



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 06:05 pm GMT

PDB ID : 6G2D
EMDB ID : EMD-4342
Title : Citrate-induced acetyl-CoA carboxylase (ACC-Cit) filament at 5.4 Å resolution
Authors : Hunkeler, M.; Hagmann, A.; Stutfeld, 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

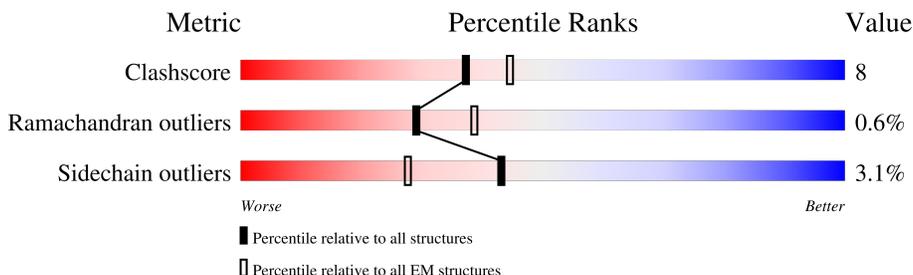
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	
1	C	2407	
1	D	2407	
1	F	2407	

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

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...

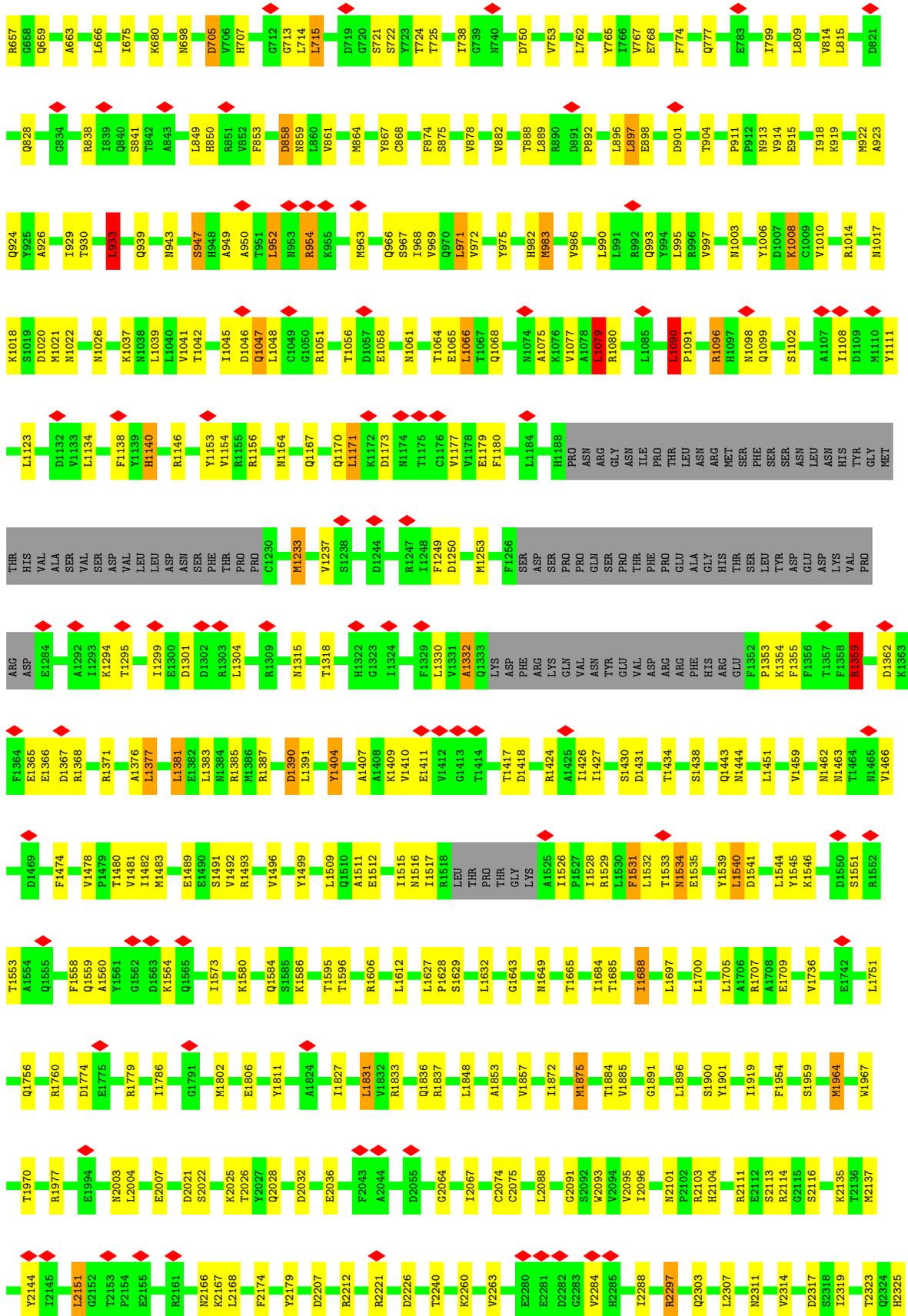
Continued from previous page...

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



HIS
SER
VAL
ILE
GLU
GLU
ASN
ILE
LYS
CYS
ILE
SER
ARG
ASP
TYR
VAL
LEU
LYS
GLN
ILE
ARG
SER
LEU
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 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	B	0.42	0/5209	0.95	13/7030 (0.2%)
1	C	0.40	1/17302 (0.0%)	0.88	34/23432 (0.1%)
1	D	0.42	2/17302 (0.0%)	0.94	59/23432 (0.3%)
1	F	0.42	0/5284	0.96	12/7131 (0.2%)
All	All	0.41	3/45097 (0.0%)	0.92	118/61025 (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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1526	ILE	C-N	7.03	1.47	1.34
1	D	1527	PRO	CB-CG	-5.58	1.22	1.50
1	C	1138	PHE	CA-C	5.14	1.66	1.52

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	971	LEU	CA-CB-CG	13.49	146.33	115.30
1	D	1526	ILE	C-N-CD	-13.29	91.36	120.60
1	D	585	GLY	N-CA-C	12.22	143.64	113.10
1	D	222	LEU	CA-CB-CG	10.98	140.56	115.30
1	D	1527	PRO	C-N-CA	10.94	149.04	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	222	LEU	CA-CB-CG	9.88	138.01	115.30
1	D	1381	LEU	CA-CB-CG	9.12	136.27	115.30
1	F	933	LEU	CA-CB-CG	9.12	136.26	115.30
1	D	1382	GLU	C-N-CA	8.96	144.11	121.70
1	D	1527	PRO	CA-N-CD	-8.85	99.11	111.50
1	D	1079	LEU	CA-CB-CG	8.80	135.54	115.30
1	D	1085	LEU	CB-CG-CD2	8.72	125.83	111.00
1	D	1384	ASN	C-N-CA	8.24	142.31	121.70
1	D	971	LEU	CA-CB-CG	7.96	133.61	115.30
1	D	1478	VAL	CG1-CB-CG2	7.77	123.33	110.90
1	D	1250	ASP	CB-CG-OD1	7.71	125.24	118.30
1	F	1090	LEU	CA-CB-CG	7.71	133.03	115.30
1	D	1423	VAL	CG1-CB-CG2	7.55	122.99	110.90
1	C	2179	TYR	CB-CG-CD2	-7.54	116.47	121.00
1	F	933	LEU	CB-CG-CD1	7.47	123.70	111.00
1	C	2151	LEU	CB-CG-CD2	-7.42	98.39	111.00
1	D	974	ARG	CA-CB-CG	7.41	129.70	113.40
1	C	1079	LEU	CA-CB-CG	7.34	132.18	115.30
1	C	286	TYR	CA-CB-CG	7.17	127.02	113.40
1	C	1367	ASP	CB-CG-OD1	7.14	124.73	118.30
1	C	1359	ARG	CA-CB-CG	7.13	129.08	113.40
1	C	983	MET	CA-CB-CG	7.01	125.22	113.30
1	D	1134	LEU	CB-CA-C	7.00	123.51	110.20
1	B	971	LEU	CA-CB-CG	6.96	131.30	115.30
1	C	1831	LEU	CA-CB-CG	6.88	131.13	115.30
1	D	1391	LEU	CB-CG-CD2	6.87	122.67	111.00
1	C	2179	TYR	CB-CG-CD1	6.85	125.11	121.00
1	D	1288	ILE	CG1-CB-CG2	6.84	126.44	111.40
1	D	983	MET	CA-CB-CG	6.83	124.91	113.30
1	D	1451	LEU	CA-CB-CG	6.80	130.95	115.30
1	D	286	TYR	CA-CB-CG	6.77	126.26	113.40
1	D	1130	ILE	CG1-CB-CG2	6.71	126.16	111.40
1	C	223	LEU	CA-CB-CG	6.67	130.64	115.30
1	D	1449	LEU	CB-CG-CD1	6.61	122.24	111.00
1	D	1124	ILE	CG1-CB-CG2	6.49	125.69	111.40
1	D	223	LEU	CA-CB-CG	6.48	130.20	115.30
1	D	1368	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	B	1158	TYR	CA-CB-CG	6.36	125.49	113.40
1	D	1539	TYR	CB-CG-CD2	-6.33	117.20	121.00
1	C	540	TYR	CB-CG-CD1	-6.24	117.26	121.00
1	F	858	ASP	CB-CG-OD1	6.21	123.89	118.30
1	C	1964	MET	CA-CB-CG	6.16	123.77	113.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	952	LEU	CA-CB-CG	6.16	129.47	115.30
1	C	2151	LEU	CB-CG-CD1	6.14	121.44	111.00
1	D	1964	MET	CA-CB-CG	6.13	123.73	113.30
1	D	897	LEU	CA-CB-CG	6.12	129.37	115.30
1	D	1517	ILE	C-N-CA	6.09	136.94	121.70
1	F	896	LEU	CA-CB-CG	6.08	129.28	115.30
1	F	1449	LEU	CB-CG-CD1	6.03	121.25	111.00
1	C	858	ASP	CB-CG-OD1	6.02	123.72	118.30
1	D	1367	ASP	CB-CG-OD1	5.99	123.69	118.30
1	C	1964	MET	CB-CG-SD	5.98	130.33	112.40
1	D	374	PHE	CB-CG-CD1	-5.97	116.62	120.80
1	D	1504	TRP	CB-CA-C	5.91	122.21	110.40
1	C	889	LEU	CA-CB-CG	5.86	128.77	115.30
1	C	1140	HIS	CB-CA-C	5.78	121.97	110.40
1	C	933	LEU	CA-CB-CG	5.78	128.60	115.30
1	C	588	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	F	1233	MET	CA-CB-CG	5.73	123.04	113.30
1	C	1368	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	D	899	LEU	CA-CB-CG	5.72	128.47	115.30
1	D	637	LEU	CB-CG-CD2	-5.69	101.33	111.00
1	D	111	ARG	CA-CB-CG	5.67	125.87	113.40
1	D	540	TYR	CB-CG-CD1	-5.66	117.61	121.00
1	B	1140	HIS	CB-CA-C	5.62	121.64	110.40
1	C	540	TYR	CB-CG-CD2	5.62	124.37	121.00
1	D	1403	LEU	CA-CB-CG	5.59	128.16	115.30
1	D	1508	VAL	CG1-CB-CG2	-5.57	101.99	110.90
1	D	666	LEU	CB-CG-CD1	5.56	120.45	111.00
1	C	1404	TYR	CA-CB-CG	5.55	123.95	113.40
1	D	1130	ILE	C-N-CA	5.54	135.56	121.70
1	D	1509	LEU	CA-CB-CG	5.53	128.01	115.30
1	B	858	ASP	CB-CG-OD1	5.50	123.25	118.30
1	B	1090	LEU	CA-CB-CG	5.48	127.89	115.30
1	D	374	PHE	CB-CG-CD2	5.47	124.63	120.80
1	B	1318	THR	OG1-CB-CG2	5.46	122.56	110.00
1	D	657	ARG	CA-CB-CG	5.46	125.41	113.40
1	C	1531	PHE	CB-CG-CD2	5.45	124.62	120.80
1	C	815	LEU	CA-CB-CG	5.43	127.80	115.30
1	C	715	LEU	CA-CB-CG	5.42	127.78	115.30
1	D	666	LEU	CB-CG-CD2	-5.41	101.81	111.00
1	B	1442	LEU	CA-CB-CG	5.37	127.65	115.30
1	D	1403	LEU	CB-CG-CD1	5.36	120.12	111.00
1	C	867	TYR	CA-CB-CG	-5.36	103.21	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1232	ARG	CG-CD-NE	5.36	123.05	111.80
1	D	1368	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	B	990	LEU	CA-CB-CG	5.35	127.60	115.30
1	C	896	LEU	CA-CB-CG	5.33	127.56	115.30
1	D	974	ARG	N-CA-CB	5.31	120.15	110.60
1	D	1451	LEU	CB-CG-CD1	5.29	119.99	111.00
1	D	1485	PRO	N-CA-C	5.28	125.83	112.10
1	D	952	LEU	CA-CB-CG	5.26	127.39	115.30
1	B	1079	LEU	CA-CB-CG	5.24	127.36	115.30
1	C	1390	ASP	N-CA-C	-5.24	96.85	111.00
1	D	540	TYR	CB-CG-CD2	5.23	124.14	121.00
1	C	1090	LEU	CA-CB-CG	5.22	127.32	115.30
1	B	1568	LEU	CB-CG-CD2	5.21	119.86	111.00
1	D	1128	THR	OG1-CB-CG2	5.20	121.97	110.00
1	B	1428	ARG	N-CA-CB	-5.19	101.25	110.60
1	D	1250	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	F	1368	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	F	1137	PHE	C-N-CA	-5.16	108.81	121.70
1	D	382	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	C	1233	MET	CA-CB-CG	5.10	121.97	113.30
1	C	1531	PHE	CB-CG-CD1	-5.05	117.26	120.80
1	F	971	LEU	CA-CB-CG	5.05	126.91	115.30
1	B	896	LEU	CA-CB-CG	5.04	126.89	115.30
1	D	561	PHE	CB-CG-CD2	-5.03	117.28	120.80
1	F	909	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	D	561	PHE	CB-CG-CD1	5.02	124.31	120.80
1	C	990	LEU	CA-CB-CG	5.01	126.83	115.30
1	B	1367	ASP	CB-CG-OD1	5.01	122.81	118.30
1	D	896	LEU	CA-CB-CG	5.00	126.81	115.30

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
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
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	108	0
1	C	16940	16841	16897	255	0
1	D	16940	16842	16897	282	0
1	F	5186	5194	5214	113	0
All	All	44178	43991	44142	728	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 8.

All (728) 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:F:1123:LEU:O	1:F:1156:ARG:NH1	2.15	0.80
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
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:B:898:GLU:OE1	1:B:975:TYR:OH	2.01	0.75
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:357:HIS:HD1	1:D:378:CYS:HG	1.38	0.69
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:838:ARG:O	1:C:841:SER:OG	2.10	0.62
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:F:1172:LYS:O	1:F:1175:THR:OG1	2.12	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: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:D:184:ASN:HA	1:D:188:ALA:HB3	1.82	0.61
1:B:1020:ASP:OD1	1:B:1021:MET:N	2.32	0.61
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: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: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:C:404:MET:O	1:C:425:TYR:OH	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:1967:TRP:O	1:D:2025:LYS:NZ	2.32	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:275:SER:OG	1:D:414:MET:O	2.14	0.59
1:D:1836:GLN:OE1	1:D:2028:GLN:NE2	2.36	0.59
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:721:SER:HG	1:D:722:SER:H	1.51	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:1700:LEU:HD22	1:D:1802:MET:HE1	1.87	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:C:1045:ILE:O	1:C:1048:LEU:C	2.43	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:C:569:GLU:OE2	1:C:573:ASN:ND2	2.29	0.56
1:C:418:VAL:O	1:C:419:SER:OG	2.17	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
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:D:287:GLU:O	1:D:290:TYR:C	2.43	0.56
1:C:939:GLN:O	1:C:943:ASN:ND2	2.39	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:1253:MET:HE1	1:C:1318:THR:HG22	1.87	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: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
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: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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:C:982:HIS:O	1:C:986:VAL:HG12	2.08	0.52
1:C:1099:GLN:O	1:C:1102:SER:OG	2.19	0.52
1:C:1359:ARG:N	1:C:1365:GLU:O	2.42	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:B:1124:ILE:C	1:B:1125:LEU:HD22	2.30	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:C:2022:SER:O	1:C:2026:THR:OG1	2.20	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1295:THR:OG1	1:B:1332:ALA:O	2.28	0.51
1:C:724:THR:HG21	1:D:170:LYS:CG	2.40	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: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: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
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:293:ASP:OD1	1:D:293:ASP:N	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: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: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:F:1323:GLY:C	1:F:1324:ILE:HD12	2.32	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:1294:LYS:O	1:C:1295:THR:OG1	2.27	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:B:1578:VAL:HG12	1:B:1580:LYS:H	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:1480:THR:O	1:F:1480:THR:OG1	2.29	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
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:2311:ASN:O	1:D:2314:VAL:HG22	2.13	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:1164:ASN:C	1:F:1165:SER:HG	2.15	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:1071:LYS:O	1:F:1074:ASN:C	2.51	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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: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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1039:LEU:O	1:C:1042:THR:OG1	2.14	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:996:ARG:NH1	1:D:1027:TYR:OH	2.47	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: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:1164:ASN:O	1:D:1165:SER:OG	2.32	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: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:B:1431:ASP:C	1:B:1432:LEU:HD12	2.36	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1480:THR:O	1:C:1480:THR:OG1	2.31	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: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:D:1064:THR:O	1:D:1068:GLN:NE2	2.44	0.45
1:D:1071:LYS:O	1:D:1074:ASN:C	2.55	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: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: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: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:D:1545:TYR:OH	1:D:1567:PRO:O	2.24	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: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:D:1700:LEU:HD22	1:D:1802:MET:HE3	1.96	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:C:529:LEU:H	1:C:540:TYR:HA	1.84	0.43
1:C:1170:GLN:C	1:C:1171:LEU:HD12	2.39	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:1480:THR:O	1:B:1480:THR:OG1	2.28	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: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: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:713:GLY:C	1:C:714:LEU:HD12	2.39	0.42
1:C:1875:MET:N	1:C:1875:MET:SD	2.92	0.42
1:D:1046:ASP:OD2	1:D:1080:ARG:NH1	2.52	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:766:ILE:HG22	1:D:779:TYR:C	2.39	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:287:GLU:O	1:C:290:TYR:C	2.58	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:C:534:ASN:HB3	1:C:537:VAL:HG23	2.01	0.42
1:D:864:MET:O	1:D:1037:LYS:NZ	2.51	0.42
1:D:1845:HIS:C	1:D:1846:LEU:HD22	2.40	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:527:GLN:CD	1:D:529:LEU:HD21	2.40	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:D:894:LEU:HB3	1:D:895:PRO:HD3	2.00	0.42
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:939:GLN:CD	1:F:943:ASN:HD21	2.19	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: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:1474:PHE:C	1:D:1475:LEU:HD12	2.41	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: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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:593:TYR:HA	1:C:596:LYS:HZ2	1.86	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:1774:ASP:O	1:C:1779:ARG:NH1	2.54	0.40
1:D:612:TRP:C	1:D:616:LEU:HD23	2.42	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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%)	15	54
1	C	2107/2407 (88%)	1908 (91%)	191 (9%)	8 (0%)	34	72
1	D	2107/2407 (88%)	1901 (90%)	193 (9%)	13 (1%)	25	65
1	F	620/2407 (26%)	521 (84%)	91 (15%)	8 (1%)	12	48
All	All	5443/9628 (56%)	4852 (89%)	556 (10%)	35 (1%)	29	65

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1087	ALA
1	B	1304	LEU
1	B	1365	GLU
1	C	1304	LEU
1	D	1527	PRO
1	F	1087	ALA
1	C	211	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 [i](#)

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%)	552 (97%)	19 (3%)	38 61
1	C	1855/2108 (88%)	1806 (97%)	49 (3%)	46 67
1	D	1855/2108 (88%)	1800 (97%)	55 (3%)	41 63

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	579/2108 (28%)	552 (95%)	27 (5%)	26	52
All	All	4860/8432 (58%)	4710 (97%)	150 (3%)	43	62

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	857	LEU
1	B	889	LEU
1	B	897	LEU
1	B	947	SER
1	B	1090	LEU
1	B	1309	ARG
1	B	1354	LYS
1	B	1359	ARG
1	B	1368	ARG
1	B	1381	LEU
1	B	1417	THR
1	B	1438	SER
1	B	1444	ASN
1	B	1463	ASN
1	B	1531	PHE
1	B	1534	ASN
1	B	1540	LEU
1	B	1546	LYS
1	B	1577	TYR
1	C	223	LEU
1	C	529	LEU
1	C	637	LEU
1	C	652	LEU
1	C	655	LEU
1	C	698	ASN
1	C	705	ASP
1	C	828	GLN
1	C	875	SER
1	C	897	LEU
1	C	915	GLU
1	C	933	LEU
1	C	947	SER
1	C	954	ARG
1	C	983	MET
1	C	1008	LYS
1	C	1017	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1065	GLU
1	C	1066	LEU
1	C	1079	LEU
1	C	1090	LEU
1	C	1096	ARG
1	C	1250	ASP
1	C	1354	LYS
1	C	1359	ARG
1	C	1381	LEU
1	C	1417	THR
1	C	1438	SER
1	C	1444	ASN
1	C	1463	ASN
1	C	1531	PHE
1	C	1534	ASN
1	C	1540	LEU
1	C	1649	ASN
1	C	1848	LEU
1	C	1875	MET
1	C	1964	MET
1	C	1970	THR
1	C	2003	ASN
1	C	2116	SER
1	C	2135	LYS
1	C	2137	MET
1	C	2151	LEU
1	C	2221	ARG
1	C	2240	THR
1	C	2297	ARG
1	C	2326	ILE
1	C	2327	SER
1	C	2333	GLU
1	D	223	LEU
1	D	439	ASN
1	D	451	MET
1	D	532	ARG
1	D	652	LEU
1	D	655	LEU
1	D	657	ARG
1	D	698	ASN
1	D	715	LEU
1	D	747	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	791	LEU
1	D	897	LEU
1	D	899	LEU
1	D	915	GLU
1	D	947	SER
1	D	954	ARG
1	D	974	ARG
1	D	1017	ASN
1	D	1079	LEU
1	D	1096	ARG
1	D	1170	GLN
1	D	1175	THR
1	D	1233	MET
1	D	1236	MET
1	D	1250	ASP
1	D	1354	LYS
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	1444	ASN
1	D	1449	LEU
1	D	1451	LEU
1	D	1463	ASN
1	D	1475	LEU
1	D	1478	VAL
1	D	1513	LEU
1	D	1531	PHE
1	D	1534	ASN
1	D	1540	LEU
1	D	1575	THR
1	D	1649	ASN
1	D	1875	MET
1	D	1964	MET
1	D	1970	THR
1	D	2003	ASN
1	D	2116	SER
1	D	2135	LYS
1	D	2221	ARG
1	D	2240	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	2297	ARG
1	D	2326	ILE
1	D	2327	SER
1	F	851	ARG
1	F	864	MET
1	F	897	LEU
1	F	899	LEU
1	F	909	ARG
1	F	915	GLU
1	F	933	LEU
1	F	947	SER
1	F	1065	GLU
1	F	1066	LEU
1	F	1090	LEU
1	F	1096	ARG
1	F	1244	ASP
1	F	1250	ASP
1	F	1289	LEU
1	F	1319	LEU
1	F	1326	ARG
1	F	1354	LYS
1	F	1381	LEU
1	F	1417	THR
1	F	1438	SER
1	F	1444	ASN
1	F	1449	LEU
1	F	1463	ASN
1	F	1478	VAL
1	F	1534	ASN
1	F	1540	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
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	1114	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1287	HIS
1	B	1313	GLN
1	B	1315	ASN
1	B	1333	GLN
1	B	1388	ASN
1	B	1443	GLN
1	B	1444	ASN
1	B	1463	ASN
1	B	1476	ASN
1	B	1534	ASN
1	B	1565	GLN
1	B	1569	HIS
1	C	165	ASN
1	C	225	ASN
1	C	280	ASN
1	C	354	GLN
1	C	698	ASN
1	C	859	ASN
1	C	862	ASN
1	C	943	ASN
1	C	966	GLN
1	C	1017	ASN
1	C	1026	ASN
1	C	1119	ASN
1	C	1429	HIS
1	C	1443	GLN
1	C	1444	ASN
1	C	1462	ASN
1	C	1463	ASN
1	C	1476	ASN
1	C	1534	ASN
1	C	2003	ASN
1	C	2028	GLN
1	C	2045	ASN
1	D	225	ASN
1	D	280	ASN
1	D	354	GLN
1	D	698	ASN
1	D	707	HIS
1	D	862	ASN
1	D	943	ASN
1	D	964	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	966	GLN
1	D	1017	ASN
1	D	1026	ASN
1	D	1114	GLN
1	D	1443	GLN
1	D	1444	ASN
1	D	1463	ASN
1	D	1534	ASN
1	D	1946	GLN
1	D	2003	ASN
1	D	2028	GLN
1	D	2045	ASN
1	F	859	ASN
1	F	862	ASN
1	F	865	ASN
1	F	1170	GLN
1	F	1181	GLN
1	F	1402	HIS
1	F	1444	ASN
1	F	1462	ASN
1	F	1463	ASN
1	F	1534	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

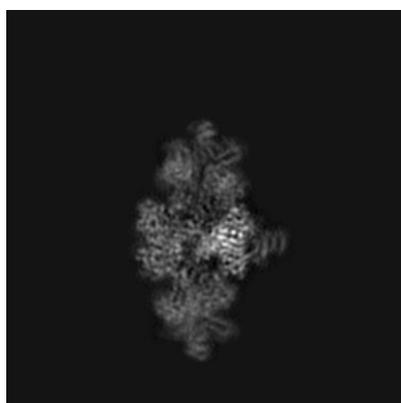
6 Map visualisation [i](#)

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

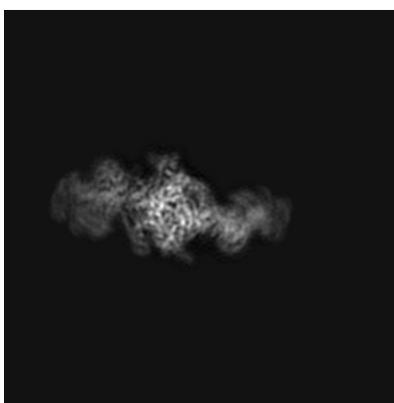
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

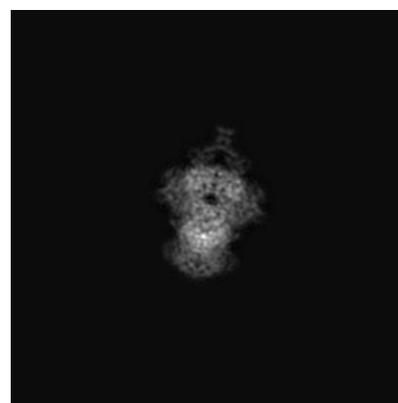
6.1.1 Primary map



X



Y



Z

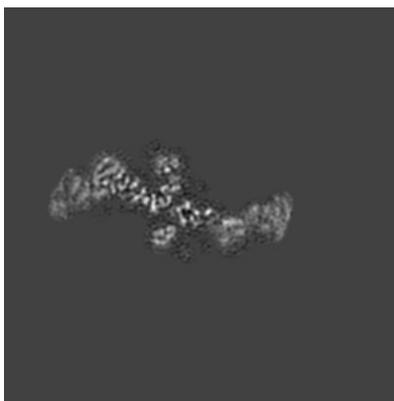
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 225



Y Index: 225

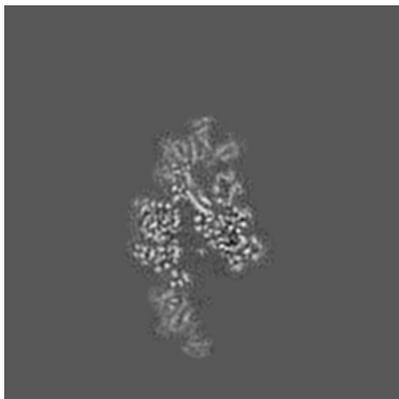


Z Index: 225

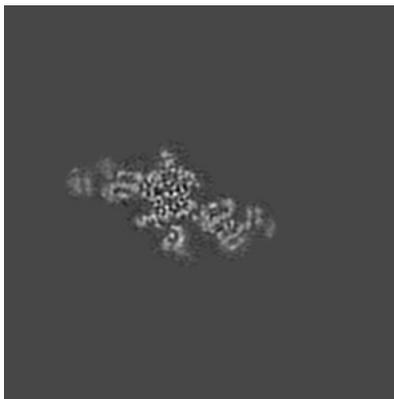
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

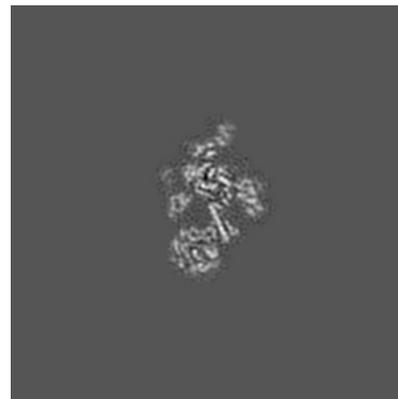
6.3.1 Primary map



X Index: 217



Y Index: 247



Z Index: 177

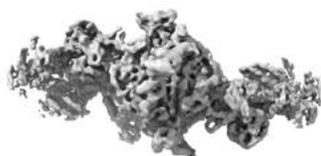
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 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.

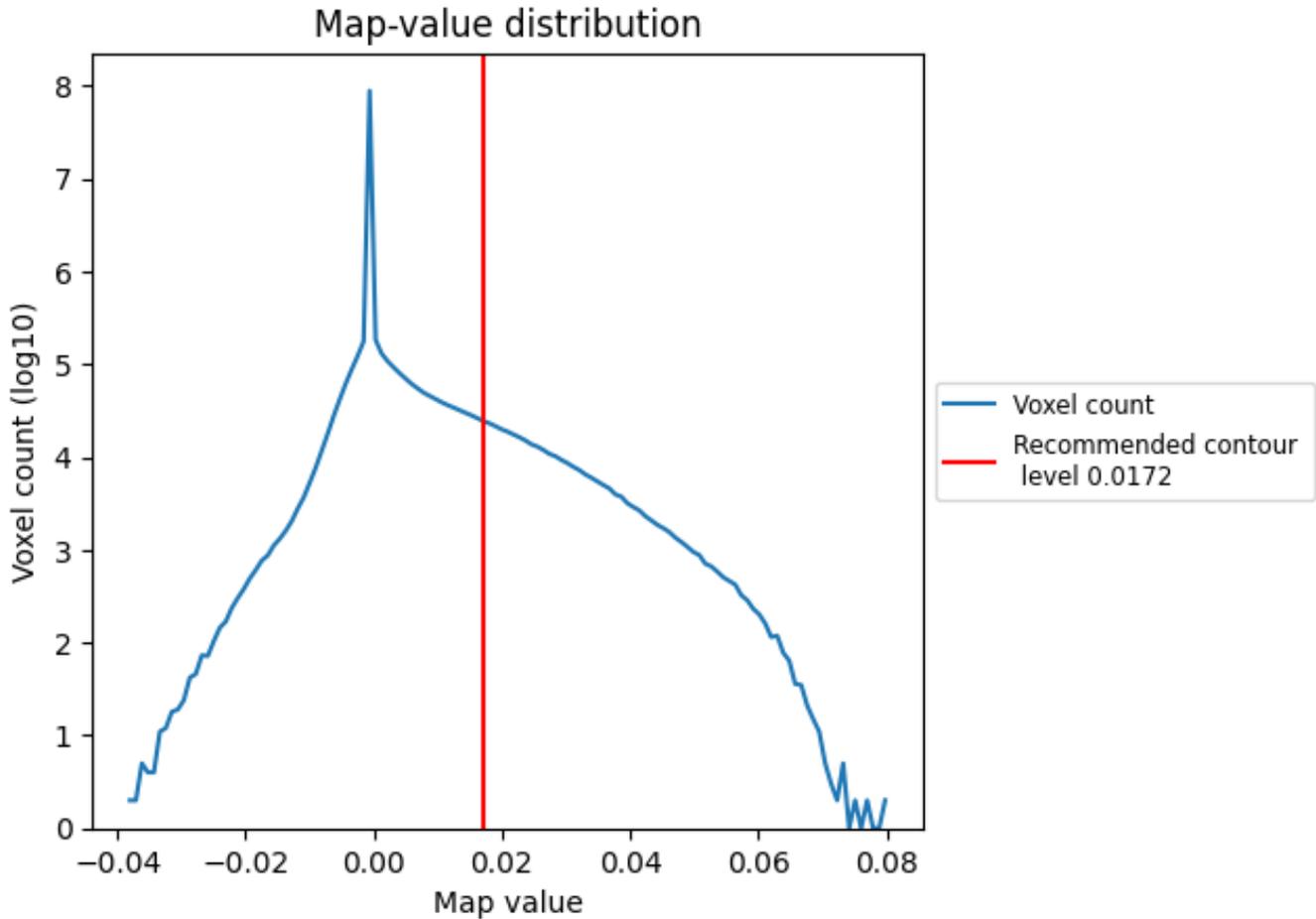
6.5 Mask visualisation

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

7 Map analysis [i](#)

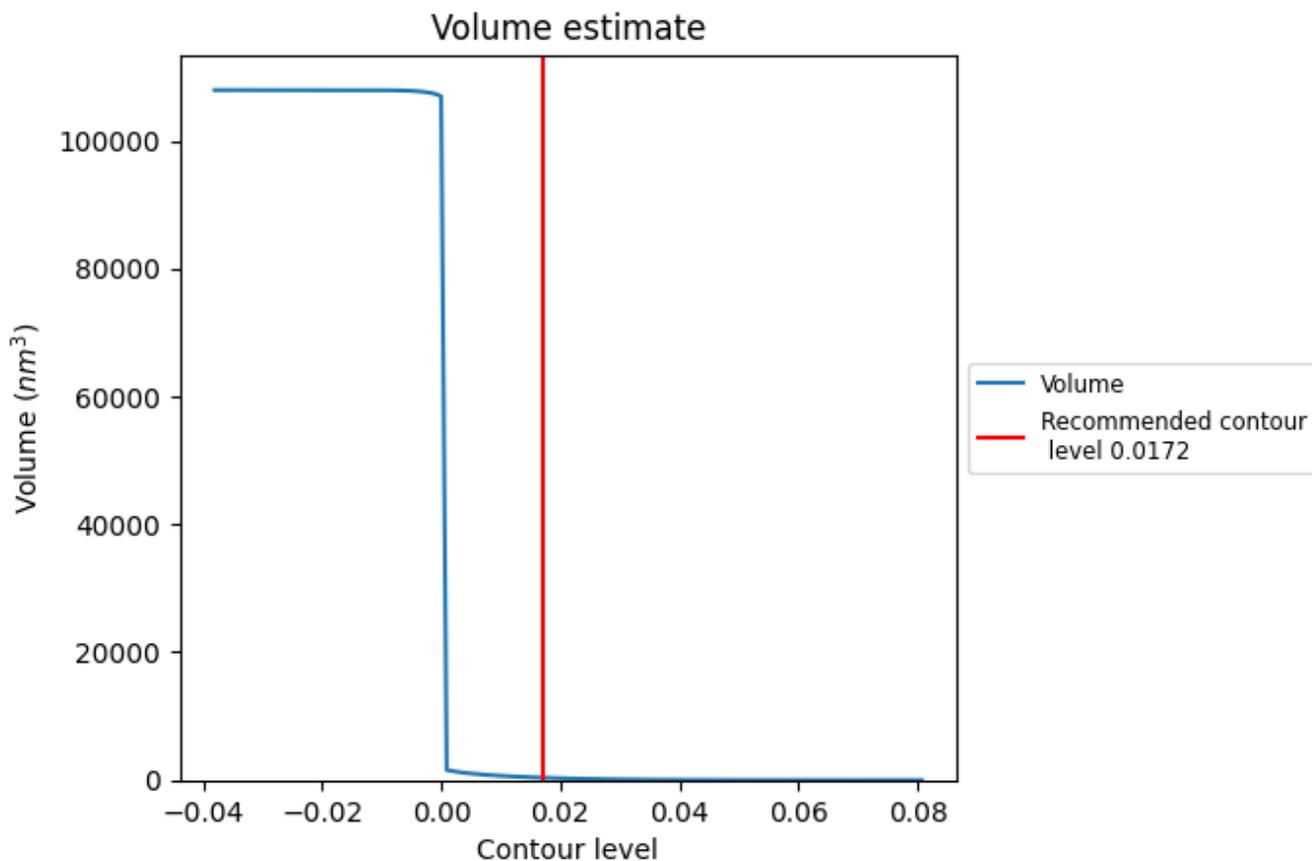
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

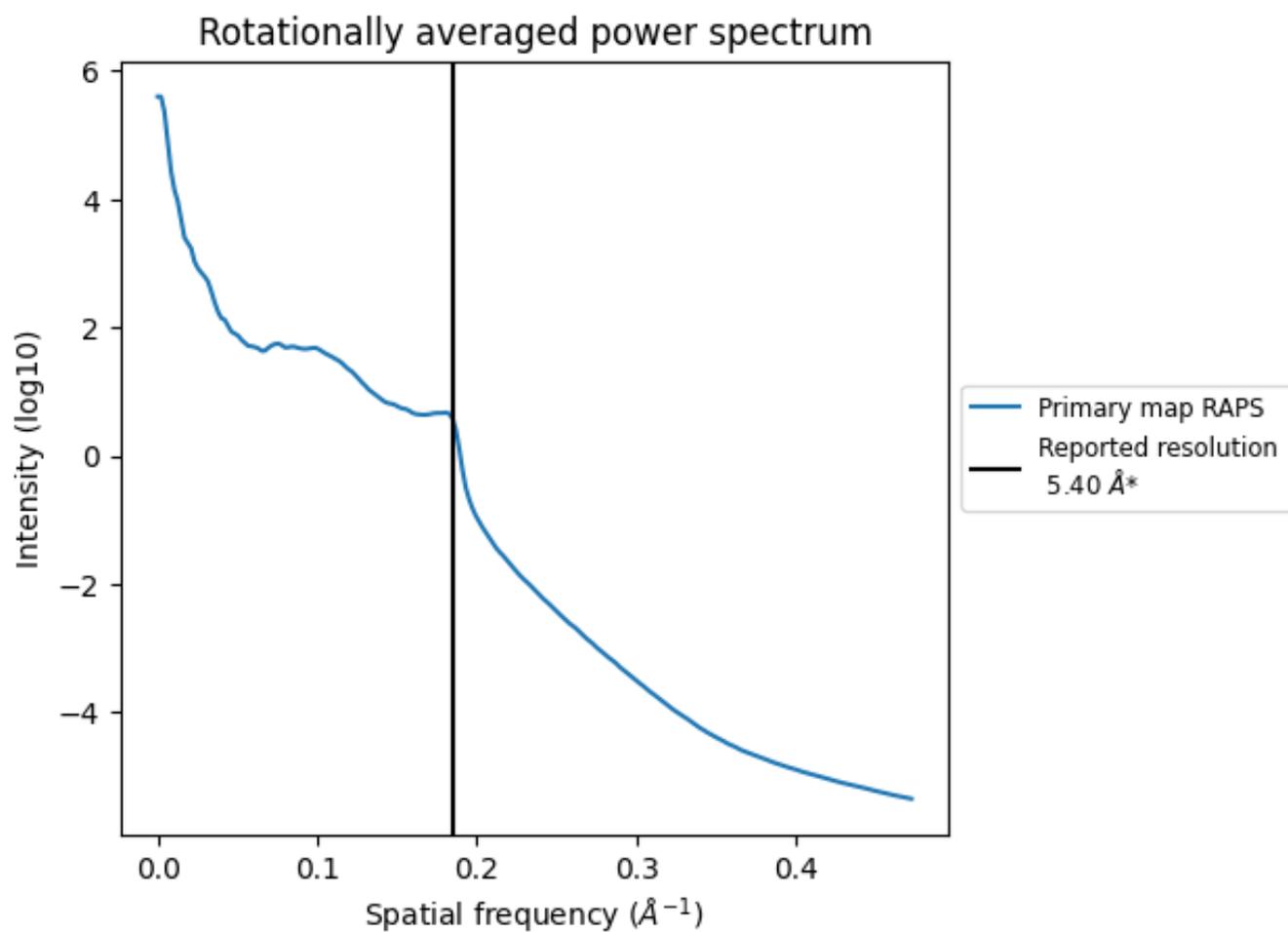
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 370 nm^3 ; 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.185\AA^{-1}

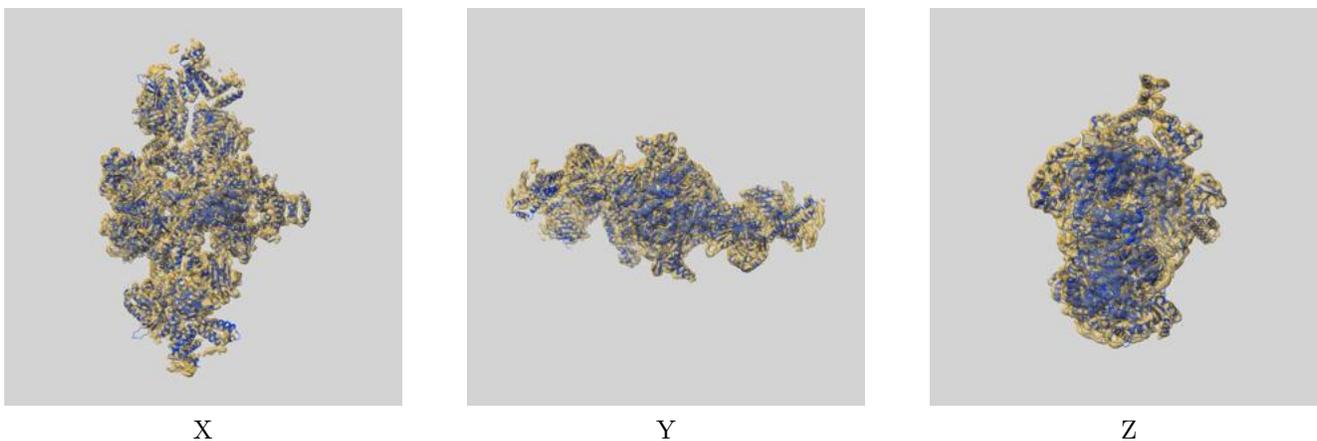
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

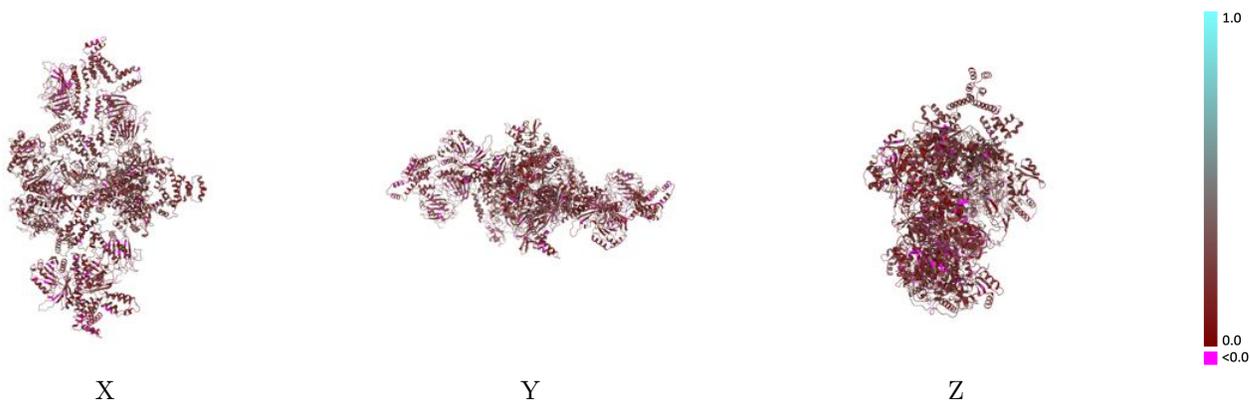
This section contains information regarding the fit between EMDB map EMD-4342 and PDB model 6G2D. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



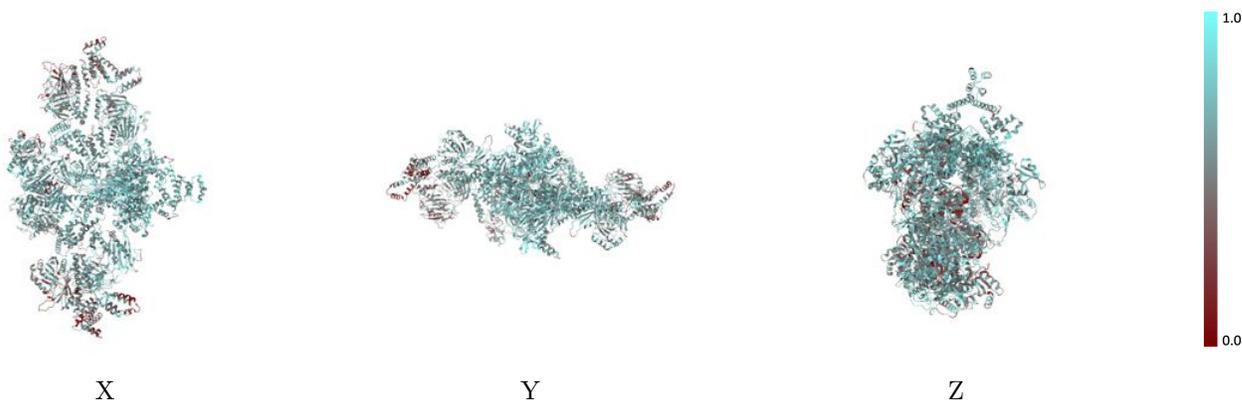
The images above show the 3D surface view of the map at the recommended contour level 0.0172 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



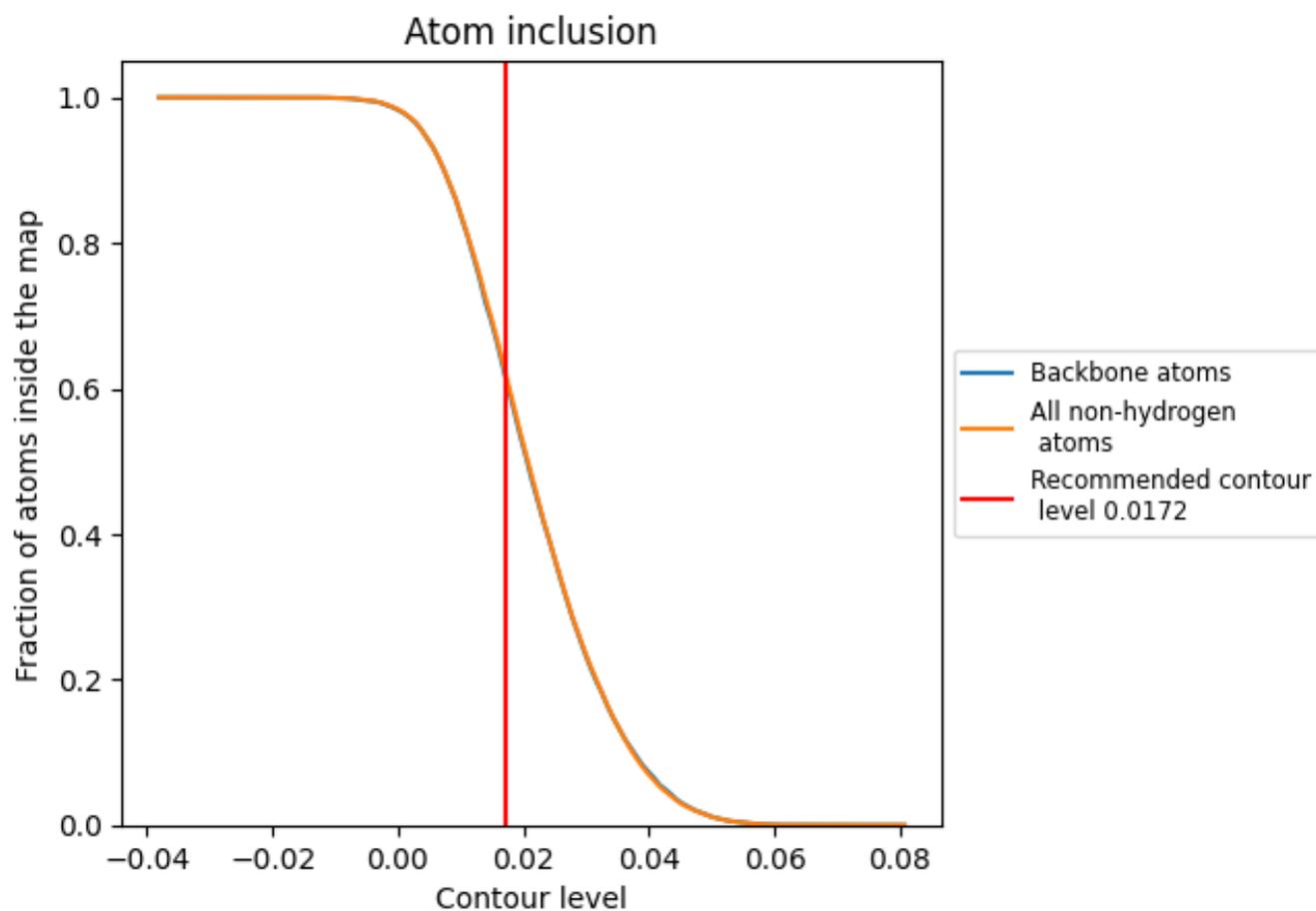
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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	 0.6199	 0.2160
B	 0.5194	 0.1810
C	 0.6712	 0.2260
D	 0.6747	 0.2280
F	 0.4604	 0.1760

