



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 06:36 AM UTC

PDB ID : 6G2D / pdb_00006g2d
EMDB ID : EMD-4342
Title : Citrate-induced acetyl-CoA carboxylase (ACC-Cit) filament at 5.4 Å resolution
Authors : Hunkeler, M.; Hagmann, A.; Stüttfeld, E.; Chami, M.; Stahlberg, H.; Maier, T.
Deposited on : 2018-03-23
Resolution : 5.40 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

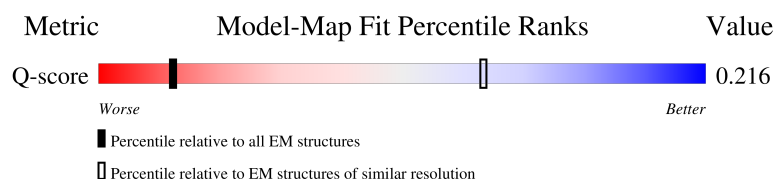
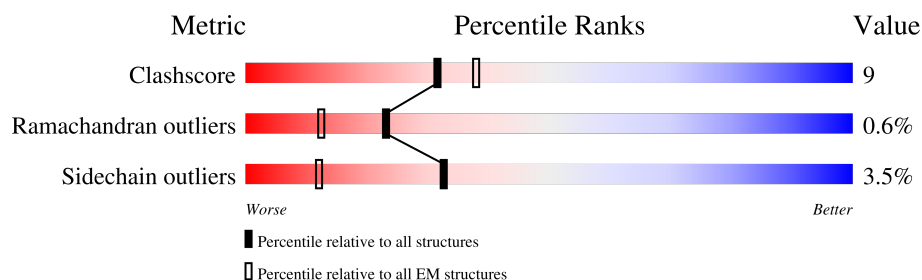
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.40 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	538 (4.90 - 5.90)

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	B	2407	8% 18% 8% . 74%
1	C	2407	7% 69% 17% . 12%
1	D	2407	7% 68% 18% . 12%
1	F	2407	10% 18% 7% . 74%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 88169 atoms, of which 43991 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 Acetyl-CoA carboxylase 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	B	625	Total	C	H	N	O	S	0	0
			10226	3267	5114	888	922	35		
1	C	2121	Total	C	H	N	O	S	0	0
			33781	10771	16841	2945	3124	100		
1	D	2121	Total	C	H	N	O	S	0	0
			33782	10771	16842	2945	3124	100		
1	F	634	Total	C	H	N	O	S	0	0
			10380	3310	5194	905	936	35		

There are 244 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-60	MET	-	initiating methionine	UNP Q13085
B	-59	ALA	-	expression tag	UNP Q13085
B	-58	HIS	-	expression tag	UNP Q13085
B	-57	HIS	-	expression tag	UNP Q13085
B	-56	HIS	-	expression tag	UNP Q13085
B	-55	HIS	-	expression tag	UNP Q13085
B	-54	HIS	-	expression tag	UNP Q13085
B	-53	HIS	-	expression tag	UNP Q13085
B	-52	HIS	-	expression tag	UNP Q13085
B	-51	HIS	-	expression tag	UNP Q13085
B	-50	HIS	-	expression tag	UNP Q13085
B	-49	HIS	-	expression tag	UNP Q13085
B	-48	GLY	-	expression tag	UNP Q13085
B	-47	SER	-	expression tag	UNP Q13085
B	-46	THR	-	expression tag	UNP Q13085
B	-45	SER	-	expression tag	UNP Q13085
B	-44	GLY	-	expression tag	UNP Q13085
B	-43	SER	-	expression tag	UNP Q13085
B	-42	GLY	-	expression tag	UNP Q13085
B	-41	GLU	-	expression tag	UNP Q13085
B	-40	GLN	-	expression tag	UNP Q13085
B	-39	LYS	-	expression tag	UNP Q13085

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-38	LEU	-	expression tag	UNP Q13085
B	-37	ILE	-	expression tag	UNP Q13085
B	-36	SER	-	expression tag	UNP Q13085
B	-35	GLU	-	expression tag	UNP Q13085
B	-34	GLU	-	expression tag	UNP Q13085
B	-33	ASP	-	expression tag	UNP Q13085
B	-32	LEU	-	expression tag	UNP Q13085
B	-31	GLY	-	expression tag	UNP Q13085
B	-30	SER	-	expression tag	UNP Q13085
B	-29	THR	-	expression tag	UNP Q13085
B	-28	SER	-	expression tag	UNP Q13085
B	-27	GLY	-	expression tag	UNP Q13085
B	-26	SER	-	expression tag	UNP Q13085
B	-25	GLY	-	expression tag	UNP Q13085
B	-24	ASP	-	expression tag	UNP Q13085
B	-23	TYR	-	expression tag	UNP Q13085
B	-22	LYS	-	expression tag	UNP Q13085
B	-21	ASP	-	expression tag	UNP Q13085
B	-20	ASP	-	expression tag	UNP Q13085
B	-19	ASP	-	expression tag	UNP Q13085
B	-18	ASP	-	expression tag	UNP Q13085
B	-17	LYS	-	expression tag	UNP Q13085
B	-16	LEU	-	expression tag	UNP Q13085
B	-15	THR	-	expression tag	UNP Q13085
B	-14	SER	-	expression tag	UNP Q13085
B	-13	LEU	-	expression tag	UNP Q13085
B	-12	TYR	-	expression tag	UNP Q13085
B	-11	LYS	-	expression tag	UNP Q13085
B	-10	LYS	-	expression tag	UNP Q13085
B	-9	ALA	-	expression tag	UNP Q13085
B	-8	GLY	-	expression tag	UNP Q13085
B	-7	LEU	-	expression tag	UNP Q13085
B	-6	GLU	-	expression tag	UNP Q13085
B	-5	ASN	-	expression tag	UNP Q13085
B	-4	LEU	-	expression tag	UNP Q13085
B	-3	TYR	-	expression tag	UNP Q13085
B	-2	PHE	-	expression tag	UNP Q13085
B	-1	GLN	-	expression tag	UNP Q13085
B	0	GLY	-	expression tag	UNP Q13085
C	-60	MET	-	initiating methionine	UNP Q13085
C	-59	ALA	-	expression tag	UNP Q13085
C	-58	HIS	-	expression tag	UNP Q13085

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-57	HIS	-	expression tag	UNP Q13085
C	-56	HIS	-	expression tag	UNP Q13085
C	-55	HIS	-	expression tag	UNP Q13085
C	-54	HIS	-	expression tag	UNP Q13085
C	-53	HIS	-	expression tag	UNP Q13085
C	-52	HIS	-	expression tag	UNP Q13085
C	-51	HIS	-	expression tag	UNP Q13085
C	-50	HIS	-	expression tag	UNP Q13085
C	-49	HIS	-	expression tag	UNP Q13085
C	-48	GLY	-	expression tag	UNP Q13085
C	-47	SER	-	expression tag	UNP Q13085
C	-46	THR	-	expression tag	UNP Q13085
C	-45	SER	-	expression tag	UNP Q13085
C	-44	GLY	-	expression tag	UNP Q13085
C	-43	SER	-	expression tag	UNP Q13085
C	-42	GLY	-	expression tag	UNP Q13085
C	-41	GLU	-	expression tag	UNP Q13085
C	-40	GLN	-	expression tag	UNP Q13085
C	-39	LYS	-	expression tag	UNP Q13085
C	-38	LEU	-	expression tag	UNP Q13085
C	-37	ILE	-	expression tag	UNP Q13085
C	-36	SER	-	expression tag	UNP Q13085
C	-35	GLU	-	expression tag	UNP Q13085
C	-34	GLU	-	expression tag	UNP Q13085
C	-33	ASP	-	expression tag	UNP Q13085
C	-32	LEU	-	expression tag	UNP Q13085
C	-31	GLY	-	expression tag	UNP Q13085
C	-30	SER	-	expression tag	UNP Q13085
C	-29	THR	-	expression tag	UNP Q13085
C	-28	SER	-	expression tag	UNP Q13085
C	-27	GLY	-	expression tag	UNP Q13085
C	-26	SER	-	expression tag	UNP Q13085
C	-25	GLY	-	expression tag	UNP Q13085
C	-24	ASP	-	expression tag	UNP Q13085
C	-23	TYR	-	expression tag	UNP Q13085
C	-22	LYS	-	expression tag	UNP Q13085
C	-21	ASP	-	expression tag	UNP Q13085
C	-20	ASP	-	expression tag	UNP Q13085
C	-19	ASP	-	expression tag	UNP Q13085
C	-18	ASP	-	expression tag	UNP Q13085
C	-17	LYS	-	expression tag	UNP Q13085
C	-16	LEU	-	expression tag	UNP Q13085

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-15	THR	-	expression tag	UNP Q13085
C	-14	SER	-	expression tag	UNP Q13085
C	-13	LEU	-	expression tag	UNP Q13085
C	-12	TYR	-	expression tag	UNP Q13085
C	-11	LYS	-	expression tag	UNP Q13085
C	-10	LYS	-	expression tag	UNP Q13085
C	-9	ALA	-	expression tag	UNP Q13085
C	-8	GLY	-	expression tag	UNP Q13085
C	-7	LEU	-	expression tag	UNP Q13085
C	-6	GLU	-	expression tag	UNP Q13085
C	-5	ASN	-	expression tag	UNP Q13085
C	-4	LEU	-	expression tag	UNP Q13085
C	-3	TYR	-	expression tag	UNP Q13085
C	-2	PHE	-	expression tag	UNP Q13085
C	-1	GLN	-	expression tag	UNP Q13085
C	0	GLY	-	expression tag	UNP Q13085
D	-60	MET	-	initiating methionine	UNP Q13085
D	-59	ALA	-	expression tag	UNP Q13085
D	-58	HIS	-	expression tag	UNP Q13085
D	-57	HIS	-	expression tag	UNP Q13085
D	-56	HIS	-	expression tag	UNP Q13085
D	-55	HIS	-	expression tag	UNP Q13085
D	-54	HIS	-	expression tag	UNP Q13085
D	-53	HIS	-	expression tag	UNP Q13085
D	-52	HIS	-	expression tag	UNP Q13085
D	-51	HIS	-	expression tag	UNP Q13085
D	-50	HIS	-	expression tag	UNP Q13085
D	-49	HIS	-	expression tag	UNP Q13085
D	-48	GLY	-	expression tag	UNP Q13085
D	-47	SER	-	expression tag	UNP Q13085
D	-46	THR	-	expression tag	UNP Q13085
D	-45	SER	-	expression tag	UNP Q13085
D	-44	GLY	-	expression tag	UNP Q13085
D	-43	SER	-	expression tag	UNP Q13085
D	-42	GLY	-	expression tag	UNP Q13085
D	-41	GLU	-	expression tag	UNP Q13085
D	-40	GLN	-	expression tag	UNP Q13085
D	-39	LYS	-	expression tag	UNP Q13085
D	-38	LEU	-	expression tag	UNP Q13085
D	-37	ILE	-	expression tag	UNP Q13085
D	-36	SER	-	expression tag	UNP Q13085
D	-35	GLU	-	expression tag	UNP Q13085

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-34	GLU	-	expression tag	UNP Q13085
D	-33	ASP	-	expression tag	UNP Q13085
D	-32	LEU	-	expression tag	UNP Q13085
D	-31	GLY	-	expression tag	UNP Q13085
D	-30	SER	-	expression tag	UNP Q13085
D	-29	THR	-	expression tag	UNP Q13085
D	-28	SER	-	expression tag	UNP Q13085
D	-27	GLY	-	expression tag	UNP Q13085
D	-26	SER	-	expression tag	UNP Q13085
D	-25	GLY	-	expression tag	UNP Q13085
D	-24	ASP	-	expression tag	UNP Q13085
D	-23	TYR	-	expression tag	UNP Q13085
D	-22	LYS	-	expression tag	UNP Q13085
D	-21	ASP	-	expression tag	UNP Q13085
D	-20	ASP	-	expression tag	UNP Q13085
D	-19	ASP	-	expression tag	UNP Q13085
D	-18	ASP	-	expression tag	UNP Q13085
D	-17	LYS	-	expression tag	UNP Q13085
D	-16	LEU	-	expression tag	UNP Q13085
D	-15	THR	-	expression tag	UNP Q13085
D	-14	SER	-	expression tag	UNP Q13085
D	-13	LEU	-	expression tag	UNP Q13085
D	-12	TYR	-	expression tag	UNP Q13085
D	-11	LYS	-	expression tag	UNP Q13085
D	-10	LYS	-	expression tag	UNP Q13085
D	-9	ALA	-	expression tag	UNP Q13085
D	-8	GLY	-	expression tag	UNP Q13085
D	-7	LEU	-	expression tag	UNP Q13085
D	-6	GLU	-	expression tag	UNP Q13085
D	-5	ASN	-	expression tag	UNP Q13085
D	-4	LEU	-	expression tag	UNP Q13085
D	-3	TYR	-	expression tag	UNP Q13085
D	-2	PHE	-	expression tag	UNP Q13085
D	-1	GLN	-	expression tag	UNP Q13085
D	0	GLY	-	expression tag	UNP Q13085
F	-60	MET	-	initiating methionine	UNP Q13085
F	-59	ALA	-	expression tag	UNP Q13085
F	-58	HIS	-	expression tag	UNP Q13085
F	-57	HIS	-	expression tag	UNP Q13085
F	-56	HIS	-	expression tag	UNP Q13085
F	-55	HIS	-	expression tag	UNP Q13085
F	-54	HIS	-	expression tag	UNP Q13085

Continued on next page...

Continued from previous page...

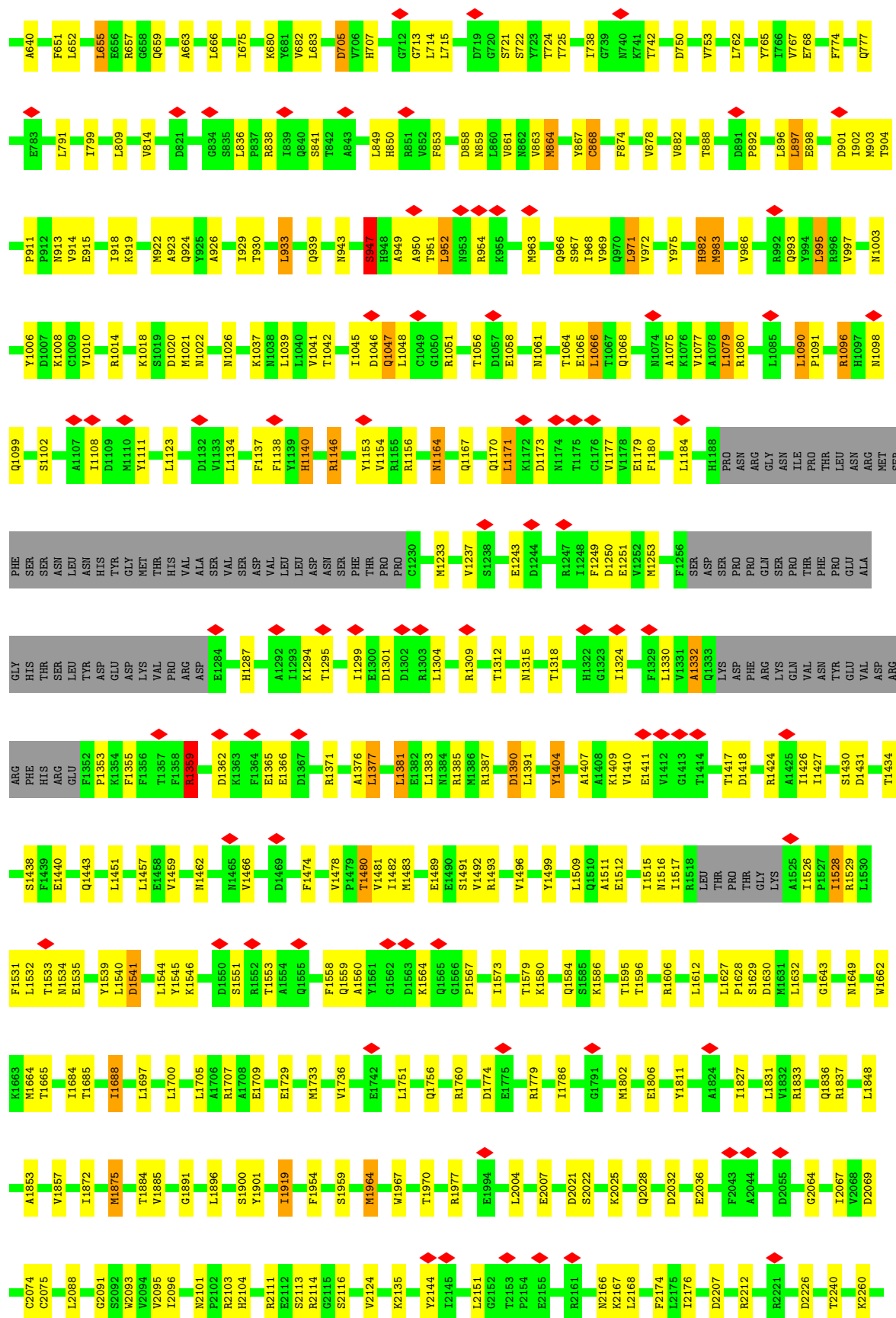
Chain	Residue	Modelled	Actual	Comment	Reference
F	-53	HIS	-	expression tag	UNP Q13085
F	-52	HIS	-	expression tag	UNP Q13085
F	-51	HIS	-	expression tag	UNP Q13085
F	-50	HIS	-	expression tag	UNP Q13085
F	-49	HIS	-	expression tag	UNP Q13085
F	-48	GLY	-	expression tag	UNP Q13085
F	-47	SER	-	expression tag	UNP Q13085
F	-46	THR	-	expression tag	UNP Q13085
F	-45	SER	-	expression tag	UNP Q13085
F	-44	GLY	-	expression tag	UNP Q13085
F	-43	SER	-	expression tag	UNP Q13085
F	-42	GLY	-	expression tag	UNP Q13085
F	-41	GLU	-	expression tag	UNP Q13085
F	-40	GLN	-	expression tag	UNP Q13085
F	-39	LYS	-	expression tag	UNP Q13085
F	-38	LEU	-	expression tag	UNP Q13085
F	-37	ILE	-	expression tag	UNP Q13085
F	-36	SER	-	expression tag	UNP Q13085
F	-35	GLU	-	expression tag	UNP Q13085
F	-34	GLU	-	expression tag	UNP Q13085
F	-33	ASP	-	expression tag	UNP Q13085
F	-32	LEU	-	expression tag	UNP Q13085
F	-31	GLY	-	expression tag	UNP Q13085
F	-30	SER	-	expression tag	UNP Q13085
F	-29	THR	-	expression tag	UNP Q13085
F	-28	SER	-	expression tag	UNP Q13085
F	-27	GLY	-	expression tag	UNP Q13085
F	-26	SER	-	expression tag	UNP Q13085
F	-25	GLY	-	expression tag	UNP Q13085
F	-24	ASP	-	expression tag	UNP Q13085
F	-23	TYR	-	expression tag	UNP Q13085
F	-22	LYS	-	expression tag	UNP Q13085
F	-21	ASP	-	expression tag	UNP Q13085
F	-20	ASP	-	expression tag	UNP Q13085
F	-19	ASP	-	expression tag	UNP Q13085
F	-18	ASP	-	expression tag	UNP Q13085
F	-17	LYS	-	expression tag	UNP Q13085
F	-16	LEU	-	expression tag	UNP Q13085
F	-15	THR	-	expression tag	UNP Q13085
F	-14	SER	-	expression tag	UNP Q13085
F	-13	LEU	-	expression tag	UNP Q13085
F	-12	TYR	-	expression tag	UNP Q13085

Continued on next page...

Continued from previous page...

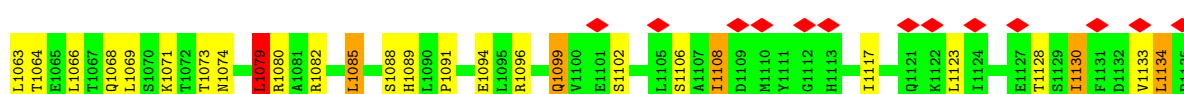
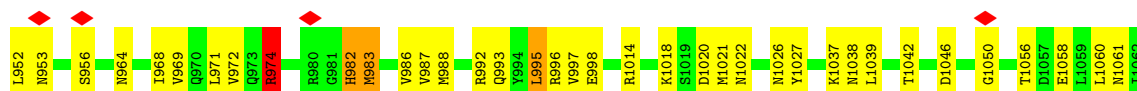
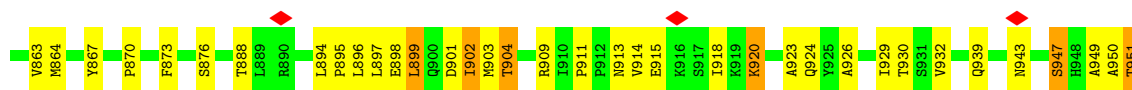
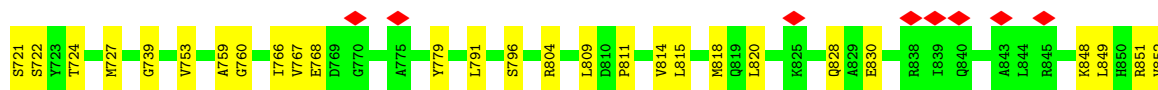
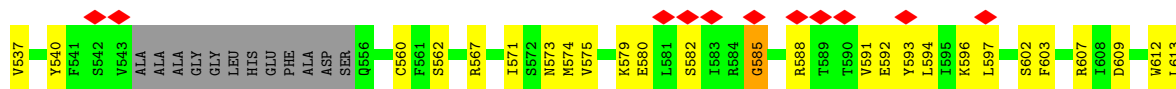
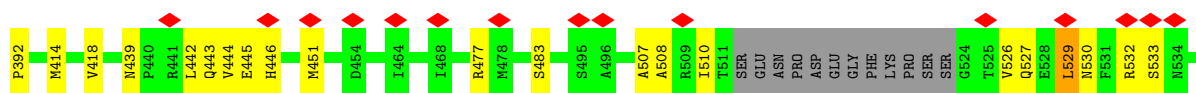
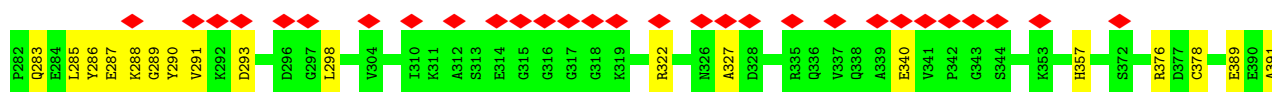
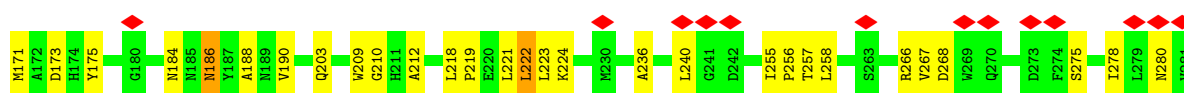
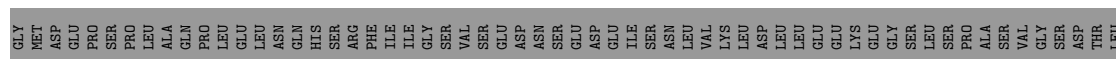
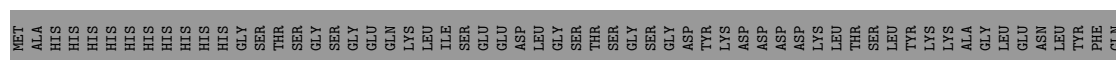
Chain	Residue	Modelled	Actual	Comment	Reference
F	-11	LYS	-	expression tag	UNP Q13085
F	-10	LYS	-	expression tag	UNP Q13085
F	-9	ALA	-	expression tag	UNP Q13085
F	-8	GLY	-	expression tag	UNP Q13085
F	-7	LEU	-	expression tag	UNP Q13085
F	-6	GLU	-	expression tag	UNP Q13085
F	-5	ASN	-	expression tag	UNP Q13085
F	-4	LEU	-	expression tag	UNP Q13085
F	-3	TYR	-	expression tag	UNP Q13085
F	-2	PHE	-	expression tag	UNP Q13085
F	-1	GLN	-	expression tag	UNP Q13085
F	0	GLY	-	expression tag	UNP Q13085

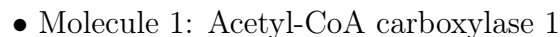






● Molecule 1: Acetyl-CoA carboxylase 1



[illegible]

--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--	--



HIS
SER
VAL
ILE
GLU
GLU
ASN
ILE
LYS
CYS
ILE
SER
ARG
ASP
TYR
VAL
LEU
LYS
GLN
ILE
ARG
SER
VAL
GLN
ALA
ASN
PRO
GLU
VAL
ALA
MET
ASP
SER
ILE
ILE
HIS
MET
THR
GLN
HIS
ILE
SER
PRO
THR
GLN
ARG
ALA
GLU
VAL
ILE
ARG
ILE
LEU
SER
THR
MET
ASP
SER
PRO

SER
THR

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	131062	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 ($e^-/\text{\AA}^2$)	40.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.081	Depositor
Minimum map value	-0.038	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0172	Depositor
Map size (Å)	476.09998, 476.09998, 476.09998	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.058, 1.058, 1.058	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	B	0.40	0/5209	1.07	11/7030 (0.2%)
1	C	0.38	2/17302 (0.0%)	0.97	29/23432 (0.1%)
1	D	0.40	2/17302 (0.0%)	1.06	74/23432 (0.3%)
1	F	0.40	0/5284	1.06	9/7131 (0.1%)
All	All	0.39	4/45097 (0.0%)	1.03	123/61025 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	8
1	C	0	16
1	D	0	16
1	F	0	10
All	All	0	50

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1138	PHE	CA-C	10.11	1.66	1.52
1	D	1526	ILE	C-N	5.88	1.47	1.33
1	D	1527	PRO	CB-CG	-5.52	1.22	1.49
1	C	1138	PHE	N-CA	5.24	1.52	1.46

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1527	PRO	CA-C-N	20.21	149.04	123.17
1	D	1527	PRO	C-N-CA	20.21	149.04	123.17
1	D	585	GLY	N-CA-C	12.85	143.64	113.18
1	D	1382	GLU	CA-C-N	12.63	144.11	122.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1382	GLU	C-N-CA	12.63	144.11	122.26
1	D	1384	ASN	CA-C-N	11.01	142.31	122.38
1	D	1384	ASN	C-N-CA	11.01	142.31	122.38
1	D	1526	ILE	CA-C-N	10.78	133.32	119.84
1	D	1526	ILE	C-N-CA	10.78	133.32	119.84
1	D	1527	PRO	CA-N-CD	-9.21	99.11	112.00
1	C	971	LEU	CA-CB-CG	8.58	146.33	116.30
1	D	1517	ILE	CA-C-N	8.46	136.94	121.70
1	D	1517	ILE	C-N-CA	8.46	136.94	121.70
1	D	1526	ILE	C-N-CD	-8.20	91.36	125.00
1	D	974	ARG	CA-CB-CG	7.80	129.70	114.10
1	D	1094	GLU	CA-C-N	7.70	133.75	120.58
1	D	1094	GLU	C-N-CA	7.70	133.75	120.58
1	C	1359	ARG	CA-CB-CG	7.49	129.08	114.10
1	C	286	TYR	CA-CB-CG	7.29	127.02	113.90
1	D	529	LEU	N-CA-C	7.24	120.57	108.20
1	D	1156	ARG	CA-C-N	7.20	132.54	120.88
1	D	1156	ARG	C-N-CA	7.20	132.54	120.88
1	D	222	LEU	CA-CB-CG	6.93	140.56	116.30
1	D	1526	ILE	CA-C-O	-6.87	110.74	119.95
1	D	286	TYR	CA-CB-CG	6.87	126.26	113.90
1	D	289	GLY	N-CA-C	-6.83	104.22	113.37
1	D	1134	LEU	CB-CA-C	6.77	123.51	110.17
1	B	1318	THR	OG1-CB-CG2	6.63	122.56	109.30
1	D	1485	PRO	N-CA-C	6.48	125.83	112.47
1	B	1158	TYR	CA-CB-CG	6.44	125.49	113.90
1	C	1390	ASP	N-CA-C	-6.38	96.85	108.02
1	D	1128	THR	OG1-CB-CG2	6.33	121.97	109.30
1	D	1528	ILE	N-CA-C	6.29	117.81	106.61
1	D	1418	ASP	CA-C-N	6.24	130.56	121.26
1	D	1418	ASP	C-N-CA	6.24	130.56	121.26
1	F	1243	GLU	N-CA-C	-6.23	104.41	111.14
1	C	222	LEU	CA-CB-CG	6.20	138.01	116.30
1	D	1455	ASP	CA-C-N	6.15	128.43	120.44
1	D	1455	ASP	C-N-CA	6.15	128.43	120.44
1	D	1099	GLN	CA-C-N	6.12	129.11	120.42
1	D	1099	GLN	C-N-CA	6.12	129.11	120.42
1	F	904	THR	N-CA-C	-6.12	104.89	112.90
1	C	289	GLY	N-CA-C	-6.09	105.20	113.37
1	C	868	CYS	N-CA-C	6.04	123.65	110.80
1	D	1091	PRO	N-CA-C	6.00	124.84	112.47
1	D	1130	ILE	CA-C-N	6.00	135.56	121.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1130	ILE	C-N-CA	6.00	135.56	121.52
1	D	974	ARG	N-CA-CB	5.98	120.15	110.40
1	C	867	TYR	CA-CB-CG	-5.94	103.21	113.90
1	D	1429	HIS	N-CA-C	5.92	120.01	111.02
1	D	111	ARG	CA-CB-CG	5.88	125.87	114.10
1	C	1964	MET	CB-CG-SD	5.88	130.33	112.70
1	D	283	GLN	N-CA-C	-5.82	105.44	113.18
1	C	1140	HIS	CB-CA-C	5.80	121.97	110.42
1	D	1504	TRP	CB-CA-C	5.80	122.21	110.38
1	C	1541	ASP	N-CA-C	-5.74	99.89	109.24
1	C	1243	GLU	N-CA-C	-5.74	104.94	111.14
1	C	947	SER	CA-C-N	-5.72	111.41	122.06
1	C	947	SER	C-N-CA	-5.72	111.41	122.06
1	D	1381	LEU	CA-CB-CG	5.71	136.27	116.30
1	F	933	LEU	CA-CB-CG	5.70	136.26	116.30
1	D	1478	VAL	CG1-CB-CG2	5.69	123.33	110.80
1	D	1381	LEU	N-CA-CB	5.69	118.87	109.88
1	C	1137	PHE	CA-C-N	-5.69	110.67	121.54
1	C	1137	PHE	C-N-CA	-5.69	110.67	121.54
1	C	982	HIS	N-CA-C	5.67	117.14	111.07
1	D	657	ARG	CA-CB-CG	5.66	125.41	114.10
1	B	1171	LEU	N-CA-C	5.65	118.00	109.41
1	B	1140	HIS	CB-CA-C	5.64	121.64	110.42
1	D	1541	ASP	N-CA-C	-5.63	100.06	109.24
1	C	1579	THR	N-CA-C	-5.59	99.61	108.73
1	D	1583	LEU	N-CA-C	-5.59	104.63	112.12
1	C	1404	TYR	CA-CB-CG	5.58	123.95	113.90
1	F	995	LEU	N-CA-C	-5.58	104.59	111.40
1	C	983	MET	CA-CB-CG	5.56	125.22	114.10
1	D	1423	VAL	CG1-CB-CG2	5.54	122.99	110.80
1	B	901	ASP	N-CA-C	-5.54	104.88	111.69
1	D	1089	HIS	CA-C-N	5.52	126.98	120.09
1	D	1089	HIS	C-N-CA	5.52	126.98	120.09
1	D	1079	LEU	CA-CB-CG	5.50	135.54	116.30
1	D	1402	HIS	N-CA-CB	5.50	119.38	110.42
1	F	1418	ASP	CA-C-N	5.49	132.02	121.54
1	F	1418	ASP	C-N-CA	5.49	132.02	121.54
1	D	288	LYS	N-CA-C	-5.48	105.33	112.23
1	C	836	LEU	N-CA-C	5.47	114.43	108.14
1	D	1528	ILE	CB-CA-C	-5.44	105.05	111.09
1	C	1146	ARG	CB-CG-CD	5.43	123.79	111.30
1	C	995	LEU	N-CA-C	-5.41	104.80	111.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1243	GLU	N-CA-C	-5.41	105.30	111.14
1	D	983	MET	CA-CB-CG	5.40	124.91	114.10
1	D	1527	PRO	N-CA-C	5.40	123.59	112.47
1	D	1370	TYR	CA-C-N	-5.38	113.24	120.87
1	D	1370	TYR	C-N-CA	-5.38	113.24	120.87
1	B	1507	ARG	N-CA-CB	-5.35	103.19	111.65
1	C	1359	ARG	CB-CG-CD	5.30	123.48	111.30
1	D	1502	ARG	CA-C-N	5.29	127.37	120.28
1	D	1502	ARG	C-N-CA	5.29	127.37	120.28
1	D	1288	ILE	CG1-CB-CG2	5.25	126.44	110.70
1	B	1428	ARG	N-CA-CB	-5.24	101.25	110.90
1	B	1418	ASP	CA-C-N	5.24	131.54	121.54
1	B	1418	ASP	C-N-CA	5.24	131.54	121.54
1	D	1515	ILE	N-CA-C	5.22	120.19	109.34
1	C	864	MET	N-CA-C	-5.21	106.60	113.17
1	D	1079	LEU	CB-CA-C	-5.21	101.00	110.63
1	D	526	VAL	N-CA-C	-5.16	98.26	107.18
1	D	1130	ILE	CG1-CB-CG2	5.15	126.16	110.70
1	D	982	HIS	N-CA-C	5.15	116.58	111.07
1	D	904	THR	N-CA-C	-5.13	106.18	112.90
1	D	920	LYS	CB-CA-C	5.12	118.92	110.88
1	D	974	ARG	N-CA-C	-5.12	106.54	112.89
1	B	1287	HIS	N-CA-C	5.11	117.82	109.59
1	F	901	ASP	N-CA-C	-5.10	105.41	111.69
1	C	290	TYR	CA-C-N	5.10	131.15	121.97
1	C	290	TYR	C-N-CA	5.10	131.15	121.97
1	F	1440	GLU	N-CA-CB	5.06	117.56	110.12
1	D	920	LYS	CG-CD-CE	5.06	122.94	111.30
1	D	1085	LEU	CB-CG-CD2	5.04	125.83	110.70
1	C	210	GLY	CA-C-N	5.04	131.17	121.54
1	C	210	GLY	C-N-CA	5.04	131.17	121.54
1	D	1232	ARG	CG-CD-NE	5.02	123.05	112.00
1	D	1443	GLN	CA-C-N	5.02	126.96	120.44
1	D	1443	GLN	C-N-CA	5.02	126.96	120.44
1	F	1440	GLU	CA-CB-CG	5.01	124.11	114.10

There are no chirality outliers.

All (50) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1171	LEU	Peptide
1	B	1173	ASP	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	1249	PHE	Peptide
1	B	1315	ASN	Peptide
1	B	1332	ALA	Peptide
1	B	1360	ALA	Peptide
1	B	1466	VAL	Peptide
1	B	1564	LYS	Peptide
1	C	1047	GLN	Peptide
1	C	1171	LEU	Peptide
1	C	1173	ASP	Peptide
1	C	1249	PHE	Peptide
1	C	1315	ASN	Peptide
1	C	1332	ALA	Peptide
1	C	1362	ASP	Peptide
1	C	1377	LEU	Peptide
1	C	1466	VAL	Peptide
1	C	1564	LYS	Peptide
1	C	277	ARG	Peptide
1	C	588	ARG	Peptide
1	C	750	ASP	Peptide
1	C	924	GLN	Peptide
1	C	952	LEU	Peptide
1	C	954	ARG	Peptide
1	D	1108	ILE	Peptide
1	D	1130	ILE	Peptide
1	D	1184	LEU	Peptide
1	D	1249	PHE	Peptide
1	D	1315	ASN	Peptide
1	D	1332	ALA	Peptide
1	D	1360	ALA	Peptide
1	D	1376	ALA	Peptide
1	D	1526	ILE	Peptide
1	D	1527	PRO	Peptide
1	D	210	GLY	Peptide
1	D	617	ILE	Peptide
1	D	924	GLN	Peptide
1	D	951	THR	Peptide
1	D	953	ASN	Peptide
1	D	956	SER	Peptide
1	F	1140	HIS	Peptide
1	F	1171	LEU	Peptide
1	F	1172	LYS	Peptide
1	F	1249	PHE	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	F	1315	ASN	Peptide
1	F	1332	ALA	Peptide
1	F	1376	ALA	Peptide
1	F	1377	LEU	Peptide
1	F	1564	LYS	Peptide
1	F	924	GLN	Peptide

5.2 Too-close contacts [i](#)

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	B	5112	5114	5134	112	0
1	C	16940	16841	16897	273	0
1	D	16940	16842	16897	296	0
1	F	5186	5194	5214	116	0
All	All	44178	43991	44142	764	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 9.

All (764) 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:C:1511:ALA:HB3	1:C:1532:LEU:HD12	1.36	1.07
1:C:721:SER:OG	1:D:173:ASP:O	1.92	0.86
1:C:1533:THR:OG1	1:C:1541:ASP:O	1.94	0.84
1:D:357:HIS:ND1	1:D:378:CYS:SG	2.50	0.83
1:C:1387:ARG:O	1:C:1409:LYS:NZ	2.12	0.81
1:C:173:ASP:O	1:D:721:SER:OG	1.98	0.81
1:D:1700:LEU:HD22	1:D:1802:MET:HE3	1.64	0.80
1:F:1123:LEU:O	1:F:1156:ARG:NH1	2.15	0.80
1:C:2334:VAL:HG23	1:D:2316:MET:HE1	1.66	0.77
1:B:898:GLU:OE1	1:B:975:TYR:OH	2.01	0.77
1:D:477:ARG:NE	1:D:483:SER:O	2.14	0.77
1:B:1512:GLU:OE1	1:B:1529:ARG:NH2	2.18	0.77
1:C:1003:ASN:O	1:C:1008:LYS:NZ	2.17	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:864:MET:O	1:B:1037:LYS:NZ	2.16	0.77
1:B:1123:LEU:O	1:B:1156:ARG:NH1	2.18	0.77
1:D:1900:SER:OG	1:D:1977:ARG:NH2	2.18	0.76
1:D:1533:THR:OG1	1:D:1541:ASP:O	2.02	0.76
1:C:2317:ASP:OD2	1:D:2297:ARG:NH2	2.19	0.76
1:C:864:MET:O	1:C:1037:LYS:NZ	2.19	0.75
1:F:1082:ARG:NH2	1:F:1458:GLU:OE1	2.19	0.75
1:B:1038:ASN:HD22	1:B:1073:THR:HG22	1.52	0.75
1:D:1424:ARG:NH2	1:D:1577:TYR:OH	2.20	0.74
1:D:1833:ARG:NH1	1:D:1836:GLN:OE1	2.21	0.74
1:D:1447:GLU:O	1:D:1451:LEU:HD13	1.87	0.74
1:D:1954:PHE:O	1:D:2212:ARG:NH1	2.20	0.74
1:F:1512:GLU:OE1	1:F:1529:ARG:NH2	2.20	0.74
1:D:1022:ASN:O	1:D:1026:ASN:ND2	2.20	0.74
1:F:1022:ASN:O	1:F:1026:ASN:ND2	2.20	0.74
1:B:1140:HIS:O	1:B:1146:ARG:NH2	2.20	0.74
1:C:1900:SER:OG	1:C:1977:ARG:NH2	2.20	0.74
1:F:1038:ASN:ND2	1:F:1073:THR:O	2.20	0.73
1:D:1099:GLN:O	1:D:1102:SER:OG	2.02	0.73
1:F:901:ASP:O	1:F:904:THR:OG1	2.06	0.73
1:D:588:ARG:NH2	1:D:739:GLY:O	2.21	0.73
1:C:1837:ARG:NH2	1:C:2036:GLU:OE2	2.22	0.73
1:C:2316:MET:HE1	1:D:2334:VAL:HG23	1.69	0.73
1:D:357:HIS:HD1	1:D:378:CYS:HG	1.31	0.73
1:D:943:ASN:O	1:D:947:SER:OG	2.06	0.73
1:D:873:PHE:O	1:D:876:SER:OG	2.06	0.72
1:F:1531:PHE:O	1:F:1543:SER:OG	2.07	0.72
1:C:1811:TYR:OH	1:C:2032:ASP:OD1	2.08	0.72
1:C:1041:VAL:HG11	1:C:1077:VAL:HG22	1.70	0.72
1:D:1707:ARG:NE	1:D:1806:GLU:OE2	2.23	0.71
1:D:1534:ASN:ND2	1:D:1539:TYR:O	2.24	0.71
1:C:322:ARG:NH2	1:C:340:GLU:OE2	2.23	0.71
1:C:477:ARG:NE	1:C:483:SER:O	2.17	0.71
1:F:1387:ARG:O	1:F:1409:LYS:NZ	2.23	0.71
1:D:828:GLN:OE1	1:D:830:GLU:N	2.22	0.71
1:C:139:ARG:NH2	1:D:533:SER:O	2.24	0.71
1:D:1046:ASP:O	1:D:1050:GLY:HA3	1.91	0.71
1:B:1091:PRO:O	1:B:1096:ARG:NH1	2.24	0.70
1:D:255:ILE:HG23	1:D:258:LEU:HD12	1.71	0.70
1:D:2300:VAL:O	1:D:2304:ILE:HD12	1.91	0.70
1:C:2091:GLY:O	1:C:2095:VAL:HG22	1.91	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2229:LYS:NZ	1:D:2245:GLN:OE1	2.22	0.70
1:D:596:LYS:NZ	1:D:621:VAL:O	2.25	0.70
1:D:1123:LEU:O	1:D:1156:ARG:NH1	2.25	0.70
1:D:532:ARG:NH2	1:D:580:GLU:OE2	2.24	0.69
1:D:623:ALA:O	1:D:625:ARG:NH1	2.25	0.69
1:D:376:ARG:NH2	1:D:443:GLN:OE1	2.26	0.69
1:B:1014:ARG:O	1:B:1018:LYS:HA	1.93	0.69
1:C:121:VAL:HG22	1:C:204:ALA:HB3	1.74	0.69
1:C:1700:LEU:HD22	1:C:1802:MET:HE3	1.73	0.69
1:C:1833:ARG:NH1	1:C:1836:GLN:OE1	2.25	0.69
1:D:901:ASP:O	1:D:904:THR:OG1	2.09	0.69
1:D:1038:ASN:ND2	1:D:1073:THR:O	2.25	0.69
1:D:530:ASN:ND2	1:D:537:VAL:O	2.26	0.69
1:D:1811:TYR:OH	1:D:2032:ASP:OD1	2.09	0.68
1:F:1172:LYS:O	1:F:1175:THR:OG1	2.12	0.68
1:B:1022:ASN:O	1:B:1026:ASN:ND2	2.26	0.68
1:C:567:ARG:NH2	1:C:603:PHE:O	2.26	0.68
1:C:530:ASN:O	1:C:532:ARG:NH2	2.27	0.68
1:D:1235:GLY:O	1:D:1236:MET:HE3	1.94	0.68
1:C:1079:LEU:HB3	1:C:1462:ASN:HD22	1.58	0.68
1:B:892:PRO:HG2	1:B:929:ILE:HD11	1.76	0.68
1:B:939:GLN:O	1:B:943:ASN:ND2	2.27	0.68
1:D:322:ARG:NH2	1:D:340:GLU:OE2	2.27	0.68
1:C:580:GLU:OE1	1:D:135:ARG:NH2	2.27	0.67
1:C:1022:ASN:O	1:C:1026:ASN:ND2	2.27	0.67
1:D:138:ARG:NH2	1:D:171:MET:O	2.27	0.67
1:C:1123:LEU:O	1:C:1156:ARG:NH1	2.29	0.66
1:D:287:GLU:O	1:D:290:TYR:O	2.12	0.66
1:C:655:LEU:O	1:C:1014:ARG:NH1	2.29	0.66
1:C:1427:ILE:O	1:C:1478:VAL:HG22	1.94	0.66
1:D:1082:ARG:NH1	1:D:1455:ASP:OD1	2.29	0.66
1:D:804:ARG:NH2	1:D:1745:TYR:OH	2.28	0.66
1:C:248:ILE:HG13	1:C:265:LEU:HD13	1.78	0.65
1:D:1020:ASP:OD1	1:D:1021:MET:N	2.29	0.65
1:F:1020:ASP:OD1	1:F:1021:MET:N	2.29	0.65
1:C:190:VAL:HG13	1:C:218:LEU:HD23	1.79	0.65
1:D:1177:VAL:HG13	1:D:1237:VAL:HG22	1.77	0.65
1:C:892:PRO:HB2	1:C:929:ILE:HD11	1.78	0.65
1:C:1020:ASP:OD1	1:C:1021:MET:N	2.30	0.65
1:C:1836:GLN:OE1	1:C:2028:GLN:NE2	2.29	0.65
1:B:1534:ASN:ND2	1:B:1539:TYR:O	2.29	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1039:LEU:O	1:C:1042:THR:OG1	2.14	0.65
1:C:1140:HIS:O	1:C:1146:ARG:NH2	2.30	0.64
1:D:1445:GLU:O	1:D:1449:LEU:HD13	1.97	0.64
1:F:1014:ARG:O	1:F:1018:LYS:HA	1.97	0.64
1:F:1533:THR:OG1	1:F:1541:ASP:O	2.16	0.64
1:C:1434:THR:OG1	1:C:1482:ILE:O	2.11	0.64
1:C:838:ARG:O	1:C:841:SER:OG	2.10	0.64
1:F:1382:GLU:OE2	1:F:1529:ARG:NH2	2.31	0.64
1:B:930:THR:OG1	1:D:1166:VAL:O	2.16	0.63
1:D:939:GLN:O	1:D:943:ASN:ND2	2.31	0.63
1:C:901:ASP:O	1:C:904:THR:OG1	2.17	0.63
1:D:1967:TRP:O	1:D:2025:LYS:NZ	2.32	0.63
1:D:926:ALA:O	1:D:929:ILE:HG22	1.98	0.63
1:C:2021:ASP:OD1	1:C:2022:SER:N	2.31	0.63
1:D:1700:LEU:HD22	1:D:1802:MET:CE	2.28	0.63
1:D:1457:LEU:O	1:D:1457:LEU:HD23	1.98	0.63
1:D:2021:ASP:OD1	1:D:2022:SER:N	2.31	0.63
1:B:1496:VAL:HG11	1:B:1540:LEU:HD11	1.79	0.63
1:F:1083:GLN:O	1:F:1087:ALA:HB2	1.97	0.63
1:D:2166:ASN:OD1	1:D:2167:LYS:N	2.32	0.62
1:C:571:ILE:O	1:C:575:VAL:HG23	1.99	0.62
1:B:996:ARG:NH1	1:B:1027:TYR:OH	2.33	0.62
1:D:186:ASN:N	1:D:186:ASN:OD1	2.33	0.62
1:D:760:GLY:O	1:D:809:LEU:N	2.32	0.62
1:C:355:SER:OG	1:C:426:LEU:HD11	1.99	0.62
1:D:1530:LEU:HD12	1:D:1544:LEU:HD12	1.82	0.62
1:F:1534:ASN:ND2	1:F:1539:TYR:O	2.33	0.62
1:C:705:ASP:OD1	1:C:705:ASP:N	2.30	0.62
1:F:898:GLU:OE1	1:F:975:TYR:OH	2.15	0.62
1:C:1014:ARG:O	1:C:1018:LYS:HA	1.98	0.62
1:C:1366:GLU:OE1	1:C:1371:ARG:NH2	2.32	0.62
1:F:1046:ASP:O	1:F:1050:GLY:HA3	2.00	0.62
1:C:1662:TRP:HB2	1:C:1664:MET:HE3	1.81	0.62
1:D:190:VAL:HG22	1:D:218:LEU:HD21	1.82	0.62
1:F:858:ASP:OD1	1:F:859:ASN:N	2.33	0.61
1:F:918:ILE:O	1:F:922:MET:HG2	1.99	0.61
1:F:1158:TYR:OH	1:F:1326:ARG:NH1	2.33	0.61
1:C:1045:ILE:O	1:C:1048:LEU:C	2.43	0.61
1:D:184:ASN:HA	1:D:188:ALA:HB3	1.82	0.61
1:D:1454:MET:HE1	1:D:1503:LEU:HD22	1.80	0.61
1:B:1020:ASP:OD1	1:B:1021:MET:N	2.32	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:LYS:N	1:C:203:GLN:OE1	2.32	0.61
1:C:1434:THR:HG23	1:C:1481:VAL:HB	1.83	0.61
1:D:1606:ARG:NH1	1:D:1628:PRO:O	2.32	0.61
1:D:982:HIS:O	1:D:986:VAL:HG12	2.00	0.61
1:C:858:ASP:OD1	1:C:859:ASN:N	2.33	0.61
1:C:1047:GLN:O	1:C:1048:LEU:HD22	1.99	0.61
1:D:1039:LEU:O	1:D:1042:THR:OG1	2.16	0.61
1:F:850:HIS:HB2	1:F:897:LEU:HD23	1.82	0.61
1:D:562:SER:HB3	1:D:574:MET:HE2	1.83	0.61
1:F:1014:ARG:NH1	1:F:1018:LYS:O	2.33	0.61
1:F:1079:LEU:HG	1:F:1459:VAL:HG22	1.83	0.61
1:B:1492:VAL:O	1:B:1496:VAL:HG12	2.00	0.61
1:B:902:ILE:HD13	1:B:971:LEU:HD22	1.82	0.61
1:D:1946:GLN:NE2	1:D:1949:GLN:OE1	2.34	0.61
1:D:287:GLU:O	1:D:290:TYR:C	2.43	0.60
1:D:1237:VAL:HB	1:D:1291:VAL:HG12	1.83	0.60
1:F:1545:TYR:OH	1:F:1567:PRO:O	2.19	0.60
1:D:212:ALA:HB1	1:D:218:LEU:HD11	1.82	0.60
1:D:1820:VAL:HG11	1:D:1846:LEU:HD21	1.82	0.60
1:B:1511:ALA:HB3	1:B:1532:LEU:HD12	1.83	0.60
1:D:1403:LEU:HB3	1:D:1423:VAL:HG23	1.83	0.60
1:C:850:HIS:HB2	1:C:897:LEU:HD23	1.83	0.60
1:F:1092:SER:HB3	1:F:1095:LEU:HD23	1.84	0.60
1:D:275:SER:OG	1:D:414:MET:O	2.14	0.60
1:B:961:PHE:O	1:B:965:THR:HG22	2.01	0.60
1:B:1046:ASP:O	1:B:1050:GLY:HA3	2.02	0.60
1:F:1163:LEU:HD13	1:F:1182:PHE:HB3	1.83	0.60
1:C:1492:VAL:O	1:C:1496:VAL:HG12	2.01	0.60
1:C:2166:ASN:OD1	1:C:2167:LYS:N	2.34	0.60
1:D:1085:LEU:O	1:D:1088:SER:OG	2.19	0.60
1:B:1370:TYR:HE1	1:B:1383:LEU:HD23	1.67	0.59
1:B:1177:VAL:HG13	1:B:1237:VAL:HG22	1.83	0.59
1:B:858:ASP:OD1	1:B:859:ASN:N	2.35	0.59
1:C:1534:ASN:ND2	1:C:1539:TYR:O	2.36	0.59
1:C:2074:CYS:O	1:C:2101:ASN:ND2	2.35	0.59
1:B:1374:GLU:O	1:B:1376:ALA:N	2.35	0.59
1:C:1385:ARG:NE	1:C:1573:ILE:O	2.36	0.59
1:C:1606:ARG:NH1	1:C:1628:PRO:O	2.36	0.59
1:D:389:GLU:HB2	1:D:507:ALA:HB3	1.85	0.59
1:D:508:ALA:HB3	1:D:560:CYS:SG	2.43	0.59
1:D:1836:GLN:OE1	1:D:2028:GLN:NE2	2.36	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:707:HIS:CG	1:D:162:LEU:HD21	2.36	0.59
1:C:1330:LEU:HD12	1:C:1355:PHE:CE1	2.38	0.59
1:C:1700:LEU:HD22	1:C:1802:MET:CE	2.32	0.59
1:C:1967:TRP:O	1:C:2025:LYS:NZ	2.34	0.59
1:B:1481:VAL:O	1:B:1517:ILE:HG22	2.02	0.58
1:C:926:ALA:O	1:C:929:ILE:HG22	2.02	0.58
1:D:567:ARG:NH2	1:D:603:PHE:O	2.34	0.58
1:C:1632:LEU:HD12	1:C:1665:THR:O	2.02	0.58
1:F:1445:GLU:O	1:F:1449:LEU:HD13	2.03	0.58
1:C:1377:LEU:HD12	1:C:1426:ILE:HD11	1.84	0.58
1:C:1684:ILE:O	1:C:1688:ILE:HA	2.03	0.58
1:F:1099:GLN:O	1:F:1102:SER:OG	2.16	0.58
1:F:1373:LEU:HD13	1:F:1374:GLU:N	2.18	0.58
1:D:2107:MET:SD	1:D:2107:MET:N	2.76	0.58
1:B:1167:GLN:N	1:B:1167:GLN:OE1	2.37	0.58
1:C:1167:GLN:OE1	1:C:1167:GLN:N	2.37	0.58
1:F:1094:GLU:O	1:F:1095:LEU:HD22	2.04	0.58
1:C:849:LEU:HD22	1:C:888:THR:CG2	2.34	0.57
1:D:686:THR:O	1:D:694:VAL:HG12	2.04	0.57
1:D:903:MET:HE2	1:D:918:ILE:HD11	1.86	0.57
1:B:1166:VAL:HG22	1:B:1180:PHE:CD1	2.39	0.57
1:D:1457:LEU:HD22	1:D:1506:LEU:CD1	2.33	0.57
1:F:1492:VAL:O	1:F:1496:VAL:HG12	2.04	0.57
1:F:886:MET:HE1	1:F:1048:LEU:HD22	1.87	0.57
1:B:1047:GLN:O	1:B:1048:LEU:HD22	2.04	0.57
1:C:240:LEU:HD21	1:C:415:VAL:HG11	1.85	0.57
1:C:725:THR:HG22	1:C:738:ILE:HG23	1.86	0.57
1:D:2091:GLY:O	1:D:2095:VAL:HG22	2.03	0.57
1:B:1154:VAL:HG11	1:B:1180:PHE:CZ	2.39	0.57
1:C:715:LEU:HD13	1:D:175:TYR:OH	2.05	0.57
1:C:949:ALA:O	1:C:952:LEU:HD22	2.05	0.57
1:D:947:SER:O	1:D:950:ALA:HB3	2.05	0.57
1:C:993:GLN:O	1:C:997:VAL:HG22	2.04	0.57
1:B:1253:MET:SD	1:B:1253:MET:N	2.78	0.57
1:B:1421:PHE:CE2	1:B:1460:ALA:HB1	2.40	0.57
1:D:993:GLN:O	1:D:997:VAL:HG22	2.05	0.57
1:F:864:MET:SD	1:F:993:GLN:NE2	2.78	0.57
1:B:1124:ILE:C	1:B:1125:LEU:HD22	2.30	0.56
1:C:569:GLU:OE2	1:C:573:ASN:ND2	2.29	0.56
1:C:2174:PHE:O	1:D:804:ARG:NH2	2.38	0.56
1:D:1239:PHE:CE1	1:D:1248:ILE:HD11	2.40	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:966:GLN:O	1:B:969:VAL:HG12	2.05	0.56
1:D:1504:TRP:O	1:D:1507:ARG:NH1	2.33	0.56
1:C:248:ILE:CG1	1:C:265:LEU:HD13	2.36	0.56
1:D:391:ALA:HB3	1:D:392:PRO:HD3	1.88	0.56
1:D:1737:ALA:HB3	1:D:1750:TYR:O	2.05	0.56
1:F:1113:HIS:O	1:F:1116:CYS:N	2.39	0.56
1:C:1253:MET:HE1	1:C:1318:THR:HA	1.88	0.56
1:C:939:GLN:O	1:C:943:ASN:ND2	2.39	0.56
1:C:1099:GLN:O	1:C:1102:SER:OG	2.19	0.56
1:D:721:SER:OG	1:D:722:SER:N	2.39	0.56
1:F:1052:ASP:OD2	1:F:1054:THR:OG1	2.23	0.56
1:F:1391:LEU:HD13	1:F:1404:TYR:OH	2.06	0.56
1:C:2297:ARG:NH2	1:D:2317:ASP:OD2	2.39	0.56
1:D:1383:LEU:HD13	1:D:1383:LEU:O	2.06	0.56
1:D:2016:GLN:HE21	1:D:2045:ASN:HD21	1.53	0.56
1:F:898:GLU:O	1:F:902:ILE:HD12	2.06	0.56
1:B:1184:LEU:HD22	1:B:1187:SER:HB3	1.88	0.55
1:C:1736:VAL:HG22	1:C:1751:LEU:CD2	2.36	0.55
1:D:709:LEU:HD11	1:D:715:LEU:HG	1.86	0.55
1:B:1531:PHE:O	1:B:1543:SER:OG	2.21	0.55
1:B:874:PHE:O	1:B:878:VAL:HG22	2.06	0.55
1:C:184:ASN:HA	1:C:188:ALA:HB3	1.89	0.55
1:D:418:VAL:HG12	1:D:418:VAL:O	2.06	0.55
1:D:629:MET:O	1:D:633:VAL:HG23	2.07	0.55
1:C:721:SER:OG	1:C:722:SER:N	2.39	0.55
1:C:753:VAL:HG13	1:C:814:VAL:HG13	1.88	0.55
1:D:1481:VAL:O	1:D:1517:ILE:HG22	2.06	0.55
1:C:2297:ARG:HG2	1:D:2314:VAL:HG12	1.88	0.55
1:F:1167:GLN:N	1:F:1167:GLN:OE1	2.40	0.55
1:C:132:LYS:NZ	1:C:450:GLU:OE1	2.40	0.55
1:C:1381:LEU:HD13	1:C:1383:LEU:HD22	1.89	0.55
1:C:2174:PHE:O	1:D:1745:TYR:OH	2.24	0.55
1:D:1545:TYR:OH	1:D:1567:PRO:O	2.24	0.55
1:F:1323:GLY:C	1:F:1324:ILE:HD12	2.32	0.55
1:C:1901:TYR:OH	1:C:1959:SER:O	2.19	0.55
1:D:704:VAL:HB	1:D:716:LEU:HD11	1.89	0.55
1:D:759:ALA:HB2	1:D:811:PRO:HD3	1.89	0.55
1:F:1233:MET:HB3	1:F:1287:HIS:HD1	1.72	0.55
1:D:767:VAL:HG12	1:D:768:GLU:H	1.71	0.54
1:C:162:LEU:HD21	1:D:707:HIS:HB3	1.88	0.54
1:D:442:LEU:HD11	1:D:446:HIS:CG	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1420:ARG:NH2	1:F:1578:VAL:O	2.41	0.54
1:C:1885:VAL:HG11	1:C:1891:GLY:HA2	1.88	0.54
1:D:1430:SER:OG	1:D:1431:ASP:N	2.40	0.54
1:D:1527:PRO:CB	1:D:1528:ILE:HG12	2.38	0.54
1:C:911:PRO:O	1:C:914:VAL:HG12	2.07	0.54
1:C:1729:GLU:O	1:C:1733:MET:HE3	2.08	0.54
1:D:612:TRP:O	1:D:616:LEU:HD23	2.08	0.54
1:F:1079:LEU:HD11	1:F:1462:ASN:HD22	1.72	0.54
1:C:408:ALA:HB2	1:C:425:TYR:OH	2.07	0.54
1:D:724:THR:O	1:D:739:GLY:N	2.40	0.54
1:F:1546:LYS:N	1:F:1559:GLN:O	2.40	0.54
1:C:528:GLU:HG3	1:D:532:ARG:HB3	1.90	0.53
1:B:992:ARG:HA	1:B:995:LEU:HB3	1.89	0.53
1:C:762:LEU:HD11	1:C:809:LEU:HD12	1.89	0.53
1:C:767:VAL:HG12	1:C:768:GLU:H	1.73	0.53
1:C:1134:LEU:HD21	1:C:1153:TYR:HB2	1.90	0.53
1:C:1309:ARG:O	1:C:1312:THR:OG1	2.24	0.53
1:C:1707:ARG:NE	1:C:1806:GLU:OE2	2.38	0.53
1:D:1737:ALA:HB2	1:D:1752:TYR:CD1	2.43	0.53
1:D:659:GLN:NE2	1:D:2007:GLU:OE2	2.42	0.53
1:D:903:MET:HE2	1:D:918:ILE:CD1	2.39	0.53
1:F:939:GLN:OE1	1:F:943:ASN:ND2	2.26	0.53
1:B:1496:VAL:HG21	1:B:1540:LEU:HD13	1.90	0.53
1:D:911:PRO:O	1:D:914:VAL:HG12	2.09	0.53
1:C:1580:LYS:O	1:C:1584:GLN:NE2	2.41	0.53
1:D:809:LEU:HD22	1:D:815:LEU:HD21	1.91	0.53
1:D:1366:GLU:OE1	1:D:1371:ARG:NH1	2.40	0.53
1:C:1430:SER:OG	1:C:1431:ASP:N	2.41	0.53
1:C:2088:LEU:HD12	1:C:2093:TRP:HE3	1.74	0.53
1:C:2103:ARG:NH1	1:C:2226:ASP:OD1	2.41	0.53
1:F:1071:LYS:O	1:F:1074:ASN:C	2.51	0.53
1:C:1253:MET:HE1	1:C:1318:THR:HG22	1.88	0.53
1:D:686:THR:HG21	1:D:870:PRO:HD3	1.91	0.53
1:B:1546:LYS:N	1:B:1559:GLN:O	2.42	0.53
1:C:354:GLN:NE2	1:C:355:SER:O	2.41	0.53
1:D:1184:LEU:HD11	1:D:1232:ARG:NH2	2.23	0.53
1:D:1421:PHE:CE2	1:D:1457:LEU:HD21	2.44	0.53
1:D:219:PRO:HA	1:D:222:LEU:HD23	1.91	0.52
1:D:715:LEU:HD12	1:D:715:LEU:O	2.09	0.52
1:F:926:ALA:O	1:F:929:ILE:HG22	2.09	0.52
1:F:993:GLN:O	1:F:997:VAL:HG22	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:982:HIS:O	1:C:986:VAL:HG12	2.08	0.52
1:C:1359:ARG:N	1:C:1365:GLU:O	2.42	0.52
1:C:2069:ASP:OD1	1:D:1808:SER:OG	2.24	0.52
1:B:1370:TYR:CE1	1:B:1383:LEU:HD23	2.45	0.52
1:C:1091:PRO:O	1:C:1096:ARG:NH1	2.42	0.52
1:C:170:LYS:HG2	1:D:724:THR:HG21	1.91	0.52
1:F:1107:ALA:HB1	1:F:1116:CYS:HB2	1.91	0.52
1:B:850:HIS:HB2	1:B:897:LEU:HD23	1.92	0.52
1:C:1041:VAL:CG1	1:C:1077:VAL:HG22	2.40	0.52
1:C:1509:LEU:HD12	1:C:1534:ASN:O	2.10	0.52
1:B:898:GLU:O	1:B:902:ILE:HD12	2.10	0.52
1:C:1108:ILE:O	1:C:1111:TYR:N	2.43	0.52
1:D:1480:THR:O	1:D:1480:THR:OG1	2.28	0.52
1:C:724:THR:HG21	1:D:170:LYS:HG3	1.91	0.52
1:D:1014:ARG:O	1:D:1018:LYS:HA	2.09	0.52
1:D:1167:GLN:N	1:D:1167:GLN:OE1	2.42	0.52
1:F:1079:LEU:CD1	1:F:1462:ASN:HD22	2.23	0.52
1:C:1064:THR:O	1:C:1068:GLN:NE2	2.40	0.52
1:F:1178:VAL:HG12	1:F:1236:MET:HB3	1.92	0.52
1:F:1421:PHE:CZ	1:F:1460:ALA:HB1	2.45	0.52
1:B:1056:THR:O	1:B:1058:GLU:N	2.40	0.52
1:C:1586:LYS:NZ	1:C:1685:THR:OG1	2.20	0.52
1:D:510:ILE:HD11	1:D:540:TYR:O	2.10	0.52
1:B:1014:ARG:NH1	1:B:1021:MET:SD	2.83	0.51
1:B:1295:THR:OG1	1:B:1332:ALA:O	2.28	0.51
1:C:562:SER:CB	1:C:574:MET:HE2	2.39	0.51
1:C:724:THR:HG21	1:D:170:LYS:CG	2.40	0.51
1:C:542:SER:OG	1:C:557:PHE:O	2.27	0.51
1:D:923:ALA:O	1:D:926:ALA:HB3	2.10	0.51
1:D:1627:LEU:HD22	1:D:1628:PRO:HD2	1.92	0.51
1:C:849:LEU:HD22	1:C:888:THR:HG22	1.91	0.51
1:C:971:LEU:HD22	1:C:975:TYR:CZ	2.45	0.51
1:F:947:SER:O	1:F:950:ALA:HB3	2.10	0.51
1:C:404:MET:O	1:C:425:TYR:OH	2.19	0.51
1:C:918:ILE:O	1:C:922:MET:HG2	2.10	0.51
1:C:947:SER:O	1:C:950:ALA:HB3	2.10	0.51
1:D:721:SER:HG	1:D:722:SER:H	1.58	0.51
1:D:1662:TRP:HB2	1:D:1664:MET:HE3	1.92	0.51
1:F:1431:ASP:OD1	1:F:1480:THR:N	2.40	0.51
1:D:1535:GLU:HG3	1:D:1536:SER:H	1.76	0.51
1:F:1457:LEU:HB3	1:F:1506:LEU:HD23	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:ASP:N	1:C:293:ASP:OD1	2.43	0.51
1:C:304:VAL:O	1:C:350:ARG:NH2	2.42	0.51
1:C:966:GLN:O	1:C:969:VAL:HG12	2.10	0.51
1:C:1299:ILE:O	1:C:1301:ASP:N	2.44	0.51
1:C:1756:GLN:O	1:C:1760:ARG:NH1	2.44	0.51
1:D:120:LYS:N	1:D:203:GLN:OE1	2.44	0.51
1:D:676:TYR:N	1:D:679:VAL:O	2.42	0.51
1:D:1470:CYS:HA	1:D:1509:LEU:HD23	1.92	0.51
1:C:186:ASN:OD1	1:C:186:ASN:N	2.42	0.51
1:D:209:TRP:CZ2	1:D:444:VAL:HG23	2.46	0.51
1:C:1551:SER:OG	1:C:1553:THR:O	2.28	0.51
1:C:1853:ALA:O	1:C:1857:VAL:HG23	2.09	0.51
1:D:592:GLU:OE1	1:D:625:ARG:NH1	2.43	0.51
1:B:968:ILE:O	1:B:972:VAL:HG12	2.12	0.50
1:C:1545:TYR:OH	1:C:1567:PRO:O	2.17	0.50
1:C:878:VAL:O	1:C:882:VAL:HG23	2.11	0.50
1:C:1786:ILE:O	1:D:2195:ARG:NE	2.44	0.50
1:B:1151:GLU:OE2	1:D:932:VAL:HG12	2.12	0.50
1:B:1431:ASP:C	1:B:1432:LEU:HD12	2.36	0.50
1:D:949:ALA:O	1:D:952:LEU:HD22	2.11	0.50
1:C:356:ARG:NH2	1:C:377:ASP:OD2	2.43	0.50
1:C:1046:ASP:OD1	1:C:1080:ARG:NH2	2.44	0.50
1:C:1517:ILE:HG13	1:C:1526:ILE:HD11	1.93	0.50
1:C:1443:GLN:NE2	1:C:1491:SER:OG	2.44	0.50
1:F:902:ILE:HD13	1:F:971:LEU:HD22	1.93	0.50
1:C:300:ALA:O	1:C:304:VAL:HG22	2.12	0.50
1:C:874:PHE:O	1:C:878:VAL:HG22	2.12	0.50
1:C:903:MET:HE2	1:C:918:ILE:HD11	1.94	0.50
1:B:1578:VAL:HG12	1:B:1580:LYS:H	1.77	0.50
1:C:1391:LEU:HD22	1:C:1404:TYR:OH	2.11	0.49
1:C:2096:ILE:HG22	1:C:2096:ILE:O	2.12	0.49
1:B:1295:THR:HG21	1:B:1331:VAL:HB	1.95	0.49
1:B:1330:LEU:HD12	1:B:1355:PHE:HE1	1.77	0.49
1:D:675:ILE:HA	1:D:680:LYS:HA	1.94	0.49
1:D:1071:LYS:O	1:D:1074:ASN:C	2.55	0.49
1:D:1108:ILE:HD13	1:D:1145:VAL:HB	1.94	0.49
1:D:1941:ARG:O	1:D:1951:LEU:N	2.39	0.49
1:B:1148:ALA:O	1:B:1152:VAL:HG23	2.13	0.49
1:C:898:GLU:OE1	1:C:975:TYR:OH	2.29	0.49
1:C:2303:GLN:O	1:C:2307:LEU:HD23	2.12	0.49
1:C:1330:LEU:HD21	1:C:1353:PRO:HB3	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1627:LEU:HD22	1:C:1628:PRO:HD2	1.93	0.49
1:D:898:GLU:O	1:D:902:ILE:HD12	2.13	0.49
1:F:933:LEU:HD13	1:F:933:LEU:O	2.12	0.49
1:C:913:ASN:OD1	1:C:914:VAL:N	2.45	0.49
1:C:971:LEU:HD22	1:C:975:TYR:CE2	2.48	0.49
1:D:293:ASP:OD1	1:D:293:ASP:N	2.44	0.49
1:D:2311:ASN:O	1:D:2314:VAL:HG22	2.13	0.49
1:B:1480:THR:O	1:B:1480:THR:OG1	2.28	0.49
1:C:1493:ARG:NH1	1:C:1540:LEU:HD21	2.28	0.49
1:C:1595:THR:OG1	1:C:1596:THR:N	2.45	0.49
1:D:255:ILE:O	1:D:257:THR:N	2.44	0.49
1:D:591:VAL:HA	1:D:594:LEU:HD12	1.94	0.49
1:D:1714:ILE:HD12	1:D:1817:ILE:HB	1.95	0.49
1:D:2260:LYS:O	1:D:2263:VAL:HG12	2.13	0.48
1:F:922:MET:HG3	1:F:923:ALA:N	2.27	0.48
1:D:266:ARG:H	1:D:285:LEU:HD21	1.78	0.48
1:D:1853:ALA:O	1:D:1857:VAL:HG23	2.13	0.48
1:F:1375:PRO:O	1:F:1378:ALA:HB2	2.13	0.48
1:C:1061:ASN:O	1:C:1064:THR:HG22	2.14	0.48
1:F:1319:LEU:HD21	1:F:1361:ARG:HB2	1.96	0.48
1:D:1527:PRO:HB3	1:D:1528:ILE:HG12	1.94	0.48
1:D:2096:ILE:O	1:D:2096:ILE:HG22	2.13	0.48
1:F:1517:ILE:HG13	1:F:1526:ILE:HD11	1.95	0.48
1:C:1180:PHE:O	1:C:1233:MET:HB2	2.13	0.48
1:B:1471:ASN:ND2	1:B:1507:ARG:O	2.46	0.48
1:C:721:SER:HG	1:C:722:SER:H	1.61	0.48
1:C:1170:GLN:C	1:C:1171:LEU:HD12	2.39	0.48
1:C:765:TYR:OH	1:C:799:ILE:HG21	2.14	0.48
1:D:968:ILE:O	1:D:972:VAL:HG12	2.14	0.48
1:F:1061:ASN:O	1:F:1064:THR:HG22	2.14	0.48
1:F:1165:SER:HB2	1:F:1181:GLN:HB2	1.96	0.48
1:D:753:VAL:HG13	1:D:814:VAL:HG13	1.95	0.48
1:D:1964:MET:HE3	1:D:1964:MET:H	1.78	0.48
1:F:1143:GLN:HE21	1:F:1170:GLN:NE2	2.10	0.48
1:C:1827:ILE:HD13	1:D:2094:VAL:HG11	1.96	0.47
1:D:913:ASN:OD1	1:D:914:VAL:N	2.47	0.47
1:D:1079:LEU:HD11	1:D:1462:ASN:HB3	1.96	0.47
1:F:1164:ASN:O	1:F:1165:SER:OG	2.32	0.47
1:C:1098:ASN:OD1	1:F:1098:ASN:ND2	2.46	0.47
1:C:1418:ASP:OD2	1:C:1584:GLN:NE2	2.47	0.47
1:F:878:VAL:O	1:F:882:VAL:HG23	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1391:LEU:HB2	1:F:1404:TYR:HE2	1.79	0.47
1:C:1045:ILE:O	1:C:1048:LEU:O	2.31	0.47
1:D:2325:HIS:O	1:D:2326:ILE:HG23	2.14	0.47
1:C:510:ILE:HD11	1:C:540:TYR:O	2.15	0.47
1:C:713:GLY:C	1:C:714:LEU:HD12	2.39	0.47
1:C:2284:VAL:HG12	1:C:2284:VAL:O	2.14	0.47
1:F:852:VAL:CG1	1:F:888:THR:HG21	2.45	0.47
1:F:906:VAL:HG13	1:F:909:ARG:HE	1.80	0.47
1:B:1092:SER:HB3	1:B:1095:LEU:HB3	1.96	0.47
1:B:1093:TYR:CE1	1:B:1133:VAL:HG22	2.50	0.47
1:C:236:ALA:O	1:C:240:LEU:HB2	2.15	0.47
1:C:1045:ILE:HG21	1:C:1080:ARG:HB3	1.95	0.47
1:C:1090:LEU:O	1:C:1090:LEU:HD22	2.14	0.47
1:C:1534:ASN:HD22	1:C:1535:GLU:N	2.13	0.47
1:D:766:ILE:HG22	1:D:779:TYR:C	2.39	0.47
1:D:1239:PHE:CZ	1:D:1248:ILE:HD11	2.49	0.47
1:B:926:ALA:O	1:B:929:ILE:HG22	2.14	0.47
1:B:1105:LEU:HD21	1:B:1145:VAL:HG11	1.97	0.47
1:C:1233:MET:HE3	1:C:1287:HIS:CE1	2.49	0.47
1:D:255:ILE:HG23	1:D:258:LEU:HB2	1.97	0.47
1:D:1534:ASN:HD22	1:D:1535:GLU:H	1.63	0.47
1:B:1333:GLN:OE1	1:B:1352:PHE:N	2.48	0.47
1:B:1535:GLU:HG3	1:B:1536:SER:H	1.80	0.47
1:C:592:GLU:OE2	1:C:742:THR:OG1	2.33	0.47
1:D:1774:ASP:O	1:D:1779:ARG:NH1	2.48	0.47
1:D:1824:ALA:HB3	1:D:1846:LEU:HD13	1.97	0.47
1:F:1253:MET:SD	1:F:1253:MET:N	2.87	0.47
1:F:1359:ARG:NH2	1:F:1367:ASP:OD2	2.47	0.47
1:F:1408:ALA:HB2	1:F:1418:ASP:HB2	1.95	0.47
1:B:993:GLN:O	1:B:997:VAL:HG22	2.15	0.47
1:B:1061:ASN:O	1:B:1064:THR:HG22	2.15	0.47
1:B:1064:THR:O	1:B:1068:GLN:NE2	2.43	0.47
1:B:1154:VAL:HG11	1:B:1180:PHE:CE2	2.50	0.47
1:C:2260:LYS:O	1:C:2263:VAL:HG12	2.14	0.47
1:D:1061:ASN:O	1:D:1064:THR:HG22	2.15	0.47
1:D:1442:LEU:HD13	1:D:1442:LEU:HA	1.72	0.47
1:F:1066:LEU:O	1:F:1069:LEU:HD13	2.14	0.47
1:B:1391:LEU:O	1:B:1391:LEU:HD12	2.16	0.46
1:C:2064:GLY:O	1:C:2067:ILE:HG13	2.16	0.46
1:C:2093:TRP:CD1	1:D:1797:LEU:HD13	2.49	0.46
1:D:527:GLN:CD	1:D:529:LEU:HD21	2.40	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:996:ARG:NH1	1:D:1027:TYR:OH	2.47	0.46
1:D:1845:HIS:C	1:D:1846:LEU:HD22	2.40	0.46
1:C:287:GLU:O	1:C:290:TYR:O	2.32	0.46
1:C:1512:GLU:OE1	1:C:1529:ARG:NH2	2.48	0.46
1:D:1534:ASN:HD22	1:D:1535:GLU:N	2.13	0.46
1:D:2113:SER:O	1:D:2114:ARG:NH1	2.41	0.46
1:C:287:GLU:O	1:C:290:TYR:C	2.58	0.46
1:C:919:LYS:HA	1:C:922:MET:HG2	1.97	0.46
1:D:255:ILE:HD11	1:D:266:ARG:HE	1.80	0.46
1:D:1474:PHE:C	1:D:1475:LEU:HD12	2.41	0.46
1:F:939:GLN:CD	1:F:943:ASN:HD21	2.19	0.46
1:F:1391:LEU:HB2	1:F:1404:TYR:CE2	2.50	0.46
1:B:1090:LEU:O	1:B:1090:LEU:HD22	2.15	0.46
1:B:1302:ASP:O	1:B:1306:ALA:HB2	2.16	0.46
1:D:389:GLU:HG3	1:D:445:GLU:HG2	1.97	0.46
1:B:1039:LEU:O	1:B:1042:THR:OG1	2.28	0.46
1:D:593:TYR:O	1:D:597:LEU:HD23	2.16	0.46
1:D:2284:VAL:HG12	1:D:2284:VAL:O	2.15	0.46
1:F:1418:ASP:OD2	1:F:1420:ARG:NH1	2.49	0.46
1:F:1511:ALA:HB3	1:F:1532:LEU:HD12	1.98	0.46
1:B:1289:LEU:HB3	1:B:1324:ILE:HD11	1.98	0.46
1:C:219:PRO:HA	1:C:222:LEU:HD23	1.98	0.46
1:D:1330:LEU:HD22	1:D:1355:PHE:CE1	2.51	0.46
1:C:762:LEU:CD1	1:C:809:LEU:HD12	2.45	0.46
1:C:1006:TYR:O	1:C:1010:VAL:HG23	2.15	0.46
1:C:2095:VAL:HG23	1:C:2096:ILE:HG12	1.97	0.46
1:D:638:HIS:ND1	1:D:727:MET:HB2	2.31	0.46
1:F:1301:ASP:OD1	1:F:1302:ASP:N	2.48	0.46
1:B:1496:VAL:HG21	1:B:1540:LEU:CD1	2.44	0.46
1:C:2111:ARG:NH1	1:C:2207:ASP:OD1	2.49	0.46
1:C:2319:ILE:O	1:C:2323:THR:N	2.47	0.46
1:D:849:LEU:HD22	1:D:888:THR:HG22	1.97	0.46
1:F:1154:VAL:HG13	1:F:1180:PHE:CE1	2.50	0.46
1:B:1424:ARG:HA	1:B:1474:PHE:HB3	1.98	0.46
1:C:969:VAL:HA	1:C:972:VAL:HG12	1.98	0.46
1:D:1434:THR:HG22	1:D:1482:ILE:HG23	1.97	0.46
1:B:943:ASN:O	1:B:947:SER:OG	2.28	0.45
1:C:1051:ARG:NH2	1:F:1109:ASP:O	2.50	0.45
1:D:920:LYS:O	1:D:923:ALA:HB3	2.14	0.45
1:D:1352:PHE:HB3	1:D:1353:PRO:HD3	1.98	0.45
1:D:1421:PHE:CD2	1:D:1457:LEU:HD21	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1424:ARG:HG2	1:D:1474:PHE:HB3	1.99	0.45
1:B:1411:GLU:OE2	1:B:1412:VAL:HG22	2.16	0.45
1:D:256:PRO:O	1:D:257:THR:OG1	2.35	0.45
1:F:923:ALA:O	1:F:926:ALA:HB3	2.17	0.45
1:C:248:ILE:HG12	1:C:265:LEU:HD22	1.99	0.45
1:C:1056:THR:O	1:C:1058:GLU:N	2.42	0.45
1:C:1612:LEU:HD22	1:C:1896:LEU:HB3	1.99	0.45
1:D:2319:ILE:O	1:D:2323:THR:N	2.47	0.45
1:B:936:PHE:O	1:B:938:SER:N	2.42	0.45
1:D:221:LEU:HA	1:D:224:LYS:HG2	1.97	0.45
1:D:612:TRP:C	1:D:616:LEU:HD23	2.42	0.45
1:D:2296:SER:O	1:D:2300:VAL:HG23	2.16	0.45
1:C:637:LEU:HA	1:C:640:ALA:HB3	1.98	0.45
1:D:1299:ILE:HG22	1:D:1299:ILE:O	2.16	0.45
1:C:1451:LEU:HD21	1:C:1499:TYR:CE2	2.51	0.45
1:D:2017:VAL:HG11	1:D:2050:SER:HB3	1.98	0.45
1:F:1154:VAL:HG13	1:F:1180:PHE:CZ	2.51	0.45
1:F:1249:PHE:CE1	1:F:1253:MET:HE2	2.52	0.45
1:D:1064:THR:O	1:D:1068:GLN:NE2	2.44	0.45
1:F:913:ASN:OD1	1:F:914:VAL:N	2.49	0.45
1:F:939:GLN:O	1:F:943:ASN:ND2	2.50	0.45
1:D:1330:LEU:HD11	1:D:1353:PRO:CB	2.46	0.45
1:F:919:LYS:HA	1:F:922:MET:HG2	1.98	0.45
1:F:1330:LEU:HD13	1:F:1355:PHE:CD1	2.52	0.45
1:C:593:TYR:HA	1:C:596:LYS:HZ2	1.82	0.45
1:C:2113:SER:O	1:C:2114:ARG:NH1	2.44	0.45
1:D:818:MET:SD	1:D:818:MET:N	2.90	0.45
1:D:1134:LEU:HD23	1:D:1137:PHE:CE1	2.51	0.45
1:F:1481:VAL:O	1:F:1517:ILE:HG22	2.17	0.45
1:C:562:SER:HB2	1:C:574:MET:HE2	1.99	0.44
1:C:774:PHE:N	1:C:777:GLN:OE1	2.47	0.44
1:C:1515:ILE:CG2	1:C:1528:ILE:HD11	2.47	0.44
1:D:1309:ARG:NH1	1:D:1366:GLU:OE2	2.49	0.44
1:D:1545:TYR:HA	1:D:1560:ALA:HA	1.98	0.44
1:B:1166:VAL:HG22	1:B:1180:PHE:HD1	1.81	0.44
1:C:715:LEU:HD13	1:D:175:TYR:CZ	2.52	0.44
1:C:1177:VAL:HG13	1:C:1237:VAL:HG22	2.00	0.44
1:B:1055:LEU:HD13	1:B:1056:THR:N	2.33	0.44
1:C:190:VAL:HG13	1:C:218:LEU:CD2	2.47	0.44
1:C:575:VAL:HG12	1:C:579:LYS:NZ	2.33	0.44
1:D:298:LEU:HD22	1:D:327:ALA:HB1	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:909:ARG:HH11	1:D:964:ASN:HB3	1.82	0.44
1:F:1177:VAL:HG13	1:F:1237:VAL:HG22	1.98	0.44
1:C:562:SER:HB3	1:C:574:MET:HE2	1.98	0.44
1:C:922:MET:HG3	1:C:923:ALA:N	2.32	0.44
1:C:995:LEU:HD12	1:C:1066:LEU:HD22	1.98	0.44
1:D:767:VAL:HG12	1:D:768:GLU:N	2.32	0.44
1:D:1517:ILE:HG12	1:D:1527:PRO:CD	2.48	0.44
1:C:767:VAL:HG12	1:C:768:GLU:N	2.32	0.44
1:C:1705:LEU:HD11	1:C:1709:GLU:OE2	2.17	0.44
1:D:848:LYS:O	1:D:852:VAL:HG23	2.17	0.44
1:D:1919:ILE:HG21	1:D:2216:TYR:CD2	2.53	0.44
1:C:858:ASP:HA	1:C:861:VAL:HG12	1.99	0.44
1:D:1060:LEU:HA	1:D:1063:LEU:HB2	1.99	0.44
1:B:933:LEU:HB3	1:D:1117:ILE:HG12	1.99	0.44
1:F:852:VAL:HG11	1:F:888:THR:HG21	2.00	0.44
1:B:1360:ALA:HB2	1:B:1365:GLU:HA	2.00	0.44
1:B:1545:TYR:HA	1:B:1560:ALA:HA	2.00	0.44
1:C:1167:GLN:NE2	1:C:1179:GLU:OE1	2.51	0.44
1:C:1919:ILE:HD12	1:C:1919:ILE:H	1.82	0.44
1:D:638:HIS:CE1	1:D:727:MET:HB2	2.53	0.44
1:D:1301:ASP:OD1	1:D:1302:ASP:N	2.51	0.44
1:D:2137:MET:HE2	1:D:2179:TYR:CD2	2.53	0.44
1:F:1481:VAL:HG22	1:F:1515:ILE:HD11	1.99	0.44
1:B:886:MET:SD	1:B:1048:LEU:HD21	2.58	0.44
1:B:961:PHE:CE2	1:B:965:THR:HG21	2.52	0.44
1:C:849:LEU:HD22	1:C:888:THR:HG21	2.00	0.44
1:C:1390:ASP:N	1:C:1407:ALA:O	2.33	0.44
1:C:1872:ILE:HB	1:C:1884:THR:HG21	1.99	0.44
1:D:1369:ILE:CD1	1:D:1391:LEU:HD21	2.47	0.44
1:F:1424:ARG:HG2	1:F:1474:PHE:HB3	2.00	0.44
1:B:1482:ILE:O	1:B:1482:ILE:HG22	2.18	0.43
1:C:474:LYS:NZ	1:C:484:PRO:O	2.49	0.43
1:D:2288:ILE:HD12	1:D:2288:ILE:H	1.83	0.43
1:C:442:LEU:HD11	1:C:446:HIS:CG	2.53	0.43
1:C:1643:GLY:HA3	1:C:1697:LEU:HD21	2.00	0.43
1:D:1421:PHE:CD2	1:D:1457:LEU:HD11	2.53	0.43
1:B:939:GLN:OE1	1:B:976:ARG:NH1	2.50	0.43
1:C:963:MET:HA	1:C:966:GLN:HG2	2.01	0.43
1:D:2173:GLU:HA	1:D:2176:ILE:HD12	1.99	0.43
1:F:969:VAL:HA	1:F:972:VAL:HG12	1.99	0.43
1:F:1233:MET:HE2	1:F:1287:HIS:ND1	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:529:LEU:H	1:C:540:TYR:HA	1.84	0.43
1:C:2288:ILE:HD12	1:C:2288:ILE:H	1.83	0.43
1:D:571:ILE:O	1:D:575:VAL:HG23	2.18	0.43
1:D:682:VAL:C	1:D:683:LEU:HD12	2.43	0.43
1:D:988:MET:HE1	1:D:1058:GLU:HB3	2.00	0.43
1:D:1164:ASN:OD1	1:D:1164:ASN:N	2.52	0.43
1:D:1457:LEU:HD13	1:D:1506:LEU:HD11	2.01	0.43
1:B:1038:ASN:ND2	1:B:1074:ASN:OD1	2.51	0.43
1:C:629:MET:O	1:C:633:VAL:HG23	2.18	0.43
1:C:682:VAL:C	1:C:683:LEU:HD12	2.44	0.43
1:C:707:HIS:CD2	1:C:715:LEU:HD11	2.52	0.43
1:B:980:ARG:O	1:B:984:LYS:HG3	2.19	0.43
1:C:574:MET:O	1:C:577:ALA:HB3	2.19	0.43
1:C:1079:LEU:HB2	1:C:1459:VAL:HG22	2.00	0.43
1:C:1294:LYS:HA	1:C:1332:ALA:HB3	2.01	0.43
1:B:856:VAL:HG21	1:B:884:ARG:HB3	1.99	0.43
1:C:1410:VAL:HG12	1:C:1411:GLU:N	2.34	0.43
1:D:1177:VAL:HG13	1:D:1237:VAL:CG2	2.45	0.43
1:D:1935:ARG:NH2	1:D:1972:VAL:HG11	2.33	0.43
1:C:923:ALA:O	1:C:926:ALA:HB3	2.19	0.43
1:D:1528:ILE:HA	1:D:1545:TYR:O	2.18	0.43
1:B:919:LYS:HA	1:B:922:MET:HG2	2.00	0.43
1:C:442:LEU:HD11	1:C:446:HIS:CB	2.49	0.43
1:C:659:GLN:NE2	1:C:2007:GLU:OE2	2.52	0.43
1:C:933:LEU:HD21	1:F:1155:ARG:HD2	2.01	0.43
1:C:968:ILE:O	1:C:972:VAL:HG12	2.19	0.43
1:C:1546:LYS:N	1:C:1559:GLN:O	2.52	0.43
1:D:1102:SER:O	1:D:1106:SER:OG	2.30	0.43
1:D:1528:ILE:CA	1:D:1545:TYR:O	2.67	0.43
1:B:1418:ASP:OD2	1:B:1420:ARG:NH1	2.52	0.43
1:C:1164:ASN:OD1	1:C:1164:ASN:N	2.49	0.43
1:C:2311:ASN:O	1:C:2314:VAL:HG22	2.19	0.43
1:D:864:MET:O	1:D:1037:LYS:NZ	2.51	0.43
1:D:895:PRO:O	1:D:899:LEU:HD23	2.19	0.43
1:D:969:VAL:HA	1:D:972:VAL:HG12	2.00	0.43
1:D:1434:THR:CG2	1:D:1482:ILE:HG23	2.49	0.43
1:B:878:VAL:O	1:B:882:VAL:HG23	2.19	0.42
1:B:1155:ARG:O	1:B:1159:ILE:HB	2.19	0.42
1:D:2119:GLU:OE1	1:D:2121:GLU:N	2.51	0.42
1:B:1237:VAL:HB	1:B:1291:VAL:HG12	2.01	0.42
1:C:1875:MET:N	1:C:1875:MET:SD	2.92	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1046:ASP:OD2	1:D:1080:ARG:NH1	2.52	0.42
1:D:1964:MET:HE3	1:D:1964:MET:N	2.34	0.42
1:D:2181:GLN:O	1:D:2184:VAL:HG22	2.19	0.42
1:C:528:GLU:HG2	1:C:540:TYR:HB3	2.00	0.42
1:D:1330:LEU:HD13	1:D:1355:PHE:CD1	2.54	0.42
1:B:1037:LYS:O	1:B:1041:VAL:HG23	2.19	0.42
1:C:528:GLU:CG	1:D:532:ARG:HB3	2.50	0.42
1:C:659:GLN:NE2	1:C:2004:LEU:O	2.51	0.42
1:C:663:ALA:O	1:C:666:LEU:HD23	2.18	0.42
1:C:930:THR:HG22	1:C:930:THR:O	2.19	0.42
1:F:963:MET:HA	1:F:966:GLN:HG2	2.01	0.42
1:B:1165:SER:HB2	1:B:1181:GLN:HB2	2.00	0.42
1:C:1154:VAL:HG13	1:C:1180:PHE:CE1	2.55	0.42
1:C:1627:LEU:HD12	1:C:1629:SER:OG	2.19	0.42
1:D:609:ASP:OD1	1:D:612:TRP:N	2.52	0.42
1:D:1134:LEU:HD23	1:D:1137:PHE:HE1	1.84	0.42
1:D:1165:SER:HB2	1:D:1181:GLN:HB3	2.01	0.42
1:D:1481:VAL:HG22	1:D:1515:ILE:HD11	2.02	0.42
1:D:2064:GLY:O	1:D:2067:ILE:HG13	2.19	0.42
1:C:1545:TYR:HA	1:C:1560:ALA:HA	2.02	0.42
1:D:613:LEU:O	1:D:617:ILE:HD12	2.20	0.42
1:D:1239:PHE:HB3	1:D:1293:ILE:HG22	2.02	0.42
1:B:1066:LEU:HD11	1:B:1077:VAL:CG1	2.50	0.42
1:C:537:VAL:HG13	1:C:562:SER:HB2	2.01	0.42
1:C:675:ILE:HA	1:C:680:LYS:HA	2.01	0.42
1:F:885:LEU:HD11	1:F:889:LEU:HD12	2.01	0.42
1:F:896:LEU:HA	1:F:899:LEU:HD23	2.01	0.42
1:F:1062:ILE:HD12	1:F:1062:ILE:H	1.85	0.42
1:B:901:ASP:O	1:B:904:THR:OG1	2.36	0.42
1:C:534:ASN:HB3	1:C:537:VAL:HG23	2.01	0.42
1:F:1180:PHE:HB2	1:F:1234:GLY:HA3	2.02	0.42
1:F:1377:LEU:CD1	1:F:1426:ILE:HD11	2.49	0.42
1:F:1390:ASP:HB2	1:F:1409:LYS:HB3	2.01	0.42
1:D:1410:VAL:HG12	1:D:1411:GLU:N	2.34	0.42
1:D:1919:ILE:HD12	1:D:1919:ILE:H	1.85	0.42
1:F:1164:ASN:OD1	1:F:1164:ASN:N	2.51	0.42
1:F:1299:ILE:HG22	1:F:1299:ILE:O	2.19	0.42
1:F:1454:MET:HB2	1:F:1506:LEU:HD21	2.00	0.42
1:F:1549:THR:HG22	1:F:1554:ALA:HA	2.00	0.42
1:B:1047:GLN:C	1:B:1048:LEU:HD22	2.45	0.42
1:D:894:LEU:HB3	1:D:895:PRO:HD3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:930:THR:HG22	1:D:930:THR:O	2.20	0.42
1:D:1923:ILE:O	1:D:2209:LYS:NZ	2.53	0.42
1:D:2095:VAL:HG23	1:D:2096:ILE:HG12	2.02	0.42
1:F:965:THR:HG23	1:F:965:THR:O	2.20	0.42
1:F:1306:ALA:HA	1:F:1309:ARG:HE	1.84	0.42
1:D:1066:LEU:O	1:D:1069:LEU:HD13	2.20	0.41
1:D:1071:LYS:O	1:D:1074:ASN:N	2.53	0.41
1:D:1627:LEU:HD12	1:D:1629:SER:OG	2.19	0.41
1:D:2275:GLU:O	1:D:2279:THR:HG23	2.20	0.41
1:B:1294:LYS:O	1:B:1295:THR:OG1	2.33	0.41
1:C:164:ALA:HB1	1:C:525:THR:HG21	2.02	0.41
1:C:221:LEU:HA	1:C:224:LYS:HG2	2.02	0.41
1:C:1294:LYS:O	1:C:1295:THR:OG1	2.27	0.41
1:C:1954:PHE:O	1:C:2212:ARG:NH1	2.52	0.41
1:D:278:ILE:CG2	1:D:280:ASN:HD22	2.33	0.41
1:D:1515:ILE:O	1:D:1527:PRO:HG2	2.20	0.41
1:D:1517:ILE:H	1:D:1527:PRO:HD2	1.84	0.41
1:B:1164:ASN:OD1	1:B:1164:ASN:N	2.48	0.41
1:D:1133:VAL:HG11	1:D:1332:ALA:HB2	2.01	0.41
1:C:1424:ARG:HG2	1:C:1474:PHE:HB3	2.03	0.41
1:C:1489:GLU:HA	1:C:1492:VAL:HG12	2.02	0.41
1:C:1534:ASN:HD22	1:C:1535:GLU:H	1.66	0.41
1:C:2075:CYS:O	1:C:2104:HIS:NE2	2.53	0.41
1:D:1056:THR:O	1:D:1058:GLU:N	2.51	0.41
1:D:1527:PRO:HB2	1:D:1528:ILE:HG12	2.02	0.41
1:F:1424:ARG:HA	1:F:1474:PHE:HB3	2.02	0.41
1:F:1535:GLU:HG3	1:F:1536:SER:H	1.85	0.41
1:B:878:VAL:HB	1:B:1040:LEU:HD11	2.03	0.41
1:B:1534:ASN:HD22	1:B:1535:GLU:N	2.18	0.41
1:D:255:ILE:CD1	1:D:266:ARG:HE	2.34	0.41
1:D:1457:LEU:HD22	1:D:1506:LEU:HD11	2.01	0.41
1:D:2137:MET:HE2	1:D:2179:TYR:HD2	1.84	0.41
1:B:1410:VAL:HG12	1:B:1411:GLU:N	2.36	0.41
1:C:657:ARG:HE	1:C:2007:GLU:CG	2.34	0.41
1:C:1827:ILE:O	1:C:1831:LEU:HD13	2.21	0.41
1:D:579:LYS:O	1:D:582:SER:OG	2.34	0.41
1:D:1405:LEU:HD12	1:D:1421:PHE:HE1	1.86	0.41
1:D:2323:THR:HG22	1:D:2323:THR:O	2.21	0.41
1:F:1014:ARG:CZ	1:F:1021:MET:HE1	2.51	0.41
1:B:1388:ASN:HD22	1:B:1576:PRO:HB2	1.86	0.41
1:B:1506:LEU:HD12	1:B:1506:LEU:N	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:ASP:OD2	1:D:851:ARG:NH2	2.54	0.41
1:C:1075:ALA:O	1:C:1079:LEU:HD12	2.20	0.41
1:C:1528:ILE:HB	1:C:1544:LEU:HD21	2.03	0.41
1:D:585:GLY:HA2	1:D:588:ARG:HD2	2.01	0.41
1:D:651:PHE:O	1:D:655:LEU:HB2	2.21	0.41
1:D:1595:THR:OG1	1:D:1596:THR:N	2.54	0.41
1:B:1009:CYS:O	1:B:1013:LEU:HD23	2.21	0.41
1:C:651:PHE:O	1:C:655:LEU:HB2	2.21	0.41
1:C:657:ARG:HE	1:C:2007:GLU:CD	2.29	0.41
1:C:1480:THR:HA	1:C:1516:ASN:O	2.21	0.41
1:C:2323:THR:HG22	1:C:2323:THR:O	2.20	0.41
1:C:2325:HIS:O	1:C:2326:ILE:HG23	2.20	0.41
1:D:537:VAL:HG21	1:D:573:ASN:HB3	2.01	0.41
1:D:1154:VAL:HG22	1:D:1236:MET:SD	2.61	0.41
1:F:1293:ILE:HD11	1:F:1331:VAL:HG12	2.03	0.41
1:C:967:SER:O	1:C:971:LEU:HB2	2.21	0.41
1:C:2144:TYR:CD1	1:C:2168:LEU:HD11	2.55	0.41
1:D:529:LEU:H	1:D:540:TYR:HA	1.86	0.41
1:D:602:SER:OG	1:D:607:ARG:NH2	2.53	0.41
1:D:1133:VAL:HG23	1:D:1353:PRO:CG	2.51	0.41
1:D:1184:LEU:HD11	1:D:1232:ARG:CZ	2.51	0.41
1:D:2304:ILE:O	1:D:2308:VAL:HG23	2.21	0.41
1:F:1410:VAL:HG12	1:F:1411:GLU:N	2.36	0.41
1:B:997:VAL:HG23	1:B:998:GLU:N	2.36	0.41
1:B:1533:THR:OG1	1:B:1541:ASP:O	2.31	0.41
1:C:405:GLU:O	1:C:409:VAL:HG23	2.21	0.41
1:C:511:THR:C	1:C:590:THR:HG21	2.46	0.41
1:C:1545:TYR:CG	1:C:1558:PHE:HB3	2.56	0.41
1:B:1055:LEU:HD12	1:B:1060:LEU:HG	2.02	0.40
1:C:173:ASP:O	1:D:722:SER:N	2.42	0.40
1:D:236:ALA:O	1:D:240:LEU:HB2	2.21	0.40
1:D:992:ARG:HA	1:D:995:LEU:HB3	2.03	0.40
1:D:1794:PRO:HB3	1:D:1797:LEU:HD12	2.03	0.40
1:F:1324:ILE:HD12	1:F:1324:ILE:N	2.36	0.40
1:C:418:VAL:O	1:C:419:SER:OG	2.17	0.40
1:C:1774:ASP:O	1:C:1779:ARG:NH1	2.54	0.40
1:B:1387:ARG:HE	1:B:1576:PRO:HG3	1.86	0.40
1:D:267:VAL:HG12	1:D:268:ASP:N	2.36	0.40
1:D:971:LEU:HA	1:D:974:ARG:HD3	2.03	0.40
1:D:1289:LEU:O	1:D:1327:LEU:HA	2.21	0.40
1:D:2323:THR:HG23	1:D:2326:ILE:HD11	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1297:CYS:SG	1:B:1298:ASP:N	2.94	0.40
1:C:533:SER:O	1:D:139:ARG:NE	2.52	0.40
1:D:796:SER:O	1:D:820:LEU:HD22	2.22	0.40
1:D:997:VAL:HG23	1:D:998:GLU:N	2.36	0.40
1:F:922:MET:HG3	1:F:923:ALA:H	1.86	0.40
1:F:1382:GLU:O	1:F:1424:ARG:NH2	2.53	0.40
1:B:1302:ASP:O	1:B:1306:ALA:CB	2.70	0.40
1:B:1309:ARG:O	1:B:1312:THR:OG1	2.33	0.40
1:C:1299:ILE:HD12	1:C:1299:ILE:H	1.86	0.40
1:C:1434:THR:HG21	1:C:1483:MET:HB2	2.02	0.40
1:D:689:SER:HB3	1:D:692:SER:HB2	2.04	0.40
1:D:983:MET:O	1:D:987:VAL:HG12	2.22	0.40
1:D:1546:LYS:O	1:D:1558:PHE:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	609/2407 (25%)	522 (86%)	81 (13%)	6 (1%)	12	47
1	C	2107/2407 (88%)	1908 (91%)	191 (9%)	8 (0%)	30	67
1	D	2107/2407 (88%)	1901 (90%)	193 (9%)	13 (1%)	21	59
1	F	620/2407 (26%)	521 (84%)	91 (15%)	8 (1%)	9	40
All	All	5443/9628 (56%)	4852 (89%)	556 (10%)	35 (1%)	23	59

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1087	ALA
1	B	1304	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1365	GLU
1	C	1304	LEU
1	D	1527	PRO
1	F	1087	ALA
1	C	211	HIS
1	D	291	VAL
1	D	667	LEU
1	D	867	TYR
1	F	1172	LYS
1	B	937	PRO
1	C	291	VAL
1	C	868	CYS
1	C	1376	ALA
1	D	1564	LYS
1	D	1580	LYS
1	D	1376	ALA
1	D	1400	LYS
1	D	1560	ALA
1	D	1581	ASP
1	F	937	PRO
1	F	994	TYR
1	F	1113	HIS
1	F	1173	ASP
1	C	419	SER
1	F	938	SER
1	F	1376	ALA
1	B	1360	ALA
1	C	853	PHE
1	D	1146	ARG
1	D	1360	ALA
1	C	1688	ILE
1	D	1688	ILE
1	B	1412	VAL

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	B	571/2108 (27%)	549 (96%)	22 (4%)	28	49
1	C	1855/2108 (88%)	1801 (97%)	54 (3%)	37	57
1	D	1855/2108 (88%)	1796 (97%)	59 (3%)	34	55
1	F	579/2108 (28%)	546 (94%)	33 (6%)	18	39
All	All	4860/8432 (58%)	4692 (96%)	168 (4%)	32	53

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	857	LEU
1	B	863	VAL
1	B	889	LEU
1	B	896	LEU
1	B	897	LEU
1	B	902	ILE
1	B	947	SER
1	B	995	LEU
1	B	1090	LEU
1	B	1164	ASN
1	B	1359	ARG
1	B	1381	LEU
1	B	1417	THR
1	B	1438	SER
1	B	1440	GLU
1	B	1457	LEU
1	B	1480	THR
1	B	1528	ILE
1	B	1531	PHE
1	B	1546	LYS
1	B	1568	LEU
1	B	1577	TYR
1	C	186	ASN
1	C	223	LEU
1	C	529	LEU
1	C	581	LEU
1	C	637	LEU
1	C	652	LEU
1	C	655	LEU
1	C	705	ASP
1	C	791	LEU
1	C	863	VAL
1	C	896	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	897	LEU
1	C	902	ILE
1	C	915	GLU
1	C	933	LEU
1	C	947	SER
1	C	951	THR
1	C	983	MET
1	C	1065	GLU
1	C	1066	LEU
1	C	1079	LEU
1	C	1090	LEU
1	C	1096	ARG
1	C	1164	ASN
1	C	1184	LEU
1	C	1250	ASP
1	C	1251	GLU
1	C	1324	ILE
1	C	1359	ARG
1	C	1381	LEU
1	C	1417	THR
1	C	1438	SER
1	C	1440	GLU
1	C	1457	LEU
1	C	1480	THR
1	C	1528	ILE
1	C	1531	PHE
1	C	1630	ASP
1	C	1649	ASN
1	C	1848	LEU
1	C	1875	MET
1	C	1919	ILE
1	C	1964	MET
1	C	1970	THR
1	C	2116	SER
1	C	2124	VAL
1	C	2135	LYS
1	C	2151	LEU
1	C	2176	ILE
1	C	2240	THR
1	C	2326	ILE
1	C	2327	SER
1	C	2333	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	2334	VAL
1	D	170	LYS
1	D	186	ASN
1	D	223	LEU
1	D	439	ASN
1	D	451	MET
1	D	637	LEU
1	D	652	LEU
1	D	655	LEU
1	D	666	LEU
1	D	715	LEU
1	D	791	LEU
1	D	863	VAL
1	D	896	LEU
1	D	897	LEU
1	D	899	LEU
1	D	902	ILE
1	D	915	GLU
1	D	947	SER
1	D	951	THR
1	D	974	ARG
1	D	995	LEU
1	D	1079	LEU
1	D	1096	ARG
1	D	1164	ASN
1	D	1175	THR
1	D	1250	ASP
1	D	1310	GLU
1	D	1324	ILE
1	D	1377	LEU
1	D	1381	LEU
1	D	1391	LEU
1	D	1403	LEU
1	D	1417	THR
1	D	1438	SER
1	D	1440	GLU
1	D	1449	LEU
1	D	1451	LEU
1	D	1457	LEU
1	D	1475	LEU
1	D	1478	VAL
1	D	1480	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	1508	VAL
1	D	1513	LEU
1	D	1531	PHE
1	D	1575	THR
1	D	1630	ASP
1	D	1649	ASN
1	D	1875	MET
1	D	1919	ILE
1	D	1964	MET
1	D	1970	THR
1	D	2116	SER
1	D	2124	VAL
1	D	2176	ILE
1	D	2240	THR
1	D	2308	VAL
1	D	2326	ILE
1	D	2327	SER
1	D	2334	VAL
1	F	863	VAL
1	F	864	MET
1	F	896	LEU
1	F	897	LEU
1	F	899	LEU
1	F	902	ILE
1	F	909	ARG
1	F	915	GLU
1	F	933	LEU
1	F	947	SER
1	F	951	THR
1	F	995	LEU
1	F	1065	GLU
1	F	1066	LEU
1	F	1090	LEU
1	F	1095	LEU
1	F	1164	ASN
1	F	1175	THR
1	F	1244	ASP
1	F	1250	ASP
1	F	1289	LEU
1	F	1319	LEU
1	F	1324	ILE
1	F	1326	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	1381	LEU
1	F	1417	THR
1	F	1438	SER
1	F	1440	GLU
1	F	1449	LEU
1	F	1457	LEU
1	F	1478	VAL
1	F	1480	THR
1	F	1528	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	859	ASN
1	B	862	ASN
1	B	865	ASN
1	B	943	ASN
1	B	964	ASN
1	B	966	GLN
1	B	1033	GLN
1	B	1038	ASN
1	B	1083	GLN
1	B	1287	HIS
1	B	1313	GLN
1	B	1333	GLN
1	B	1398	ASN
1	B	1402	HIS
1	B	1444	ASN
1	B	1463	ASN
1	B	1476	ASN
1	B	1534	ASN
1	B	1569	HIS
1	C	165	ASN
1	C	185	ASN
1	C	280	ASN
1	C	283	GLN
1	C	354	GLN
1	C	403	HIS
1	C	530	ASN
1	C	559	HIS
1	C	638	HIS
1	C	659	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	698	ASN
1	C	859	ASN
1	C	939	GLN
1	C	943	ASN
1	C	966	GLN
1	C	1119	ASN
1	C	1143	GLN
1	C	1287	HIS
1	C	1402	HIS
1	C	1443	GLN
1	C	1444	ASN
1	C	1462	ASN
1	C	1463	ASN
1	C	1534	ASN
1	C	1569	HIS
1	C	1732	HIS
1	C	1768	HIS
1	C	2003	ASN
1	C	2012	GLN
1	C	2013	GLN
1	C	2028	GLN
1	C	2045	ASN
1	C	2146	HIS
1	C	2180	HIS
1	C	2190	HIS
1	C	2285	HIS
1	C	2291	ASN
1	D	270	GLN
1	D	280	ASN
1	D	325	ASN
1	D	559	HIS
1	D	698	ASN
1	D	827	GLN
1	D	862	ASN
1	D	943	ASN
1	D	964	ASN
1	D	966	GLN
1	D	1017	ASN
1	D	1170	GLN
1	D	1181	GLN
1	D	1398	ASN
1	D	1444	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	1463	ASN
1	D	1534	ASN
1	D	1735	HIS
1	D	1946	GLN
1	D	2003	ASN
1	D	2013	GLN
1	D	2028	GLN
1	D	2045	ASN
1	D	2146	HIS
1	D	2291	ASN
1	F	859	ASN
1	F	862	ASN
1	F	900	GLN
1	F	928	ASN
1	F	1074	ASN
1	F	1170	GLN
1	F	1402	HIS
1	F	1444	ASN
1	F	1462	ASN
1	F	1534	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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.

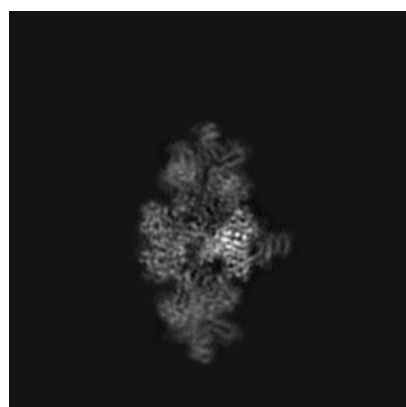
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4342. These allow visual inspection of the internal detail of the map and identification of artifacts.

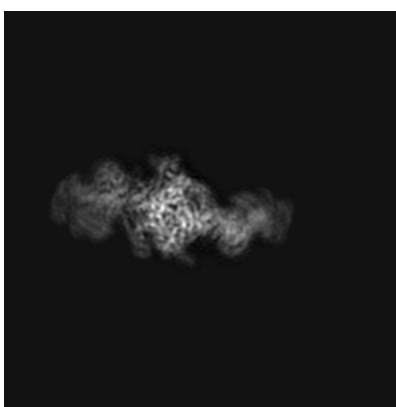
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

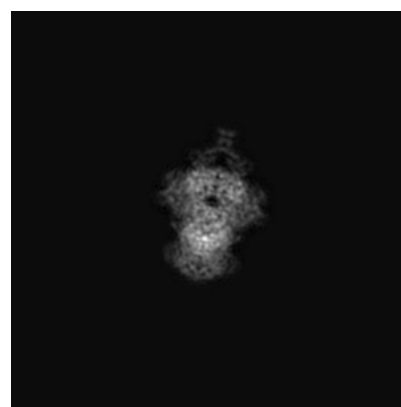
6.1.1 Primary map



X



Y

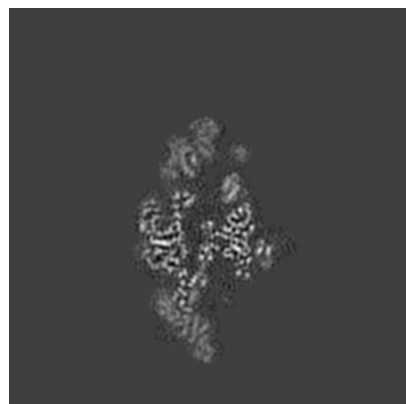


Z

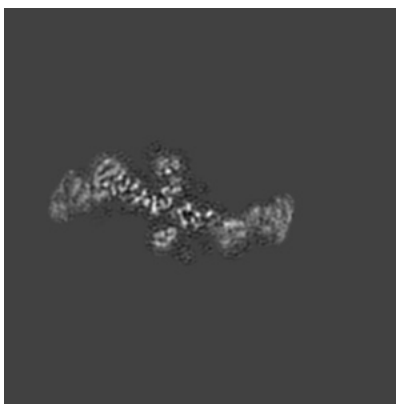
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 225



Y Index: 225

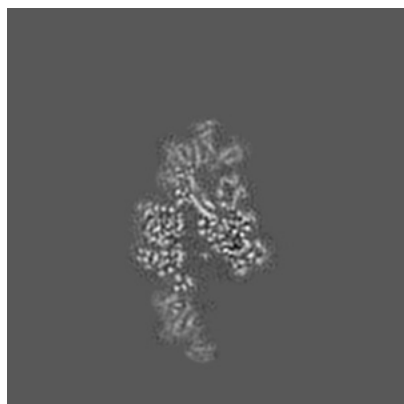


Z Index: 225

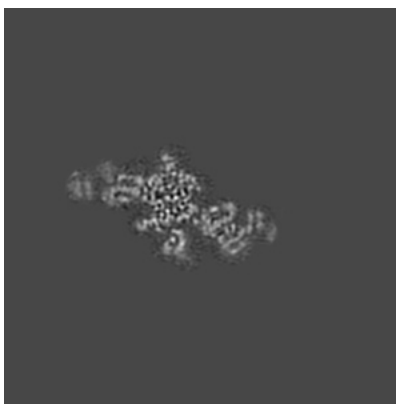
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

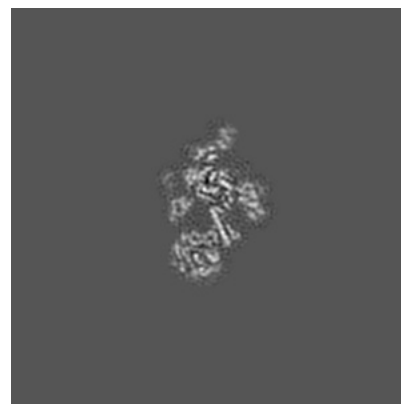
6.3.1 Primary map



X Index: 217



Y Index: 247

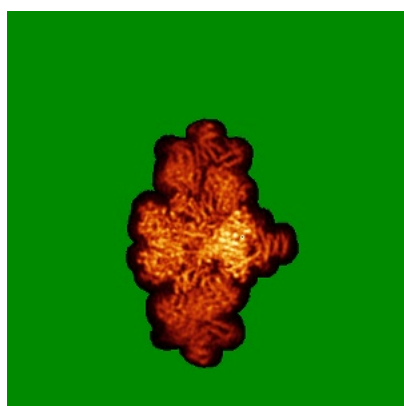


Z Index: 177

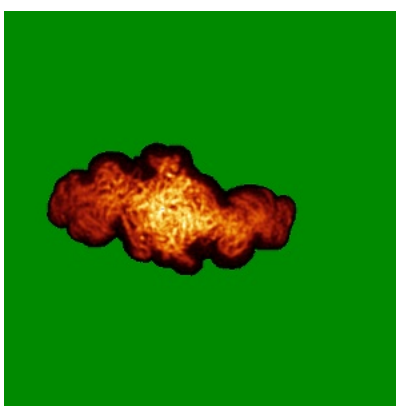
The images above show the largest variance slices of the map in three orthogonal directions.

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

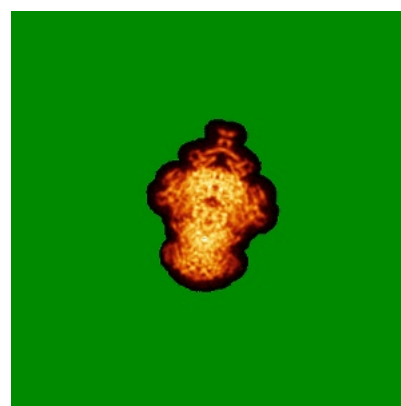
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0172. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

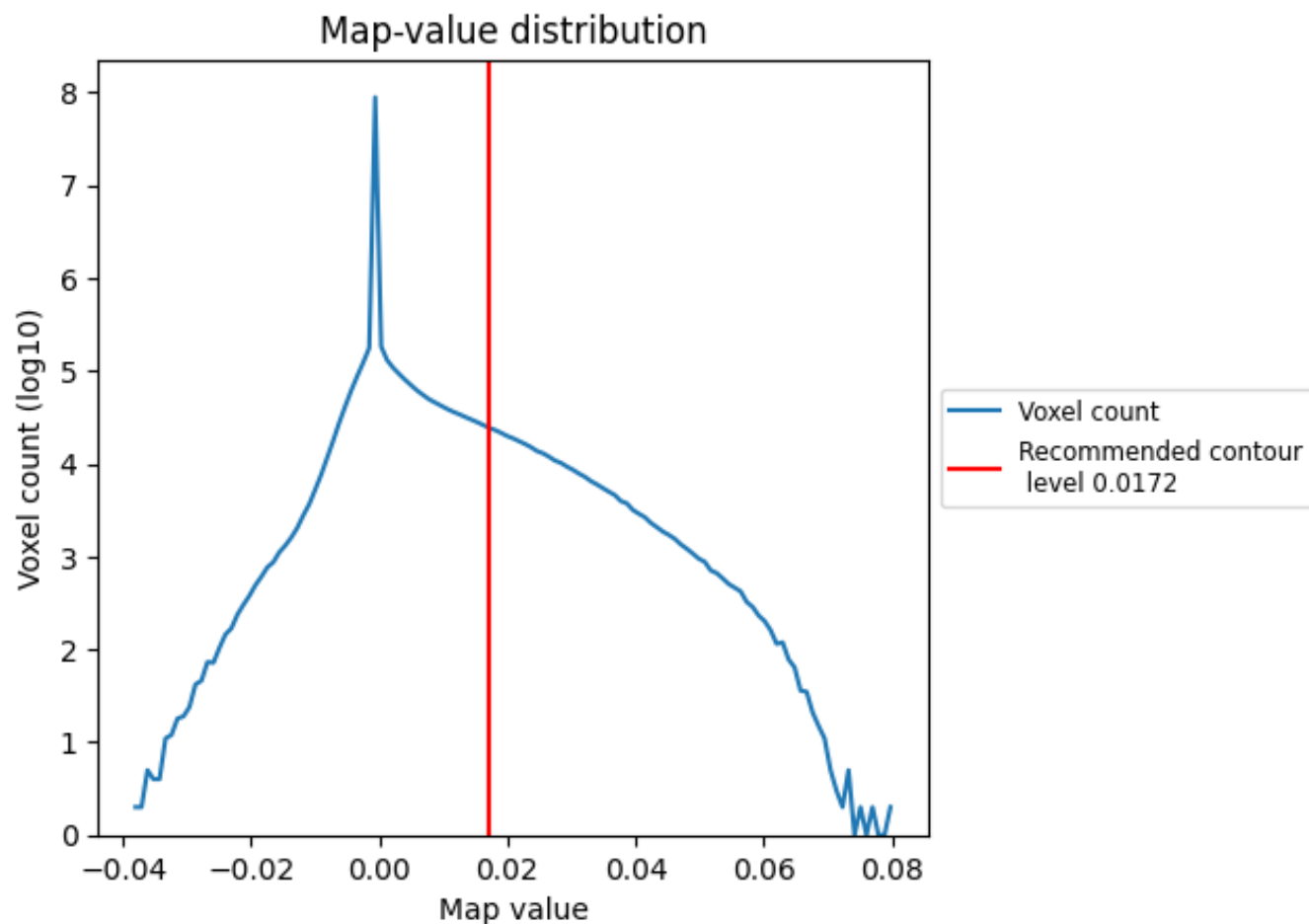
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

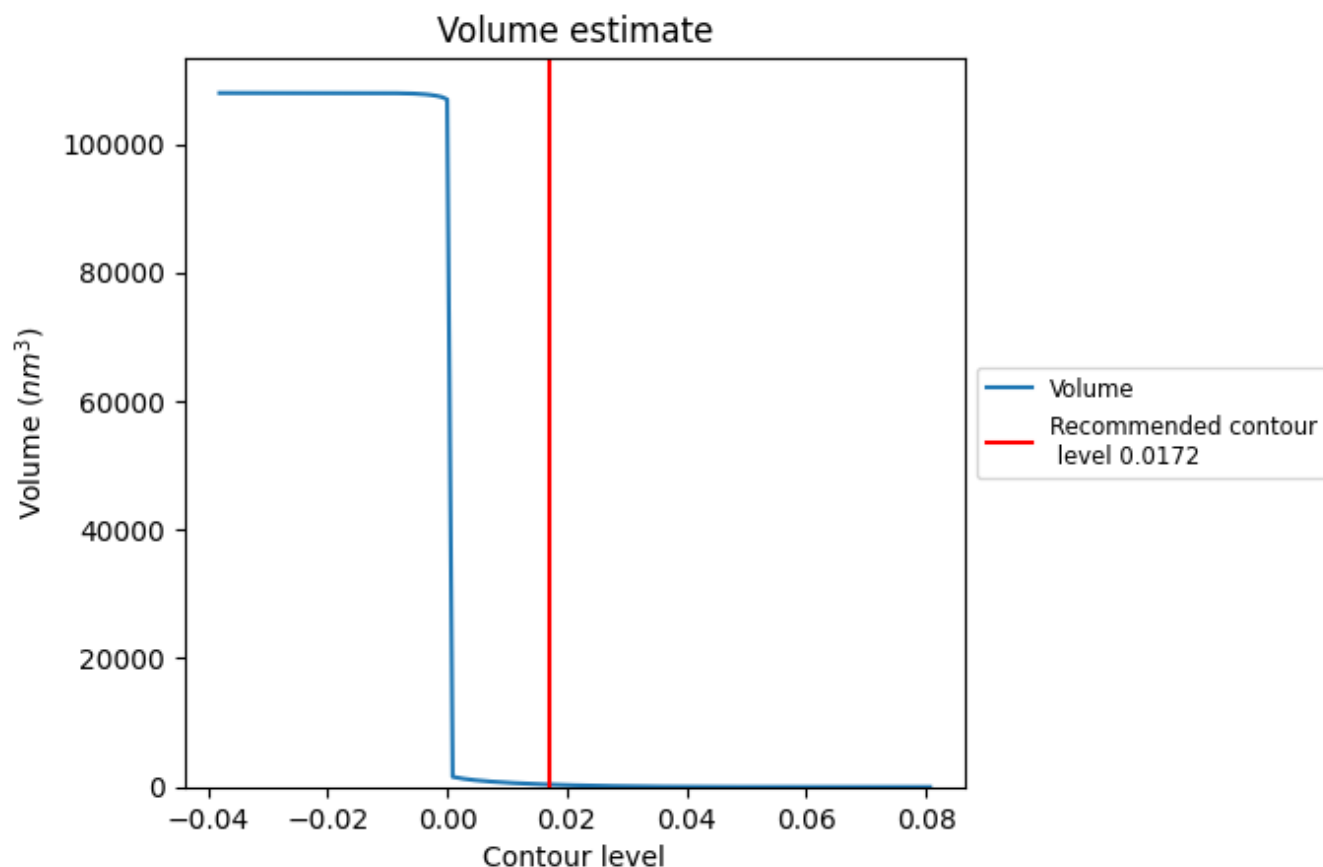
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

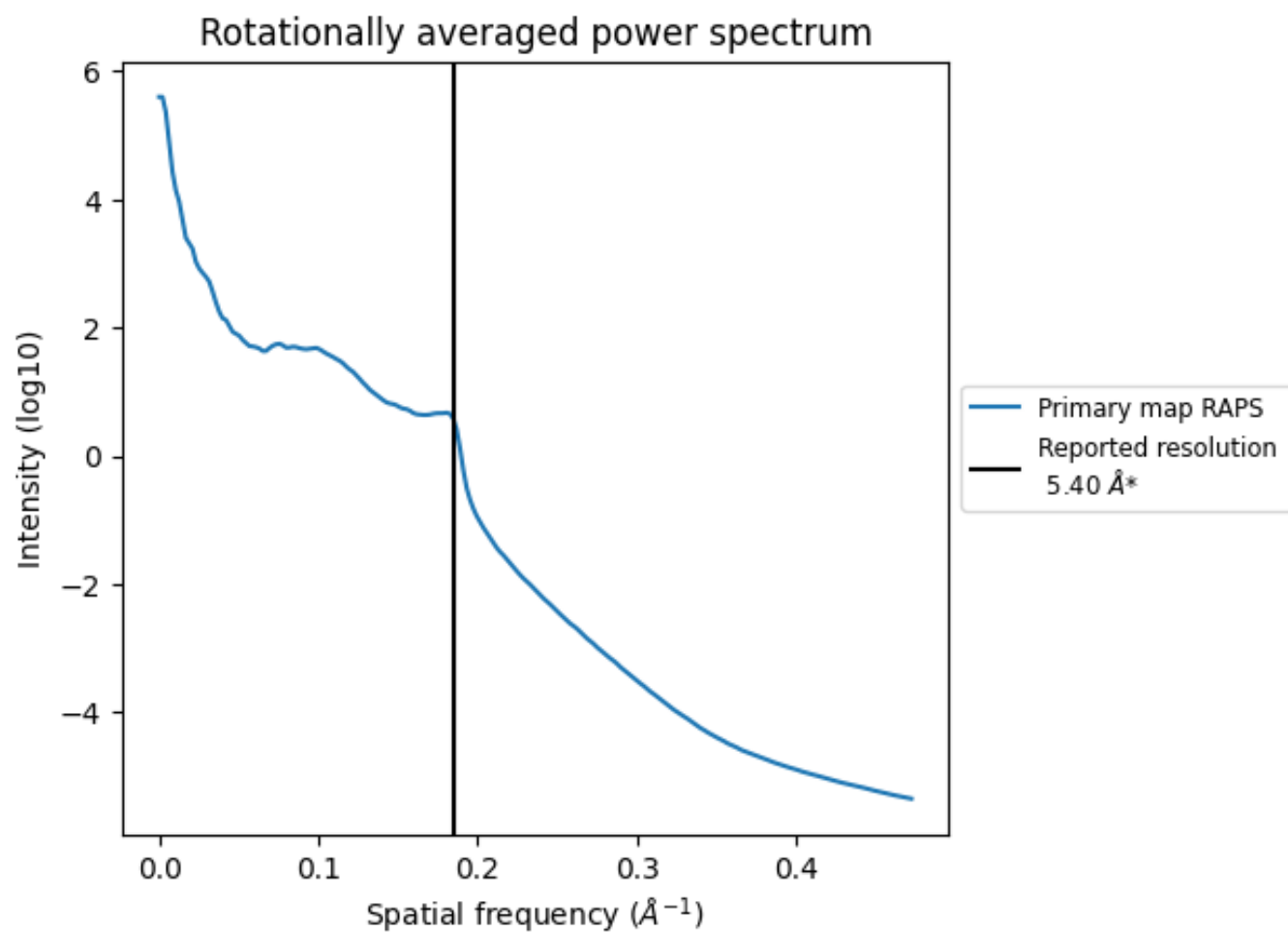
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 370 nm³; this corresponds to an approximate mass of 334 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 0.185 Å⁻¹

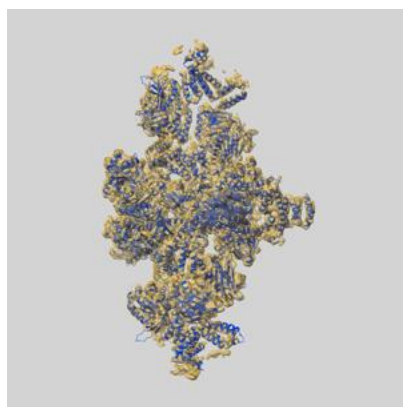
8 Fourier-Shell correlation

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

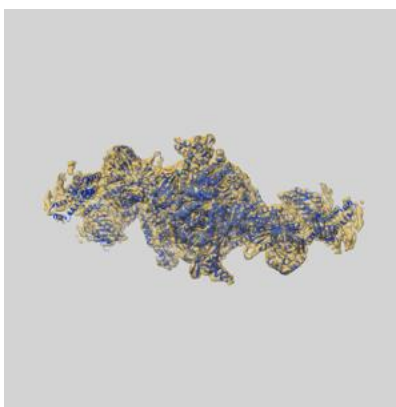
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4342 and PDB model 6G2D. Per-residue inclusion information can be found in section 3 on page 10.

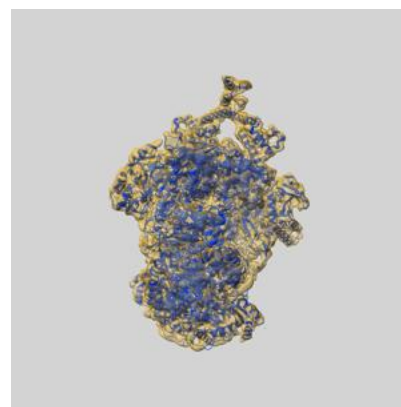
9.1 Map-model overlay [i](#)



X



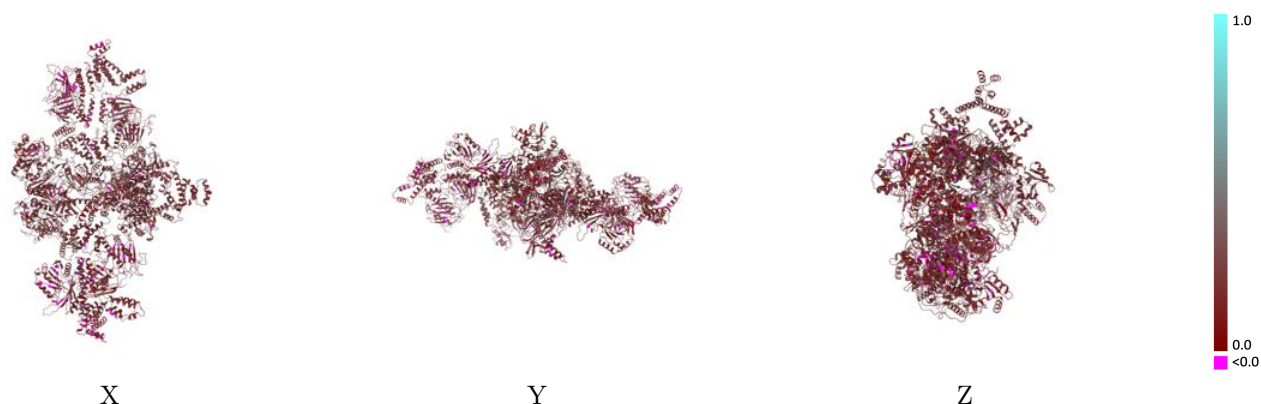
Y



Z

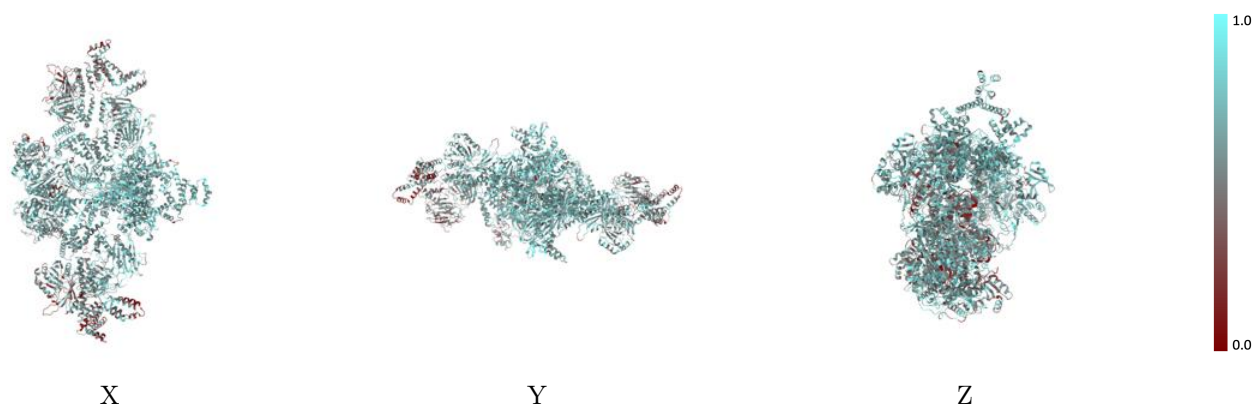
The images above show the 3D surface view of the map at the recommended contour level 0.0172 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



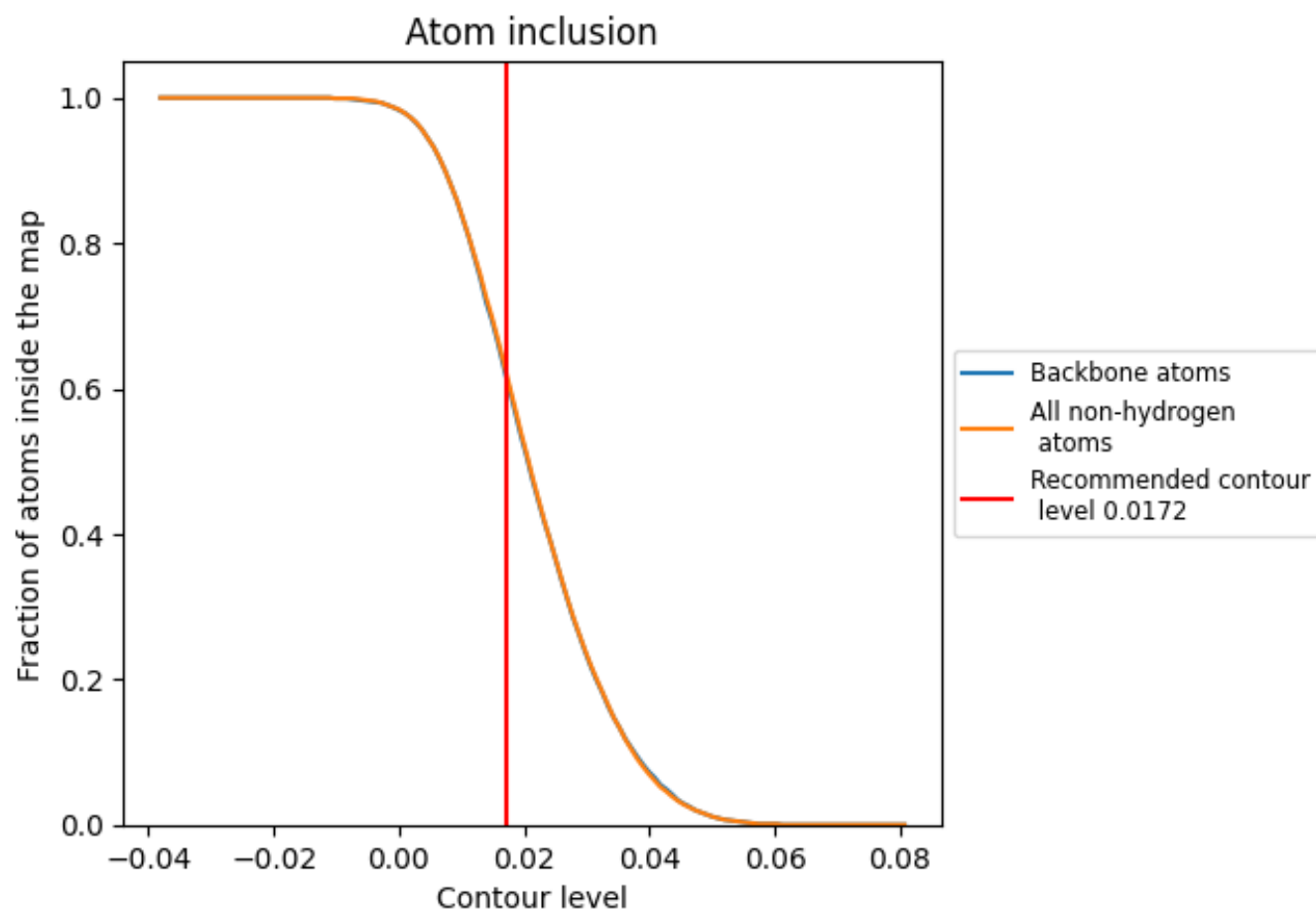
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0172).

9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0172) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6200	0.2160
B	0.5190	0.1810
C	0.6710	0.2260
D	0.6750	0.2280
F	0.4600	0.1760

