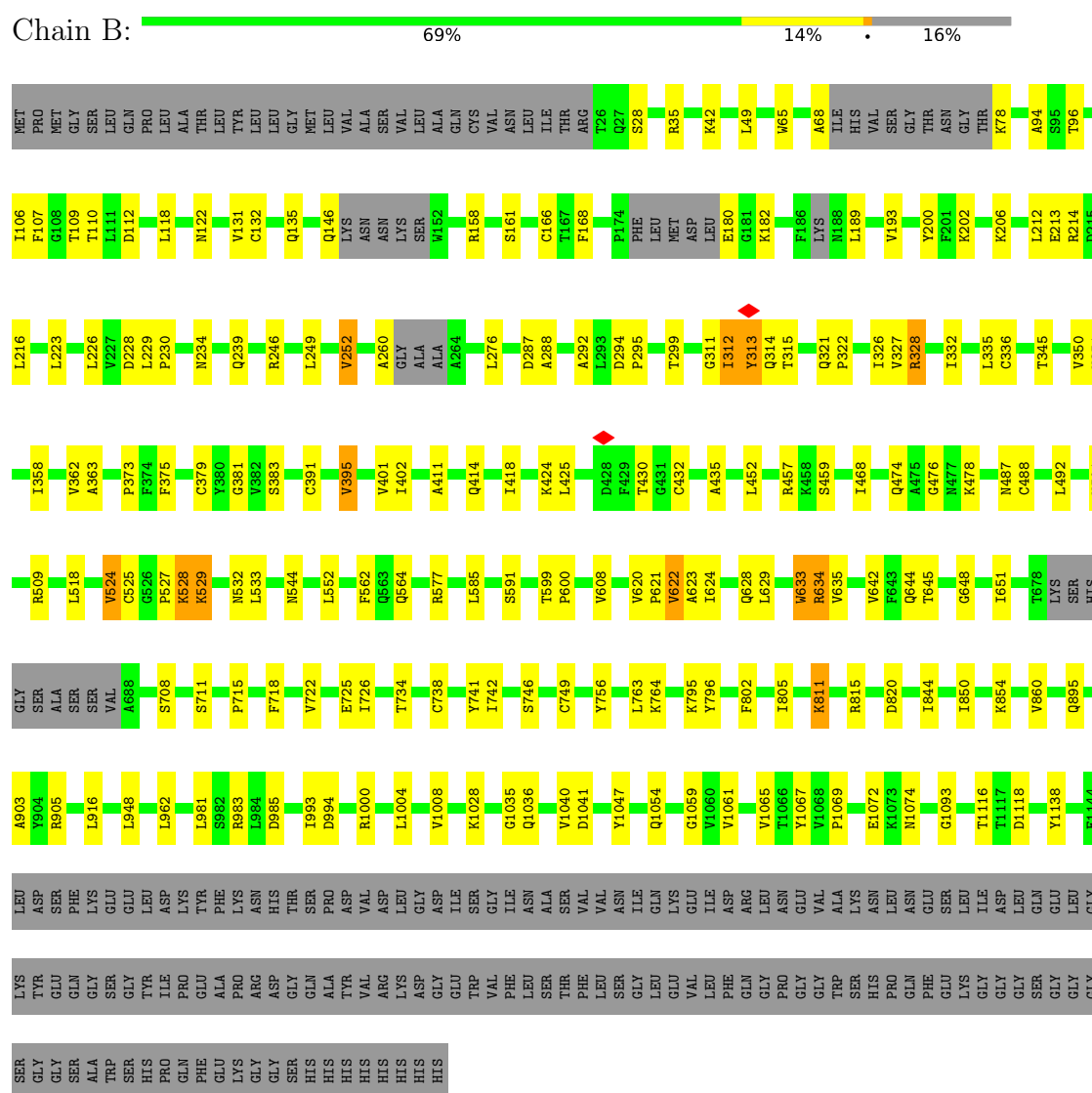
- Molecule 3 is a protein called CYFN1006-2 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	218	Total	C	N	O	S	0	0
			1646	1050	268	320	8		
3	H	218	Total	C	N	O	S	0	0
			1646	1050	268	320	8		
3	I	218	Total	C	N	O	S	0	0
			1646	1050	268	320	8		
3	M	218	Total	C	N	O	S	0	0
			1646	1050	268	320	8		
3	N	218	Total	C	N	O	S	0	0
			1646	1050	268	320	8		
3	O	218	Total	C	N	O	S	0	0
			1646	1050	268	320	8		

3 Residue-property plots

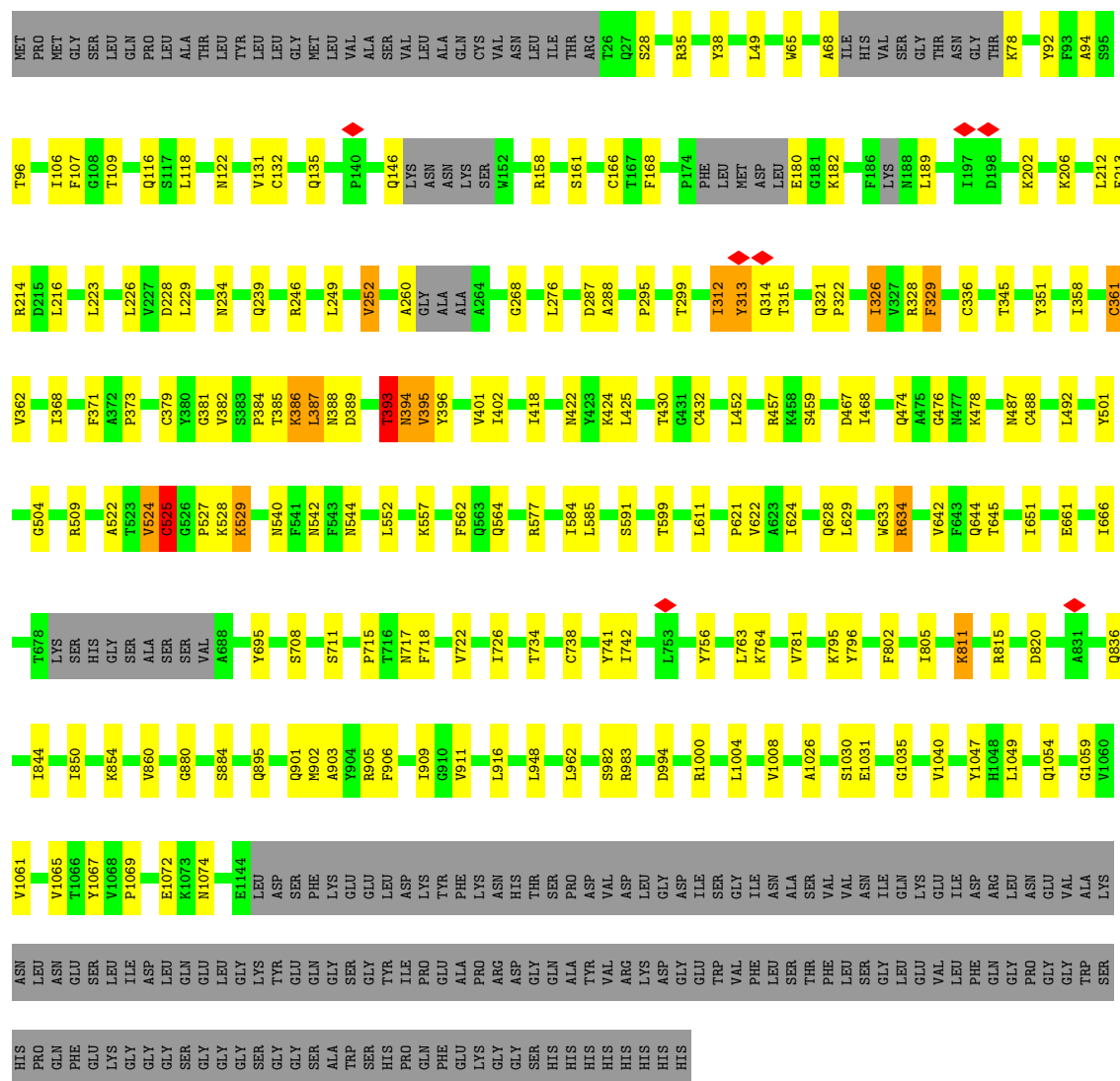
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Spike glycoprotein,Fibritin,Expression Tag

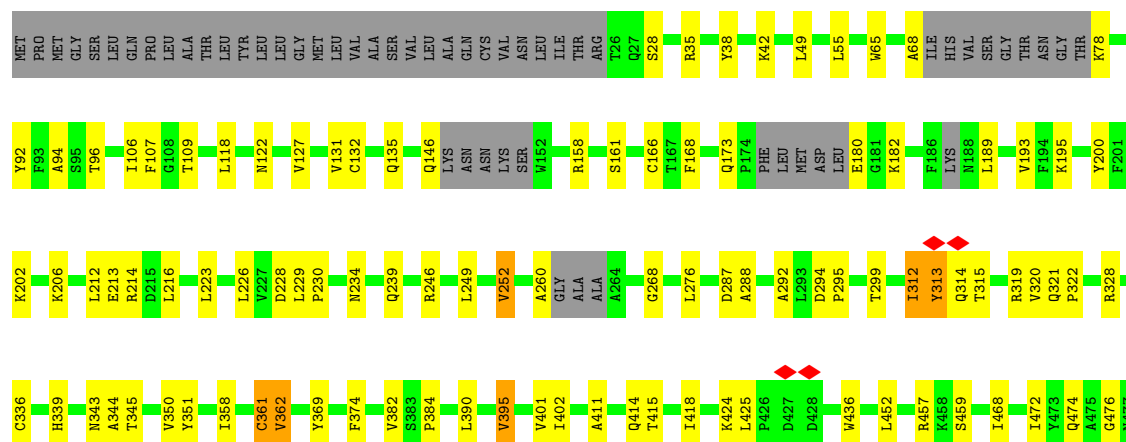


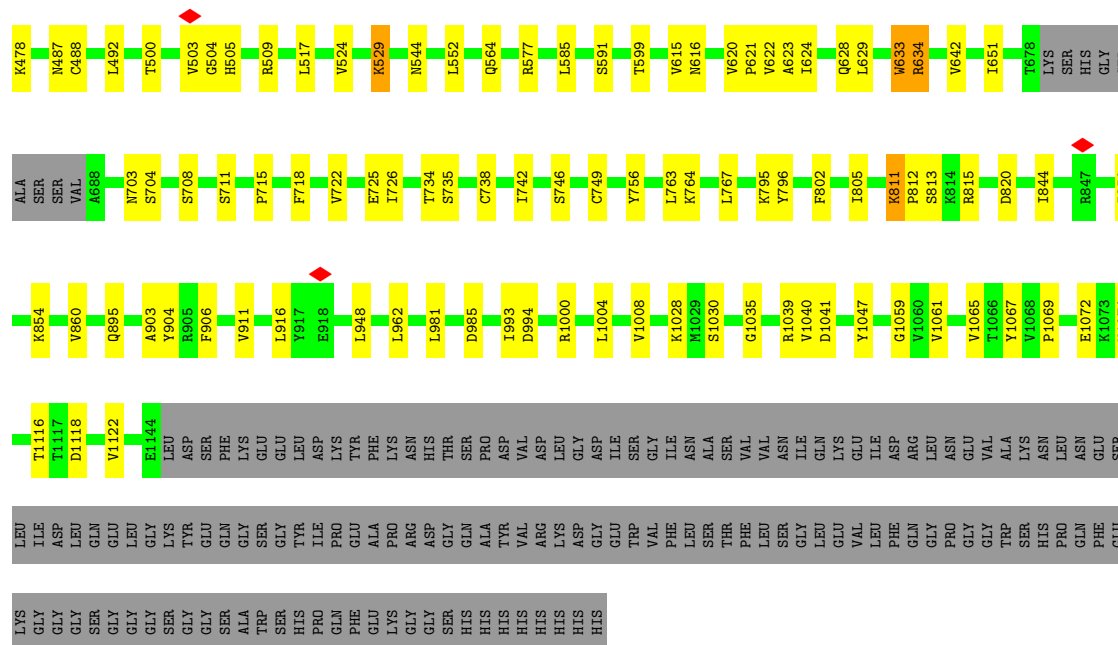
• Molecule 1: Spike glycoprotein,Fibritin,Expression Tag



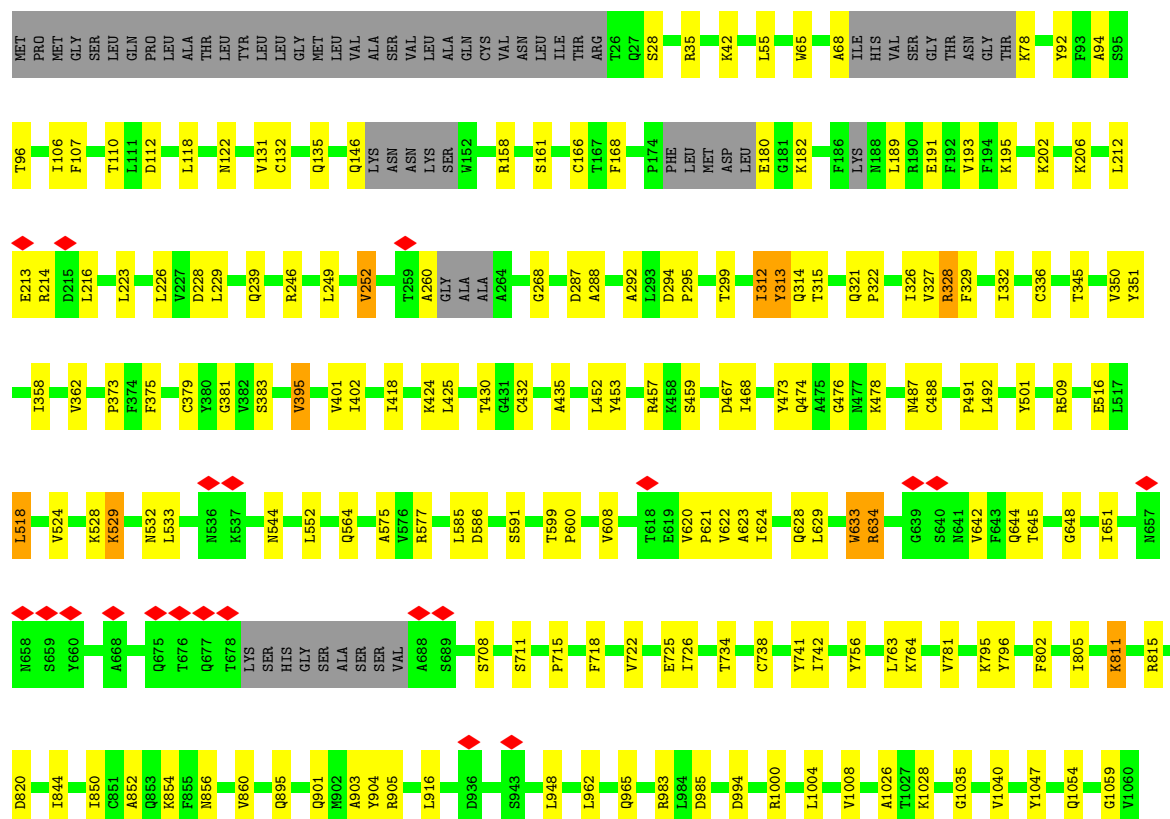


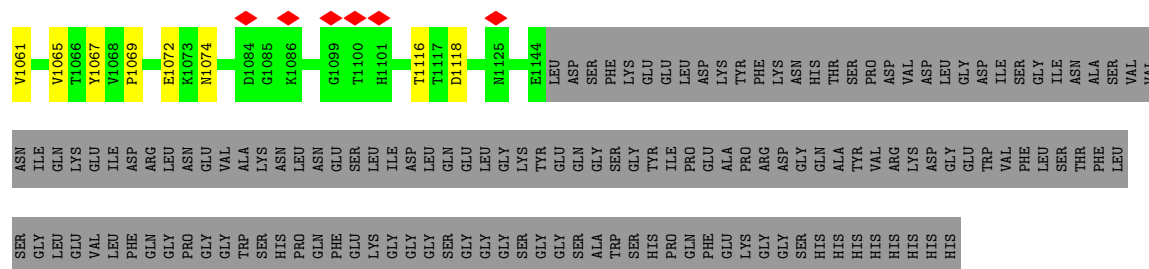
• Molecule 1: Spike glycoprotein,Fibritin,Expression Tag



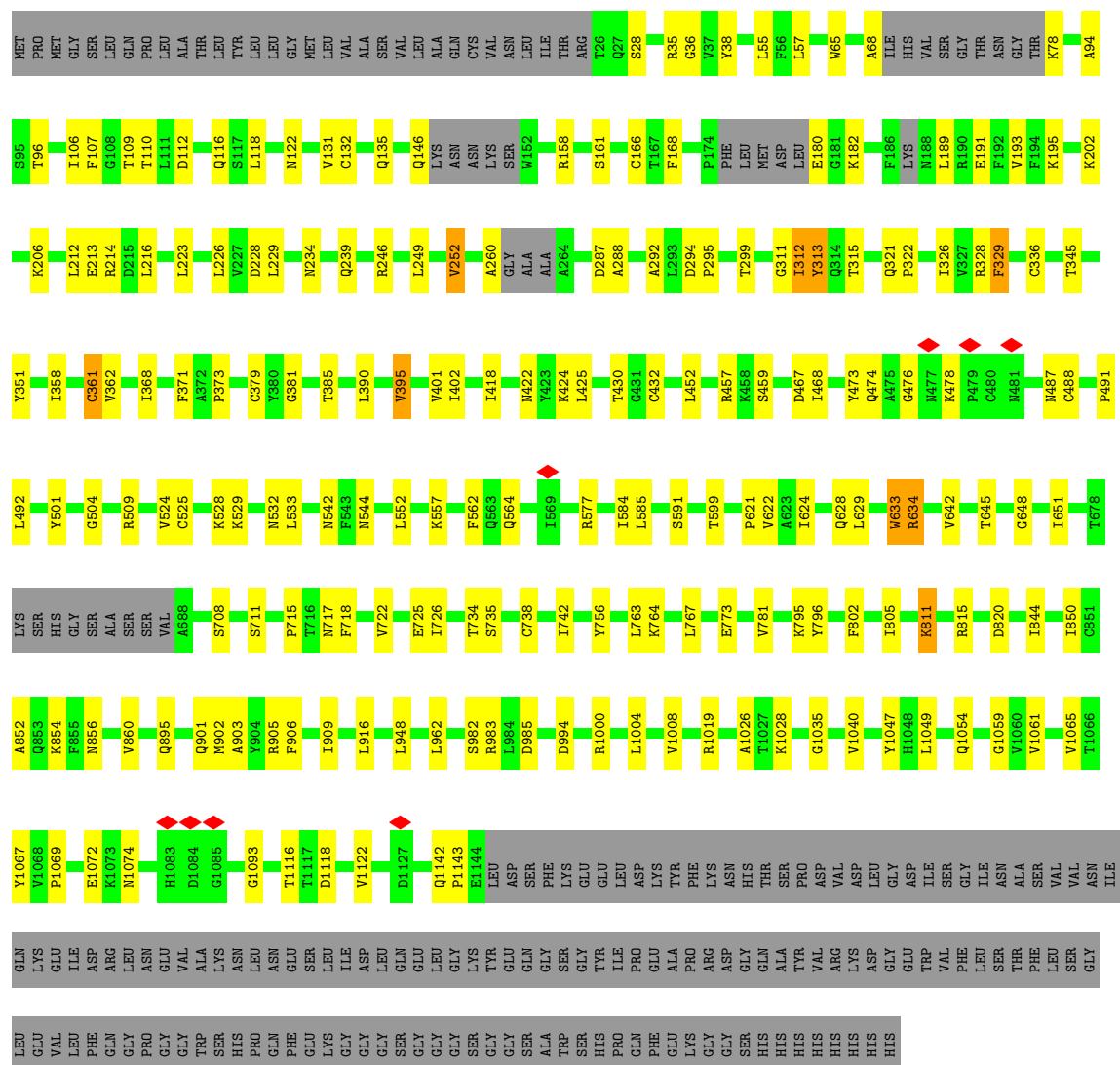


• Molecule 1: Spike glycoprotein,Fibritin,Expression Tag





• Molecule 1: Spike glycoprotein,Fibritin,Expression Tag



• Molecule 1: Spike glycoprotein,Fibritin,Expression Tag



THR
GLU
CYS
SER

• Molecule 2: CYFN1006-2 light chain

Chain L: 

GLN S2 S9 P15 I21 S22 C23 W41 L52 M53 I54 Y55 E56 V57 N65 R75 S88 S89 G93 L94 Y107 V116 M123 I157 Y161 P162 T166 A171 S174 K187 N190 N191 Y193 A194 A195 L201 T222 VAL

GLU
LYS
THR
VAL
ALA
PRO
THR
GLU
CYS
SER

• Molecule 2: CYFN1006-2 light chain

Chain P: 

GLN S2 C23 W41 Y42 L52 M53 I54 Y55 E56 V57 N65 R75 A87 G93 Y107 V116 T122 T125 V126 K131 T137 A148 N149 L156 P162 G163 A164 V165 T166 A171 D172 S173 S174 P175 V175 K177 A178 K187 N190 N191 K192

Y193 A194 L201 T202 P203 E204 S208 T217 H218 E219 G220 S221 T222 VAL GLU LYS THR VAL ALA PRO THR GLU CYS SER

• Molecule 2: CYFN1006-2 light chain

Chain Q: 

GLN S2 S9 P15 I21 S22 C23 W41 L52 M53 I54 Y55 E56 V57 N65 R75 S88 S89 G93 L94 Y107 R115 V116 M123 I157 Y161 P162 T166 A171 S174 N190 N191 K192 A195 L201 T222 VAL GLU LYS

THR
VAL
ALA
PRO
THR
GLU
CYS
SER

• Molecule 2: CYFN1006-2 light chain

Chain R: 

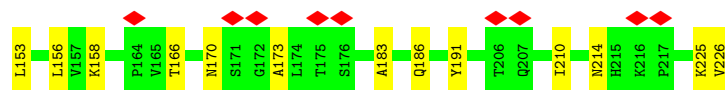
GLN S2 A3 S9 P15 G16 Q17 I21 S22 C23 W41 L52 M53 I54 Y55 E56 V57 N65 R75 N85 T86 A87 S88 L89 G93 L94 Y107 R115 V116 M123 P141 L146 Q147 A148 N149 L153 I157 Y161 P162 T166 A171

S174 K187 N190 N191 K192 Y193 A194 A195 L199 S200 L201 T202 P203 T222 VAL GLU LYS THR VAL ALA PRO THR GLU CYS SER

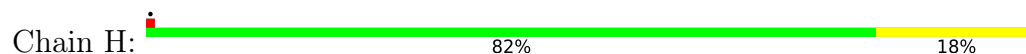
• Molecule 3: CYFN1006-2 heavy chain

Chain G: 

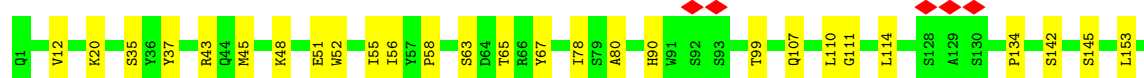
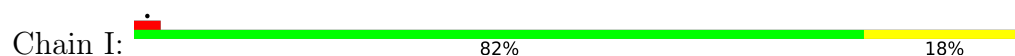
Q1 E11 V12 K13 K14 P15 S35 Y36 Y37 G40 R43 K44 Q44 T222 K48 E51 W52 I55 I56 Y57 P58 G59 D62 S63 D64 T65 I78 D81 K82 T99 Q107 L110 G111 I113 L114 T125 V126 S127 K132 F137 S142 S145



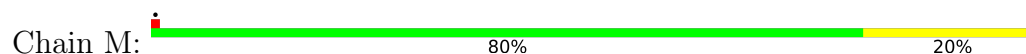
- Molecule 3: CYFN1006-2 heavy chain



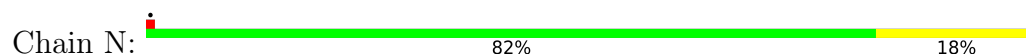
- Molecule 3: CYFN1006-2 heavy chain



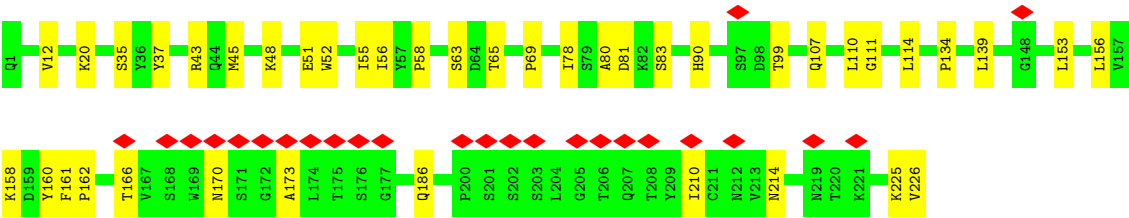
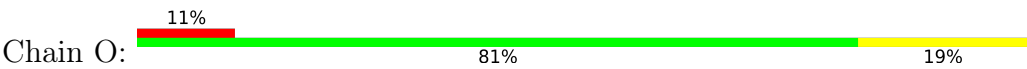
- Molecule 3: CYFN1006-2 heavy chain



- Molecule 3: CYFN1006-2 heavy chain



- Molecule 3: CYFN1006-2 heavy chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	66958	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)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.852	Depositor
Minimum map value	-0.698	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	571.2, 571.2, 571.2	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.19, 1.19, 1.19	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	1/8707 (0.0%)	0.32	3/11856 (0.0%)
1	B	0.09	0/8707	0.27	0/11856
1	C	0.09	0/8707	0.27	0/11856
1	D	0.09	0/8707	0.25	0/11856
1	E	0.09	0/8707	0.26	0/11856
1	F	0.09	0/8707	0.27	0/11856
2	J	0.08	0/1540	0.27	0/2101
2	K	0.08	0/1540	0.24	0/2101
2	L	0.08	0/1540	0.25	0/2101
2	P	0.09	0/1540	0.26	0/2101
2	Q	0.08	0/1540	0.25	0/2101
2	R	0.09	0/1540	0.27	0/2101
3	G	0.09	0/1691	0.26	0/2302
3	H	0.08	0/1691	0.22	0/2302
3	I	0.08	0/1691	0.22	0/2302
3	M	0.09	0/1691	0.26	0/2302
3	N	0.08	0/1691	0.22	0/2302
3	O	0.08	0/1691	0.22	0/2302
All	All	0.11	1/71628 (0.0%)	0.27	3/97554 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	393	THR	CA-C	-10.52	1.47	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	386	LYS	N-CA-C	-9.51	101.19	113.17
1	A	389	ASP	N-CA-C	-5.93	107.86	114.62
1	A	525	CYS	N-CA-C	5.35	122.19	110.80

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	8502	0	8290	117	0
1	B	8502	0	8290	110	0
1	C	8502	0	8290	112	0
1	D	8502	0	8290	118	0
1	E	8502	0	8290	106	0
1	F	8502	0	8290	103	0
2	J	1502	0	1445	17	0
2	K	1502	0	1445	13	0
2	L	1502	0	1445	15	0
2	P	1502	0	1445	14	0
2	Q	1502	0	1445	14	0
2	R	1502	0	1445	19	0
3	G	1646	0	1615	23	0
3	H	1646	0	1615	20	0
3	I	1646	0	1615	20	0
3	M	1646	0	1615	23	0
3	N	1646	0	1615	20	0
3	O	1646	0	1615	21	0
All	All	69900	0	68100	823	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 (823) 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:A:322:PRO:HD3	1:A:629:LEU:HB3	1.66	0.77
1:E:322:PRO:HD3	1:E:629:LEU:HB3	1.66	0.77
1:D:322:PRO:HD3	1:D:629:LEU:HB3	1.68	0.76
1:B:322:PRO:HD3	1:B:629:LEU:HB3	1.66	0.76
1:D:361:CYS:H	1:D:524:VAL:HG12	1.52	0.74
1:C:336:CYS:HB2	1:C:362:VAL:H	1.53	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:564:GLN:HG3	1:B:577:ARG:HB3	1.69	0.73
1:F:336:CYS:HB2	1:F:362:VAL:H	1.54	0.73
1:D:564:GLN:HG3	1:D:577:ARG:HB3	1.71	0.72
1:E:564:GLN:HG3	1:E:577:ARG:HB3	1.70	0.72
1:A:564:GLN:HG3	1:A:577:ARG:HB3	1.72	0.71
1:D:116:GLN:HE21	1:F:468:ILE:HD11	1.55	0.71
1:A:116:GLN:HE21	1:C:468:ILE:HD11	1.56	0.70
3:G:37:TYR:HA	3:G:107:GLN:HE21	1.57	0.69
1:A:1047:TYR:HB2	1:A:1067:TYR:HB3	1.75	0.68
1:F:322:PRO:HD3	1:F:629:LEU:HB3	1.75	0.68
3:M:37:TYR:HA	3:M:107:GLN:HE21	1.57	0.68
1:D:1047:TYR:HB2	1:D:1067:TYR:HB3	1.74	0.68
1:C:295:PRO:HG3	1:C:634:ARG:HD2	1.75	0.68
1:A:299:THR:HG21	1:A:599:THR:HG21	1.74	0.68
3:I:37:TYR:HA	3:I:107:GLN:HE21	1.59	0.67
1:F:1047:TYR:HB2	1:F:1067:TYR:HB3	1.76	0.67
1:E:1047:TYR:HB2	1:E:1067:TYR:HB3	1.76	0.67
1:C:322:PRO:HD3	1:C:629:LEU:HB3	1.77	0.66
1:A:295:PRO:HG3	1:A:634:ARG:HD2	1.75	0.66
1:D:544:ASN:ND2	1:D:564:GLN:OE1	2.28	0.66
1:C:299:THR:HG21	1:C:599:THR:HG21	1.77	0.66
1:D:478:LYS:HE3	1:D:487:ASN:HD21	1.60	0.66
3:N:56:ILE:HG22	3:N:65:THR:HG22	1.78	0.66
3:O:37:TYR:HA	3:O:107:GLN:HE21	1.61	0.65
1:B:763:LEU:HD22	1:B:1008:VAL:HG21	1.77	0.65
1:B:1047:TYR:HB2	1:B:1067:TYR:HB3	1.79	0.65
1:A:393:THR:HG23	1:A:522:ALA:HA	1.78	0.65
1:B:315:THR:HB	1:C:764:LYS:HD3	1.77	0.65
1:A:328:ARG:HG3	1:A:542:ASN:HB3	1.78	0.64
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	1.79	0.64
3:I:56:ILE:HG22	3:I:65:THR:HG22	1.79	0.64
1:A:478:LYS:HE3	1:A:487:ASN:HD21	1.60	0.64
1:D:1035:GLY:HA3	1:F:1040:VAL:HG21	1.79	0.64
3:H:56:ILE:HG22	3:H:65:THR:HG22	1.80	0.64
1:F:299:THR:HG21	1:F:599:THR:HG21	1.79	0.64
2:Q:190:ASN:OD1	2:Q:192:LYS:NZ	2.28	0.64
1:C:1047:TYR:HB2	1:C:1067:TYR:HB3	1.78	0.64
1:E:299:THR:HG21	1:E:599:THR:HG21	1.80	0.64
1:D:328:ARG:HG3	1:D:542:ASN:HB3	1.78	0.63
1:C:321:GLN:HE21	1:C:591:SER:H	1.47	0.63
1:D:299:THR:HG21	1:D:599:THR:HG21	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	1.80	0.63
3:O:56:ILE:HG22	3:O:65:THR:HG22	1.81	0.63
1:E:381:GLY:HA3	1:E:430:THR:HG23	1.81	0.63
3:G:56:ILE:HG22	3:G:65:THR:HG22	1.80	0.63
1:E:764:LYS:HD3	1:D:315:THR:HB	1.81	0.63
1:B:132:CYS:SG	1:B:166:CYS:N	2.72	0.62
2:P:190:ASN:OD1	2:P:192:LYS:NZ	2.33	0.62
1:B:1035:GLY:HA3	1:A:1040:VAL:HG21	1.80	0.62
1:A:68:ALA:HA	1:A:78:LYS:HA	1.81	0.62
1:A:1035:GLY:HA3	1:C:1040:VAL:HG21	1.82	0.62
2:J:190:ASN:OD1	2:J:192:LYS:NZ	2.33	0.62
1:B:312:ILE:HD12	1:B:313:TYR:H	1.63	0.62
1:C:131:VAL:HB	1:C:168:PHE:HB3	1.82	0.62
1:E:478:LYS:HE3	1:E:487:ASN:HD21	1.64	0.62
3:M:56:ILE:HG22	3:M:65:THR:HG22	1.81	0.62
1:C:132:CYS:SG	1:C:166:CYS:N	2.73	0.61
2:J:52:LEU:HD11	2:J:55:TYR:HB3	1.81	0.61
1:E:315:THR:HB	1:F:764:LYS:HD3	1.80	0.61
2:P:23:CYS:HB3	2:P:87:ALA:HB3	1.83	0.61
1:C:564:GLN:HG3	1:C:577:ARG:HB3	1.82	0.61
1:B:725:GLU:OE2	1:B:1028:LYS:NZ	2.33	0.61
1:A:642:VAL:HG12	1:A:651:ILE:HG12	1.82	0.61
1:A:312:ILE:HD12	1:A:313:TYR:H	1.65	0.61
2:K:190:ASN:OD1	2:K:192:LYS:NZ	2.28	0.61
2:Q:23:CYS:HB3	2:Q:87:ALA:HB3	1.82	0.61
1:F:295:PRO:HG3	1:F:634:ARG:HD2	1.83	0.61
1:A:345:THR:O	1:A:509:ARG:NH1	2.34	0.61
1:A:764:LYS:HD3	1:C:315:THR:HB	1.83	0.60
1:C:452:LEU:HD13	1:C:492:LEU:HB3	1.83	0.60
2:R:190:ASN:OD1	2:R:192:LYS:NZ	2.33	0.60
2:L:23:CYS:HB3	2:L:87:ALA:HB3	1.83	0.60
1:A:132:CYS:SG	1:A:166:CYS:N	2.74	0.60
1:B:35:ARG:HD2	1:B:216:LEU:HD13	1.84	0.60
1:B:381:GLY:HA3	1:B:430:THR:HG23	1.83	0.60
1:E:1040:VAL:HG21	1:F:1035:GLY:HA3	1.84	0.60
1:D:763:LEU:HD22	1:D:1008:VAL:HG21	1.83	0.60
1:F:312:ILE:HD12	1:F:313:TYR:H	1.66	0.60
1:E:312:ILE:HD12	1:E:313:TYR:H	1.66	0.60
1:E:132:CYS:SG	1:E:166:CYS:N	2.74	0.60
1:B:478:LYS:HE3	1:B:487:ASN:HD21	1.66	0.60
1:A:28:SER:HB2	1:A:65:TRP:HB3	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:452:LEU:HD13	1:F:492:LEU:HB3	1.84	0.60
1:E:107:PHE:HB2	1:E:118:LEU:HB3	1.84	0.60
1:E:131:VAL:HB	1:E:168:PHE:HB3	1.83	0.60
2:P:52:LEU:HD11	2:P:55:TYR:HB3	1.84	0.60
1:F:763:LEU:HD22	1:F:1008:VAL:HG21	1.83	0.60
2:J:23:CYS:HB3	2:J:87:ALA:HB3	1.84	0.60
1:D:68:ALA:HA	1:D:78:LYS:HA	1.83	0.60
1:F:132:CYS:SG	1:F:166:CYS:N	2.74	0.60
1:A:544:ASN:ND2	1:A:564:GLN:OE1	2.34	0.60
2:R:52:LEU:HD11	2:R:55:TYR:HB3	1.83	0.60
1:B:122:ASN:ND2	1:B:180:GLU:O	2.34	0.59
1:B:68:ALA:HA	1:B:78:LYS:HA	1.83	0.59
1:B:1040:VAL:HG21	1:C:1035:GLY:HA3	1.84	0.59
1:D:132:CYS:SG	1:D:166:CYS:N	2.75	0.59
1:D:312:ILE:HD12	1:D:313:TYR:H	1.66	0.59
1:D:345:THR:O	1:D:509:ARG:NH1	2.35	0.59
3:H:37:TYR:HA	3:H:107:GLN:HE21	1.68	0.59
1:E:28:SER:HB2	1:E:65:TRP:HB3	1.84	0.59
1:D:295:PRO:HG3	1:D:634:ARG:HD2	1.83	0.59
1:C:642:VAL:HG12	1:C:651:ILE:HG12	1.84	0.59
1:E:763:LEU:HD22	1:E:1008:VAL:HG21	1.84	0.59
3:M:45:MET:HB2	3:M:48:LYS:HB2	1.85	0.59
3:I:56:ILE:HD12	3:I:80:ALA:HB2	1.85	0.59
1:E:68:ALA:HA	1:E:78:LYS:HA	1.85	0.59
1:D:501:TYR:HE1	3:O:63:SER:HB2	1.67	0.59
2:K:21:ILE:HD12	2:K:89:LEU:HD23	1.85	0.59
1:C:68:ALA:HA	1:C:78:LYS:HA	1.83	0.59
1:C:312:ILE:HD12	1:C:313:TYR:H	1.67	0.59
1:E:1035:GLY:HA3	1:D:1040:VAL:HG21	1.84	0.59
1:D:107:PHE:HB2	1:D:118:LEU:HB3	1.85	0.59
2:R:23:CYS:HB3	2:R:87:ALA:HB3	1.85	0.59
1:F:122:ASN:ND2	1:F:180:GLU:O	2.36	0.59
1:F:564:GLN:HG3	1:F:577:ARG:HB3	1.84	0.59
1:B:345:THR:O	1:B:509:ARG:NH1	2.36	0.59
1:A:321:GLN:HE21	1:A:591:SER:H	1.51	0.59
1:E:122:ASN:ND2	1:E:180:GLU:O	2.36	0.59
2:K:23:CYS:HB3	2:K:87:ALA:HB3	1.85	0.58
2:L:190:ASN:OD1	2:L:192:LYS:NZ	2.34	0.58
3:G:45:MET:HB2	3:G:48:LYS:HB2	1.85	0.58
1:C:478:LYS:HE3	1:C:487:ASN:HD21	1.68	0.58
1:F:478:LYS:HE3	1:F:487:ASN:HD21	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1054:GLN:HB2	1:D:1061:VAL:HB	1.84	0.58
1:C:361:CYS:H	1:C:524:VAL:HG22	1.68	0.58
1:B:299:THR:HG21	1:B:599:THR:HG21	1.85	0.58
1:A:107:PHE:HB2	1:A:118:LEU:HB3	1.86	0.58
1:D:524:VAL:HG23	1:D:525:CYS:H	1.69	0.58
2:L:75:ARG:NH1	2:L:93:GLY:O	2.37	0.58
1:B:764:LYS:HD3	1:A:315:THR:HB	1.86	0.58
3:I:45:MET:HB2	3:I:48:LYS:HB2	1.86	0.58
1:D:381:GLY:HA3	1:D:430:THR:HG23	1.85	0.58
1:B:28:SER:HB2	1:B:65:TRP:HB3	1.84	0.58
1:D:642:VAL:HG12	1:D:651:ILE:HG12	1.85	0.58
1:A:131:VAL:HB	1:A:168:PHE:HB3	1.84	0.57
1:A:742:ILE:O	1:A:1000:ARG:NH2	2.37	0.57
2:K:75:ARG:NH1	2:K:93:GLY:O	2.37	0.57
1:E:634:ARG:O	1:E:634:ARG:NE	2.37	0.57
1:D:634:ARG:O	1:D:634:ARG:NE	2.36	0.57
1:D:781:VAL:HG22	1:D:1026:ALA:HB2	1.85	0.57
1:B:107:PHE:HB2	1:B:118:LEU:HB3	1.86	0.57
1:B:726:ILE:HG12	1:B:1061:VAL:HG22	1.86	0.57
1:B:131:VAL:HB	1:B:168:PHE:HB3	1.85	0.57
2:R:75:ARG:NH1	2:R:93:GLY:O	2.38	0.57
1:F:642:VAL:HG12	1:F:651:ILE:HG12	1.86	0.57
1:B:742:ILE:O	1:B:1000:ARG:NH2	2.37	0.57
1:E:452:LEU:HD13	1:E:492:LEU:HB3	1.86	0.57
1:B:94:ALA:HB1	1:B:189:LEU:HD11	1.86	0.57
1:B:295:PRO:HG3	1:B:634:ARG:HD2	1.85	0.57
1:A:122:ASN:ND2	1:A:180:GLU:O	2.38	0.57
1:D:94:ALA:HB1	1:D:189:LEU:HD11	1.87	0.57
1:D:122:ASN:ND2	1:D:180:GLU:O	2.37	0.57
3:O:210:ILE:HA	3:O:225:LYS:HA	1.87	0.57
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.87	0.57
1:E:35:ARG:HD2	1:E:216:LEU:HD13	1.86	0.57
1:E:345:THR:O	1:E:509:ARG:NH1	2.37	0.57
1:A:634:ARG:O	1:A:634:ARG:NE	2.38	0.57
2:Q:75:ARG:NH1	2:Q:93:GLY:O	2.38	0.57
1:F:424:LYS:NZ	1:F:425:LEU:O	2.38	0.57
1:E:292:ALA:HB1	1:E:633:TRP:HB2	1.87	0.57
1:E:642:VAL:HG12	1:E:651:ILE:HG12	1.86	0.57
1:C:94:ALA:HB1	1:C:189:LEU:HD11	1.87	0.56
1:F:811:LYS:NZ	1:F:820:ASP:OD2	2.38	0.56
1:B:206:LYS:HB2	1:B:223:LEU:HA	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:PRO:HG3	1:A:504:GLY:HA3	1.86	0.56
3:O:134:PRO:HB3	3:O:160:TYR:HB3	1.87	0.56
1:B:424:LYS:NZ	1:B:425:LEU:O	2.38	0.56
2:J:75:ARG:NH1	2:J:93:GLY:O	2.38	0.56
1:D:726:ILE:HG12	1:D:1061:VAL:HG22	1.87	0.56
3:N:153:LEU:HD23	3:N:226:VAL:HG13	1.87	0.56
3:O:45:MET:HB2	3:O:48:LYS:HB2	1.87	0.56
1:B:642:VAL:HG12	1:B:651:ILE:HG12	1.87	0.56
1:C:107:PHE:HB2	1:C:118:LEU:HB3	1.88	0.56
1:D:718:PHE:HA	1:D:1069:PRO:HA	1.86	0.56
1:C:28:SER:HB2	1:C:65:TRP:HB3	1.86	0.56
1:C:815:ARG:NE	1:C:820:ASP:OD1	2.39	0.56
1:D:361:CYS:N	1:D:524:VAL:HG12	2.18	0.56
1:D:373:PRO:HB3	1:F:504:GLY:HA3	1.88	0.56
1:B:452:LEU:HD13	1:B:492:LEU:HB3	1.88	0.56
1:C:742:ILE:O	1:C:1000:ARG:NH2	2.39	0.56
1:E:1074:ASN:OD1	1:F:895:GLN:NE2	2.39	0.56
1:F:107:PHE:HB2	1:F:118:LEU:HB3	1.88	0.56
1:F:321:GLN:HE21	1:F:591:SER:H	1.53	0.56
1:B:895:GLN:NE2	1:A:1074:ASN:OD1	2.39	0.56
1:A:49:LEU:HB3	1:A:276:LEU:HD11	1.88	0.56
2:L:52:LEU:HD11	2:L:55:TYR:HB3	1.87	0.56
1:C:122:ASN:ND2	1:C:180:GLU:O	2.39	0.56
1:F:35:ARG:HD2	1:F:216:LEU:HD13	1.88	0.56
1:E:726:ILE:HG12	1:E:1061:VAL:HG22	1.88	0.55
2:P:75:ARG:NH1	2:P:93:GLY:O	2.39	0.55
1:E:895:GLN:NE2	1:D:1074:ASN:OD1	2.40	0.55
1:A:385:THR:HG1	1:C:415:THR:HG1	1.53	0.55
1:D:457:ARG:NH2	1:D:459:SER:O	2.36	0.55
1:B:815:ARG:NE	1:B:820:ASP:OD1	2.39	0.55
1:B:1074:ASN:OD1	1:C:895:GLN:NE2	2.40	0.55
1:C:424:LYS:NZ	1:C:425:LEU:O	2.39	0.55
3:M:158:LYS:NZ	3:M:186:GLN:OE1	2.38	0.55
1:F:28:SER:HB2	1:F:65:TRP:HB3	1.88	0.55
1:E:718:PHE:HA	1:E:1069:PRO:HA	1.89	0.55
1:D:385:THR:HG1	1:F:415:THR:HG1	1.51	0.55
1:F:815:ARG:NE	1:F:820:ASP:OD1	2.39	0.55
3:G:158:LYS:NZ	3:G:186:GLN:OE1	2.38	0.55
1:E:94:ALA:HB1	1:E:189:LEU:HD11	1.89	0.55
2:Q:21:ILE:HD12	2:Q:89:LEU:HD23	1.89	0.55
1:B:802:PHE:HD1	1:B:805:ILE:HD11	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ALA:HB1	1:A:189:LEU:HD11	1.89	0.55
1:A:948:LEU:HD21	1:A:1059:GLY:HA3	1.87	0.55
3:H:45:MET:HB2	3:H:48:LYS:HB2	1.88	0.55
1:D:206:LYS:HB2	1:D:223:LEU:HA	1.88	0.55
1:D:764:LYS:HD3	1:F:315:THR:HB	1.89	0.55
1:A:158:ARG:HB3	1:A:252:VAL:HG13	1.89	0.55
1:E:206:LYS:HB2	1:E:223:LEU:HA	1.89	0.55
1:D:28:SER:HB2	1:D:65:TRP:HB3	1.89	0.55
1:D:895:GLN:NE2	1:F:1074:ASN:OD1	2.40	0.55
1:F:68:ALA:HA	1:F:78:LYS:HA	1.89	0.55
1:F:131:VAL:HB	1:F:168:PHE:HB3	1.89	0.55
1:D:424:LYS:NZ	1:D:425:LEU:O	2.38	0.54
1:F:94:ALA:HB1	1:F:189:LEU:HD11	1.89	0.54
1:F:634:ARG:O	1:F:634:ARG:NE	2.37	0.54
1:A:895:GLN:NE2	1:C:1074:ASN:OD1	2.40	0.54
1:A:726:ILE:HG12	1:A:1061:VAL:HG22	1.89	0.54
1:C:634:ARG:O	1:C:634:ARG:NE	2.38	0.54
2:R:153:LEU:HB2	2:R:199:LEU:HB3	1.89	0.54
1:A:452:LEU:HD13	1:A:492:LEU:HB3	1.88	0.54
1:E:424:LYS:NZ	1:E:425:LEU:O	2.38	0.54
1:E:756:TYR:OH	1:E:994:ASP:OD1	2.24	0.54
1:F:350:VAL:HG11	1:F:418:ILE:HD12	1.89	0.54
1:A:501:TYR:HE1	3:I:63:SER:HB2	1.71	0.54
2:K:9:SER:HA	2:K:123:MET:H	1.72	0.54
3:O:56:ILE:HD12	3:O:80:ALA:HB2	1.90	0.54
1:F:358:ILE:HB	1:F:395:VAL:HG13	1.90	0.54
2:K:52:LEU:HD11	2:K:55:TYR:HB3	1.90	0.54
1:E:815:ARG:NE	1:E:820:ASP:OD1	2.40	0.54
3:N:45:MET:HB2	3:N:48:LYS:HB2	1.90	0.54
2:Q:9:SER:HA	2:Q:123:MET:H	1.73	0.54
1:D:452:LEU:HD13	1:D:492:LEU:HB3	1.89	0.54
1:A:718:PHE:HA	1:A:1069:PRO:HA	1.89	0.54
3:I:158:LYS:NZ	3:I:186:GLN:OE1	2.38	0.53
3:I:210:ILE:HA	3:I:225:LYS:HA	1.90	0.53
1:C:345:THR:O	1:C:509:ARG:NH1	2.41	0.53
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.90	0.53
1:C:726:ILE:HG12	1:C:1061:VAL:HG22	1.88	0.53
1:F:292:ALA:HB1	1:F:633:TRP:HB2	1.88	0.53
1:C:202:LYS:NZ	1:C:228:ASP:OD2	2.41	0.53
1:D:811:LYS:NZ	1:D:820:ASP:OD2	2.38	0.53
1:F:361:CYS:SG	1:F:362:VAL:N	2.81	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:15:PRO:HA	2:K:94:LEU:HB2	1.89	0.53
3:I:153:LEU:HD23	3:I:226:VAL:HG13	1.90	0.53
1:C:55:LEU:HB2	1:C:195:LYS:HE2	1.89	0.53
1:C:725:GLU:OE2	1:C:1028:LYS:NZ	2.34	0.53
1:E:725:GLU:OE2	1:E:1028:LYS:NZ	2.40	0.53
3:M:210:ILE:HA	3:M:225:LYS:HA	1.91	0.53
1:F:726:ILE:HG12	1:F:1061:VAL:HG22	1.90	0.53
1:A:715:PRO:HA	1:A:1072:GLU:HA	1.91	0.53
2:L:9:SER:HA	2:L:123:MET:H	1.73	0.53
3:O:158:LYS:NZ	3:O:186:GLN:OE1	2.38	0.53
3:G:210:ILE:HA	3:G:225:LYS:HA	1.90	0.53
1:E:476:GLY:HA3	1:E:487:ASN:HB2	1.91	0.53
1:B:350:VAL:HG11	1:B:418:ILE:HD12	1.89	0.53
1:B:544:ASN:ND2	1:B:564:GLN:OE1	2.42	0.53
3:N:134:PRO:HB3	3:N:160:TYR:HB3	1.91	0.53
1:F:110:THR:OG1	1:F:112:ASP:OD1	2.26	0.53
1:B:644:GLN:NE2	1:B:645:THR:O	2.42	0.53
1:E:722:VAL:HG22	1:E:1065:VAL:HG22	1.91	0.53
1:A:781:VAL:HG22	1:A:1026:ALA:HB2	1.90	0.53
1:D:361:CYS:SG	1:D:362:VAL:N	2.81	0.53
1:D:815:ARG:NE	1:D:820:ASP:OD1	2.42	0.53
3:N:56:ILE:HD13	3:N:78:ILE:HG22	1.91	0.53
1:F:206:LYS:HB2	1:F:223:LEU:HA	1.90	0.53
1:A:381:GLY:HA3	1:A:430:THR:HG23	1.91	0.53
1:A:373:PRO:HB3	1:C:504:GLY:HA3	1.90	0.52
1:C:206:LYS:HB2	1:C:223:LEU:HA	1.90	0.52
1:C:811:LYS:NZ	1:C:820:ASP:OD2	2.41	0.52
1:D:756:TYR:OH	1:D:994:ASP:OD1	2.26	0.52
1:C:358:ILE:HB	1:C:395:VAL:HG13	1.91	0.52
3:H:158:LYS:NZ	3:H:186:GLN:OE1	2.37	0.52
3:I:134:PRO:HB3	3:I:160:TYR:HB3	1.90	0.52
1:E:983:ARG:HA	1:D:390:LEU:HD11	1.91	0.52
1:A:206:LYS:HB2	1:A:223:LEU:HA	1.90	0.52
1:F:722:VAL:HG22	1:F:1065:VAL:HG22	1.91	0.52
1:B:634:ARG:NE	1:B:634:ARG:O	2.37	0.52
1:C:756:TYR:OH	1:C:994:ASP:OD1	2.26	0.52
1:E:811:LYS:NZ	1:E:820:ASP:OD2	2.38	0.52
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	1.91	0.52
1:A:906:PHE:HA	1:A:909:ILE:HG12	1.92	0.52
1:C:715:PRO:HA	1:C:1072:GLU:HA	1.91	0.52
1:D:715:PRO:HA	1:D:1072:GLU:HA	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:718:PHE:HA	1:F:1069:PRO:HA	1.91	0.52
1:E:600:PRO:HD2	1:E:608:VAL:HG12	1.92	0.52
1:F:345:THR:O	1:F:509:ARG:NH1	2.43	0.52
1:A:35:ARG:HD2	1:A:216:LEU:HD13	1.91	0.52
3:I:52:TRP:HE1	3:I:55:ILE:HG23	1.75	0.52
1:D:321:GLN:HE21	1:D:591:SER:H	1.57	0.52
1:D:722:VAL:HG22	1:D:1065:VAL:HG22	1.92	0.52
1:A:424:LYS:NZ	1:A:425:LEU:O	2.38	0.52
3:H:56:ILE:HD13	3:H:78:ILE:HG22	1.91	0.52
1:E:802:PHE:HD1	1:E:805:ILE:HD11	1.75	0.52
1:B:109:THR:OG1	1:B:234:ASN:O	2.28	0.51
1:A:815:ARG:NE	1:A:820:ASP:OD1	2.43	0.51
1:E:350:VAL:HG11	1:E:418:ILE:HD12	1.92	0.51
1:B:948:LEU:HD21	1:B:1059:GLY:HA3	1.93	0.51
1:A:756:TYR:OH	1:A:994:ASP:OD1	2.26	0.51
3:H:153:LEU:HD23	3:H:226:VAL:HG13	1.91	0.51
3:H:210:ILE:HA	3:H:225:LYS:HA	1.92	0.51
2:Q:15:PRO:HA	2:Q:94:LEU:HB2	1.91	0.51
2:R:21:ILE:HD12	2:R:89:LEU:HD23	1.93	0.51
1:F:715:PRO:HA	1:F:1072:GLU:HA	1.93	0.51
1:F:756:TYR:OH	1:F:994:ASP:OD1	2.28	0.51
1:B:756:TYR:OH	1:B:994:ASP:OD1	2.29	0.51
1:C:350:VAL:HG11	1:C:418:ILE:HD12	1.91	0.51
1:C:544:ASN:ND2	1:C:564:GLN:OE1	2.44	0.51
3:M:153:LEU:HD23	3:M:226:VAL:HG13	1.92	0.51
1:D:131:VAL:HB	1:D:168:PHE:HB3	1.91	0.51
3:I:170:ASN:HB2	3:I:173:ALA:HB3	1.93	0.51
1:C:361:CYS:SG	1:C:362:VAL:N	2.83	0.51
1:E:1054:GLN:HB2	1:E:1061:VAL:HB	1.92	0.51
3:O:170:ASN:HB2	3:O:173:ALA:HB3	1.92	0.51
3:H:134:PRO:HB3	3:H:160:TYR:HB3	1.91	0.51
1:C:718:PHE:HA	1:C:1069:PRO:HA	1.91	0.51
1:E:715:PRO:HA	1:E:1072:GLU:HA	1.92	0.51
1:D:292:ALA:HB1	1:D:633:TRP:HB2	1.92	0.51
3:N:158:LYS:NZ	3:N:186:GLN:OE1	2.37	0.51
1:F:852:ALA:O	1:F:856:ASN:ND2	2.44	0.51
1:B:718:PHE:HA	1:B:1069:PRO:HA	1.91	0.51
3:G:153:LEU:HD23	3:G:226:VAL:HG13	1.93	0.51
3:M:170:ASN:HB2	3:M:173:ALA:HB3	1.92	0.51
2:R:9:SER:HA	2:R:123:MET:H	1.76	0.51
1:F:725:GLU:OE2	1:F:1028:LYS:NZ	2.38	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:170:ASN:HB2	3:H:173:ALA:HB3	1.93	0.50
2:Q:52:LEU:HD11	2:Q:55:TYR:HB3	1.92	0.50
1:A:361:CYS:SG	1:A:362:VAL:N	2.83	0.50
1:A:457:ARG:NH2	1:A:459:SER:O	2.38	0.50
1:E:734:THR:HG22	1:E:860:VAL:HG22	1.93	0.50
1:D:802:PHE:HD1	1:D:805:ILE:HD11	1.76	0.50
3:N:210:ILE:HA	3:N:225:LYS:HA	1.93	0.50
1:A:384:PRO:O	1:A:387:LEU:HB2	2.11	0.50
1:E:96:THR:OG1	1:E:214:ARG:NH1	2.44	0.50
1:A:361:CYS:H	1:A:524:VAL:HG12	1.76	0.50
1:A:802:PHE:HD1	1:A:805:ILE:HD11	1.76	0.50
1:E:457:ARG:NH2	1:E:459:SER:O	2.38	0.50
1:D:532:ASN:OD1	1:D:533:LEU:N	2.45	0.50
1:B:457:ARG:NH2	1:B:459:SER:O	2.38	0.50
1:B:811:LYS:NZ	1:B:820:ASP:OD2	2.41	0.50
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.93	0.50
1:F:158:ARG:HB3	1:F:252:VAL:HG13	1.94	0.50
1:B:202:LYS:NZ	1:B:228:ASP:OD2	2.43	0.50
1:B:321:GLN:HE21	1:B:591:SER:H	1.60	0.50
1:D:202:LYS:NZ	1:D:228:ASP:OD2	2.42	0.50
1:F:734:THR:HG22	1:F:860:VAL:HG22	1.94	0.50
3:G:56:ILE:HD13	3:G:78:ILE:HG22	1.94	0.50
3:H:63:SER:HB2	1:C:500:THR:HG21	1.93	0.50
1:F:1054:GLN:HB2	1:F:1061:VAL:HB	1.94	0.50
2:R:141:PRO:HB2	2:R:146:LEU:HD11	1.93	0.50
2:R:171:ALA:O	2:R:174:SER:OG	2.26	0.50
1:A:983:ARG:HA	1:C:390:LEU:HD11	1.94	0.50
1:B:358:ILE:HB	1:B:395:VAL:HG13	1.92	0.49
1:B:1116:THR:OG1	1:B:1118:ASP:OD1	2.28	0.49
2:J:153:LEU:HB2	2:J:199:LEU:HB3	1.94	0.49
1:E:544:ASN:ND2	1:E:564:GLN:OE1	2.45	0.49
1:F:742:ILE:O	1:F:1000:ARG:NH2	2.45	0.49
1:A:202:LYS:NZ	1:A:228:ASP:OD2	2.43	0.49
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.94	0.49
2:K:41:TRP:N	2:K:54:ILE:O	2.41	0.49
1:D:906:PHE:HA	1:D:909:ILE:HG12	1.95	0.49
3:N:170:ASN:HB2	3:N:173:ALA:HB3	1.94	0.49
1:A:811:LYS:NZ	1:A:820:ASP:OD2	2.39	0.49
1:C:35:ARG:HD2	1:C:216:LEU:HD13	1.95	0.49
3:M:111:GLY:HA3	3:M:114:LEU:HD22	1.95	0.49
3:N:37:TYR:HA	3:N:107:GLN:HE21	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:35:ARG:NH2	1:F:191:GLU:OE2	2.46	0.49
1:B:327:VAL:H	1:B:328:ARG:HH11	1.60	0.49
1:E:55:LEU:HB2	1:E:195:LYS:HE2	1.95	0.49
3:N:35:SER:HA	3:N:58:PRO:HB2	1.95	0.49
1:E:295:PRO:HG3	1:E:634:ARG:HD2	1.93	0.49
1:E:624:ILE:HB	1:E:628:GLN:HB2	1.95	0.49
1:D:948:LEU:HD21	1:D:1059:GLY:HA3	1.94	0.49
2:Q:41:TRP:N	2:Q:54:ILE:O	2.42	0.49
1:A:246:ARG:HG3	1:A:260:ALA:HB3	1.95	0.49
1:C:369:TYR:OH	1:C:384:PRO:O	2.31	0.49
3:M:56:ILE:HD13	3:M:78:ILE:HG22	1.95	0.49
3:O:153:LEU:HD23	3:O:226:VAL:HG13	1.94	0.49
1:F:457:ARG:NH2	1:F:459:SER:O	2.40	0.49
1:F:802:PHE:HD1	1:F:805:ILE:HD11	1.78	0.49
3:G:111:GLY:HA3	3:G:114:LEU:HD22	1.95	0.49
3:H:35:SER:HA	3:H:58:PRO:HB2	1.94	0.49
2:L:41:TRP:N	2:L:54:ILE:O	2.40	0.49
1:E:321:GLN:HE21	1:E:591:SER:H	1.61	0.49
1:D:983:ARG:HA	1:F:390:LEU:HD11	1.95	0.49
3:N:63:SER:HB2	1:F:500:THR:HG21	1.93	0.49
2:L:157:ILE:HB	2:L:195:ALA:HB3	1.95	0.48
1:D:287:ASP:OD1	1:D:288:ALA:N	2.46	0.48
3:H:6:GLN:NE2	3:H:122:THR:OG1	2.46	0.48
1:E:358:ILE:HB	1:E:395:VAL:HG13	1.95	0.48
1:D:246:ARG:HG3	1:D:260:ALA:HB3	1.94	0.48
1:B:287:ASP:OD1	1:B:288:ALA:N	2.46	0.48
1:C:158:ARG:HB3	1:C:252:VAL:HG13	1.96	0.48
1:D:476:GLY:HA3	1:D:487:ASN:HB2	1.94	0.48
3:M:11:GLU:HB3	3:M:13:LYS:HE3	1.95	0.48
3:M:126:VAL:HG23	3:M:127:SER:H	1.78	0.48
2:R:157:ILE:HB	2:R:195:ALA:HB3	1.95	0.48
3:O:52:TRP:HE1	3:O:55:ILE:HG23	1.78	0.48
1:F:294:ASP:OD1	1:F:294:ASP:N	2.47	0.48
1:B:476:GLY:HA3	1:B:487:ASN:HB2	1.94	0.48
1:C:734:THR:HG22	1:C:860:VAL:HG22	1.95	0.48
1:D:624:ILE:HB	1:D:628:GLN:HB2	1.95	0.48
1:A:379:CYS:HA	1:A:432:CYS:HA	1.95	0.48
1:A:418:ILE:HA	1:A:422:ASN:HD22	1.79	0.48
3:G:170:ASN:HB2	3:G:173:ALA:HB3	1.96	0.48
1:E:202:LYS:NZ	1:E:228:ASP:OD2	2.45	0.48
3:M:43:ARG:O	3:M:51:GLU:N	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:GLN:HA	1:A:488:CYS:HB3	1.95	0.48
3:H:52:TRP:HE1	3:H:55:ILE:HG23	1.78	0.48
1:F:287:ASP:OD1	1:F:288:ALA:N	2.46	0.48
1:F:850:ILE:HG22	1:F:854:LYS:HE2	1.96	0.48
1:B:624:ILE:HB	1:B:628:GLN:HB2	1.95	0.48
1:A:476:GLY:HA3	1:A:487:ASN:HB2	1.95	0.48
3:N:166:THR:HG23	3:N:214:ASN:HB2	1.95	0.48
3:I:111:GLY:HA3	3:I:114:LEU:HD22	1.96	0.48
1:D:38:TYR:OH	1:D:55:LEU:O	2.27	0.48
1:D:96:THR:OG1	1:D:214:ARG:NH1	2.47	0.48
1:D:401:VAL:HG22	1:D:509:ARG:HG2	1.95	0.48
1:F:544:ASN:ND2	1:F:564:GLN:OE1	2.47	0.48
3:H:43:ARG:O	3:H:51:GLU:N	2.45	0.48
1:C:344:ALA:O	1:C:509:ARG:NH2	2.46	0.48
1:C:401:VAL:HG22	1:C:509:ARG:HG2	1.95	0.48
1:C:948:LEU:HD21	1:C:1059:GLY:HA3	1.96	0.48
2:Q:171:ALA:O	2:Q:174:SER:OG	2.26	0.48
1:F:246:ARG:HG3	1:F:260:ALA:HB3	1.96	0.48
1:C:529:LYS:H	1:C:529:LYS:HG2	1.48	0.48
1:D:734:THR:HG22	1:D:860:VAL:HG22	1.96	0.48
1:A:902:MET:HE3	1:A:1049:LEU:HD13	1.96	0.47
1:D:457:ARG:NH1	1:D:467:ASP:OD2	2.47	0.47
1:D:552:LEU:HD12	1:D:585:LEU:HB3	1.95	0.47
1:B:741:TYR:OH	1:B:962:LEU:O	2.30	0.47
1:A:661:GLU:O	1:A:695:TYR:OH	2.30	0.47
1:C:457:ARG:NH2	1:C:459:SER:O	2.38	0.47
3:I:20:LYS:HB2	3:I:90:HIS:HD2	1.79	0.47
1:C:850:ILE:HG22	1:C:854:LYS:HE2	1.96	0.47
3:N:52:TRP:HE1	3:N:55:ILE:HG23	1.79	0.47
1:B:600:PRO:HD2	1:B:608:VAL:HG12	1.96	0.47
3:G:15:PRO:HD3	3:G:126:VAL:HB	1.96	0.47
3:H:142:SER:HG	3:H:145:SER:HG	1.62	0.47
1:D:850:ILE:HG22	1:D:854:LYS:HE2	1.96	0.47
1:B:850:ILE:HG22	1:B:854:LYS:HE2	1.96	0.47
1:A:529:LYS:HB2	1:A:529:LYS:HE2	1.35	0.47
1:C:49:LEU:HB3	1:C:276:LEU:HD11	1.96	0.47
1:C:287:ASP:OD1	1:C:288:ALA:N	2.48	0.47
1:E:246:ARG:HG3	1:E:260:ALA:HB3	1.95	0.47
1:B:501:TYR:HA	3:G:63:SER:HB2	1.96	0.47
1:A:741:TYR:OH	1:A:962:LEU:O	2.30	0.47
1:D:962:LEU:HD11	1:D:1004:LEU:HD23	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:314:GLN:OE1	1:F:315:THR:N	2.43	0.47
1:B:246:ARG:HG3	1:B:260:ALA:HB3	1.97	0.47
1:A:106:ILE:HD11	1:A:239:GLN:HB3	1.96	0.47
1:A:734:THR:HG22	1:A:860:VAL:HG22	1.97	0.47
3:G:126:VAL:HG23	3:G:127:SER:H	1.79	0.47
3:H:166:THR:HG23	3:H:214:ASN:HB2	1.95	0.47
1:C:292:ALA:HB1	1:C:633:TRP:HB2	1.95	0.47
1:E:35:ARG:NH2	1:E:191:GLU:OE2	2.48	0.47
1:E:501:TYR:HA	3:M:63:SER:HB2	1.96	0.47
1:D:158:ARG:HB3	1:D:252:VAL:HG13	1.96	0.47
1:F:202:LYS:NZ	1:F:228:ASP:OD2	2.46	0.47
1:A:368:ILE:HA	1:A:371:PHE:HD2	1.79	0.47
3:I:166:THR:HG23	3:I:214:ASN:HB2	1.96	0.47
1:E:314:GLN:OE1	1:E:315:THR:N	2.45	0.47
1:D:195:LYS:HD2	1:D:202:LYS:HD2	1.97	0.47
1:D:358:ILE:HB	1:D:395:VAL:HG13	1.95	0.47
1:D:742:ILE:O	1:D:1000:ARG:NH2	2.48	0.47
1:E:287:ASP:OD1	1:E:288:ALA:N	2.47	0.47
1:F:962:LEU:HD11	1:F:1004:LEU:HD23	1.97	0.47
1:B:106:ILE:HD11	1:B:239:GLN:HB3	1.97	0.47
2:K:157:ILE:HB	2:K:195:ALA:HB3	1.97	0.47
1:F:476:GLY:HA3	1:F:487:ASN:HB2	1.97	0.47
1:A:624:ILE:HB	1:A:628:GLN:HB2	1.96	0.46
1:A:850:ILE:HG22	1:A:854:LYS:HE2	1.97	0.46
1:E:474:GLN:HA	1:E:488:CYS:HB3	1.97	0.46
1:E:852:ALA:O	1:E:856:ASN:ND2	2.48	0.46
3:M:137:PHE:HB2	3:M:156:LEU:HB3	1.96	0.46
2:Q:157:ILE:HB	2:Q:195:ALA:HB3	1.95	0.46
1:F:1116:THR:OG1	1:F:1118:ASP:OD1	2.29	0.46
1:A:457:ARG:NH1	1:A:467:ASP:OD2	2.47	0.46
1:E:552:LEU:HD12	1:E:585:LEU:HB3	1.97	0.46
1:D:294:ASP:N	1:D:294:ASP:OD1	2.46	0.46
3:O:56:ILE:HD13	3:O:78:ILE:HG22	1.97	0.46
1:B:529:LYS:HB2	1:B:529:LYS:HE2	1.48	0.46
1:B:981:LEU:HD21	1:B:993:ILE:HD11	1.98	0.46
1:E:327:VAL:H	1:E:328:ARG:HH11	1.63	0.46
2:J:131:LYS:HD2	2:J:162:PRO:HG3	1.97	0.46
1:C:106:ILE:HD11	1:C:239:GLN:HB3	1.96	0.46
1:D:379:CYS:HA	1:D:432:CYS:HA	1.97	0.46
3:M:15:PRO:HD3	3:M:126:VAL:HB	1.98	0.46
3:N:6:GLN:NE2	3:N:122:THR:OG1	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:15:PRO:HA	2:R:94:LEU:HB2	1.97	0.46
1:A:903:ALA:HB2	1:A:916:LEU:HD22	1.97	0.46
1:A:983:ARG:HB3	1:C:382:VAL:HG12	1.96	0.46
1:F:106:ILE:HD11	1:F:239:GLN:HB3	1.98	0.46
1:F:401:VAL:HG22	1:F:509:ARG:HG2	1.97	0.46
1:F:624:ILE:HB	1:F:628:GLN:HB2	1.97	0.46
1:A:962:LEU:HD11	1:A:1004:LEU:HD23	1.98	0.46
1:E:962:LEU:HD11	1:E:1004:LEU:HD23	1.98	0.46
2:P:171:ALA:O	2:P:174:SER:OG	2.26	0.46
1:C:38:TYR:OH	1:C:55:LEU:O	2.26	0.46
1:B:158:ARG:HB3	1:B:252:VAL:HG13	1.98	0.46
1:B:379:CYS:HA	1:B:432:CYS:HA	1.97	0.46
1:E:106:ILE:HD11	1:E:239:GLN:HB3	1.97	0.46
1:E:742:ILE:O	1:E:1000:ARG:NH2	2.49	0.46
1:D:717:ASN:OD1	1:D:718:PHE:N	2.44	0.46
1:D:725:GLU:OE2	1:D:1028:LYS:NZ	2.42	0.46
2:P:42:TYR:OH	3:M:114:LEU:O	2.33	0.46
1:F:708:SER:HB3	1:F:711:SER:HB3	1.97	0.46
1:A:880:GLY:O	1:A:884:SER:OG	2.30	0.46
1:C:314:GLN:OE1	1:C:315:THR:N	2.44	0.46
2:P:137:THR:HB	2:P:156:LEU:HB2	1.98	0.46
1:A:287:ASP:OD1	1:A:288:ALA:N	2.49	0.46
1:C:411:ALA:HB3	1:C:414:GLN:HG3	1.98	0.46
1:B:363:ALA:HB2	1:B:524:VAL:HG12	1.98	0.45
1:B:528:LYS:HB3	1:B:529:LYS:H	1.65	0.45
1:A:180:GLU:HG2	1:A:226:LEU:HD21	1.98	0.45
1:E:110:THR:OG1	1:E:112:ASP:OD1	2.28	0.45
1:D:418:ILE:HA	1:D:422:ASN:HD22	1.82	0.45
3:M:52:TRP:HE1	3:M:55:ILE:HG23	1.81	0.45
3:O:20:LYS:HB2	3:O:90:HIS:HD2	1.81	0.45
2:J:116:VAL:HG13	3:G:113:ILE:HD12	1.98	0.45
3:G:11:GLU:HB3	3:G:13:LYS:HE3	1.97	0.45
3:G:142:SER:HG	3:G:145:SER:HG	1.63	0.45
1:C:135:GLN:HB3	1:C:161:SER:HB2	1.98	0.45
1:C:1116:THR:OG1	1:C:1118:ASP:OD1	2.28	0.45
1:E:850:ILE:HG22	1:E:854:LYS:HE2	1.99	0.45
1:D:474:GLN:HA	1:D:488:CYS:HB3	1.99	0.45
1:F:369:TYR:OH	1:F:384:PRO:O	2.35	0.45
1:B:708:SER:HB3	1:B:711:SER:HB3	1.97	0.45
1:A:1054:GLN:HB2	1:A:1061:VAL:HB	1.98	0.45
3:I:56:ILE:HD13	3:I:78:ILE:HG22	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:294:ASP:OD1	1:E:294:ASP:N	2.49	0.45
1:D:1116:THR:OG1	1:D:1118:ASP:OD1	2.29	0.45
1:A:49:LEU:HD23	1:A:276:LEU:HD21	1.98	0.45
2:P:116:VAL:HG13	3:M:113:ILE:HD12	1.98	0.45
1:B:411:ALA:HB3	1:B:414:GLN:HG3	1.99	0.45
3:G:43:ARG:O	3:G:51:GLU:N	2.44	0.45
1:D:708:SER:HB3	1:D:711:SER:HB3	1.98	0.45
3:O:111:GLY:HA3	3:O:114:LEU:HD22	1.98	0.45
1:A:109:THR:OG1	1:A:234:ASN:O	2.30	0.45
1:C:624:ILE:HB	1:C:628:GLN:HB2	1.97	0.45
1:C:795:LYS:HG2	1:C:796:TYR:H	1.82	0.45
1:E:92:TYR:N	1:E:268:GLY:O	2.46	0.45
1:E:708:SER:HB3	1:E:711:SER:HB3	1.98	0.45
1:D:903:ALA:HB2	1:D:916:LEU:HD22	1.98	0.45
3:M:35:SER:HA	3:M:58:PRO:HB2	1.98	0.45
1:F:985:ASP:OD1	1:F:985:ASP:N	2.50	0.45
1:A:708:SER:HB3	1:A:711:SER:HB3	1.99	0.45
1:C:708:SER:HB3	1:C:711:SER:HB3	1.99	0.45
1:E:373:PRO:HG3	1:D:504:GLY:HA3	1.99	0.45
1:E:781:VAL:HG22	1:E:1026:ALA:HB2	1.99	0.45
1:D:106:ILE:HD11	1:D:239:GLN:HB3	1.97	0.45
1:B:49:LEU:HB3	1:B:276:LEU:HD11	1.98	0.45
1:B:795:LYS:HG2	1:B:796:TYR:H	1.82	0.45
1:A:351:TYR:HD2	1:A:468:ILE:HA	1.82	0.45
1:C:620:VAL:HG13	1:C:623:ALA:HB3	1.98	0.45
1:E:158:ARG:HB3	1:E:252:VAL:HG13	1.99	0.45
2:R:41:TRP:N	2:R:54:ILE:O	2.42	0.45
3:O:139:LEU:HD21	3:O:156:LEU:HD12	1.98	0.45
3:O:161:PHE:HB3	3:O:162:PRO:HD3	1.99	0.45
1:F:344:ALA:O	1:F:509:ARG:NH2	2.49	0.45
1:F:948:LEU:HD21	1:F:1059:GLY:HA3	1.99	0.45
1:B:401:VAL:HG22	1:B:509:ARG:HG2	1.99	0.45
3:G:52:TRP:HE1	3:G:55:ILE:HG23	1.82	0.45
1:E:948:LEU:HD21	1:E:1059:GLY:HA3	1.99	0.45
1:D:368:ILE:HA	1:D:371:PHE:HD2	1.82	0.45
1:F:158:ARG:HH21	1:F:252:VAL:HG22	1.82	0.45
1:A:552:LEU:HD12	1:A:585:LEU:HB3	1.98	0.45
2:L:187:LYS:HG2	2:L:194:ALA:HB2	1.98	0.45
1:E:904:TYR:OH	1:D:1093:GLY:O	2.35	0.45
1:D:351:TYR:HD2	1:D:468:ILE:HA	1.82	0.45
3:O:43:ARG:O	3:O:51:GLU:N	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:411:ALA:HB3	1:F:414:GLN:HG3	1.99	0.45
1:B:42:LYS:HG2	1:A:562:PHE:HD2	1.82	0.44
1:A:135:GLN:HB3	1:A:161:SER:HB2	1.99	0.44
1:A:393:THR:HB	1:A:394:ASN:H	1.26	0.44
1:C:474:GLN:HA	1:C:488:CYS:HB3	1.97	0.44
1:B:734:THR:HG22	1:B:860:VAL:HG22	1.99	0.44
1:A:557:LYS:HB2	1:A:584:ILE:HG21	1.99	0.44
1:A:906:PHE:HB3	1:A:911:VAL:HB	1.99	0.44
1:C:246:ARG:HG3	1:C:260:ALA:HB3	1.99	0.44
1:E:457:ARG:NH1	1:E:467:ASP:OD2	2.50	0.44
1:B:383:SER:OG	1:C:985:ASP:N	2.50	0.44
1:A:394:ASN:HB2	1:A:396:TYR:CE2	2.53	0.44
2:J:41:TRP:N	2:J:54:ILE:O	2.44	0.44
1:D:983:ARG:HB3	1:F:382:VAL:HG12	2.00	0.44
1:B:905:ARG:HH21	1:B:1036:GLN:HB2	1.83	0.44
1:A:92:TYR:N	1:A:268:GLY:O	2.45	0.44
3:H:161:PHE:HB3	3:H:162:PRO:HD3	1.99	0.44
1:E:529:LYS:HD2	1:E:529:LYS:HA	1.38	0.44
1:D:110:THR:OG1	1:D:112:ASP:OD1	2.29	0.44
1:A:314:GLN:OE1	1:A:315:THR:N	2.46	0.44
1:E:795:LYS:HG2	1:E:796:TYR:H	1.83	0.44
1:B:351:TYR:HD2	1:B:468:ILE:HA	1.82	0.44
1:A:96:THR:OG1	1:A:214:ARG:NH1	2.51	0.44
1:E:1028:LYS:HE3	1:E:1028:LYS:HB2	1.88	0.44
1:D:158:ARG:HH21	1:D:252:VAL:HG22	1.83	0.44
1:D:852:ALA:O	1:D:856:ASN:ND2	2.51	0.44
1:A:358:ILE:HB	1:A:395:VAL:HG13	1.99	0.44
3:I:161:PHE:HB3	3:I:162:PRO:HD3	1.99	0.44
1:E:135:GLN:HB3	1:E:161:SER:HB2	1.99	0.44
3:N:43:ARG:O	3:N:51:GLU:N	2.45	0.44
1:B:474:GLN:HA	1:B:488:CYS:HB3	1.98	0.44
1:A:795:LYS:HG2	1:A:796:TYR:H	1.83	0.44
1:C:127:VAL:HG12	1:C:173:GLN:H	1.83	0.44
1:C:374:PHE:HD1	1:C:436:TRP:HB3	1.83	0.44
1:E:741:TYR:OH	1:E:962:LEU:O	2.32	0.44
1:B:158:ARG:HH21	1:B:252:VAL:HG22	1.83	0.43
3:G:166:THR:HG23	3:G:214:ASN:HB2	2.00	0.43
2:K:171:ALA:O	2:K:174:SER:OG	2.26	0.43
3:H:111:GLY:HA3	3:H:114:LEU:HD22	2.00	0.43
3:I:43:ARG:O	3:I:51:GLU:N	2.46	0.43
1:C:802:PHE:HD1	1:C:805:ILE:HD11	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:401:VAL:HG22	1:E:509:ARG:HG2	1.99	0.43
1:E:516:GLU:HG3	1:E:518:LEU:HG	1.99	0.43
1:F:620:VAL:HG13	1:F:623:ALA:HB3	1.99	0.43
1:F:795:LYS:HG2	1:F:796:TYR:H	1.83	0.43
1:B:292:ALA:HB1	1:B:633:TRP:HB2	2.00	0.43
1:B:375:PHE:N	1:B:435:ALA:O	2.44	0.43
1:B:552:LEU:HD12	1:B:585:LEU:HB3	1.99	0.43
1:D:312:ILE:H	1:D:312:ILE:HG13	1.45	0.43
1:D:982:SER:HB3	1:F:390:LEU:HD21	2.00	0.43
3:N:142:SER:HG	3:N:145:SER:HG	1.62	0.43
1:B:391:CYS:HA	1:B:525:CYS:HA	1.99	0.43
2:J:141:PRO:HB2	2:J:146:LEU:HD12	2.01	0.43
1:C:703:ASN:OD1	1:C:704:SER:N	2.52	0.43
1:D:373:PRO:HG3	1:F:505:HIS:CG	2.53	0.43
2:J:137:THR:HB	2:J:156:LEU:HB2	2.00	0.43
3:G:40:GLY:HA3	3:G:55:ILE:HG22	2.01	0.43
3:G:137:PHE:O	3:G:156:LEU:N	2.43	0.43
1:C:552:LEU:HD12	1:C:585:LEU:HB3	2.00	0.43
1:E:312:ILE:H	1:E:312:ILE:HG13	1.45	0.43
1:D:901:GLN:O	1:D:905:ARG:HG2	2.18	0.43
3:M:215:HIS:HD2	3:M:218:SER:HB3	1.83	0.43
1:F:374:PHE:HD1	1:F:436:TRP:HB3	1.83	0.43
1:C:200:TYR:HA	1:C:230:PRO:HA	2.00	0.43
1:E:180:GLU:HG2	1:E:226:LEU:HD21	2.01	0.43
1:E:351:TYR:HD2	1:E:468:ILE:HA	1.83	0.43
1:F:474:GLN:HA	1:F:488:CYS:HB3	2.00	0.43
1:C:180:GLU:HG2	1:C:226:LEU:HD21	2.00	0.43
1:C:962:LEU:HD11	1:C:1004:LEU:HD23	2.01	0.43
1:E:158:ARG:HH21	1:E:252:VAL:HG22	1.83	0.43
1:A:312:ILE:H	1:A:312:ILE:HG13	1.44	0.43
1:A:909:ILE:HD13	1:A:1049:LEU:HD21	2.01	0.43
1:C:812:PRO:O	1:C:813:SER:OG	2.34	0.43
1:E:645:THR:OG1	1:E:648:GLY:O	2.34	0.43
1:D:902:MET:HE3	1:D:1049:LEU:HD13	2.00	0.43
1:B:985:ASP:OD1	1:B:985:ASP:N	2.52	0.43
1:B:1093:GLY:O	1:C:904:TYR:OH	2.35	0.43
2:K:115:ARG:HH21	3:H:69:PRO:HD3	1.84	0.43
1:E:379:CYS:HA	1:E:432:CYS:HA	2.01	0.43
3:N:161:PHE:HB3	3:N:162:PRO:HD3	2.00	0.43
1:B:1041:ASP:HB2	1:C:1030:SER:HB2	2.00	0.43
3:I:142:SER:HG	3:I:145:SER:HG	1.60	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:TYR:N	1:C:268:GLY:O	2.45	0.43
1:E:644:GLN:NE2	1:E:645:THR:O	2.52	0.43
1:E:985:ASP:OD1	1:E:985:ASP:N	2.52	0.43
1:D:985:ASP:OD1	1:F:383:SER:OG	2.34	0.43
2:P:131:LYS:HD2	2:P:162:PRO:HG3	2.01	0.43
1:A:717:ASN:OD1	1:A:718:PHE:N	2.44	0.43
1:A:982:SER:HB3	1:C:390:LEU:HD21	2.01	0.43
1:C:319:ARG:HH22	1:C:615:VAL:HG21	1.84	0.43
1:E:620:VAL:HG13	1:E:623:ALA:HB3	2.01	0.43
3:M:183:ALA:HB1	3:M:191:TYR:HB3	2.01	0.43
2:Q:56:GLU:HG3	2:Q:65:ASN:OD1	2.19	0.43
2:R:107:TYR:HB3	2:R:116:VAL:HG12	2.00	0.43
1:C:158:ARG:HH21	1:C:252:VAL:HG22	1.84	0.42
1:C:339:HIS:O	1:C:343:ASN:N	2.50	0.42
1:C:903:ALA:HB2	1:C:916:LEU:HD22	2.00	0.42
1:E:329:PHE:CZ	1:E:533:LEU:HB2	2.54	0.42
1:E:473:TYR:H	1:E:491:PRO:HD3	1.84	0.42
1:E:903:ALA:HB2	1:E:916:LEU:HD22	2.01	0.42
1:D:109:THR:OG1	1:D:234:ASN:O	2.35	0.42
1:D:795:LYS:HG2	1:D:796:TYR:H	1.84	0.42
1:B:135:GLN:HB3	1:B:161:SER:HB2	2.01	0.42
1:B:962:LEU:HD11	1:B:1004:LEU:HD23	2.01	0.42
1:B:1054:GLN:HB2	1:B:1061:VAL:HB	2.01	0.42
1:A:811:LYS:HE2	1:A:811:LYS:HB3	1.89	0.42
2:L:21:ILE:HD12	2:L:89:LEU:HD23	2.01	0.42
1:D:773:GLU:OE2	1:D:1019:ARG:HD3	2.19	0.42
3:O:166:THR:HG23	3:O:214:ASN:HB2	2.01	0.42
1:F:575:ALA:HA	1:F:586:ASP:HA	2.00	0.42
1:F:741:TYR:OH	1:F:962:LEU:O	2.33	0.42
1:B:180:GLU:HG2	1:B:226:LEU:HD21	2.00	0.42
1:A:836:GLN:HE22	1:C:616:ASN:HD22	1.67	0.42
3:G:35:SER:HA	3:G:58:PRO:HB2	2.00	0.42
1:D:180:GLU:HG2	1:D:226:LEU:HD21	2.01	0.42
3:M:166:THR:HG23	3:M:214:ASN:HB2	1.99	0.42
1:B:532:ASN:OD1	1:B:533:LEU:N	2.52	0.42
1:B:645:THR:OG1	1:B:648:GLY:O	2.34	0.42
1:B:903:ALA:HB2	1:B:916:LEU:HD22	2.01	0.42
3:G:137:PHE:HB2	3:G:156:LEU:HB3	2.02	0.42
1:E:42:LYS:HG2	1:D:562:PHE:HD2	1.84	0.42
1:E:1116:THR:OG1	1:E:1118:ASP:OD1	2.30	0.42
1:D:311:GLY:N	1:D:599:THR:O	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:557:LYS:HB2	1:D:584:ILE:HG21	2.01	0.42
1:F:180:GLU:HG2	1:F:226:LEU:HD21	1.99	0.42
1:B:193:VAL:HG23	1:B:223:LEU:HD22	2.00	0.42
1:B:312:ILE:H	1:B:312:ILE:HG13	1.43	0.42
1:B:622:VAL:HG21	1:B:635:VAL:HG13	2.01	0.42
1:A:611:LEU:HD22	1:A:666:ILE:HG23	2.01	0.42
1:E:375:PHE:N	1:E:435:ALA:O	2.47	0.42
1:A:901:GLN:O	1:A:905:ARG:HG2	2.20	0.42
2:J:125:THR:OG1	2:J:126:VAL:N	2.53	0.42
2:J:187:LYS:HG2	2:J:194:ALA:HB2	2.01	0.42
2:L:56:GLU:HG3	2:L:65:ASN:OD1	2.19	0.42
1:C:906:PHE:HB3	1:C:911:VAL:HB	2.01	0.42
1:A:158:ARG:HH21	1:A:252:VAL:HG22	1.84	0.42
2:R:56:GLU:HG3	2:R:65:ASN:OD1	2.19	0.42
1:B:96:THR:OG1	1:B:214:ARG:NH1	2.53	0.42
1:A:38:TYR:HB3	1:A:223:LEU:HB2	2.01	0.42
1:A:212:LEU:HG	1:A:213:GLU:H	1.85	0.42
2:L:15:PRO:HA	2:L:94:LEU:HB2	2.02	0.42
2:L:171:ALA:O	2:L:174:SER:OG	2.26	0.42
1:C:294:ASP:OD1	1:C:294:ASP:N	2.51	0.42
1:C:351:TYR:CE1	1:C:452:LEU:HB2	2.54	0.42
2:P:41:TRP:N	2:P:54:ILE:O	2.46	0.42
1:F:96:THR:OG1	1:F:214:ARG:NH1	2.53	0.42
2:J:51:LYS:HE3	2:J:53:MET:HE3	2.02	0.42
1:F:123:ASN:OD1	1:F:124:ALA:N	2.46	0.42
1:C:476:GLY:HA3	1:C:487:ASN:HB2	2.01	0.41
1:D:35:ARG:HD2	1:D:216:LEU:HD13	2.00	0.41
1:D:735:SER:HA	1:D:767:LEU:HD13	2.02	0.41
2:P:107:TYR:HB3	2:P:116:VAL:HG12	2.02	0.41
2:J:144:GLU:HA	2:R:147:GLN:CD	2.44	0.41
1:D:193:VAL:HG23	1:D:223:LEU:HD22	2.02	0.41
1:D:329:PHE:CZ	1:D:533:LEU:HB2	2.55	0.41
2:P:125:THR:OG1	2:P:126:VAL:N	2.53	0.41
2:R:149:ASN:HA	2:R:203:PRO:HG3	2.01	0.41
1:F:781:VAL:HG22	1:F:1026:ALA:HB2	2.01	0.41
1:B:212:LEU:HG	1:B:213:GLU:H	1.85	0.41
1:B:294:ASP:N	1:B:294:ASP:OD1	2.53	0.41
1:A:329:PHE:HD1	1:A:329:PHE:HA	1.76	0.41
1:A:1031:GLU:OE2	1:C:1039:ARG:NE	2.44	0.41
3:I:35:SER:HA	3:I:58:PRO:HB2	2.01	0.41
1:E:212:LEU:HG	1:E:213:GLU:H	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:418:ILE:HD11	1:E:453:TYR:HB2	2.02	0.41
1:E:575:ALA:HA	1:E:586:ASP:HA	2.01	0.41
1:D:35:ARG:NH2	1:D:191:GLU:OE2	2.53	0.41
1:D:135:GLN:HB3	1:D:161:SER:HB2	2.02	0.41
1:B:314:GLN:OE1	1:B:315:THR:N	2.46	0.41
2:Q:161:TYR:HB3	2:Q:162:PRO:HD3	2.02	0.41
1:B:983:ARG:HB3	1:A:382:VAL:HG12	2.03	0.41
2:J:107:TYR:HB3	2:J:116:VAL:HG12	2.03	0.41
3:I:67:TYR:HE1	3:I:78:ILE:HG13	1.85	0.41
1:C:193:VAL:HG23	1:C:223:LEU:HD22	2.03	0.41
1:C:746:SER:HB3	1:C:749:CYS:HB3	2.03	0.41
1:D:985:ASP:OD1	1:D:985:ASP:N	2.53	0.41
2:Q:115:ARG:HH21	3:N:69:PRO:HD3	1.85	0.41
2:R:187:LYS:HG2	2:R:194:ALA:HB2	2.03	0.41
1:B:620:VAL:HG13	1:B:623:ALA:HB3	2.01	0.41
1:B:629:LEU:H	1:B:629:LEU:HD23	1.86	0.41
1:B:1116:THR:HG22	1:B:1138:TYR:HB3	2.03	0.41
1:D:473:TYR:H	1:D:491:PRO:HD3	1.84	0.41
1:F:127:VAL:HG12	1:F:173:GLN:H	1.86	0.41
1:F:529:LYS:HA	1:F:529:LYS:HD3	1.62	0.41
1:B:110:THR:OG1	1:B:112:ASP:OD1	2.27	0.41
1:B:562:PHE:HD2	1:C:42:LYS:HG2	1.85	0.41
2:K:56:GLU:HG3	2:K:65:ASN:OD1	2.21	0.41
1:C:981:LEU:HD21	1:C:993:ILE:HD11	2.01	0.41
1:F:600:PRO:HD2	1:F:608:VAL:HG12	2.03	0.41
1:A:1030:SER:HB2	1:C:1041:ASP:HB2	2.03	0.41
3:H:81:ASP:OD1	3:H:83:SER:OG	2.37	0.41
2:L:157:ILE:O	2:L:195:ALA:N	2.54	0.41
1:C:96:THR:OG1	1:C:214:ARG:NH1	2.54	0.41
1:E:965:GLN:HE22	1:F:758:SER:H	1.69	0.41
2:P:56:GLU:HG3	2:P:65:ASN:OD1	2.21	0.41
2:R:115:ARG:HH21	3:O:69:PRO:HD3	1.85	0.41
1:F:146:GLN:HE21	1:F:146:GLN:HB2	1.62	0.41
1:B:351:TYR:CE1	1:B:452:LEU:HB2	2.56	0.41
1:C:212:LEU:HG	1:C:213:GLU:H	1.85	0.41
1:E:193:VAL:HG23	1:E:223:LEU:HD22	2.03	0.41
1:E:532:ASN:OD1	1:E:533:LEU:N	2.54	0.41
1:D:212:LEU:HG	1:D:213:GLU:H	1.85	0.41
2:R:161:TYR:HB3	2:R:162:PRO:HD3	2.02	0.41
3:O:81:ASP:OD1	3:O:83:SER:OG	2.35	0.41
1:F:339:HIS:O	1:F:343:ASN:N	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:641:ASN:HB3	1:F:652:GLY:H	1.86	0.41
1:B:1028:LYS:HB2	1:B:1028:LYS:HE3	1.86	0.41
1:A:815:ARG:HE	1:A:820:ASP:HA	1.86	0.41
2:J:157:ILE:HB	2:J:195:ALA:HB3	2.02	0.41
1:C:735:SER:HA	1:C:767:LEU:HD13	2.02	0.41
1:D:36:GLY:HA3	1:D:57:LEU:HB3	2.02	0.41
2:P:187:LYS:HG2	2:P:194:ALA:HB2	2.03	0.41
3:M:40:GLY:HA3	3:M:55:ILE:HG22	2.02	0.41
2:Q:107:TYR:HB3	2:Q:116:VAL:HG12	2.03	0.41
3:N:215:HIS:HD2	3:N:218:SER:HB3	1.85	0.41
1:F:351:TYR:CE1	1:F:452:LEU:HB2	2.55	0.41
1:D:645:THR:OG1	1:D:648:GLY:O	2.37	0.40
3:N:111:GLY:HA3	3:N:114:LEU:HD22	2.03	0.40
1:A:326:ILE:HG22	1:A:540:ASN:HB2	2.03	0.40
1:A:644:GLN:NE2	1:A:645:THR:O	2.54	0.40
2:L:107:TYR:HB3	2:L:116:VAL:HG12	2.01	0.40
2:L:161:TYR:HB3	2:L:162:PRO:HD3	2.03	0.40
1:E:383:SER:OG	1:F:985:ASP:N	2.54	0.40
1:E:901:GLN:O	1:E:905:ARG:HG2	2.21	0.40
1:D:1142:GLN:HB2	1:D:1143:PRO:HD3	2.03	0.40
1:F:212:LEU:HG	1:F:213:GLU:H	1.86	0.40
1:F:472:ILE:HG22	1:F:488:CYS:HB2	2.03	0.40
1:B:311:GLY:N	1:B:599:THR:O	2.47	0.40
1:A:373:PRO:HG3	1:C:505:HIS:CG	2.56	0.40
1:A:524:VAL:HB	1:A:525:CYS:H	1.60	0.40
1:C:109:THR:OG1	1:C:234:ASN:O	2.30	0.40
1:C:351:TYR:HD2	1:C:468:ILE:HA	1.87	0.40
1:D:811:LYS:HE2	1:D:811:LYS:HB3	1.89	0.40
2:J:56:GLU:HG3	2:J:65:ASN:OD1	2.20	0.40
1:D:815:ARG:HE	1:D:820:ASP:HA	1.87	0.40
3:O:35:SER:HA	3:O:58:PRO:HB2	2.03	0.40
1:B:200:TYR:HA	1:B:230:PRO:HA	2.03	0.40
1:B:746:SER:HB3	1:B:749:CYS:HB3	2.03	0.40
3:G:183:ALA:HB1	3:G:191:TYR:HB3	2.03	0.40
2:K:21:ILE:HB	2:K:89:LEU:HB3	2.04	0.40
1:C:472:ILE:HG22	1:C:488:CYS:HB2	2.03	0.40
1:F:746:SER:HB3	1:F:749:CYS:HB3	2.02	0.40
1:F:903:ALA:HB2	1:F:916:LEU:HD22	2.04	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	1073/1295 (83%)	1028 (96%)	41 (4%)	4 (0%)	30	64
1	B	1073/1295 (83%)	1039 (97%)	32 (3%)	2 (0%)	43	74
1	C	1073/1295 (83%)	1032 (96%)	40 (4%)	1 (0%)	48	80
1	D	1073/1295 (83%)	1036 (97%)	36 (3%)	1 (0%)	48	80
1	E	1073/1295 (83%)	1041 (97%)	31 (3%)	1 (0%)	48	80
1	F	1073/1295 (83%)	1039 (97%)	33 (3%)	1 (0%)	48	80
2	J	201/215 (94%)	195 (97%)	6 (3%)	0	100	100
2	K	201/215 (94%)	194 (96%)	7 (4%)	0	100	100
2	L	201/215 (94%)	195 (97%)	6 (3%)	0	100	100
2	P	201/215 (94%)	193 (96%)	8 (4%)	0	100	100
2	Q	201/215 (94%)	194 (96%)	7 (4%)	0	100	100
2	R	201/215 (94%)	192 (96%)	9 (4%)	0	100	100
3	G	216/218 (99%)	208 (96%)	8 (4%)	0	100	100
3	H	216/218 (99%)	207 (96%)	9 (4%)	0	100	100
3	I	216/218 (99%)	208 (96%)	8 (4%)	0	100	100
3	M	216/218 (99%)	207 (96%)	9 (4%)	0	100	100
3	N	216/218 (99%)	207 (96%)	9 (4%)	0	100	100
3	O	216/218 (99%)	208 (96%)	8 (4%)	0	100	100
All	All	8940/10368 (86%)	8623 (96%)	307 (3%)	10 (0%)	49	80

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	524	VAL
1	B	527	PRO
1	A	525	CYS
1	A	527	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	621	PRO
1	B	621	PRO
1	A	621	PRO
1	C	621	PRO
1	E	621	PRO
1	D	621	PRO

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	948/1118 (85%)	922 (97%)	26 (3%)	39	60
1	B	948/1118 (85%)	923 (97%)	25 (3%)	40	61
1	C	948/1118 (85%)	925 (98%)	23 (2%)	43	63
1	D	948/1118 (85%)	926 (98%)	22 (2%)	44	63
1	E	948/1118 (85%)	924 (98%)	24 (2%)	42	62
1	F	948/1118 (85%)	921 (97%)	27 (3%)	38	59
2	J	168/179 (94%)	163 (97%)	5 (3%)	36	57
2	K	168/179 (94%)	165 (98%)	3 (2%)	51	67
2	L	168/179 (94%)	165 (98%)	3 (2%)	51	67
2	P	168/179 (94%)	163 (97%)	5 (3%)	36	57
2	Q	168/179 (94%)	165 (98%)	3 (2%)	51	67
2	R	168/179 (94%)	165 (98%)	3 (2%)	51	67
3	G	184/184 (100%)	178 (97%)	6 (3%)	33	56
3	H	184/184 (100%)	181 (98%)	3 (2%)	55	69
3	I	184/184 (100%)	181 (98%)	3 (2%)	55	69
3	M	184/184 (100%)	178 (97%)	6 (3%)	33	56
3	N	184/184 (100%)	181 (98%)	3 (2%)	55	69
3	O	184/184 (100%)	181 (98%)	3 (2%)	55	69
All	All	7800/8886 (88%)	7607 (98%)	193 (2%)	42	62

All (193) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	146	GLN
1	B	182	LYS
1	B	229	LEU
1	B	249	LEU
1	B	252	VAL
1	B	312	ILE
1	B	313	TYR
1	B	326	ILE
1	B	328	ARG
1	B	332	ILE
1	B	335	LEU
1	B	336	CYS
1	B	362	VAL
1	B	395	VAL
1	B	402	ILE
1	B	518	LEU
1	B	524	VAL
1	B	528	LYS
1	B	529	LYS
1	B	622	VAL
1	B	633	TRP
1	B	634	ARG
1	B	738	CYS
1	B	811	LYS
1	B	844	ILE
1	A	146	GLN
1	A	182	LYS
1	A	229	LEU
1	A	249	LEU
1	A	252	VAL
1	A	312	ILE
1	A	313	TYR
1	A	326	ILE
1	A	329	PHE
1	A	336	CYS
1	A	361	CYS
1	A	386	LYS
1	A	387	LEU
1	A	388	ASN
1	A	393	THR
1	A	394	ASN
1	A	395	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	402	ILE
1	A	528	LYS
1	A	529	LYS
1	A	622	VAL
1	A	633	TRP
1	A	634	ARG
1	A	738	CYS
1	A	811	LYS
1	A	844	ILE
2	J	53	MET
2	J	147	GLN
2	J	166	THR
2	J	187	LYS
2	J	201	LEU
3	G	12	VAL
3	G	99	THR
3	G	110	LEU
3	G	125	THR
3	G	126	VAL
3	G	132	LYS
2	K	53	MET
2	K	166	THR
2	K	201	LEU
3	H	12	VAL
3	H	99	THR
3	H	110	LEU
2	L	53	MET
2	L	166	THR
2	L	201	LEU
3	I	12	VAL
3	I	99	THR
3	I	110	LEU
1	C	146	GLN
1	C	182	LYS
1	C	229	LEU
1	C	249	LEU
1	C	252	VAL
1	C	312	ILE
1	C	313	TYR
1	C	320	VAL
1	C	328	ARG
1	C	361	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	362	VAL
1	C	395	VAL
1	C	402	ILE
1	C	503	VAL
1	C	517	LEU
1	C	529	LYS
1	C	622	VAL
1	C	633	TRP
1	C	634	ARG
1	C	738	CYS
1	C	811	LYS
1	C	844	ILE
1	C	1122	VAL
1	E	146	GLN
1	E	182	LYS
1	E	229	LEU
1	E	249	LEU
1	E	252	VAL
1	E	312	ILE
1	E	313	TYR
1	E	326	ILE
1	E	328	ARG
1	E	332	ILE
1	E	336	CYS
1	E	362	VAL
1	E	395	VAL
1	E	402	ILE
1	E	518	LEU
1	E	524	VAL
1	E	528	LYS
1	E	529	LYS
1	E	622	VAL
1	E	633	TRP
1	E	634	ARG
1	E	738	CYS
1	E	811	LYS
1	E	844	ILE
1	D	146	GLN
1	D	182	LYS
1	D	229	LEU
1	D	249	LEU
1	D	252	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	312	ILE
1	D	313	TYR
1	D	326	ILE
1	D	329	PHE
1	D	336	CYS
1	D	361	CYS
1	D	395	VAL
1	D	402	ILE
1	D	528	LYS
1	D	529	LYS
1	D	622	VAL
1	D	633	TRP
1	D	634	ARG
1	D	738	CYS
1	D	811	LYS
1	D	844	ILE
1	D	1122	VAL
2	P	53	MET
2	P	122	THR
2	P	166	THR
2	P	187	LYS
2	P	201	LEU
3	M	12	VAL
3	M	99	THR
3	M	110	LEU
3	M	125	THR
3	M	126	VAL
3	M	132	LYS
2	Q	53	MET
2	Q	166	THR
2	Q	201	LEU
3	N	12	VAL
3	N	99	THR
3	N	110	LEU
2	R	53	MET
2	R	166	THR
2	R	201	LEU
3	O	12	VAL
3	O	99	THR
3	O	110	LEU
1	F	146	GLN
1	F	182	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	229	LEU
1	F	249	LEU
1	F	252	VAL
1	F	312	ILE
1	F	313	TYR
1	F	320	VAL
1	F	328	ARG
1	F	335	LEU
1	F	362	VAL
1	F	395	VAL
1	F	402	ILE
1	F	503	VAL
1	F	517	LEU
1	F	525	CYS
1	F	528	LYS
1	F	529	LYS
1	F	530	SER
1	F	531	THR
1	F	622	VAL
1	F	633	TRP
1	F	634	ARG
1	F	738	CYS
1	F	811	LYS
1	F	844	ILE
1	F	1122	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (156) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	27	GLN
1	B	88	ASN
1	B	122	ASN
1	B	185	ASN
1	B	321	GLN
1	B	414	GLN
1	B	422	ASN
1	B	487	ASN
1	B	493	GLN
1	B	544	ASN
1	B	564	GLN
1	B	607	GLN
1	B	613	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	677	GLN
1	B	690	GLN
1	B	762	GLN
1	B	836	GLN
1	B	957	GLN
1	B	1011	GLN
1	B	1064	HIS
1	A	27	GLN
1	A	88	ASN
1	A	116	GLN
1	A	122	ASN
1	A	185	ASN
1	A	321	GLN
1	A	414	GLN
1	A	439	ASN
1	A	487	ASN
1	A	493	GLN
1	A	532	ASN
1	A	613	GLN
1	A	677	GLN
1	A	762	GLN
1	A	836	GLN
1	A	955	ASN
1	A	957	GLN
1	A	1005	GLN
1	A	1011	GLN
1	A	1106	GLN
2	J	147	GLN
2	J	191	ASN
2	J	218	HIS
3	G	6	GLN
3	G	90	HIS
3	G	107	GLN
3	G	120	GLN
2	K	45	HIS
2	K	95	GLN
2	K	218	HIS
3	H	6	GLN
2	L	218	HIS
3	I	72	GLN
3	I	75	GLN
3	I	90	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	I	107	GLN
1	C	27	GLN
1	C	88	ASN
1	C	122	ASN
1	C	185	ASN
1	C	321	GLN
1	C	394	ASN
1	C	414	GLN
1	C	417	ASN
1	C	487	ASN
1	C	493	GLN
1	C	536	ASN
1	C	544	ASN
1	C	564	GLN
1	C	607	GLN
1	C	613	GLN
1	C	677	GLN
1	C	690	GLN
1	C	762	GLN
1	C	836	GLN
1	C	949	GLN
1	C	955	ASN
1	C	957	GLN
1	C	1002	GLN
1	C	1011	GLN
1	C	1106	GLN
1	E	27	GLN
1	E	88	ASN
1	E	122	ASN
1	E	185	ASN
1	E	321	GLN
1	E	331	ASN
1	E	414	GLN
1	E	422	ASN
1	E	487	ASN
1	E	493	GLN
1	E	544	ASN
1	E	564	GLN
1	E	607	GLN
1	E	613	GLN
1	E	677	GLN
1	E	762	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	955	ASN
1	E	957	GLN
1	E	965	GLN
1	E	1005	GLN
1	E	1011	GLN
1	D	27	GLN
1	D	88	ASN
1	D	100	ASN
1	D	116	GLN
1	D	122	ASN
1	D	185	ASN
1	D	321	GLN
1	D	394	ASN
1	D	414	GLN
1	D	439	ASN
1	D	487	ASN
1	D	493	GLN
1	D	519	HIS
1	D	544	ASN
1	D	607	GLN
1	D	613	GLN
1	D	677	GLN
1	D	762	GLN
1	D	955	ASN
1	D	957	GLN
1	D	1002	GLN
1	D	1011	GLN
2	P	95	GLN
2	P	191	ASN
2	P	218	HIS
3	M	6	GLN
3	M	107	GLN
3	M	120	GLN
2	Q	218	HIS
2	R	95	GLN
3	O	72	GLN
3	O	90	HIS
3	O	107	GLN
1	F	27	GLN
1	F	88	ASN
1	F	122	ASN
1	F	185	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	321	GLN
1	F	331	ASN
1	F	422	ASN
1	F	487	ASN
1	F	493	GLN
1	F	536	ASN
1	F	544	ASN
1	F	564	GLN
1	F	607	GLN
1	F	613	GLN
1	F	677	GLN
1	F	690	GLN
1	F	762	GLN
1	F	955	ASN
1	F	957	GLN
1	F	965	GLN
1	F	1011	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 ⓘ

There are no chain breaks in this entry.

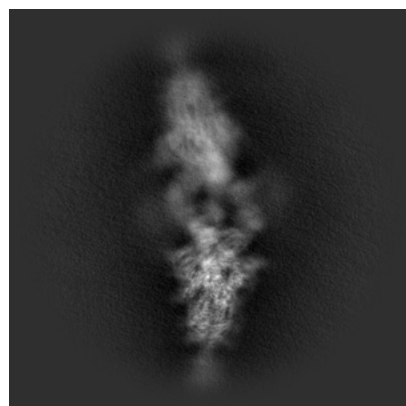
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39805. These allow visual inspection of the internal detail of the map and identification of artifacts.

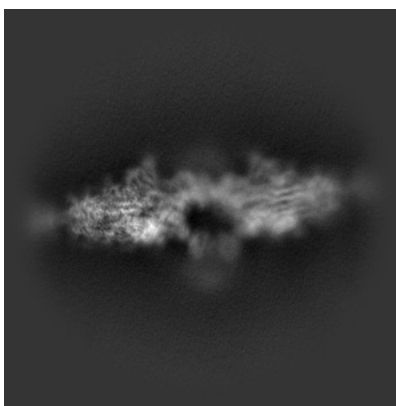
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

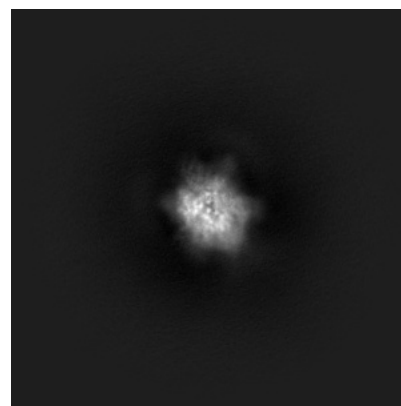
6.1.1 Primary map



X

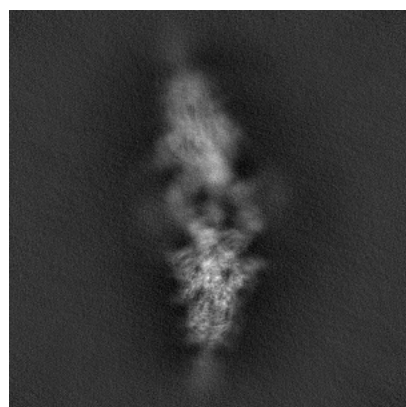


Y

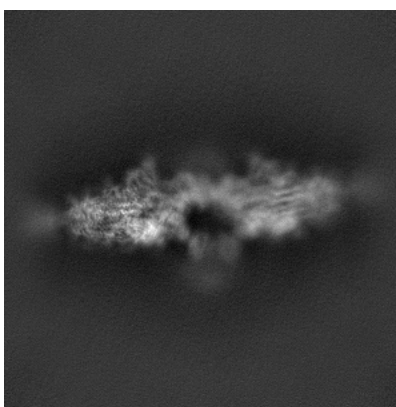


Z

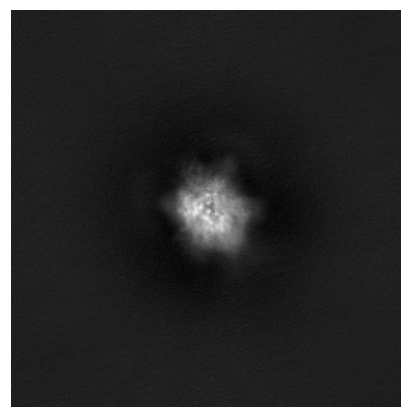
6.1.2 Raw map



X



Y

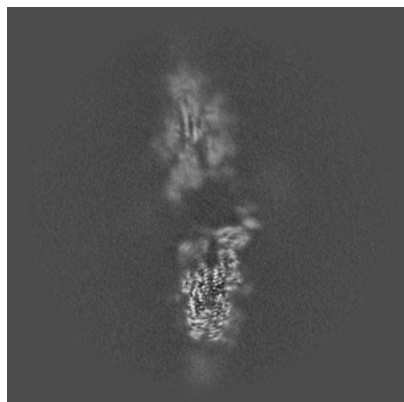


Z

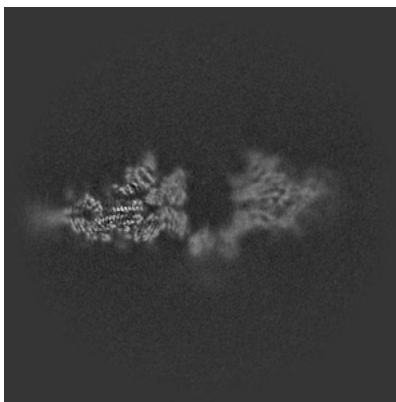
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

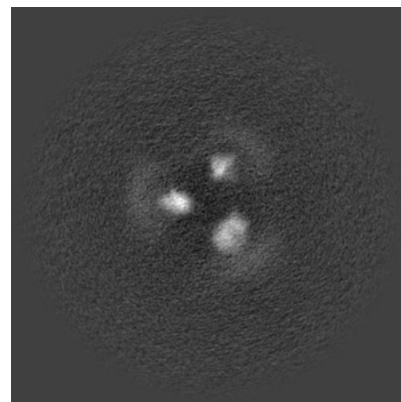
6.2.1 Primary map



X Index: 240



Y Index: 240

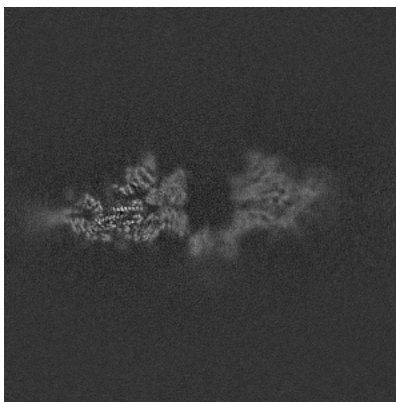


Z Index: 240

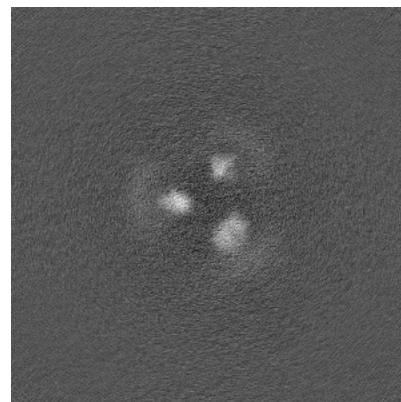
6.2.2 Raw map



X Index: 240



Y Index: 240

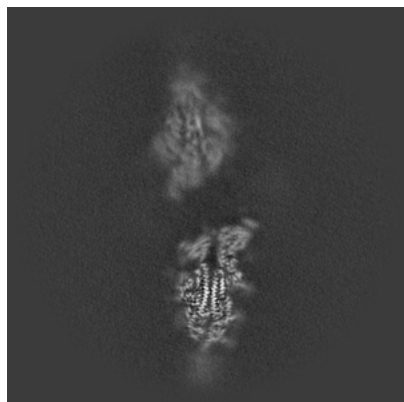


Z Index: 240

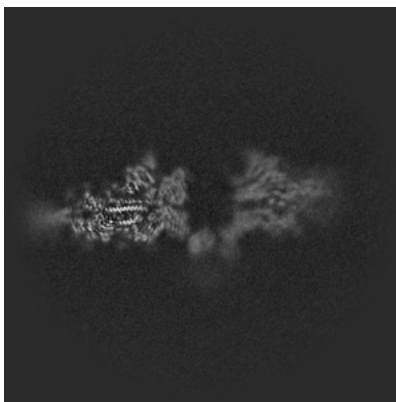
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

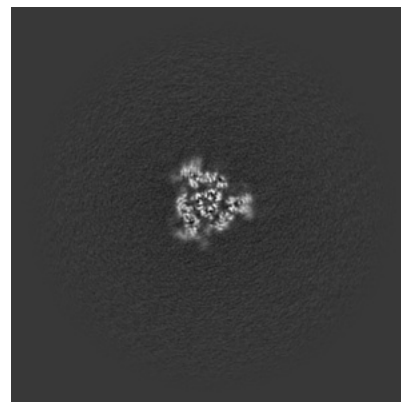
6.3.1 Primary map



X Index: 236

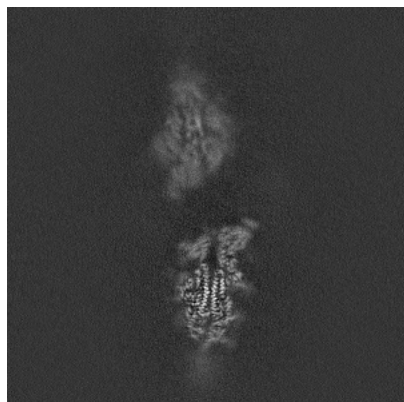


Y Index: 238



Z Index: 158

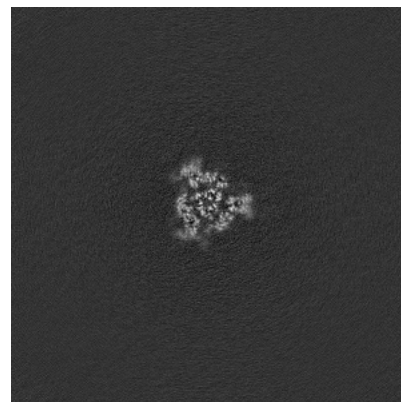
6.3.2 Raw map



X Index: 236



Y Index: 248

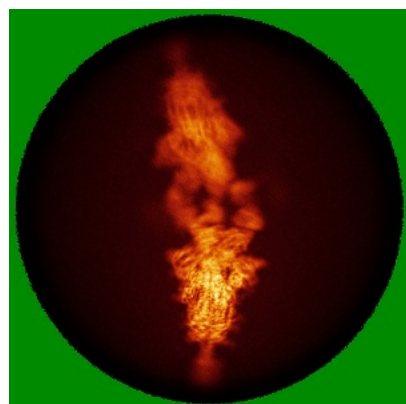


Z Index: 158

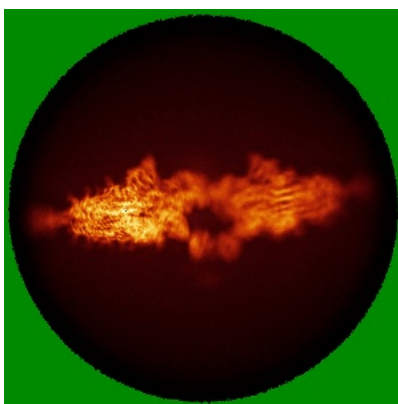
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

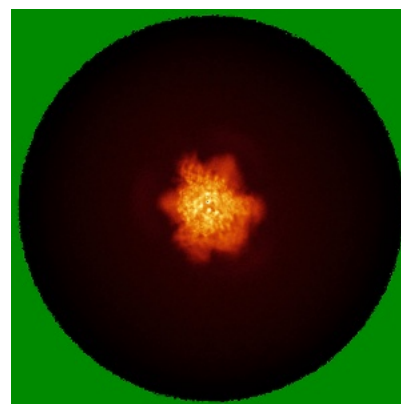
6.4.1 Primary map



X

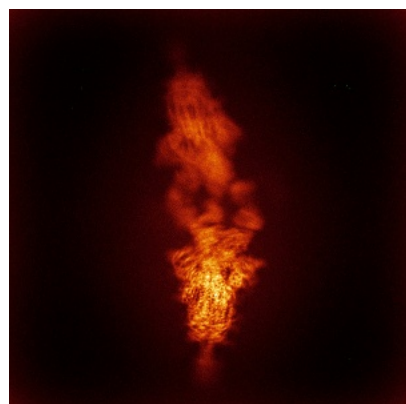


Y

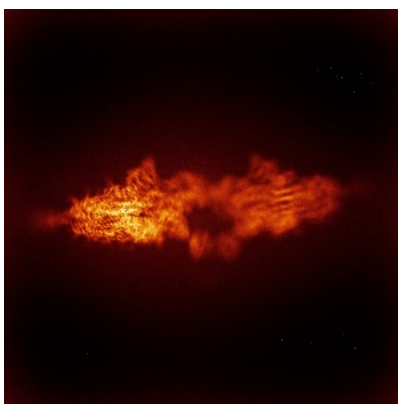


Z

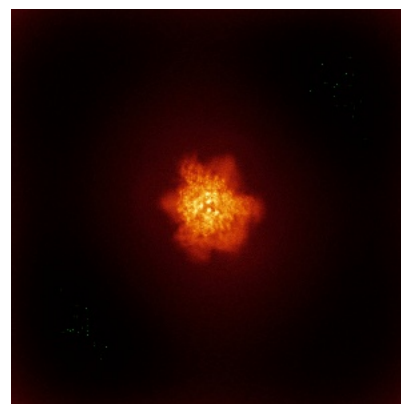
6.4.2 Raw map



X



Y

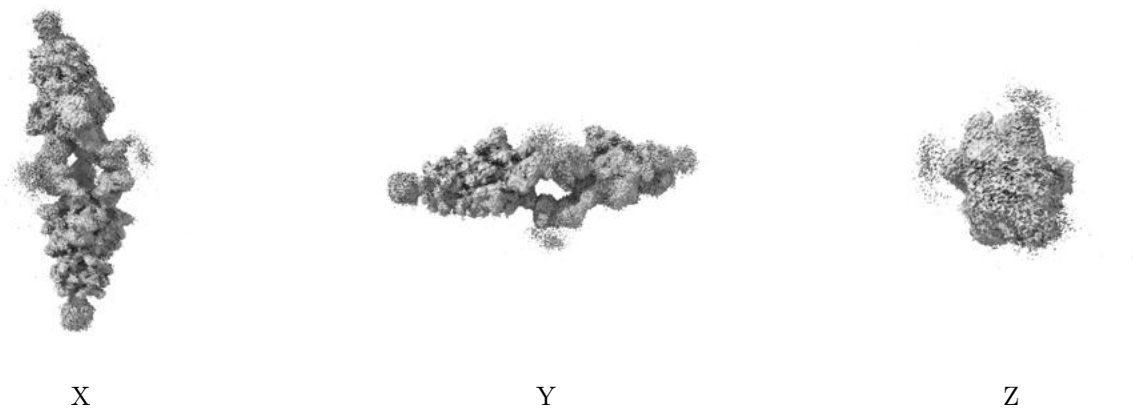


Z

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.

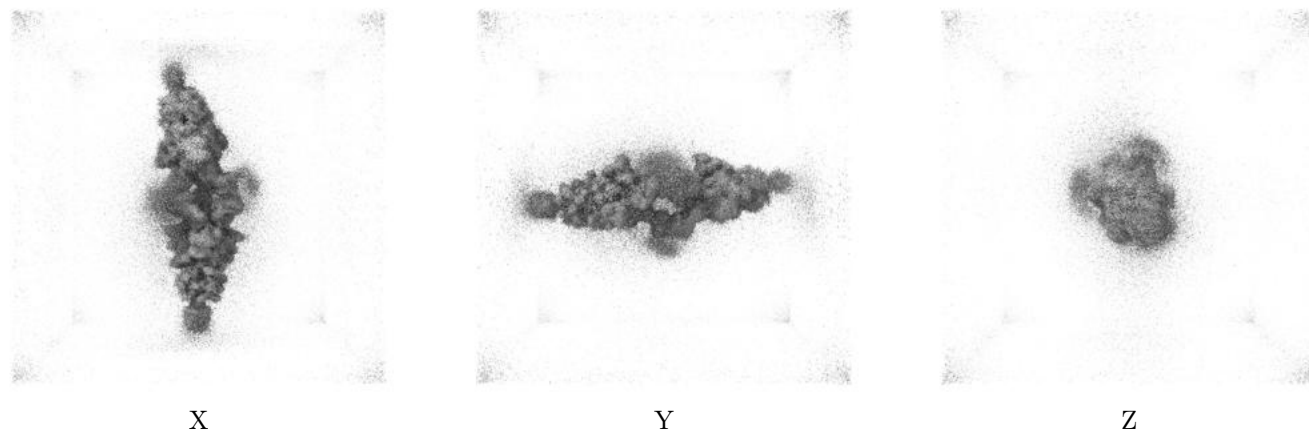
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. 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.

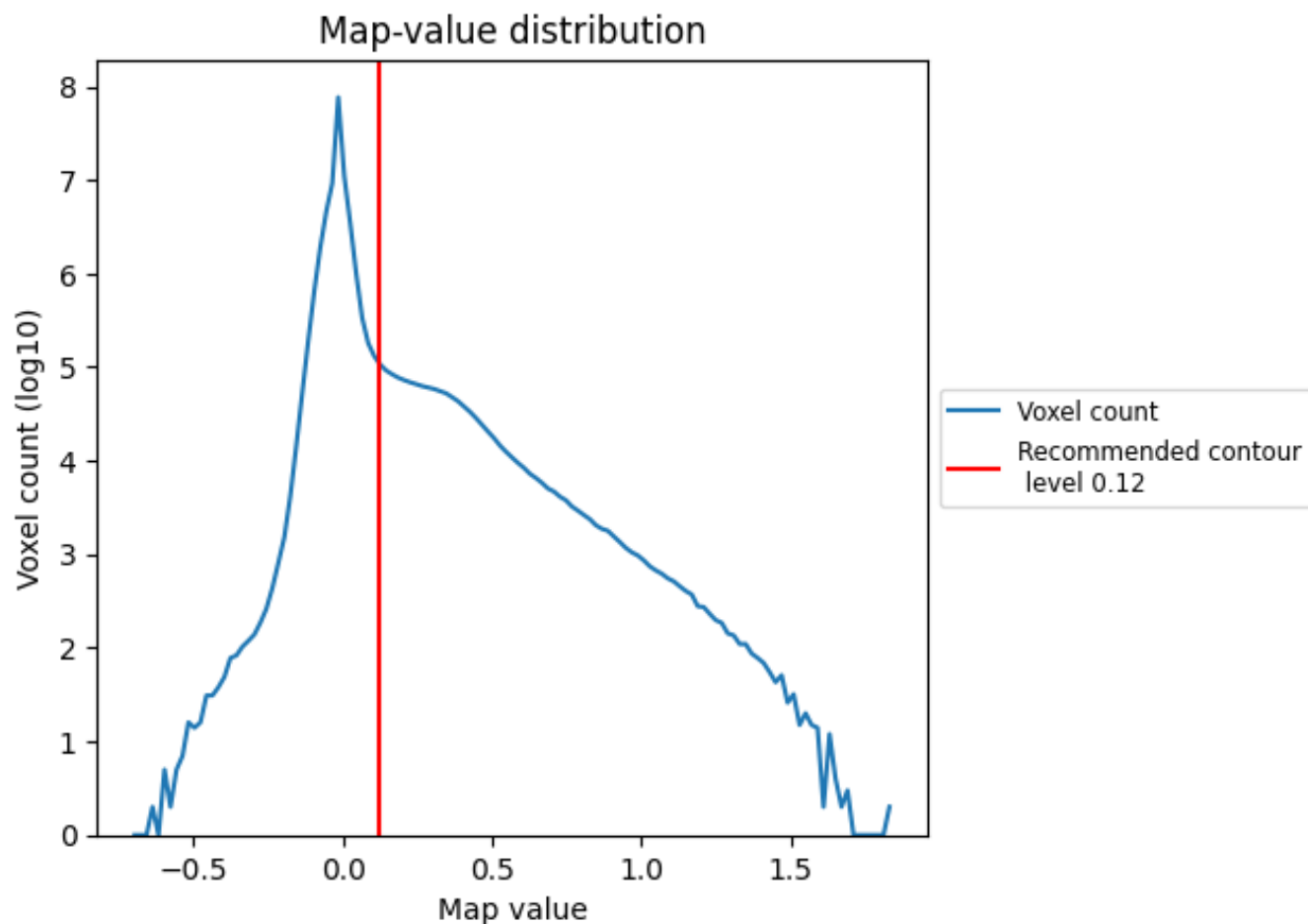
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

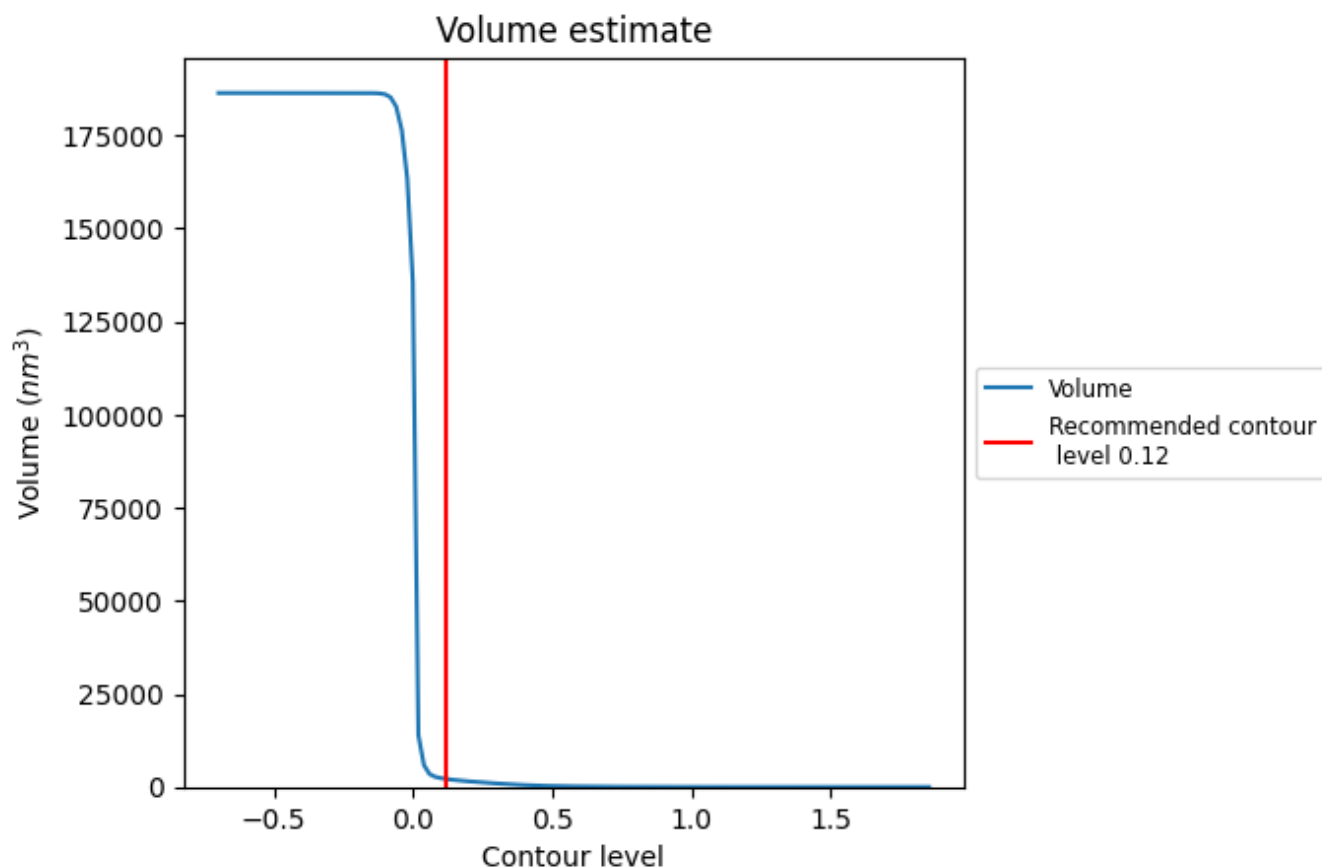
This section contains the results of statistical analysis of the map.

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.

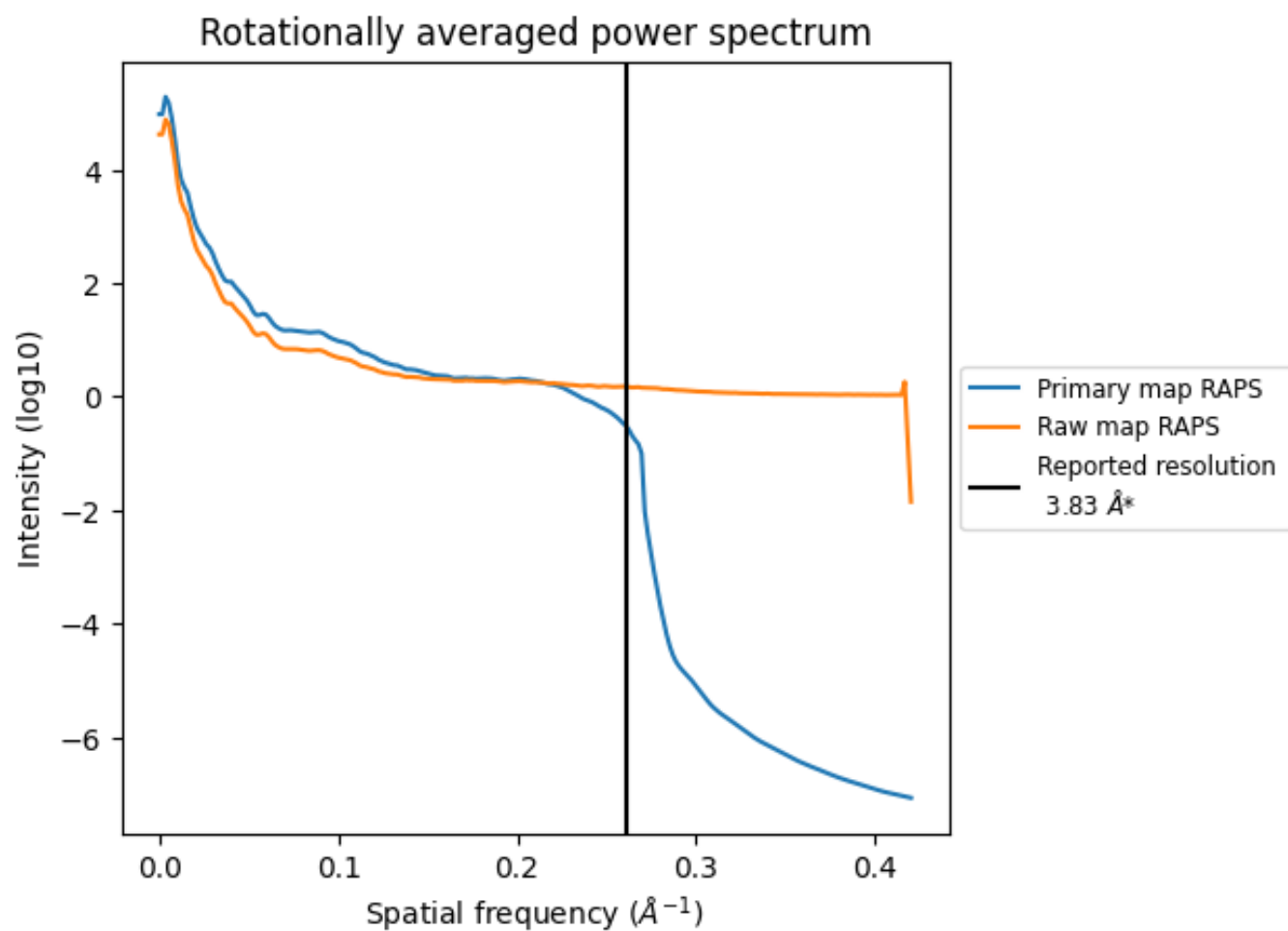
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2130 nm^3 ; this corresponds to an approximate mass of 1924 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 ⓘ

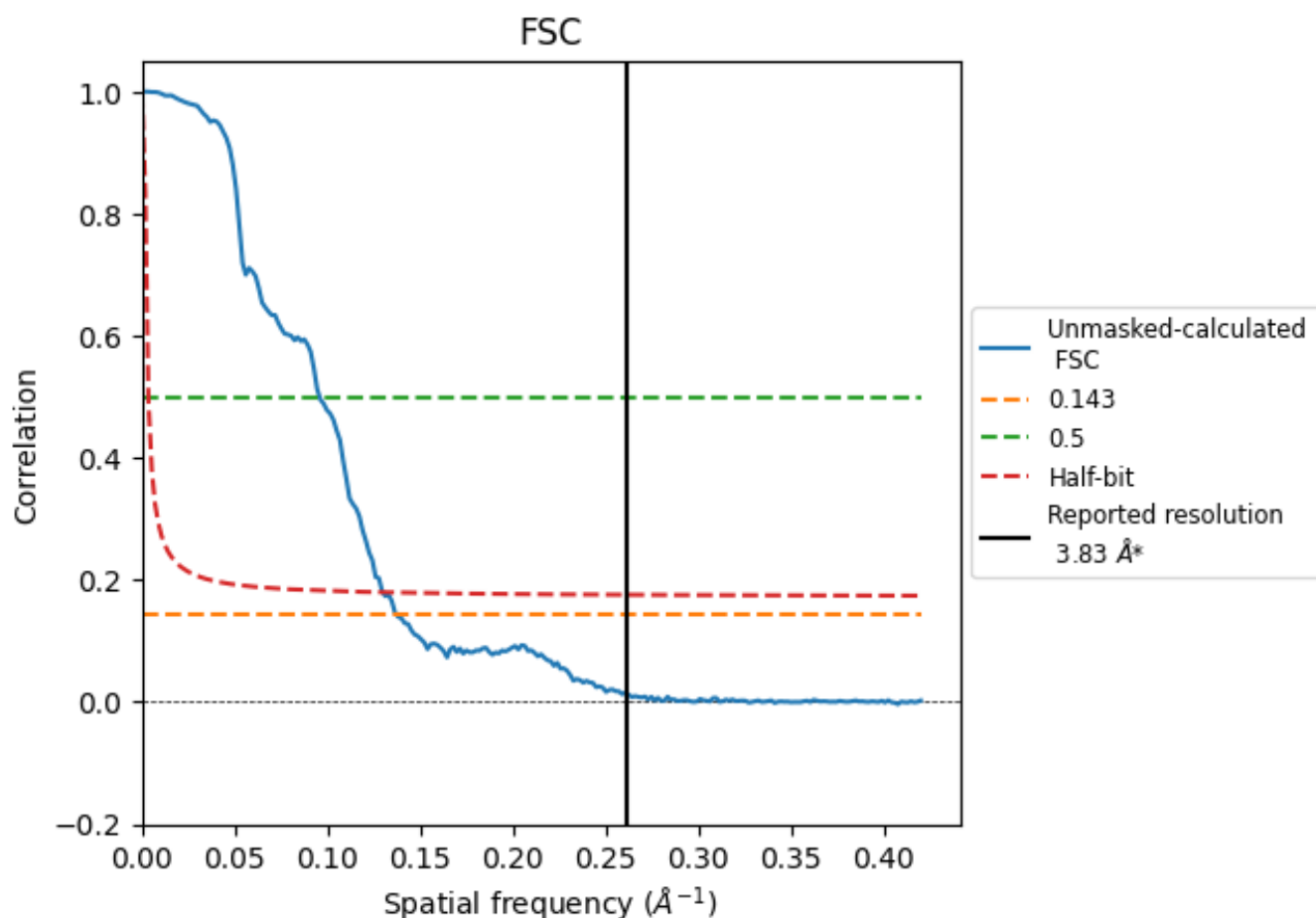


*Reported resolution corresponds to spatial frequency of 0.261 Å⁻¹

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 0.261 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

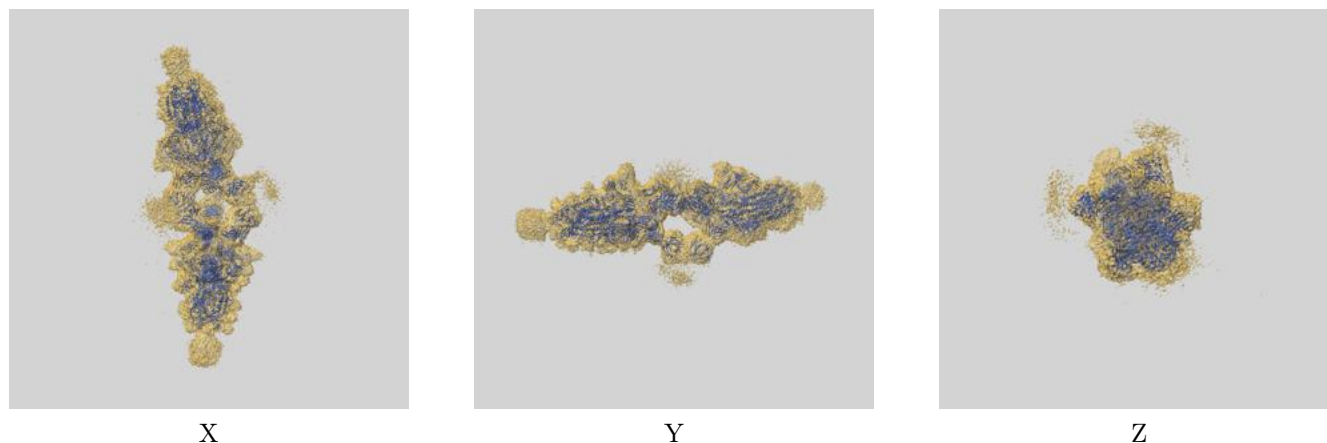
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.83	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.29	10.44	7.70

*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 7.29 differs from the reported value 3.83 by more than 10 %

9 Map-model fit [i](#)

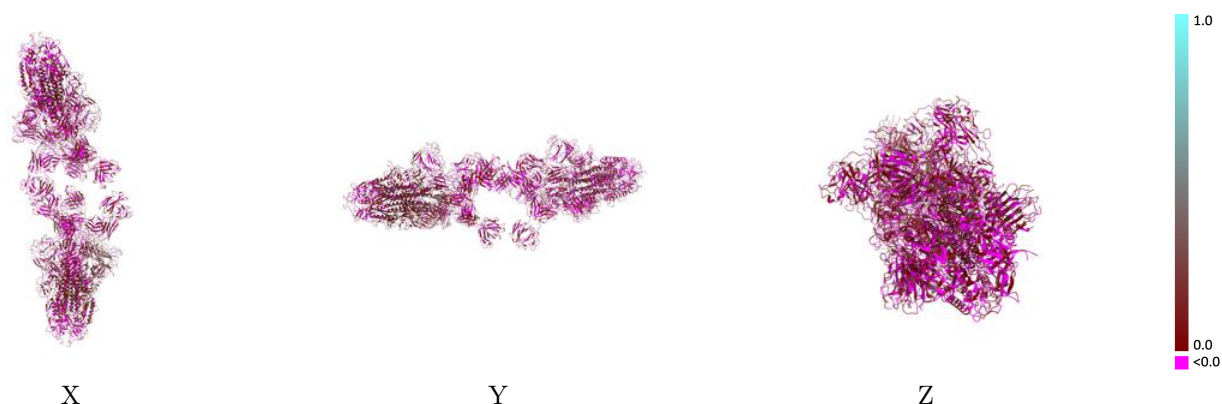
This section contains information regarding the fit between EMDB map EMD-39805 and PDB model 8Z6U. Per-residue inclusion information can be found in section [3](#) on page [17](#).

9.1 Map-model overlay [i](#)



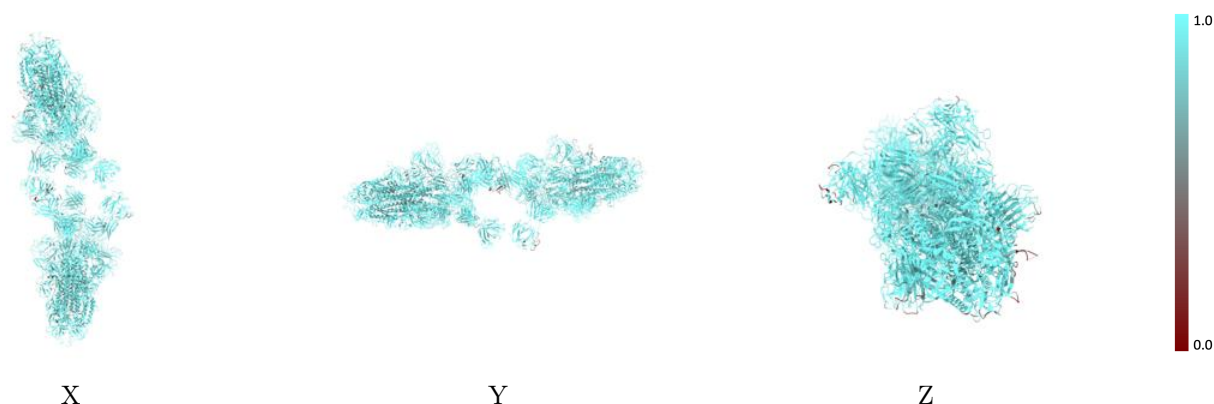
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



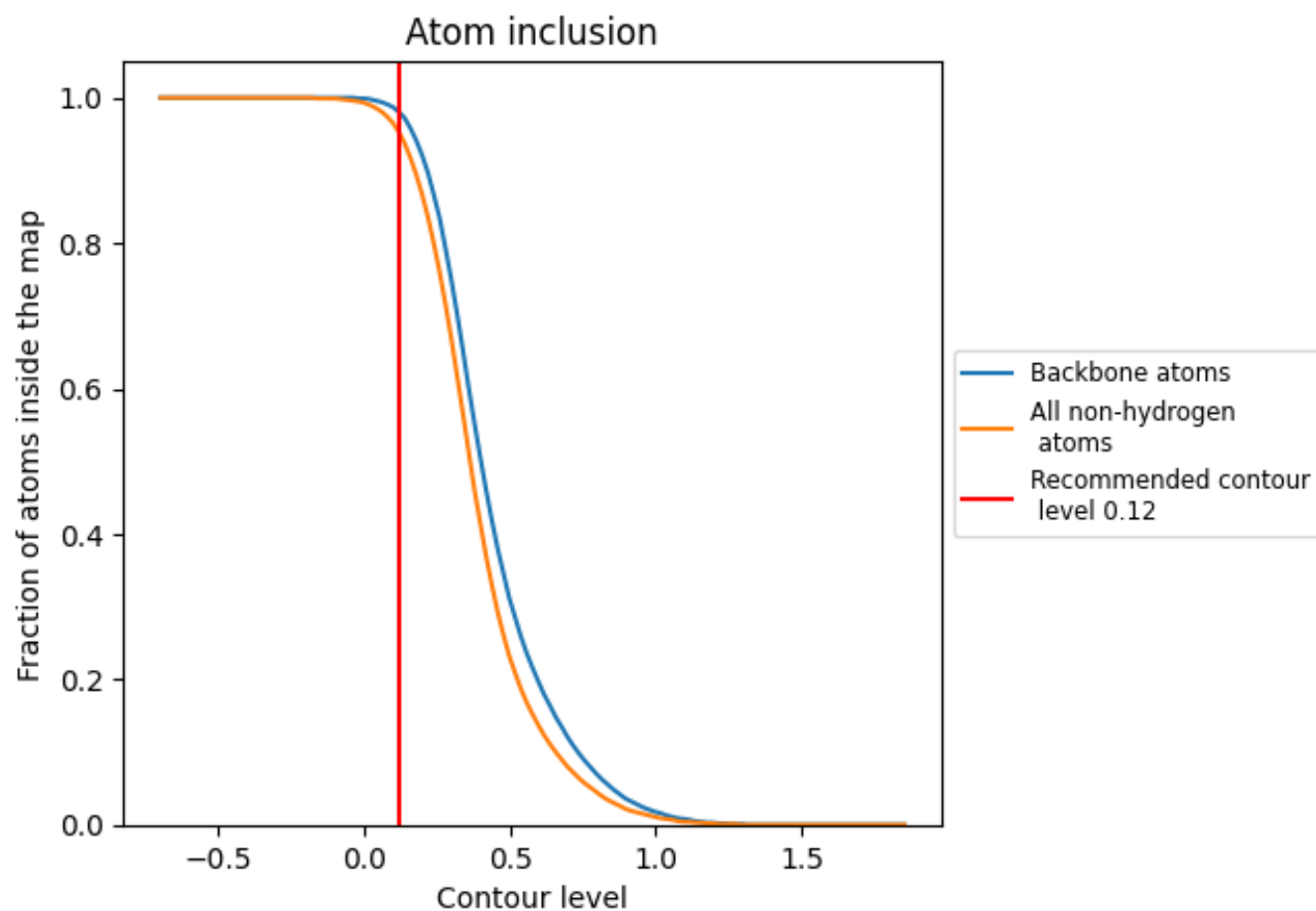
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 95% 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	 0.9520	 0.0780
A	 0.9350	 0.1090
B	 0.9580	 0.1540
C	 0.9330	 0.0990
D	 0.9760	 0.0640
E	 0.9430	 0.0520
F	 0.9610	 0.0560
G	 0.9120	 0.0290
H	 0.9670	 0.0580
I	 0.9620	 0.0370
J	 0.9680	 0.0170
K	 0.9510	 0.0950
L	 0.9910	 0.0800
M	 0.9820	 0.0570
N	 0.9820	 0.0300
O	 0.8680	 0.0300
P	 0.9050	 0.0540
Q	 0.9820	 0.0770
R	 0.9650	 0.0110

