



Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 01:56 AM JST

PDB ID : 7CXM
EMDB ID : EMD-30492
Title : Architecture of a SARS-CoV-2 mini replication and transcription complex
Authors : Yan, L.; Zhang, Y.; Ge, J.; Zheng, L.; Gao, Y.; Wang, T.; Jia, Z.; Wang, H.;
Huang, Y.; Li, M.; Wang, Q.; Rao, Z.; Lou, Z.
Deposited on : 2020-09-02
Resolution : 2.90 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) : 2.31.3

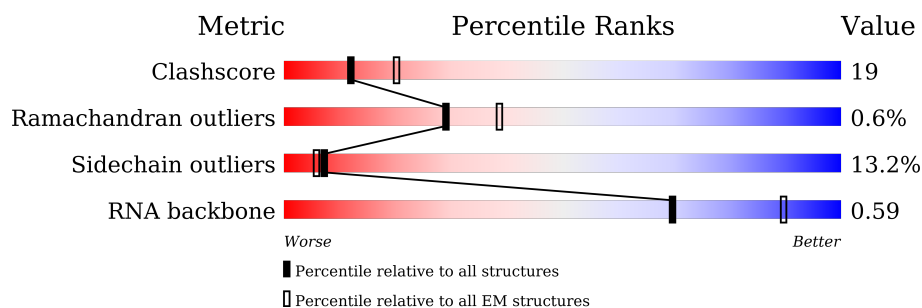
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	942	 73% 20% 5% • •
2	B	198	 6% 59% 31% 5% • 6%
2	D	198	 59% 29% 5% • 6%
3	C	83	 61% 24% • 13%
4	I	25	 40% 52% 8%
5	J	58	 28% 17% 55%
6	L	6	 33% 83% 17%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	E	601	<div><div></div><div>6%</div><div>50%</div><div>41%</div><div>8%</div><div>.</div></div>
7	F	601	<div><div></div><div>35%</div><div>38%</div><div>50%</div><div>10%</div><div>..</div></div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 21295 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	926	Total	C	N	O	S	0	0
			7458	4763	1252	1389	54		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	910	ASN	ASP	engineered mutation	UNP P0DTD1
A	933	HIS	-	expression tag	UNP P0DTD1
A	934	HIS	-	expression tag	UNP P0DTD1
A	935	HIS	-	expression tag	UNP P0DTD1
A	936	HIS	-	expression tag	UNP P0DTD1
A	937	HIS	-	expression tag	UNP P0DTD1
A	938	HIS	-	expression tag	UNP P0DTD1
A	939	HIS	-	expression tag	UNP P0DTD1
A	940	HIS	-	expression tag	UNP P0DTD1
A	941	HIS	-	expression tag	UNP P0DTD1
A	942	HIS	-	expression tag	UNP P0DTD1

- Molecule 2 is a protein called Non-structural protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	187	Total	C	N	O	S	0	0
			1396	872	240	273	11		
2	D	186	Total	C	N	O	S	0	0
			1414	889	242	272	11		

- Molecule 3 is a protein called Non-structural protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	72	Total	C	N	O	S	0	0
			553	349	91	107	6		

- Molecule 4 is a RNA chain called RNA (25-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	25	Total	C	N	O	P	0	0
			545	242	105	173	25		

- Molecule 5 is a RNA chain called RNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	26	Total	C	N	O	P	0	0
			545	244	92	183	26		

- Molecule 6 is a RNA chain called RNA (5'-R(P*UP*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	6	Total	C	N	O	P	0	0
			128	58	24	40	6		

- Molecule 7 is a protein called Helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	596	Total	C	N	O	S	0	0
			4630	2940	787	869	34		
7	E	596	Total	C	N	O	S	0	0
			4618	2935	781	869	33		

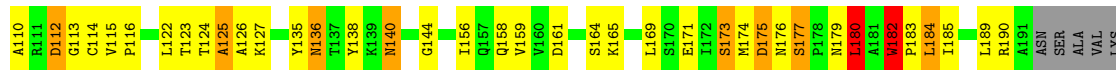
- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
8	A	2	Total	Zn	0
			2	2	
8	F	3	Total	Zn	0
			3	3	
8	E	3	Total	Zn	0
			3	3	



• Molecule 2: Non-structural protein 8

Chain D: 59% 29% 5% • 6%



• Molecule 3: Non-structural protein 7

Chain C: 61% 24% • 13%



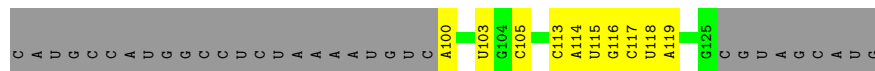
• Molecule 4: RNA (25-MER)

Chain I: 40% 52% 8%



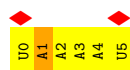
• Molecule 5: RNA (26-MER)

Chain J: 28% 17% 55%



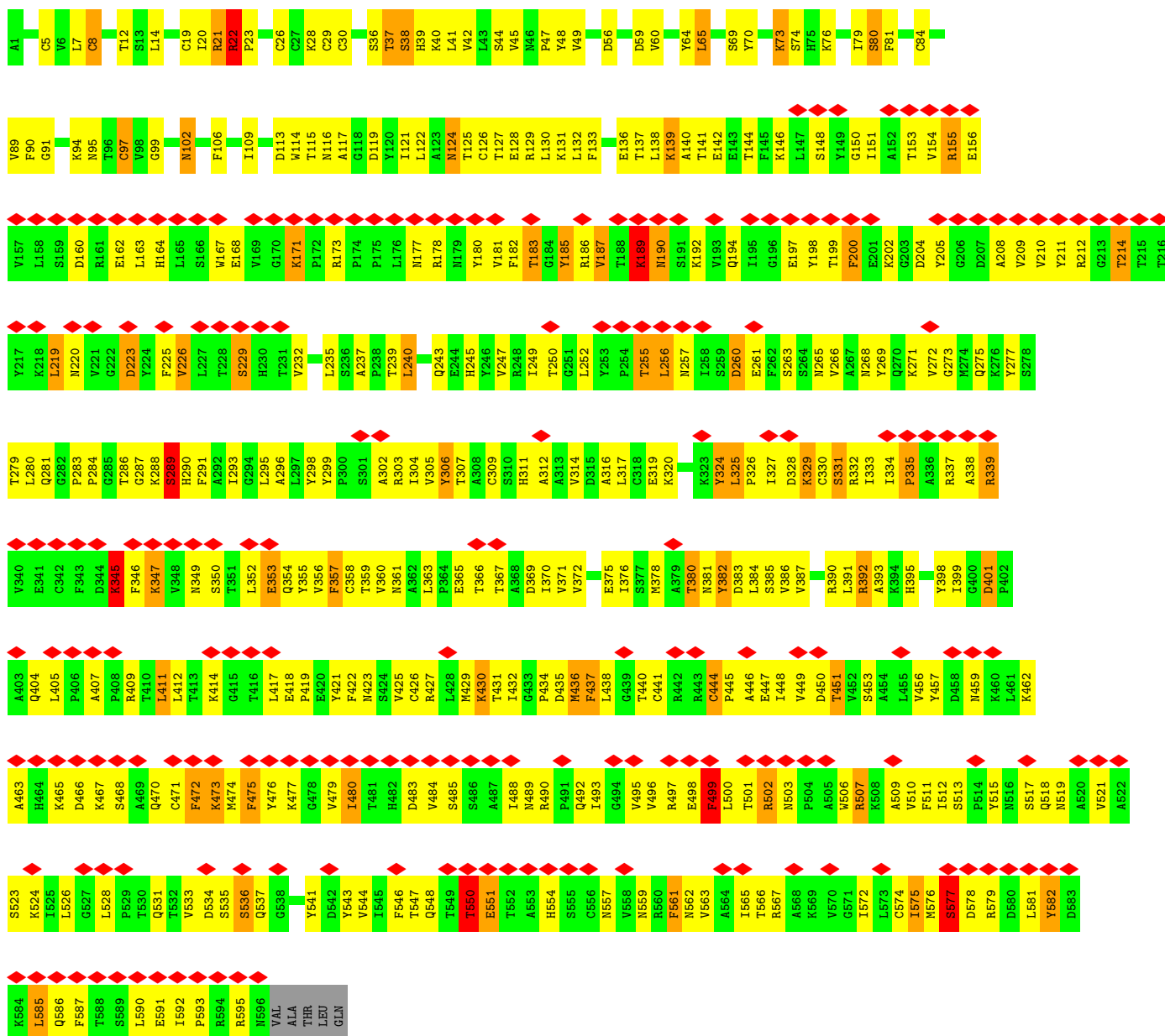
• Molecule 6: RNA (5'-R(P*UP*UP*UP*UP*UP*U)-3')

Chain L: 33% 83% 17%

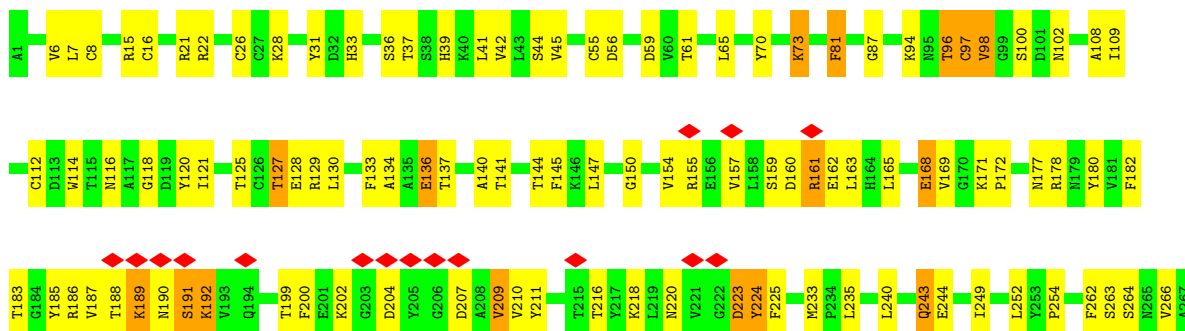


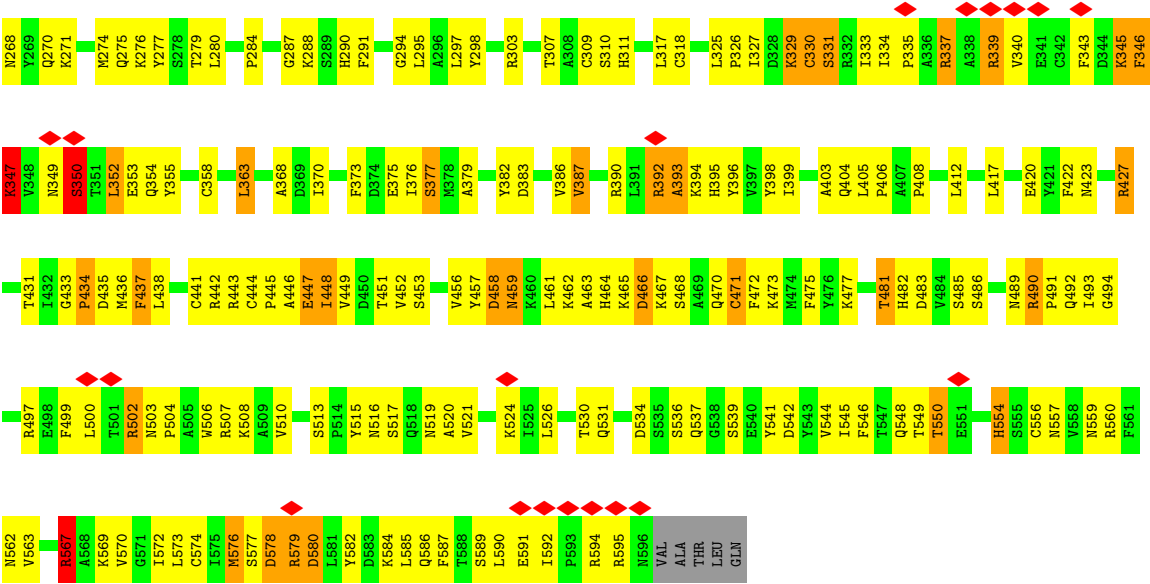
• Molecule 7: Helicase

Chain F: 35% 38% 50% 10% ••



• Molecule 7: Helicase





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	384727	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.006	Depositor
Minimum map value	-0.890	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.25	Depositor
Map size (\AA)	367.36, 367.36, 367.36	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.71	6/7647 (0.1%)	0.84	55/10379 (0.5%)
2	B	0.47	0/1414	0.88	12/1922 (0.6%)
2	D	0.54	0/1433	1.06	15/1944 (0.8%)
3	C	0.43	0/556	0.66	1/749 (0.1%)
4	I	0.61	0/611	0.79	0/953
5	J	0.65	0/606	0.80	0/940
6	L	0.24	0/143	0.70	0/220
7	E	0.32	0/4722	0.77	17/6430 (0.3%)
7	F	0.29	0/4734	0.78	25/6443 (0.4%)
All	All	0.53	6/21866 (0.0%)	0.83	125/29980 (0.4%)

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	A	0	1
7	F	0	1
All	All	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	346	TYR	CE1-CZ	-8.16	1.27	1.38
1	A	273	TYR	CE1-CZ	-6.84	1.29	1.38
1	A	606	TYR	CE1-CZ	-5.73	1.31	1.38
1	A	346	TYR	CG-CD1	-5.30	1.32	1.39
1	A	346	TYR	CB-CG	-5.13	1.44	1.51
1	A	606	TYR	CE2-CZ	-5.04	1.31	1.38

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	126	ALA	N-CA-CB	-17.75	85.25	110.10
2	D	125	ALA	CB-CA-C	-16.89	84.76	110.10
7	E	347	LYS	N-CA-CB	15.21	137.99	110.60
2	B	142	CYS	N-CA-C	-13.70	74.01	111.00
7	E	458	ASP	CB-CA-C	13.24	136.87	110.40
1	A	904	SER	N-CA-CB	-12.66	91.51	110.50
1	A	345	GLY	N-CA-C	12.26	143.74	113.10
7	E	459	ASN	N-CA-CB	-12.08	88.85	110.60
1	A	665	GLU	N-CA-CB	12.02	132.23	110.60
7	F	36	SER	CB-CA-C	-12.01	87.28	110.10
7	E	458	ASP	N-CA-C	-11.98	78.65	111.00
1	A	664	SER	N-CA-C	-11.57	79.76	111.00
1	A	346	TYR	CB-CA-C	-11.55	87.30	110.40
1	A	344	THR	N-CA-C	-11.53	79.88	111.00
7	E	393	ALA	N-CA-CB	11.38	126.03	110.10
7	F	36	SER	N-CA-C	11.00	140.69	111.00
7	E	346	PHE	N-CA-C	10.87	140.35	111.00
1	A	344	THR	CB-CA-C	10.46	139.85	111.60
2	D	125	ALA	N-CA-C	10.42	139.14	111.00
7	F	189	LYS	CB-CA-C	10.38	131.16	110.40
1	A	608	ASP	N-CA-C	-10.36	83.03	111.00
1	A	81	GLN	CB-CA-C	-10.28	89.84	110.40
1	A	383	ALA	CB-CA-C	10.13	125.29	110.10
1	A	397	SER	CB-CA-C	-10.09	90.92	110.10
7	F	21	ARG	N-CA-C	-9.99	84.03	111.00
7	F	350	SER	N-CA-CB	-9.83	95.75	110.50
7	E	392	ARG	CB-CA-C	9.43	129.26	110.40
2	B	182	TRP	N-CA-C	9.33	136.18	111.00
2	D	182	TRP	N-CA-C	9.20	135.85	111.00
7	F	190	ASN	N-CA-CB	-8.89	94.59	110.60
7	E	443	ARG	N-CA-CB	-8.78	94.80	110.60
2	D	85	SER	N-CA-CB	-8.64	97.53	110.50
2	D	184	LEU	CB-CA-C	-8.61	93.85	110.20
2	B	142	CYS	N-CA-CB	8.57	126.03	110.60
1	A	119	LEU	CB-CA-C	-8.52	94.01	110.20
7	F	37	THR	N-CA-CB	8.52	126.49	110.30
7	F	189	LYS	N-CA-C	-8.49	88.08	111.00
7	F	345	LYS	N-CA-CB	-8.40	95.48	110.60
1	A	50	LYS	CB-CA-C	-8.31	93.79	110.40
7	F	289	SER	CB-CA-C	-8.24	94.44	110.10
1	A	904	SER	N-CA-C	8.22	133.20	111.00
1	A	40	ASP	CB-CA-C	8.03	126.46	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	384	SER	N-CA-CB	-8.00	98.50	110.50
7	E	442	ARG	CB-CA-C	7.88	126.15	110.40
1	A	41	LYS	N-CA-CB	-7.83	96.50	110.60
1	A	929	THR	N-CA-CB	7.65	124.83	110.30
1	A	292	GLN	CB-CA-C	7.64	125.68	110.40
7	E	191	SER	N-CA-C	7.60	131.52	111.00
7	F	436	MET	CB-CA-C	7.45	125.31	110.40
2	D	183	PRO	N-CA-C	-7.40	92.86	112.10
7	F	437	PHE	N-CA-CB	7.27	123.69	110.60
1	A	382	ALA	CB-CA-C	-7.26	99.20	110.10
2	B	41	SER	CB-CA-C	-7.22	96.37	110.10
2	B	7	SER	N-CA-CB	-7.21	99.68	110.50
7	E	392	ARG	N-CA-C	-7.20	91.55	111.00
2	B	143	ASP	N-CA-C	-7.12	91.77	111.00
1	A	12	CYS	CA-CB-SG	-7.11	101.20	114.00
1	A	51	THR	N-CA-CB	-7.08	96.84	110.30
2	B	142	CYS	CB-CA-C	7.06	124.52	110.40
7	E	526	LEU	CB-CA-C	-7.02	96.86	110.20
7	E	434	PRO	N-CA-C	-6.96	94.01	112.10
7	E	346	PHE	CB-CA-C	-6.88	96.65	110.40
1	A	608	ASP	CB-CA-C	6.85	124.09	110.40
1	A	777	ALA	CB-CA-C	6.84	120.35	110.10
1	A	609	VAL	N-CA-C	-6.83	92.57	111.00
2	D	9	LEU	N-CA-C	-6.79	92.66	111.00
7	F	22	ARG	N-CA-CB	-6.61	98.71	110.60
2	D	180	LEU	CB-CG-CD2	6.58	122.18	111.00
1	A	346	TYR	N-CA-C	6.57	128.73	111.00
7	F	37	THR	N-CA-C	-6.56	93.30	111.00
7	F	349	ASN	CB-CA-C	6.53	123.47	110.40
1	A	384	SER	N-CA-C	6.51	128.57	111.00
1	A	107	ASP	CB-CA-C	-6.47	97.46	110.40
1	A	928	HIS	N-CA-C	-6.40	93.71	111.00
1	A	648	LEU	N-CA-C	6.36	128.16	111.00
1	A	346	TYR	N-CA-CB	-6.33	99.21	110.60
1	A	609	VAL	N-CA-CB	6.28	125.32	111.50
2	D	8	SER	N-CA-C	-6.22	94.21	111.00
1	A	120	THR	N-CA-CB	-6.21	98.50	110.30
2	B	6	PHE	CB-CA-C	6.18	122.77	110.40
2	B	141	THR	N-CA-C	6.17	127.64	111.00
1	A	403	ASN	N-CA-C	6.15	127.61	111.00
1	A	927	PRO	N-CA-C	6.15	128.09	112.10
2	D	114	CYS	N-CA-C	-6.15	94.40	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	499	PHE	N-CA-CB	-6.14	99.55	110.60
1	A	402	THR	CB-CA-C	-6.14	95.03	111.60
7	E	443	ARG	N-CA-C	6.11	127.51	111.00
1	A	903	TYR	N-CA-C	-6.11	94.51	111.00
2	D	156	ILE	CB-CA-C	-6.10	99.39	111.60
2	D	179	ASN	N-CA-C	6.06	127.37	111.00
7	F	436	MET	N-CA-C	-5.92	95.02	111.00
1	A	647	SER	CB-CA-C	-5.90	98.89	110.10
1	A	257	VAL	N-CA-C	5.90	126.92	111.00
2	B	143	ASP	N-CA-CB	5.89	121.20	110.60
7	F	480	ILE	CB-CA-C	-5.79	100.03	111.60
1	A	903	TYR	CB-CA-C	-5.77	98.86	110.40
7	F	550	THR	CB-CA-C	-5.76	96.04	111.60
1	A	292	GLN	N-CA-C	-5.75	95.47	111.00
1	A	258	ASP	C-N-CA	5.71	135.98	121.70
1	A	403	ASN	N-CA-CB	-5.68	100.38	110.60
1	A	41	LYS	N-CA-C	5.68	126.32	111.00
2	B	173	SER	CB-CA-C	-5.63	99.41	110.10
7	F	345	LYS	N-CA-C	5.60	126.11	111.00
7	F	551	GLU	N-CA-CB	-5.59	100.54	110.60
1	A	108	GLY	N-CA-C	-5.59	99.12	113.10
2	D	179	ASN	N-CA-CB	-5.54	100.62	110.60
1	A	398	VAL	N-CA-CB	-5.54	99.32	111.50
1	A	753	PHE	N-CA-CB	-5.53	100.65	110.60
3	C	25	SER	N-CA-CB	-5.52	102.21	110.50
7	F	350	SER	N-CA-C	5.44	125.70	111.00
1	A	17	ALA	N-CA-CB	-5.43	102.49	110.10
1	A	398	VAL	N-CA-C	5.42	125.63	111.00
1	A	797	ALA	N-CA-CB	-5.32	102.66	110.10
7	F	551	GLU	N-CA-C	5.31	125.34	111.00
2	B	174	MET	N-CA-C	5.30	125.30	111.00
7	E	189	LYS	C-N-CA	5.28	134.89	121.70
1	A	850	THR	N-CA-C	-5.26	96.79	111.00
7	F	499	PHE	N-CA-C	5.22	125.10	111.00
1	A	51	THR	N-CA-C	5.18	124.98	111.00
1	A	665	GLU	N-CA-C	-5.17	97.03	111.00
1	A	235	ASP	N-CA-C	5.15	124.91	111.00
1	A	96	VAL	N-CA-C	-5.14	97.11	111.00
7	E	567	ARG	N-CA-C	5.14	124.87	111.00
2	D	158	GLN	CB-CA-C	5.13	120.67	110.40
7	F	8	CYS	N-CA-CB	-5.06	101.50	110.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	17	ALA	Peptide
7	F	189	LYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7458	0	7193	142	0
2	B	1396	0	1365	44	0
2	D	1414	0	1416	46	0
3	C	553	0	585	12	0
4	I	545	0	272	20	0
5	J	545	0	281	10	0
6	L	128	0	65	4	0
7	E	4618	0	4564	222	0
7	F	4630	0	4585	316	0
8	A	2	0	0	0	0
8	E	3	0	0	0	0
8	F	3	0	0	0	0
All	All	21295	0	20326	795	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 19.

All (795) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:HIS:CD2	1:A:76:THR:CG2	1.84	1.58
1:A:75:HIS:CD2	1:A:76:THR:HG23	1.53	1.35
7:F:434:PRO:HB2	7:F:436:MET:O	1.22	1.30
1:A:260:ASP:OD2	1:A:263:LYS:NZ	1.71	1.22
2:D:182:TRP:HE3	2:D:182:TRP:O	1.31	1.14
7:E:8:CYS:SG	7:E:98:VAL:O	2.06	1.13
1:A:75:HIS:NE2	1:A:76:THR:CG2	2.11	1.13
1:A:75:HIS:CD2	1:A:76:THR:HG22	1.66	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:5:CYS:SG	7:F:26:CYS:HB3	1.93	1.07
7:E:189:LYS:HB2	7:E:190:ASN:HB2	1.38	1.04
2:B:182:TRP:HE3	2:B:182:TRP:O	1.39	1.04
7:F:189:LYS:H	7:F:190:ASN:HB2	1.13	1.04
7:F:330:CYS:O	7:F:356:VAL:HA	1.59	1.00
1:A:851:ASP:OD2	1:A:854:LEU:CD1	2.09	0.99
1:A:900:LEU:O	1:A:903:TYR:O	1.82	0.97
7:F:5:CYS:SG	7:F:26:CYS:N	2.37	0.96
7:F:19:CYS:SG	7:F:39:HIS:HE1	1.90	0.94
1:A:75:HIS:NE2	1:A:76:THR:HG21	1.81	0.94
1:A:851:ASP:OD2	1:A:854:LEU:HD11	1.66	0.94
2:D:182:TRP:O	2:D:182:TRP:CE3	2.20	0.93
2:D:180:LEU:HD22	2:D:180:LEU:H	1.35	0.90
1:A:540:THR:OG1	1:A:665:GLU:OE1	1.90	0.89
2:B:182:TRP:O	2:B:182:TRP:CE3	2.25	0.89
7:F:434:PRO:CB	7:F:436:MET:O	2.16	0.89
7:F:498:GLU:O	7:F:502:ARG:NE	2.05	0.87
7:F:5:CYS:SG	7:F:26:CYS:CB	2.62	0.87
7:F:311:HIS:HE1	7:F:334:ILE:HD11	1.39	0.86
7:F:5:CYS:SG	7:F:26:CYS:CA	2.64	0.86
7:F:474:MET:HA	7:F:575:ILE:HA	1.59	0.83
7:F:426:CYS:HA	7:F:429:MET:HG2	1.62	0.82
7:F:189:LYS:N	7:F:190:ASN:HB2	1.93	0.81
7:F:401:ASP:HB3	7:F:404:GLN:HB2	1.59	0.81
7:F:177:ASN:HB3	7:F:180:TYR:HB2	1.61	0.81
7:F:239:THR:HG23	7:F:240:LEU:HD23	1.62	0.80
7:E:459:ASN:ND2	7:E:459:ASN:H	1.79	0.80
1:A:909:ASN:O	1:A:909:ASN:ND2	2.14	0.80
7:E:7:LEU:HB3	7:E:100:SER:OG	1.82	0.79
7:E:96:THR:O	7:E:96:THR:HG23	1.79	0.79
7:F:330:CYS:HB2	7:F:353:GLU:HG3	1.64	0.79
1:A:75:HIS:HD2	1:A:76:THR:HG23	0.94	0.79
2:D:180:LEU:H	2:D:180:LEU:CD2	1.91	0.78
6:L:0:U:H5'	7:E:485:SER:HB3	1.64	0.78
7:F:317:LEU:HG	7:F:357:PHE:HD2	1.48	0.77
1:A:75:HIS:O	1:A:76:THR:O	2.01	0.77
7:F:332:ARG:HE	7:F:347:LYS:HZ3	1.33	0.77
2:D:125:ALA:O	2:D:189:LEU:HD23	1.84	0.77
1:A:17:ALA:HB1	1:A:19:LEU:HG	1.68	0.75
2:D:174:MET:SD	2:D:174:MET:N	2.60	0.75
7:E:16:CYS:SG	7:E:33:HIS:CD2	2.79	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:191:SER:O	7:E:191:SER:OG	1.98	0.74
7:F:284:PRO:HG2	7:F:566:THR:HG21	1.68	0.74
7:E:521:VAL:HA	7:E:524:LYS:HB2	1.67	0.74
7:E:445:PRO:HG3	7:E:570:VAL:HA	1.69	0.74
1:A:105:ARG:HA	1:A:109:ASP:O	1.88	0.74
7:F:187:VAL:CG2	7:F:189:LYS:O	2.36	0.74
7:E:544:VAL:HB	7:E:572:ILE:HG22	1.70	0.74
7:E:477:LYS:NZ	7:E:549:THR:O	2.21	0.73
2:B:42:LEU:O	2:B:46:LYS:HG2	1.89	0.73
7:F:448:ILE:HD11	7:F:470:GLN:HE22	1.54	0.73
7:F:293:ILE:HG12	7:F:324:TYR:HB2	1.72	0.72
7:F:492:GLN:HG2	7:F:575:ILE:HD12	1.70	0.72
7:F:472:PHE:HB2	7:F:474:MET:HG3	1.72	0.72
7:F:37:THR:O	7:F:40:LYS:NZ	2.21	0.72
7:F:260:ASP:O	7:F:263:SER:HB3	1.89	0.72
6:L:2:A:C6	7:E:408:PRO:HD2	2.24	0.72
1:A:235:ASP:O	1:A:239:SER:OG	2.08	0.71
1:A:851:ASP:OD2	1:A:854:LEU:HD12	1.89	0.71
1:A:24:THR:OG1	1:A:25:GLY:N	2.22	0.71
7:F:445:PRO:HG2	7:F:448:ILE:HG13	1.71	0.71
2:D:184:LEU:C	2:D:185:ILE:HD12	2.10	0.71
4:I:12:C:H2'	4:I:13:G:H8	1.55	0.71
7:E:363:LEU:O	7:E:390:ARG:NH1	2.24	0.71
7:E:578:ASP:OD1	7:E:582:TYR:N	2.23	0.70
7:F:181:VAL:HG21	7:F:339:ARG:HG2	1.72	0.70
7:E:451:THR:HG22	7:E:586:GLN:HB2	1.71	0.70
7:F:178:ARG:HH21	7:F:312:ALA:HB2	1.56	0.70
7:F:483:ASP:H	7:F:488:ILE:HD13	1.56	0.69
1:A:160:LYS:O	1:A:161:ASP:HB2	1.92	0.69
7:F:296:ALA:O	7:F:355:TYR:OH	2.08	0.69
2:D:173:SER:OG	2:D:175:ASP:OD1	2.11	0.69
7:F:8:CYS:SG	7:F:99:GLY:N	2.65	0.69
7:E:503:ASN:HB3	7:E:506:TRP:HB2	1.73	0.69
7:F:448:ILE:HG23	7:F:565:ILE:HG22	1.75	0.69
7:E:582:TYR:HA	7:E:585:LEU:HB2	1.75	0.68
7:F:360:VAL:HA	7:F:363:LEU:HD12	1.75	0.68
7:E:157:VAL:HA	7:E:163:LEU:HG	1.76	0.68
7:F:316:ALA:HA	7:F:319:GLU:HB3	1.76	0.68
7:F:477:LYS:HG3	7:F:492:GLN:HB2	1.74	0.67
1:A:928:HIS:O	1:A:929:THR:OG1	2.12	0.67
2:D:100:ASN:HB3	2:D:103:LEU:HD12	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:519:ASN:ND2	7:E:530:THR:OG1	2.28	0.67
7:F:48:TYR:OH	7:F:90:PHE:O	2.12	0.66
7:F:331:SER:H	7:F:332:ARG:CZ	2.08	0.66
1:A:910:ASN:OD1	1:A:910:ASN:N	2.28	0.66
7:F:289:SER:HB2	7:F:320:LYS:HE3	1.76	0.66
1:A:75:HIS:CG	1:A:76:THR:HG22	2.28	0.66
7:F:370:ILE:HA	7:F:395:HIS:O	1.96	0.66
7:F:381:ASN:ND2	7:F:423:ASN:OD1	2.28	0.66
7:F:329:LYS:HD3	7:F:332:ARG:HH22	1.61	0.66
1:A:60:ASP:OD1	1:A:61:GLU:N	2.28	0.66
7:F:243:GLN:HE22	7:F:277:TYR:H	1.44	0.66
2:D:125:ALA:O	2:D:189:LEU:CD2	2.44	0.66
2:B:25:ALA:HB1	2:B:34:VAL:HG13	1.76	0.65
7:F:146:LYS:HD2	7:F:229:SER:HB2	1.77	0.65
7:E:382:TYR:O	7:E:386:VAL:HG23	1.96	0.65
7:E:343:PHE:HD2	7:E:345:LYS:H	1.44	0.65
7:F:187:VAL:HG22	7:F:189:LYS:O	1.96	0.65
7:F:330:CYS:SG	7:F:347:LYS:NZ	2.60	0.65
7:E:37:THR:HG22	7:E:39:HIS:H	1.61	0.65
7:E:470:GLN:HE21	7:E:572:ILE:HD12	1.62	0.65
2:D:185:ILE:HD12	2:D:185:ILE:N	2.12	0.65
5:J:118:U:H2'	5:J:119:A:C8	2.31	0.65
7:F:510:VAL:HG11	7:F:531:GLN:HB2	1.76	0.65
1:A:569:ARG:NH1	5:J:103:U:OP2	2.29	0.65
7:F:546:PHE:HB2	7:F:572:ILE:HD11	1.78	0.65
2:D:136:ASN:N	2:D:136:ASN:OD1	2.30	0.65
7:F:591:GLU:HB3	7:F:593:PRO:HD2	1.79	0.65
7:E:59:ASP:OD1	7:E:61:THR:OG1	2.15	0.64
7:E:475:PHE:HE2	7:E:492:GLN:HA	1.61	0.64
2:B:50:ASP:OD2	2:B:51:ARG:NH2	2.21	0.64
2:D:171:GLU:O	2:D:176:ASN:ND2	2.30	0.64
2:D:22:TYR:HD2	2:D:38:LEU:HB3	1.63	0.64
7:F:557:ASN:O	7:F:561:PHE:HB2	1.98	0.64
2:D:123:THR:HG22	2:D:125:ALA:H	1.63	0.64
1:A:105:ARG:HH12	1:A:108:GLY:HA2	1.63	0.63
7:F:199:THR:O	7:F:211:TYR:HA	1.98	0.63
7:F:421:TYR:HA	7:F:427:ARG:HH21	1.63	0.63
7:E:456:VAL:HG21	7:E:562:ASN:HD22	1.64	0.63
7:F:470:GLN:HE21	7:F:572:ILE:HG22	1.62	0.63
7:E:330:CYS:SG	7:E:331:SER:N	2.71	0.63
7:F:467:LYS:HB2	7:F:468:SER:HB3	1.81	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:499:PHE:HE2	7:E:502:ARG:HH11	1.45	0.62
7:F:150:GLY:HA3	7:F:171:LYS:HE3	1.80	0.62
2:D:173:SER:O	2:D:177:SER:OG	2.13	0.62
7:E:515:TYR:HE2	7:E:549:THR:HG21	1.64	0.62
2:B:9:LEU:HD22	2:B:52:ASP:O	1.99	0.62
7:F:476:TYR:HB2	7:F:579:ARG:HH12	1.64	0.62
7:E:7:LEU:HD23	7:E:102:ASN:HB2	1.81	0.62
7:E:459:ASN:H	7:E:459:ASN:HD22	1.46	0.62
7:F:513:SER:OG	7:F:519:ASN:ND2	2.33	0.62
2:D:104:ASN:O	2:D:108:ASN:ND2	2.27	0.62
7:F:14:LEU:HD21	7:F:91:GLY:HA3	1.82	0.62
7:F:440:THR:OG1	7:F:462:LYS:O	2.15	0.62
7:F:521:VAL:HA	7:F:524:LYS:HG2	1.80	0.62
7:F:390:ARG:HA	7:F:390:ARG:NH1	2.14	0.62
1:A:503:GLY:O	1:A:507:ASN:ND2	2.33	0.62
7:F:235:LEU:HD22	7:F:385:SER:HB2	1.82	0.62
1:A:759:SER:O	4:I:35:G:O3'	2.16	0.61
1:A:540:THR:CB	1:A:665:GLU:OE1	2.48	0.61
7:F:129:ARG:HA	7:F:129:ARG:NE	2.14	0.61
7:F:156:GLU:HB3	7:F:164:HIS:HB3	1.81	0.61
7:E:490:ARG:H	7:E:491:PRO:HD2	1.65	0.61
7:F:187:VAL:HG23	7:F:190:ASN:H	1.65	0.61
1:A:75:HIS:NE2	1:A:76:THR:HG22	1.95	0.61
7:E:456:VAL:HG21	7:E:562:ASN:ND2	2.16	0.61
7:E:542:ASP:HA	7:E:569:LYS:HB2	1.81	0.61
7:E:441:CYS:HB3	7:E:463:ALA:HB2	1.82	0.60
4:I:25:C:H2'	4:I:26:U:C6	2.35	0.60
7:F:548:GLN:HE22	7:F:574:CYS:HB3	1.66	0.60
7:F:268:ASN:O	7:F:271:LYS:HB2	2.00	0.60
7:F:21:ARG:HH11	7:F:136:GLU:HB2	1.66	0.60
7:F:453:SER:HB3	7:F:459:ASN:HA	1.84	0.60
7:F:69:SER:OG	7:F:70:TYR:N	2.34	0.60
7:F:339:ARG:H	7:F:339:ARG:HD2	1.65	0.60
7:F:503:ASN:HB2	7:F:506:TRP:HB2	1.82	0.60
7:E:554:HIS:O	7:E:560:ARG:NH1	2.32	0.60
7:E:189:LYS:N	7:E:190:ASN:O	2.34	0.60
7:F:286:THR:HG22	7:F:441:CYS:HA	1.83	0.59
7:E:243:GLN:OE1	7:E:275:GLN:NE2	2.32	0.59
7:E:333:ILE:HG22	7:E:334:ILE:HG13	1.84	0.59
7:F:286:THR:OG1	7:F:287:GLY:N	2.35	0.59
7:E:536:SER:OG	7:E:537:GLN:N	2.33	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:ASP:OD1	1:A:608:ASP:O	2.21	0.59
7:E:481:THR:O	7:E:481:THR:OG1	2.21	0.59
1:A:663:LEU:HG	1:A:663:LEU:O	2.01	0.59
2:D:90:MET:O	2:D:94:MET:HG3	2.02	0.59
7:F:26:CYS:N	7:F:29:CYS:SG	2.75	0.59
7:F:444:CYS:SG	7:F:449:VAL:HG23	2.43	0.59
4:I:23:U:H2'	4:I:24:G:H8	1.68	0.59
7:F:287:GLY:HA3	7:F:438:LEU:HD21	1.85	0.59
7:F:303:ARG:HA	7:F:354:GLN:HB2	1.84	0.59
7:F:334:ILE:HG23	7:F:337:ARG:H	1.68	0.59
7:E:280:LEU:HB3	7:E:399:ILE:HG22	1.85	0.59
7:E:433:GLY:O	7:E:434:PRO:C	2.41	0.59
1:A:653:TYR:O	1:A:657:ASN:ND2	2.33	0.58
2:B:59:LEU:HD23	7:F:79:ILE:HD11	1.85	0.58
5:J:118:U:H2'	5:J:119:A:H8	1.68	0.58
7:F:265:ASN:HD22	7:F:291:PHE:HA	1.68	0.58
7:E:373:PHE:HB3	7:E:398:TYR:HD1	1.68	0.58
7:E:379:ALA:O	7:E:423:ASN:ND2	2.27	0.58
1:A:11:VAL:C	1:A:13:GLY:H	2.06	0.58
1:A:855:MET:HG2	1:A:858:ARG:HD3	1.83	0.58
1:A:605:VAL:C	1:A:607:SER:H	2.07	0.58
7:F:311:HIS:HA	7:F:314:VAL:HG13	1.85	0.58
7:F:404:GLN:HG2	7:F:405:LEU:HG	1.85	0.58
7:E:44:SER:OG	7:E:45:VAL:N	2.37	0.58
7:E:339:ARG:H	7:E:339:ARG:HD2	1.69	0.58
7:E:576:MET:SD	7:E:577:SER:N	2.77	0.58
3:C:68:ILE:HD12	3:C:68:ILE:H	1.69	0.58
7:F:390:ARG:HA	7:F:390:ARG:HH11	1.69	0.57
2:D:51:ARG:HH22	4:I:18:U:H4'	1.69	0.57
5:J:113:C:H2'	5:J:114:A:C8	2.38	0.57
7:E:475:PHE:CE2	7:E:492:GLN:HA	2.38	0.57
7:F:447:GLU:O	7:F:451:THR:OG1	2.20	0.57
1:A:51:THR:O	1:A:51:THR:OG1	2.22	0.57
1:A:884:TYR:O	1:A:888:ILE:HG13	2.04	0.57
7:F:484:VAL:HG22	7:F:485:SER:H	1.68	0.57
7:F:548:GLN:OE1	7:F:548:GLN:N	2.37	0.57
2:B:98:LEU:O	2:B:100:ASN:N	2.32	0.57
7:F:245:HIS:HA	7:F:275:GLN:HA	1.87	0.57
7:F:334:ILE:HD12	7:F:337:ARG:HB2	1.85	0.57
1:A:661:GLN:O	1:A:665:GLU:HG2	2.04	0.57
1:A:874:ASN:OD1	1:A:875:GLN:N	2.34	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ASP:OD1	1:A:165:PHE:N	2.37	0.57
1:A:257:VAL:HG12	1:A:263:LYS:HD2	1.87	0.57
7:F:311:HIS:CE1	7:F:334:ILE:HD11	2.29	0.57
7:E:162:GLU:HB3	7:E:210:VAL:HG12	1.85	0.57
1:A:848:VAL:O	1:A:850:THR:N	2.34	0.57
2:B:25:ALA:HB2	2:B:38:LEU:HD12	1.86	0.57
7:F:154:VAL:H	7:F:155:ARG:HH21	1.51	0.57
7:F:511:PHE:CZ	7:F:547:THR:HG21	2.40	0.57
7:F:512:ILE:HG12	7:F:546:PHE:HA	1.85	0.57
7:E:477:LYS:HB3	7:E:489:ASN:ND2	2.20	0.57
7:F:21:ARG:O	7:F:23:PRO:HD3	2.04	0.56
7:F:44:SER:OG	7:F:45:VAL:N	2.28	0.56
7:E:472:PHE:CG	7:E:585:LEU:HD23	2.40	0.56
7:F:474:MET:SD	7:F:576:MET:HB3	2.45	0.56
7:F:383:ASP:HA	7:F:386:VAL:HG22	1.87	0.56
7:E:447:GLU:O	7:E:451:THR:HG23	2.06	0.56
2:B:125:ALA:O	2:B:190:ARG:NH2	2.36	0.56
7:F:5:CYS:HG	7:F:26:CYS:HB3	1.69	0.56
7:F:128:GLU:O	7:F:131:LYS:HB2	2.06	0.56
1:A:402:THR:OG1	1:A:403:ASN:N	2.39	0.56
7:E:580:ASP:N	7:E:580:ASP:OD1	2.38	0.56
7:F:255:THR:OG1	7:F:298:TYR:O	2.20	0.56
1:A:11:VAL:C	1:A:13:GLY:N	2.58	0.56
7:F:124:ASN:HB3	7:F:427:ARG:HH22	1.69	0.56
4:I:21:C:H2'	4:I:22:A:C8	2.41	0.56
7:F:304:ILE:HG23	7:F:370:ILE:HG23	1.88	0.56
7:F:562:ASN:OD1	7:F:566:THR:OG1	2.24	0.55
1:A:358:ASP:OD1	1:A:533:ARG:NH1	2.39	0.55
7:F:204:ASP:O	7:F:523:SER:HB3	2.06	0.55
7:F:476:TYR:CD1	7:F:577:SER:HB2	2.41	0.55
1:A:260:ASP:CB	1:A:263:LYS:HG3	2.37	0.55
7:F:288:LYS:O	7:F:290:HIS:N	2.39	0.55
7:E:144:THR:HA	7:E:147:LEU:HD13	1.87	0.55
7:F:563:VAL:O	7:F:567:ARG:NH2	2.40	0.55
1:A:153:ASP:OD1	1:A:153:ASP:N	2.39	0.55
7:F:309:CYS:N	7:F:375:GLU:OE1	2.38	0.55
7:F:358:CYS:SG	7:F:359:THR:N	2.79	0.55
1:A:74:ARG:HD3	1:A:111:VAL:HG11	1.89	0.55
7:E:471:CYS:HB3	7:E:590:LEU:HG	1.89	0.55
7:F:7:LEU:HD12	7:F:29:CYS:HB2	1.89	0.54
7:E:280:LEU:HB2	7:E:436:MET:SD	2.48	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:ASP:OD1	2:B:101:ASP:N	2.33	0.54
3:C:21:ARG:HG2	3:C:21:ARG:HH11	1.72	0.54
7:F:499:PHE:HA	7:F:502:ARG:HB2	1.88	0.54
7:E:445:PRO:O	7:E:449:VAL:HG13	2.07	0.54
2:D:13:ALA:O	2:D:17:THR:HG23	2.06	0.54
7:F:288:LYS:C	7:F:290:HIS:H	2.10	0.54
7:F:367:THR:OG1	7:F:392:ARG:O	2.20	0.54
2:D:180:LEU:HD22	2:D:180:LEU:N	2.15	0.54
7:F:214:THR:HB	7:F:339:ARG:HA	1.89	0.54
7:E:133:PHE:HA	7:E:136:GLU:OE1	2.08	0.54
2:B:41:SER:O	2:B:41:SER:OG	2.26	0.54
2:B:95:LEU:HD12	2:B:95:LEU:O	2.08	0.54
7:F:200:PHE:HA	7:F:210:VAL:O	2.07	0.54
7:E:585:LEU:HG	7:E:587:PHE:CD2	2.42	0.54
7:F:114:TRP:N	7:F:119:ASP:OD2	2.40	0.54
7:F:265:ASN:HB3	7:F:269:TYR:CZ	2.43	0.54
2:D:51:ARG:NH2	4:I:18:U:O2'	2.40	0.54
7:F:138:LEU:O	7:F:142:GLU:HG2	2.07	0.54
1:A:844:VAL:HG11	1:A:849:LYS:CB	2.38	0.54
7:F:496:VAL:HG21	7:F:511:PHE:HE2	1.72	0.54
7:F:347:LYS:HD3	7:F:347:LYS:H	1.73	0.54
2:D:135:TYR:O	2:D:138:TYR:N	2.41	0.53
7:E:446:ALA:O	7:E:449:VAL:HG22	2.08	0.53
1:A:109:ASP:N	1:A:109:ASP:OD1	2.41	0.53
7:F:182:PHE:HB3	7:F:225:PHE:HB3	1.90	0.53
7:F:256:LEU:HD23	7:F:256:LEU:H	1.73	0.53
7:E:331:SER:OG	7:E:331:SER:O	2.26	0.53
7:E:590:LEU:HD13	7:E:594:ARG:HG2	1.91	0.53
7:F:59:ASP:OD1	7:F:60:VAL:N	2.41	0.53
7:F:515:TYR:HB2	7:F:518:GLN:HG2	1.90	0.53
7:F:559:ASN:O	7:F:563:VAL:HG23	2.08	0.53
7:F:194:GLN:NE2	7:F:197:GLU:OE2	2.42	0.53
7:F:380:THR:H	7:F:383:ASP:HB2	1.74	0.53
7:E:26:CYS:HB2	7:E:97:CYS:SG	2.48	0.53
7:F:546:PHE:O	7:F:574:CYS:HA	2.08	0.53
7:E:294:GLY:O	7:E:297:LEU:HD23	2.08	0.53
7:E:545:ILE:HA	7:E:573:LEU:HD11	1.90	0.53
2:B:133:PRO:O	2:B:182:TRP:O	2.27	0.53
2:D:112:ASP:N	2:D:112:ASP:OD1	2.42	0.53
7:F:289:SER:O	7:F:293:ILE:HG22	2.09	0.53
6:L:1:A:O2'	7:E:534:ASP:OD2	2.19	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:287:GLY:H	7:E:438:LEU:HD21	1.74	0.52
1:A:609:VAL:HG12	1:A:610:GLU:N	2.23	0.52
1:A:851:ASP:OD1	2:D:75:ARG:NH2	2.36	0.52
7:F:106:PHE:HA	7:F:109:ILE:HD12	1.90	0.52
7:F:405:LEU:HD21	7:F:563:VAL:HG11	1.91	0.52
7:F:495:VAL:HG11	7:F:575:ILE:HG21	1.92	0.52
7:E:159:SER:OG	7:E:160:ASP:N	2.40	0.52
7:F:140:ALA:HA	7:F:232:VAL:HG21	1.90	0.52
7:F:304:ILE:HB	7:F:355:TYR:HD1	1.74	0.52
7:F:332:ARG:HD2	7:F:347:LYS:H	1.74	0.52
7:E:268:ASN:HD22	7:E:291:PHE:HZ	1.57	0.52
1:A:592:SER:HB2	5:J:105:C:H4'	1.91	0.52
7:F:547:THR:HG22	7:F:575:ILE:HD11	1.92	0.52
7:E:243:GLN:HB2	7:E:277:TYR:HE1	1.74	0.52
2:B:46:LYS:O	2:B:50:ASP:N	2.43	0.52
7:F:122:LEU:HA	7:F:125:THR:OG1	2.09	0.52
7:E:444:CYS:HB2	7:E:448:ILE:HD11	1.92	0.52
7:F:311:HIS:O	7:F:314:VAL:HG22	2.09	0.52
7:F:404:GLN:HA	7:F:563:VAL:HG21	1.91	0.52
7:F:563:VAL:HG12	7:F:567:ARG:HH22	1.73	0.52
7:E:444:CYS:SG	7:E:449:VAL:HG12	2.50	0.52
7:F:417:LEU:HD23	7:F:417:LEU:H	1.75	0.52
7:E:36:SER:O	7:E:36:SER:OG	2.24	0.52
7:E:161:ARG:HA	7:E:211:TYR:CZ	2.44	0.52
7:E:394:LYS:HG3	7:E:395:HIS:CE1	2.45	0.52
1:A:393:THR:HG21	1:A:450:ILE:HD11	1.92	0.51
4:I:23:U:H2'	4:I:24:G:C8	2.45	0.51
7:F:515:TYR:O	7:F:519:ASN:ND2	2.43	0.51
1:A:273:TYR:CD1	1:A:273:TYR:C	2.84	0.51
1:A:342:VAL:O	1:A:342:VAL:HG23	2.10	0.51
7:E:456:VAL:HG23	7:E:457:TYR:H	1.74	0.51
1:A:543:ASN:OD1	5:J:100:A:O2'	2.27	0.51
7:F:592:ILE:N	7:F:593:PRO:HD2	2.25	0.51
7:E:56:ASP:OD1	7:E:56:ASP:N	2.43	0.51
7:E:223:ASP:OD1	7:E:223:ASP:N	2.43	0.51
1:A:661:GLN:C	1:A:662:VAL:CG1	2.78	0.51
7:F:489:ASN:O	7:F:493:ILE:N	2.35	0.51
7:E:252:LEU:HD11	7:E:370:ILE:HD11	1.92	0.51
1:A:361:LEU:HD22	1:A:361:LEU:H	1.76	0.51
7:F:327:ILE:HA	7:F:328:ASP:C	2.30	0.51
2:B:66:ALA:O	2:B:69:GLN:HG3	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:185:TYR:HB2	7:E:224:TYR:CE1	2.46	0.51
7:E:347:LYS:HE2	7:E:350:SER:OG	2.11	0.51
7:E:472:PHE:HE1	7:E:587:PHE:HB2	1.76	0.51
7:E:580:ASP:O	7:E:584:LYS:HD3	2.11	0.51
2:B:161:ASP:OD1	2:B:161:ASP:N	2.44	0.50
7:F:418:GLU:HG2	7:F:419:PRO:HD2	1.93	0.50
7:E:515:TYR:CE2	7:E:549:THR:HG21	2.44	0.50
7:E:472:PHE:CE1	7:E:587:PHE:HB2	2.46	0.50
7:E:502:ARG:O	7:E:504:PRO:HD3	2.12	0.50
7:F:500:LEU:HD21	7:F:528:LEU:HD22	1.93	0.50
7:F:256:LEU:O	7:F:257:ASN:OD1	2.29	0.50
7:F:303:ARG:NH2	7:F:353:GLU:O	2.44	0.50
7:F:407:ALA:H	7:F:409:ARG:NH2	2.09	0.50
7:F:490:ARG:HA	7:F:493:ILE:HB	1.93	0.50
1:A:661:GLN:C	1:A:662:VAL:HG13	2.32	0.50
2:B:102:ALA:O	2:B:106:ILE:HG23	2.12	0.50
7:F:38:SER:O	7:F:38:SER:OG	2.30	0.50
7:F:138:LEU:HD12	7:F:139:LYS:N	2.27	0.50
7:E:383:ASP:O	7:E:387:VAL:HG12	2.11	0.50
1:A:388:LEU:HD23	1:A:397:SER:HB2	1.93	0.50
7:F:124:ASN:O	7:F:131:LYS:NZ	2.45	0.50
7:F:495:VAL:HA	7:F:595:ARG:HH22	1.77	0.50
1:A:14:VAL:HG23	1:A:14:VAL:O	2.12	0.50
1:A:75:HIS:C	1:A:76:THR:O	2.50	0.50
5:J:117:C:H2'	5:J:118:U:C6	2.47	0.50
1:A:77:PHE:CD1	1:A:77:PHE:C	2.84	0.49
7:F:304:ILE:HB	7:F:355:TYR:CD1	2.47	0.49
2:D:56:GLN:O	2:D:60:GLU:HB2	2.12	0.49
7:F:127:THR:O	7:F:131:LYS:N	2.39	0.49
7:E:303:ARG:NE	7:E:354:GLN:HA	2.26	0.49
7:F:189:LYS:H	7:F:190:ASN:CB	2.03	0.49
1:A:329:LEU:HB2	1:A:345:GLY:O	2.12	0.49
7:F:284:PRO:HD3	7:F:401:ASP:OD2	2.12	0.49
7:F:422:PHE:HD2	7:F:426:CYS:HG	1.58	0.49
7:E:220:ASN:N	7:E:220:ASN:OD1	2.45	0.49
3:C:63:GLN:OE1	3:C:63:GLN:N	2.45	0.49
4:I:17:G:O6	5:J:119:A:N6	2.44	0.49
7:F:334:ILE:HG21	7:F:338:ALA:HB2	1.93	0.49
7:E:577:SER:O	7:E:579:ARG:NH2	2.40	0.49
7:F:434:PRO:C	7:F:436:MET:H	2.16	0.49
7:E:168:GLU:HB3	7:E:171:LYS:HE2	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:VAL:HG12	1:A:610:GLU:H	1.77	0.49
7:E:490:ARG:N	7:E:491:PRO:HD2	2.27	0.49
4:I:21:C:H2'	4:I:22:A:H8	1.77	0.49
4:I:24:G:H2'	4:I:25:C:C6	2.47	0.49
7:E:262:PHE:HE1	7:E:290:HIS:CD2	2.31	0.49
7:F:446:ALA:HB3	7:F:466:ASP:HA	1.95	0.49
1:A:62:ASP:OD1	1:A:62:ASP:N	2.45	0.48
2:B:40:LYS:O	2:B:44:VAL:HG13	2.13	0.48
2:D:72:LYS:O	2:D:76:SER:HB3	2.13	0.48
7:F:187:VAL:HG23	7:F:190:ASN:N	2.28	0.48
7:E:477:LYS:NZ	7:E:548:GLN:HB2	2.28	0.48
4:I:12:C:H2'	4:I:13:G:C8	2.43	0.48
7:F:472:PHE:HB3	7:F:574:CYS:HB2	1.95	0.48
7:E:376:ILE:HG21	7:E:398:TYR:HB3	1.95	0.48
7:E:510:VAL:HG21	7:E:541:TYR:CD2	2.48	0.48
7:F:249:ILE:HB	7:F:252:LEU:HD13	1.95	0.48
7:E:140:ALA:O	7:E:144:THR:HG22	2.13	0.48
7:E:271:LYS:NZ	7:E:435:ASP:O	2.46	0.48
7:E:335:PRO:HG2	7:E:337:ARG:HH11	1.78	0.48
7:E:377:SER:O	7:E:406:PRO:HA	2.13	0.48
7:E:470:GLN:OE1	7:E:471:CYS:N	2.46	0.48
1:A:454:ASP:OD2	1:A:457:ARG:NH1	2.46	0.48
7:E:467:LYS:HE3	7:E:468:SER:HA	1.94	0.48
7:E:539:SER:H	7:E:567:ARG:HH11	1.62	0.48
7:F:79:ILE:HG23	7:F:79:ILE:O	2.14	0.48
7:F:354:GLN:HG3	7:F:355:TYR:CE1	2.48	0.48
7:E:161:ARG:O	7:E:211:TYR:CD1	2.66	0.48
7:E:490:ARG:O	7:E:493:ILE:HG22	2.14	0.48
1:A:19:LEU:HD23	1:A:19:LEU:HA	1.57	0.48
1:A:274:ASP:O	1:A:274:ASP:OD1	2.32	0.48
1:A:275:PHE:O	1:A:279:ARG:HG3	2.14	0.48
2:B:169:LEU:HD12	2:B:169:LEU:H	1.79	0.48
3:C:45:THR:O	3:C:45:THR:OG1	2.24	0.48
7:F:129:ARG:HG2	7:F:129:ARG:HH11	1.79	0.48
7:F:427:ARG:O	7:F:431:THR:HG22	2.14	0.48
7:F:501:THR:HB	7:F:502:ARG:NH1	2.28	0.48
7:E:177:ASN:HB2	7:E:180:TYR:CD1	2.48	0.48
4:I:24:G:O2'	4:I:25:C:OP1	2.29	0.48
7:F:266:VAL:HA	7:F:269:TYR:CD2	2.49	0.48
7:E:155:ARG:NH2	7:E:165:LEU:O	2.45	0.48
7:E:177:ASN:OD1	7:E:516:ASN:ND2	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:189:LYS:CB	7:E:190:ASN:HB2	2.27	0.48
2:D:101:ASP:OD1	2:D:101:ASP:N	2.45	0.47
2:D:175:ASP:OD1	2:D:175:ASP:N	2.47	0.47
7:F:404:GLN:HA	7:F:563:VAL:CG2	2.44	0.47
7:F:141:THR:O	7:F:144:THR:HG22	2.14	0.47
7:F:376:ILE:HG23	7:F:399:ILE:O	2.14	0.47
7:F:561:PHE:O	7:F:565:ILE:HG12	2.15	0.47
1:A:260:ASP:OD2	1:A:263:LYS:HG3	2.14	0.47
3:C:50:GLU:O	3:C:53:VAL:HG12	2.14	0.47
7:F:28:LYS:HG2	7:F:97:CYS:SG	2.55	0.47
7:F:280:LEU:HD23	7:F:399:ILE:HG12	1.96	0.47
7:E:150:GLY:N	7:E:172:PRO:O	2.40	0.47
7:E:448:ILE:HG22	7:E:587:PHE:HE1	1.79	0.47
7:F:299:TYR:O	7:F:355:TYR:OH	2.31	0.47
7:F:509:ALA:HA	7:F:543:TYR:HB2	1.96	0.47
7:E:502:ARG:HB2	7:E:595:ARG:HH21	1.80	0.47
1:A:605:VAL:C	1:A:607:SER:N	2.68	0.47
2:B:50:ASP:O	2:B:54:ALA:HB3	2.15	0.47
7:F:14:LEU:HD13	7:F:44:SER:HB2	1.95	0.47
7:F:151:ILE:HG22	7:F:226:VAL:HG22	1.96	0.47
7:F:156:GLU:HB3	7:F:164:HIS:CB	2.44	0.47
7:F:162:GLU:HG2	7:F:208:ALA:HB1	1.96	0.47
7:F:252:LEU:HD23	7:F:299:TYR:CZ	2.50	0.47
7:F:347:LYS:HD3	7:F:347:LYS:N	2.29	0.47
7:E:202:LYS:HA	7:E:209:VAL:HG12	1.96	0.47
7:E:244:GLU:H	7:E:276:LYS:HB2	1.79	0.47
7:E:404:GLN:HE21	7:E:537:GLN:HE21	1.61	0.47
7:E:539:SER:O	7:E:567:ARG:HD3	2.15	0.47
7:E:31:TYR:CZ	7:E:87:GLY:HA2	2.50	0.47
7:E:177:ASN:HB2	7:E:180:TYR:CE1	2.50	0.47
7:F:114:TRP:HE1	7:F:141:THR:HG21	1.80	0.47
7:F:183:THR:OG1	7:F:194:GLN:OE1	2.33	0.47
7:F:249:ILE:HG22	7:F:273:GLY:HA3	1.98	0.46
7:F:303:ARG:NH2	7:F:352:LEU:O	2.32	0.46
7:E:277:TYR:HB2	7:E:396:TYR:HB2	1.96	0.46
7:E:427:ARG:O	7:E:431:THR:HG22	2.14	0.46
7:F:133:PHE:O	7:F:137:THR:OG1	2.17	0.46
7:F:144:THR:O	7:F:148:SER:OG	2.30	0.46
1:A:273:TYR:CD1	1:A:273:TYR:O	2.68	0.46
1:A:288:LYS:HD3	1:A:289:TYR:CE1	2.50	0.46
2:D:115:VAL:HG23	2:D:116:PRO:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:586:GLN:CD	7:F:586:GLN:H	2.17	0.46
7:E:445:PRO:HB2	7:E:448:ILE:HG23	1.98	0.46
7:E:591:GLU:HG3	7:E:592:ILE:H	1.80	0.46
7:F:256:LEU:HG	7:F:257:ASN:H	1.80	0.46
7:F:563:VAL:CG1	7:F:567:ARG:HH22	2.28	0.46
7:E:591:GLU:H	7:E:594:ARG:HB3	1.80	0.46
1:A:275:PHE:N	1:A:275:PHE:CD2	2.82	0.46
2:B:111:ARG:H	2:B:111:ARG:HD3	1.81	0.46
7:F:326:PRO:HB2	7:F:328:ASP:HB2	1.97	0.46
7:F:526:LEU:HD23	7:F:526:LEU:HA	1.84	0.46
7:E:109:ILE:HD13	7:E:134:ALA:HB2	1.98	0.46
1:A:326:PHE:O	2:B:118:ASN:ND2	2.49	0.46
1:A:330:VAL:HA	1:A:343:SER:HA	1.98	0.46
1:A:514:LEU:HD21	2:B:83:VAL:HG21	1.98	0.46
1:A:848:VAL:HG13	1:A:858:ARG:HD2	1.97	0.46
7:F:132:LEU:HD11	7:F:235:LEU:HD22	1.97	0.46
7:F:269:TYR:CE1	7:F:295:LEU:HB3	2.51	0.46
7:E:162:GLU:OE2	7:E:162:GLU:N	2.48	0.46
7:E:457:TYR:C	7:E:458:ASP:O	2.44	0.46
1:A:856:ILE:O	1:A:860:VAL:HG23	2.15	0.46
7:F:39:HIS:C	7:F:40:LYS:HZ2	2.18	0.46
7:F:223:ASP:OD1	7:F:223:ASP:N	2.48	0.46
7:F:335:PRO:HD2	7:F:337:ARG:HG2	1.96	0.46
7:E:169:VAL:O	7:E:171:LYS:NZ	2.49	0.46
7:E:279:THR:O	7:E:436:MET:HB3	2.14	0.46
7:F:371:VAL:HG21	7:F:391:LEU:HD22	1.97	0.46
1:A:758:LEU:O	1:A:760:ASP:N	2.49	0.46
7:F:41:LEU:HD22	7:F:42:VAL:H	1.79	0.46
7:F:139:LYS:HD3	7:F:382:TYR:CE2	2.51	0.46
7:F:498:GLU:O	7:F:498:GLU:HG3	2.16	0.46
7:E:288:LYS:O	7:E:290:HIS:N	2.47	0.46
1:A:654:ARG:O	1:A:658:GLU:HG3	2.16	0.46
1:A:751:LYS:HB3	1:A:752:HIS:CD2	2.51	0.46
7:F:488:ILE:HG13	7:F:521:VAL:HG21	1.98	0.46
7:F:524:LYS:HE3	7:F:524:LYS:HA	1.98	0.46
7:E:270:GLN:O	7:E:274:MET:HG3	2.15	0.46
7:F:279:THR:OG1	7:F:435:ASP:OD1	2.33	0.45
7:F:288:LYS:C	7:F:290:HIS:N	2.68	0.45
7:E:120:TYR:HE2	7:E:412:LEU:HD13	1.80	0.45
7:E:502:ARG:HD2	7:E:595:ARG:HB3	1.97	0.45
7:F:332:ARG:CZ	7:F:346:PHE:HB2	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:419:PRO:HB2	7:F:430:LYS:NZ	2.31	0.45
2:D:177:SER:HA	2:D:180:LEU:HD21	1.25	0.45
7:F:202:LYS:HB3	7:F:202:LYS:HE3	1.69	0.45
1:A:80:TYR:CD1	1:A:112:PRO:HB2	2.50	0.45
7:F:115:THR:HA	7:F:411:LEU:O	2.17	0.45
7:F:307:THR:HA	7:F:358:CYS:O	2.15	0.45
7:F:375:GLU:HG2	7:F:378:MET:HB2	1.97	0.45
7:F:476:TYR:HA	7:F:577:SER:HA	1.98	0.45
7:E:28:LYS:HE3	7:E:97:CYS:O	2.16	0.45
7:E:155:ARG:HH12	7:E:207:ASP:HB2	1.81	0.45
1:A:755:MET:HG2	1:A:764:VAL:HG22	1.97	0.45
4:I:24:G:H2'	4:I:25:C:H6	1.80	0.45
7:F:473:LYS:HE3	7:F:575:ILE:HG23	1.98	0.45
7:F:536:SER:HG	7:F:567:ARG:HE	1.61	0.45
1:A:37:ILE:HG13	1:A:38:TYR:N	2.32	0.45
1:A:75:HIS:CD2	1:A:75:HIS:C	2.89	0.45
1:A:128:VAL:O	1:A:132:ARG:HG3	2.17	0.45
1:A:197:ARG:NH1	1:A:230:GLY:O	2.50	0.45
1:A:623:ASP:OD1	1:A:623:ASP:N	2.48	0.45
3:C:44:ASP:N	3:C:44:ASP:OD1	2.50	0.45
7:F:139:LYS:HD3	7:F:382:TYR:HE2	1.81	0.45
7:F:450:ASP:OD1	7:F:451:THR:N	2.49	0.45
7:E:353:GLU:HG3	7:E:355:TYR:H	1.82	0.45
7:E:549:THR:OG1	7:E:550:THR:N	2.49	0.45
7:E:41:LEU:HD12	7:E:42:VAL:H	1.81	0.45
7:E:557:ASN:HB3	7:E:560:ARG:NH1	2.32	0.45
1:A:77:PHE:O	1:A:77:PHE:HD1	2.00	0.45
1:A:391:LYS:HB3	1:A:391:LYS:HE3	1.75	0.45
7:E:235:LEU:HD21	7:E:382:TYR:CE2	2.52	0.45
7:E:517:SER:O	7:E:521:VAL:HG23	2.16	0.45
1:A:24:THR:HG21	1:A:27:SER:OG	2.17	0.45
2:B:51:ARG:NH2	4:I:16:A:O2'	2.50	0.45
7:F:474:MET:HE1	7:F:582:TYR:HB3	1.98	0.45
7:E:200:PHE:CD2	7:E:211:TYR:HB3	2.52	0.45
7:E:386:VAL:HG12	7:E:390:ARG:HD2	1.98	0.45
7:E:435:ASP:O	7:E:436:MET:HB2	2.16	0.45
7:E:519:ASN:ND2	7:E:531:GLN:O	2.50	0.45
2:D:122:LEU:HA	2:D:190:ARG:NH1	2.32	0.45
1:A:77:PHE:CD1	1:A:77:PHE:O	2.70	0.44
2:B:161:ASP:HB2	2:B:181:ALA:HB3	1.99	0.44
2:D:185:ILE:N	2:D:185:ILE:CD1	2.76	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:64:TYR:HE2	7:F:73:LYS:HB3	1.82	0.44
7:F:337:ARG:HB2	7:F:338:ALA:H	1.53	0.44
7:F:470:GLN:HB3	7:F:572:ILE:HG22	1.98	0.44
2:B:40:LYS:O	2:B:44:VAL:CG1	2.65	0.44
7:F:279:THR:HG22	7:F:398:TYR:HD2	1.82	0.44
7:E:186:ARG:O	7:E:192:LYS:HA	2.17	0.44
7:E:546:PHE:CE2	7:E:548:GLN:HG2	2.52	0.44
1:A:281:LYS:HB3	1:A:281:LYS:HE3	1.62	0.44
2:B:166:ILE:HD12	2:B:166:ILE:H	1.82	0.44
7:E:333:ILE:O	7:E:334:ILE:HG12	2.17	0.44
7:E:466:ASP:OD1	7:E:466:ASP:N	2.50	0.44
7:F:130:LEU:HD12	7:F:130:LEU:H	1.83	0.44
7:F:261:GLU:CD	7:F:261:GLU:H	2.20	0.44
7:F:306:TYR:HE1	7:F:355:TYR:HB3	1.83	0.44
7:F:390:ARG:C	7:F:392:ARG:HH22	2.20	0.44
7:F:391:LEU:CD2	7:F:393:ALA:HB2	2.47	0.44
1:A:171:ILE:HA	1:A:174:VAL:HG12	1.99	0.44
3:C:23:GLU:HA	3:C:29:TRP:HB2	2.00	0.44
2:D:176:ASN:OD1	2:D:176:ASN:N	2.47	0.44
7:F:47:PRO:HB2	7:F:49:VAL:HG22	1.99	0.44
7:E:373:PHE:HB3	7:E:398:TYR:CD1	2.51	0.44
2:D:7:SER:O	2:D:9:LEU:N	2.51	0.44
1:A:186:LEU:O	1:A:189:THR:HG22	2.17	0.44
1:A:686:THR:O	1:A:686:THR:OG1	2.26	0.44
2:B:59:LEU:HD21	7:F:81:PHE:CD1	2.53	0.44
3:C:28:LEU:HD12	3:C:28:LEU:HA	1.80	0.44
7:F:116:ASN:HB2	7:F:119:ASP:OD1	2.17	0.44
1:A:184:GLN:O	1:A:188:LYS:HG3	2.17	0.44
1:A:798:LYS:HB2	1:A:798:LYS:HE2	1.59	0.44
7:F:64:TYR:HB2	7:F:80:SER:HB2	2.00	0.44
7:E:163:LEU:HB2	7:E:211:TYR:HE1	1.83	0.44
7:E:405:LEU:H	7:E:537:GLN:HE22	1.65	0.44
7:E:453:SER:HB3	7:E:461:LEU:HB2	2.00	0.44
1:A:268:TRP:CD1	1:A:322:PRO:HD3	2.52	0.44
1:A:371:LEU:HD23	1:A:371:LEU:HA	1.88	0.44
7:E:345:LYS:HG3	7:E:346:PHE:CD2	2.53	0.44
7:E:451:THR:HG21	7:E:587:PHE:CZ	2.53	0.44
1:A:387:LEU:HD12	1:A:388:LEU:H	1.83	0.43
1:A:598:TRP:HE1	1:A:817:THR:HG1	1.66	0.43
2:D:161:ASP:HA	2:D:184:LEU:HD23	2.00	0.43
7:F:384:LEU:O	7:F:387:VAL:HG12	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:495:VAL:O	7:F:499:PHE:HB2	2.19	0.43
7:E:161:ARG:NH1	7:E:210:VAL:HB	2.32	0.43
7:E:303:ARG:NH2	7:E:352:LEU:O	2.51	0.43
7:E:403:ALA:O	7:E:559:ASN:ND2	2.51	0.43
2:B:62:MET:HA	2:B:65:GLN:HG3	1.99	0.43
3:C:47:GLU:HG3	3:C:51:LYS:HD2	2.00	0.43
7:F:185:TYR:CE1	7:F:194:GLN:HB2	2.53	0.43
7:F:272:VAL:HG11	7:F:370:ILE:HD12	2.01	0.43
7:F:330:CYS:HA	7:F:332:ARG:HH21	1.84	0.43
7:F:507:ARG:HD2	7:F:507:ARG:HA	1.85	0.43
7:E:449:VAL:HA	7:E:452:VAL:HG12	2.00	0.43
7:E:472:PHE:CD2	7:E:582:TYR:HB2	2.53	0.43
7:E:507:ARG:HA	7:E:507:ARG:NE	2.34	0.43
1:A:496:ASN:OD1	1:A:496:ASN:N	2.36	0.43
1:A:605:VAL:HG12	1:A:606:TYR:HD1	1.83	0.43
1:A:928:HIS:O	1:A:929:THR:CB	2.66	0.43
7:F:20:ILE:HG23	7:F:21:ARG:H	1.83	0.43
7:F:386:VAL:O	7:F:390:ARG:HG2	2.17	0.43
7:E:118:GLY:O	7:E:121:ILE:HG22	2.17	0.43
7:E:159:SER:OG	7:E:162:GLU:OE2	2.33	0.43
7:E:307:THR:HG23	7:E:363:LEU:HD11	2.00	0.43
7:E:394:LYS:HA	7:E:394:LYS:HD2	1.71	0.43
7:E:406:PRO:HB3	7:E:422:PHE:CZ	2.52	0.43
7:E:541:TYR:O	7:E:569:LYS:N	2.51	0.43
7:F:499:PHE:O	7:F:502:ARG:N	2.52	0.43
7:E:41:LEU:HD12	7:E:42:VAL:N	2.34	0.43
2:B:38:LEU:O	2:B:41:SER:HB3	2.19	0.43
7:F:186:ARG:NH1	7:F:220:ASN:HB2	2.34	0.43
7:F:235:LEU:CD2	7:F:385:SER:HB2	2.48	0.43
7:F:331:SER:H	7:F:332:ARG:NH2	2.15	0.43
7:E:182:PHE:HD2	7:E:200:PHE:CE1	2.37	0.43
7:E:459:ASN:ND2	7:E:459:ASN:N	2.58	0.43
2:B:95:LEU:HD12	2:B:95:LEU:C	2.38	0.43
3:C:70:LYS:HB2	3:C:70:LYS:HE2	1.54	0.43
7:F:533:VAL:HG21	7:F:563:VAL:HG12	2.00	0.43
7:E:494:GLY:HA2	7:E:497:ARG:HB2	2.01	0.43
7:E:546:PHE:HE2	7:E:548:GLN:HG2	1.84	0.43
1:A:77:PHE:C	1:A:77:PHE:HD1	2.22	0.43
1:A:912:THR:O	1:A:912:THR:OG1	2.33	0.43
5:J:114:A:C6	5:J:115:U:C4	3.07	0.43
7:F:73:LYS:HA	7:F:76:LYS:HB2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:95:ASN:H	7:F:95:ASN:ND2	2.17	0.43
7:F:162:GLU:HG3	7:F:209:VAL:O	2.18	0.43
7:F:155:ARG:HA	7:F:155:ARG:HD3	1.75	0.43
7:F:366:THR:O	7:F:391:LEU:HG	2.18	0.43
7:F:448:ILE:CG2	7:F:566:THR:HA	2.49	0.43
7:F:480:ILE:HD11	7:F:550:THR:HG23	2.01	0.43
7:F:501:THR:HB	7:F:502:ARG:CZ	2.48	0.43
7:E:134:ALA:HA	7:E:137:THR:HG22	2.01	0.43
7:E:375:GLU:N	7:E:399:ILE:O	2.51	0.43
1:A:387:LEU:HG	2:B:128:LEU:HD12	1.99	0.43
7:F:89:VAL:O	7:F:94:LYS:NZ	2.52	0.43
7:F:167:TRP:CE2	7:F:173:ARG:HG3	2.54	0.43
7:F:247:VAL:HG12	7:E:218:LYS:HG2	2.01	0.43
7:F:346:PHE:HB3	7:F:347:LYS:HD3	2.00	0.43
7:E:127:THR:OG1	7:E:128:GLU:N	2.52	0.43
1:A:555:ARG:HD2	1:A:555:ARG:HA	1.92	0.43
7:E:125:THR:O	7:E:125:THR:OG1	2.34	0.43
7:E:165:LEU:HD11	7:E:200:PHE:CE2	2.53	0.43
7:E:263:SER:OG	7:E:264:SER:N	2.50	0.43
7:E:445:PRO:HA	7:E:465:LYS:O	2.19	0.43
2:B:49:PHE:O	2:B:53:ALA:HB3	2.19	0.42
7:F:280:LEU:HD21	7:F:438:LEU:HD22	1.99	0.42
7:F:567:ARG:HG3	7:F:567:ARG:HH11	1.82	0.42
7:E:266:VAL:O	7:E:270:GLN:HG3	2.19	0.42
7:E:326:PRO:O	7:E:327:ILE:HD13	2.19	0.42
7:E:330:CYS:SG	7:E:347:LYS:HE3	2.59	0.42
7:F:22:ARG:H	7:F:22:ARG:HG2	1.43	0.42
7:F:113:ASP:O	7:F:115:THR:HG23	2.18	0.42
7:F:333:ILE:HG12	7:F:358:CYS:HA	2.01	0.42
7:F:440:THR:OG1	7:F:441:CYS:N	2.52	0.42
7:E:249:ILE:HG12	7:E:274:MET:HG2	2.01	0.42
7:E:329:LYS:HE2	7:E:345:LYS:HG2	2.00	0.42
1:A:540:THR:HB	1:A:665:GLU:OE1	2.18	0.42
4:I:26:U:H2'	4:I:27:A:H8	1.85	0.42
7:F:316:ALA:CA	7:F:319:GLU:HB3	2.47	0.42
7:F:534:ASP:OD1	7:F:535:SER:N	2.52	0.42
7:E:437:PHE:HD1	7:E:438:LEU:H	1.68	0.42
7:E:508:LYS:HE3	7:E:508:LYS:HB2	1.85	0.42
1:A:505:PRO:O	1:A:508:LYS:HD2	2.19	0.42
2:D:174:MET:O	2:D:177:SER:OG	2.36	0.42
7:F:441:CYS:HB3	7:F:463:ALA:HB2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:585:LEU:HG	7:E:587:PHE:HD2	1.82	0.42
2:B:140:ASN:OD1	2:B:140:ASN:N	2.52	0.42
7:F:293:ILE:HD11	7:F:325:LEU:HG	2.00	0.42
7:F:302:ALA:O	7:F:354:GLN:HB2	2.20	0.42
7:E:22:ARG:NH1	7:E:22:ARG:HG3	2.35	0.42
7:E:31:TYR:CE2	7:E:87:GLY:HA2	2.55	0.42
7:E:465:LYS:HE3	7:E:465:LYS:HB3	1.86	0.42
1:A:543:ASN:O	1:A:556:THR:OG1	2.27	0.42
2:B:80:ARG:O	2:B:84:THR:HG22	2.20	0.42
7:F:484:VAL:HG13	7:F:485:SER:N	2.35	0.42
7:E:65:LEU:N	7:E:81:PHE:O	2.48	0.42
2:D:159:VAL:CG1	2:D:184:LEU:HD13	2.49	0.42
7:F:41:LEU:HD22	7:F:42:VAL:N	2.34	0.42
7:F:235:LEU:HD23	7:F:237:ALA:N	2.35	0.42
7:F:422:PHE:HB2	7:F:426:CYS:CB	2.50	0.42
7:E:585:LEU:HA	7:E:585:LEU:HD12	1.75	0.42
1:A:60:ASP:N	1:A:64:ASN:O	2.46	0.42
1:A:607:SER:HB3	1:A:608:ASP:H	1.56	0.42
1:A:759:SER:O	1:A:759:SER:OG	2.38	0.42
2:D:165:LYS:HB2	2:D:165:LYS:HE2	1.75	0.42
7:F:127:THR:HG22	7:F:128:GLU:H	1.84	0.42
7:F:163:LEU:HD11	7:F:219:LEU:HD11	2.02	0.42
1:A:901:ASP:OD1	1:A:902:MET:N	2.52	0.42
1:A:909:ASN:ND2	1:A:909:ASN:N	2.65	0.42
7:F:151:ILE:HG13	7:F:168:GLU:HG3	2.02	0.42
7:F:467:LYS:HB2	7:F:467:LYS:HE2	1.68	0.42
7:E:368:ALA:HB3	7:E:393:ALA:HB2	2.02	0.42
2:B:157:GLN:O	2:B:158:GLN:HB3	2.20	0.41
7:F:250:THR:O	7:F:250:THR:OG1	2.38	0.41
7:E:114:TRP:HD1	7:E:141:THR:HG21	1.84	0.41
7:E:560:ARG:HA	7:E:563:VAL:HG22	2.02	0.41
1:A:156:TYR:OH	1:A:170:ASP:OD1	2.31	0.41
1:A:370:GLU:HA	1:A:373:VAL:HG22	2.01	0.41
1:A:849:LYS:O	1:A:850:THR:C	2.57	0.41
5:J:115:U:H2'	5:J:116:G:H8	1.86	0.41
7:F:369:ASP:O	7:F:395:HIS:N	2.53	0.41
7:E:405:LEU:HD11	7:E:560:ARG:HG2	2.01	0.41
6:L:0:U:H2'	6:L:1:A:H2	1.84	0.41
7:F:219:LEU:HD13	7:F:225:PHE:CE1	2.55	0.41
7:F:305:VAL:HB	7:F:371:VAL:HG22	2.02	0.41
7:F:39:HIS:O	7:F:40:LYS:NZ	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:102:ASN:OD1	7:F:102:ASN:N	2.53	0.41
7:F:127:THR:HB	7:F:130:LEU:HD13	2.03	0.41
7:F:339:ARG:HD2	7:F:339:ARG:N	2.32	0.41
7:F:475:PHE:HE2	7:F:492:GLN:HA	1.85	0.41
7:F:517:SER:O	7:F:521:VAL:HG22	2.20	0.41
7:E:548:GLN:HG3	7:E:576:MET:HA	2.03	0.41
1:A:726:ARG:NH2	1:A:744:GLU:OE2	2.53	0.41
3:C:27:LYS:O	3:C:31:GLN:NE2	2.53	0.41
7:F:281:GLN:O	7:F:283:PRO:HD3	2.20	0.41
7:F:451:THR:HB	7:F:585:LEU:HG	2.02	0.41
7:F:519:ASN:O	7:F:523:SER:OG	2.24	0.41
7:F:577:SER:OG	7:F:578:ASP:N	2.53	0.41
7:E:154:VAL:HG23	7:E:223:ASP:O	2.20	0.41
1:A:65:LEU:HD23	1:A:65:LEU:HA	1.88	0.41
1:A:751:LYS:HB3	1:A:752:HIS:HD2	1.85	0.41
2:B:162:ALA:HB2	2:B:183:PRO:HD2	2.02	0.41
7:F:65:LEU:HD22	7:F:65:LEU:HA	1.86	0.41
7:F:448:ILE:HG21	7:F:566:THR:HA	2.03	0.41
1:A:238:TYR:O	1:A:242:MET:HG3	2.20	0.41
1:A:303:ASP:O	1:A:307:ILE:HG13	2.21	0.41
2:D:136:ASN:O	2:D:140:ASN:ND2	2.54	0.41
7:E:254:PRO:HB3	7:E:298:TYR:CE1	2.56	0.41
7:E:331:SER:OG	7:E:333:ILE:HG13	2.21	0.41
7:E:449:VAL:O	7:E:453:SER:OG	2.27	0.41
1:A:572:HIS:O	1:A:576:LEU:HG	2.21	0.41
1:A:689:TYR:O	1:A:693:VAL:HG23	2.21	0.41
1:A:858:ARG:HG2	4:I:32:G:H5'	2.03	0.41
2:D:38:LEU:C	2:D:39:LYS:HZ3	2.24	0.41
2:D:164:SER:O	2:D:164:SER:OG	2.29	0.41
7:E:182:PHE:HB2	7:E:225:PHE:HB3	2.03	0.41
1:A:19:LEU:HD23	1:A:58:GLU:HA	2.03	0.41
1:A:28:THR:HG21	1:A:52:ASN:HA	2.03	0.41
1:A:188:LYS:HD3	1:A:214:GLY:HA3	2.03	0.41
1:A:321:PHE:HB3	1:A:322:PRO:HD2	2.03	0.41
1:A:333:ILE:HG22	1:A:361:LEU:HD12	2.02	0.41
1:A:847:ILE:O	1:A:850:THR:O	2.38	0.41
2:D:75:ARG:O	2:D:77:GLU:N	2.54	0.41
4:I:23:U:C4	4:I:24:G:N7	2.89	0.41
7:F:243:GLN:NE2	7:F:277:TYR:O	2.53	0.41
7:F:280:LEU:HD13	7:F:436:MET:HG3	2.03	0.41
7:F:306:TYR:HA	7:F:372:VAL:HG22	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:345:LYS:HB2	7:F:345:LYS:HE2	1.71	0.41
7:F:448:ILE:O	7:F:448:ILE:HG22	2.21	0.41
7:F:510:VAL:HB	7:F:544:VAL:HG12	2.03	0.41
7:F:544:VAL:O	7:F:572:ILE:HA	2.20	0.41
7:E:21:ARG:HG3	7:E:21:ARG:HH11	1.85	0.41
7:E:73:LYS:HE2	7:E:73:LYS:HB3	1.85	0.41
7:E:182:PHE:HD2	7:E:200:PHE:HE1	1.69	0.41
7:E:187:VAL:HB	7:E:192:LYS:HG2	2.02	0.41
7:E:204:ASP:OD1	7:E:204:ASP:N	2.44	0.41
7:E:345:LYS:HG3	7:E:346:PHE:CE2	2.56	0.41
7:E:405:LEU:HB2	7:E:537:GLN:OE1	2.21	0.41
7:E:417:LEU:HA	7:E:417:LEU:HD23	1.87	0.41
7:E:493:ILE:O	7:E:497:ARG:HG2	2.21	0.41
7:E:520:ALA:O	7:E:524:LYS:N	2.54	0.41
1:A:8:LEU:HD12	1:A:21:PRO:HG3	2.03	0.41
1:A:330:VAL:HG11	2:B:117:LEU:HD13	2.03	0.41
7:F:198:TYR:HD1	7:F:225:PHE:HE2	1.67	0.41
7:F:578:ASP:CG	7:F:581:LEU:HB3	2.41	0.41
1:A:749:LEU:HD23	1:A:749:LEU:HA	1.83	0.40
2:B:38:LEU:HD23	2:B:38:LEU:HA	1.69	0.40
2:B:57:ARG:HD3	2:B:57:ARG:HA	1.81	0.40
2:B:132:ILE:HA	2:B:133:PRO:HD3	1.96	0.40
4:I:25:C:H2'	4:I:26:U:H6	1.81	0.40
7:F:357:PHE:CD1	7:F:357:PHE:N	2.89	0.40
7:F:380:THR:HA	7:F:423:ASN:HD22	1.86	0.40
7:E:108:ALA:O	7:E:112:CYS:HB3	2.21	0.40
3:C:25:SER:O	3:C:25:SER:OG	2.30	0.40
2:D:97:LYS:HE3	2:D:97:LYS:HB2	1.67	0.40
7:E:486:SER:HB3	7:E:517:SER:OG	2.21	0.40
7:E:557:ASN:OD1	7:E:560:ARG:N	2.44	0.40
1:A:159:LYS:O	1:A:159:LYS:HG2	2.21	0.40
1:A:371:LEU:HB3	2:B:87:MET:SD	2.62	0.40
2:B:47:SER:O	2:B:51:ARG:HG2	2.22	0.40
2:D:9:LEU:HD21	2:D:56:GLN:HG2	2.03	0.40
4:I:18:U:H2'	4:I:19:A:C8	2.57	0.40
7:F:117:ALA:O	7:F:121:ILE:HG12	2.22	0.40
7:F:411:LEU:HD23	7:F:411:LEU:HA	1.76	0.40
7:E:406:PRO:HB3	7:E:422:PHE:CE2	2.57	0.40
2:D:144:GLY:O	2:D:169:LEU:HD11	2.22	0.40
7:F:5:CYS:SG	7:F:26:CYS:HA	2.58	0.40
7:F:20:ILE:HG23	7:F:21:ARG:N	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:79:ILE:O	7:F:79:ILE:HG13	2.20	0.40
7:F:546:PHE:HB3	7:F:574:CYS:SG	2.61	0.40
7:E:268:ASN:ND2	7:E:291:PHE:CZ	2.89	0.40
7:E:284:PRO:HD3	7:E:457:TYR:OH	2.22	0.40
7:E:497:ARG:HH11	7:E:500:LEU:HD11	1.86	0.40
7:F:376:ILE:HD13	7:F:429:MET:SD	2.62	0.40
7:F:456:VAL:HG23	7:F:457:TYR:CD2	2.56	0.40
7:E:456:VAL:HG23	7:E:457:TYR:CD2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	924/942 (98%)	863 (93%)	53 (6%)	8 (1%)	17	48
2	B	185/198 (93%)	168 (91%)	15 (8%)	2 (1%)	14	42
2	D	184/198 (93%)	168 (91%)	14 (8%)	2 (1%)	14	42
3	C	70/83 (84%)	67 (96%)	3 (4%)	0	100	100
7	E	594/601 (99%)	524 (88%)	69 (12%)	1 (0%)	47	78
7	F	594/601 (99%)	516 (87%)	75 (13%)	3 (0%)	29	61
All	All	2551/2623 (97%)	2306 (90%)	229 (9%)	16 (1%)	29	58

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	THR
1	A	161	ASP
1	A	259	THR
1	A	607	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	F	289	SER
1	A	13	GLY
1	A	160	LYS
2	B	182	TRP
7	F	335	PRO
7	F	577	SER
1	A	257	VAL
2	B	183	PRO
1	A	832	PRO
7	E	350	SER
2	D	110	ALA
2	D	113	GLY

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	A	817/833 (98%)	733 (90%)	84 (10%)	7	22
2	B	144/167 (86%)	123 (85%)	21 (15%)	3	9
2	D	149/167 (89%)	131 (88%)	18 (12%)	5	15
3	C	67/77 (87%)	62 (92%)	5 (8%)	13	37
7	E	512/523 (98%)	433 (85%)	79 (15%)	2	8
7	F	514/523 (98%)	431 (84%)	83 (16%)	2	7
All	All	2203/2290 (96%)	1913 (87%)	290 (13%)	7	12

All (290) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	14	VAL
1	A	18	ARG
1	A	20	THR
1	A	22	CYS
1	A	24	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	31	VAL
1	A	32	TYR
1	A	37	ILE
1	A	41	LYS
1	A	49	LEU
1	A	62	ASP
1	A	64	ASN
1	A	72	VAL
1	A	76	THR
1	A	77	PHE
1	A	78	SER
1	A	80	TYR
1	A	90	LEU
1	A	105	ARG
1	A	116	ARG
1	A	141	THR
1	A	160	LYS
1	A	166	VAL
1	A	167	GLU
1	A	183	ARG
1	A	189	THR
1	A	197	ARG
1	A	235	ASP
1	A	236	SER
1	A	257	VAL
1	A	258	ASP
1	A	261	LEU
1	A	270	LEU
1	A	284	ASP
1	A	293	THR
1	A	343	SER
1	A	346	TYR
1	A	361	LEU
1	A	372	LEU
1	A	384	SER
1	A	434	SER
1	A	478	LYS
1	A	481	ASP
1	A	501	SER
1	A	551	LYS
1	A	556	THR
1	A	564	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	567	THR
1	A	578	SER
1	A	592	SER
1	A	605	VAL
1	A	607	SER
1	A	614	LEU
1	A	631	ARG
1	A	648	LEU
1	A	649	SER
1	A	665	GLU
1	A	675	VAL
1	A	684	ASP
1	A	686	THR
1	A	687	THR
1	A	710	THR
1	A	714	LYS
1	A	723	LEU
1	A	739	THR
1	A	758	LEU
1	A	759	SER
1	A	760	ASP
1	A	768	SER
1	A	778	SER
1	A	783	LYS
1	A	790	ASN
1	A	801	THR
1	A	815	GLN
1	A	835	SER
1	A	836	ARG
1	A	853	THR
1	A	854	LEU
1	A	855	MET
1	A	909	ASN
1	A	912	THR
1	A	913	SER
1	A	914	ARG
2	B	15	PHE
2	B	56	GLN
2	B	58	LYS
2	B	60	GLU
2	B	62	MET
2	B	64	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	76	SER
2	B	78	ASP
2	B	80	ARG
2	B	85	SER
2	B	111	ARG
2	B	128	LEU
2	B	142	CYS
2	B	148	THR
2	B	155	GLU
2	B	158	GLN
2	B	174	MET
2	B	177	SER
2	B	180	LEU
2	B	187	THR
2	B	189	LEU
3	C	22	VAL
3	C	24	SER
3	C	34	GLN
3	C	52	MET
3	C	60	LEU
2	D	12	TYR
2	D	31	SER
2	D	32	GLU
2	D	55	MET
2	D	59	LEU
2	D	75	ARG
2	D	78	ASP
2	D	83	VAL
2	D	112	ASP
2	D	124	THR
2	D	127	LYS
2	D	136	ASN
2	D	140	ASN
2	D	173	SER
2	D	175	ASP
2	D	177	SER
2	D	180	LEU
2	D	182	TRP
7	F	12	THR
7	F	22	ARG
7	F	30	CYS
7	F	38	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	F	56	ASP
7	F	65	LEU
7	F	73	LYS
7	F	74	SER
7	F	80	SER
7	F	84	CYS
7	F	97	CYS
7	F	102	ASN
7	F	124	ASN
7	F	126	CYS
7	F	139	LYS
7	F	153	THR
7	F	155	ARG
7	F	160	ASP
7	F	171	LYS
7	F	183	THR
7	F	185	TYR
7	F	187	VAL
7	F	192	LYS
7	F	200	PHE
7	F	205	TYR
7	F	212	ARG
7	F	214	THR
7	F	219	LEU
7	F	223	ASP
7	F	226	VAL
7	F	229	SER
7	F	240	LEU
7	F	255	THR
7	F	256	LEU
7	F	260	ASP
7	F	306	TYR
7	F	324	TYR
7	F	325	LEU
7	F	329	LYS
7	F	331	SER
7	F	339	ARG
7	F	345	LYS
7	F	347	LYS
7	F	353	GLU
7	F	357	PHE
7	F	361	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	F	365	GLU
7	F	380	THR
7	F	382	TYR
7	F	392	ARG
7	F	401	ASP
7	F	411	LEU
7	F	412	LEU
7	F	414	LYS
7	F	425	VAL
7	F	430	LYS
7	F	432	ILE
7	F	437	PHE
7	F	444	CYS
7	F	451	THR
7	F	465	LYS
7	F	471	CYS
7	F	472	PHE
7	F	473	LYS
7	F	475	PHE
7	F	479	VAL
7	F	497	ARG
7	F	499	PHE
7	F	502	ARG
7	F	507	ARG
7	F	536	SER
7	F	537	GLN
7	F	541	TYR
7	F	550	THR
7	F	551	GLU
7	F	554	HIS
7	F	561	PHE
7	F	575	ILE
7	F	577	SER
7	F	582	TYR
7	F	585	LEU
7	F	587	PHE
7	F	590	LEU
7	E	6	VAL
7	E	15	ARG
7	E	55	CYS
7	E	70	TYR
7	E	73	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	E	81	PHE
7	E	94	LYS
7	E	96	THR
7	E	97	CYS
7	E	98	VAL
7	E	116	ASN
7	E	127	THR
7	E	129	ARG
7	E	130	LEU
7	E	136	GLU
7	E	145	PHE
7	E	161	ARG
7	E	168	GLU
7	E	178	ARG
7	E	183	THR
7	E	188	THR
7	E	192	LYS
7	E	199	THR
7	E	209	VAL
7	E	216	THR
7	E	223	ASP
7	E	224	TYR
7	E	233	MET
7	E	240	LEU
7	E	243	GLN
7	E	295	LEU
7	E	309	CYS
7	E	310	SER
7	E	311	HIS
7	E	317	LEU
7	E	318	CYS
7	E	325	LEU
7	E	329	LYS
7	E	330	CYS
7	E	331	SER
7	E	337	ARG
7	E	339	ARG
7	E	340	VAL
7	E	345	LYS
7	E	347	LYS
7	E	349	ASN
7	E	350	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	E	352	LEU
7	E	358	CYS
7	E	363	LEU
7	E	377	SER
7	E	387	VAL
7	E	392	ARG
7	E	420	GLU
7	E	427	ARG
7	E	437	PHE
7	E	447	GLU
7	E	448	ILE
7	E	462	LYS
7	E	464	HIS
7	E	466	ASP
7	E	471	CYS
7	E	473	LYS
7	E	481	THR
7	E	482	HIS
7	E	483	ASP
7	E	490	ARG
7	E	502	ARG
7	E	513	SER
7	E	550	THR
7	E	554	HIS
7	E	556	CYS
7	E	567	ARG
7	E	574	CYS
7	E	576	MET
7	E	578	ASP
7	E	579	ARG
7	E	580	ASP
7	E	589	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	HIS
1	A	752	HIS
1	A	909	ASN
7	F	33	HIS
7	F	311	HIS
7	F	381	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	F	470	GLN
7	F	519	ASN
7	E	404	GLN
7	E	459	ASN
7	E	516	ASN
7	E	519	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	I	24/25 (96%)	1 (4%)	1 (4%)
5	J	25/58 (43%)	0	0
6	L	5/6 (83%)	4 (80%)	0
All	All	54/89 (60%)	5 (9%)	1 (1%)

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	I	25	C
6	L	1	A
6	L	3	A
6	L	4	A
6	L	5	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	I	24	G

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

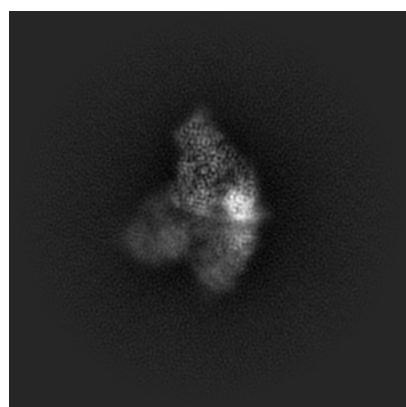
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30492. These allow visual inspection of the internal detail of the map and identification of artifacts.

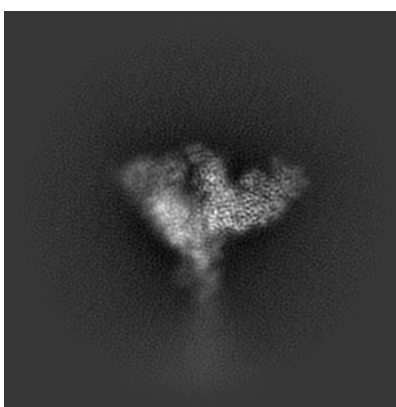
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

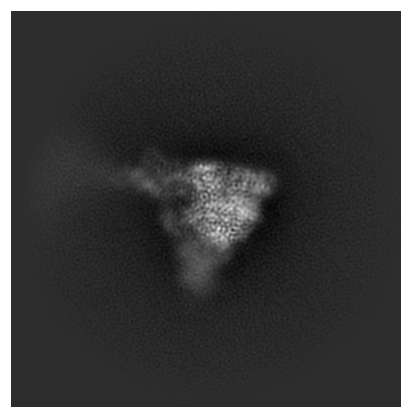
6.1.1 Primary map



X



Y

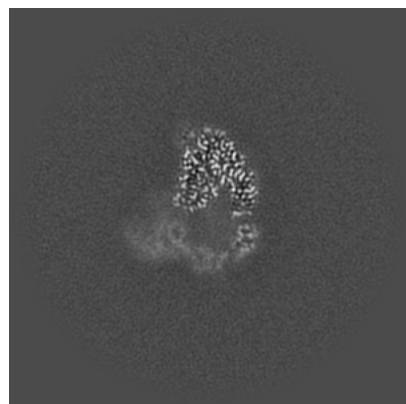


Z

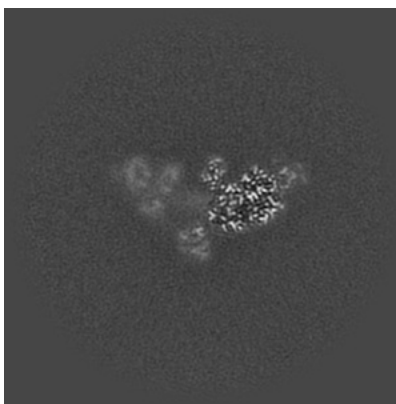
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

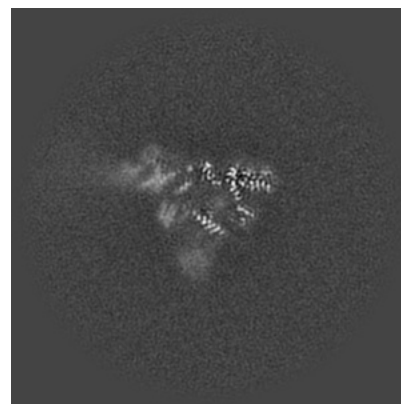
6.2.1 Primary map



X Index: 224



Y Index: 224

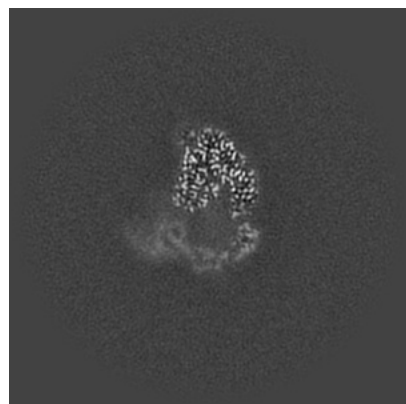


Z Index: 224

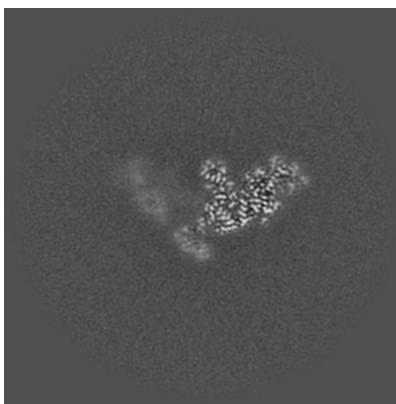
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

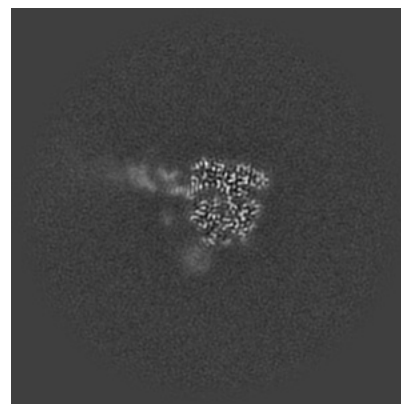
6.3.1 Primary map



X Index: 225



Y Index: 217

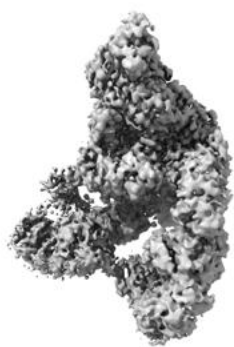


Z Index: 234

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 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

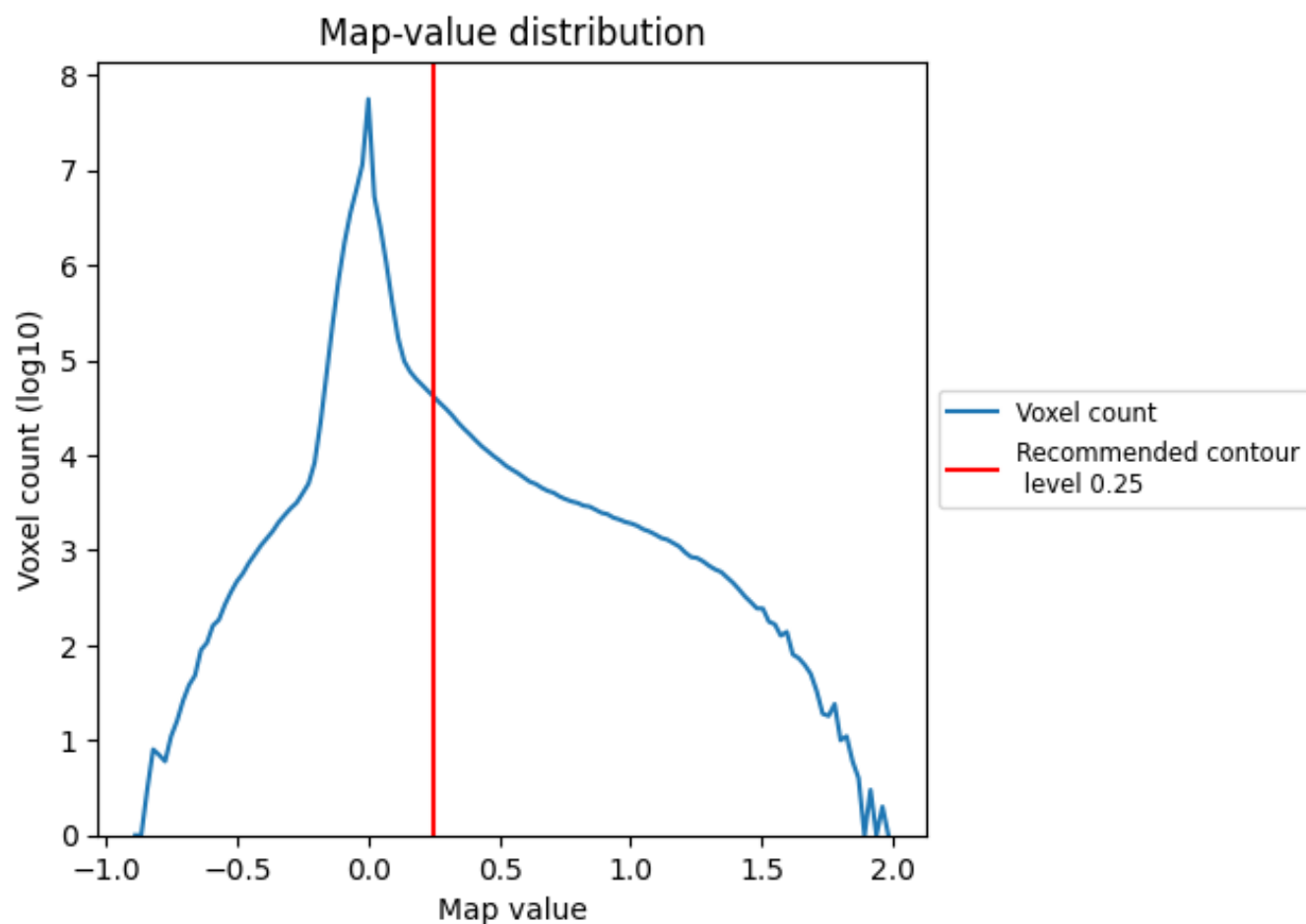
6.5 Mask visualisation

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

7 Map analysis [i](#)

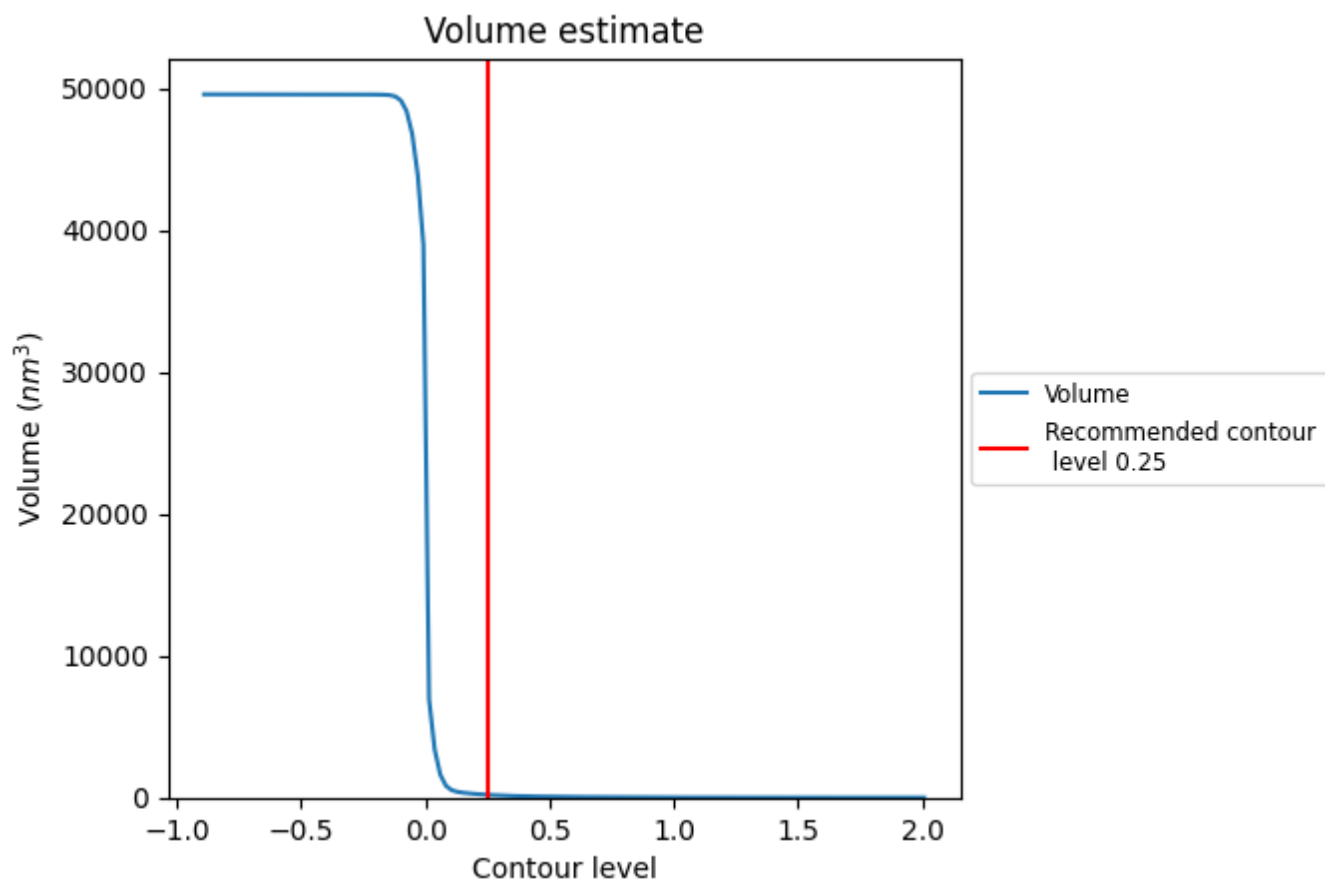
This section contains the results of statistical analysis of the map.

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.

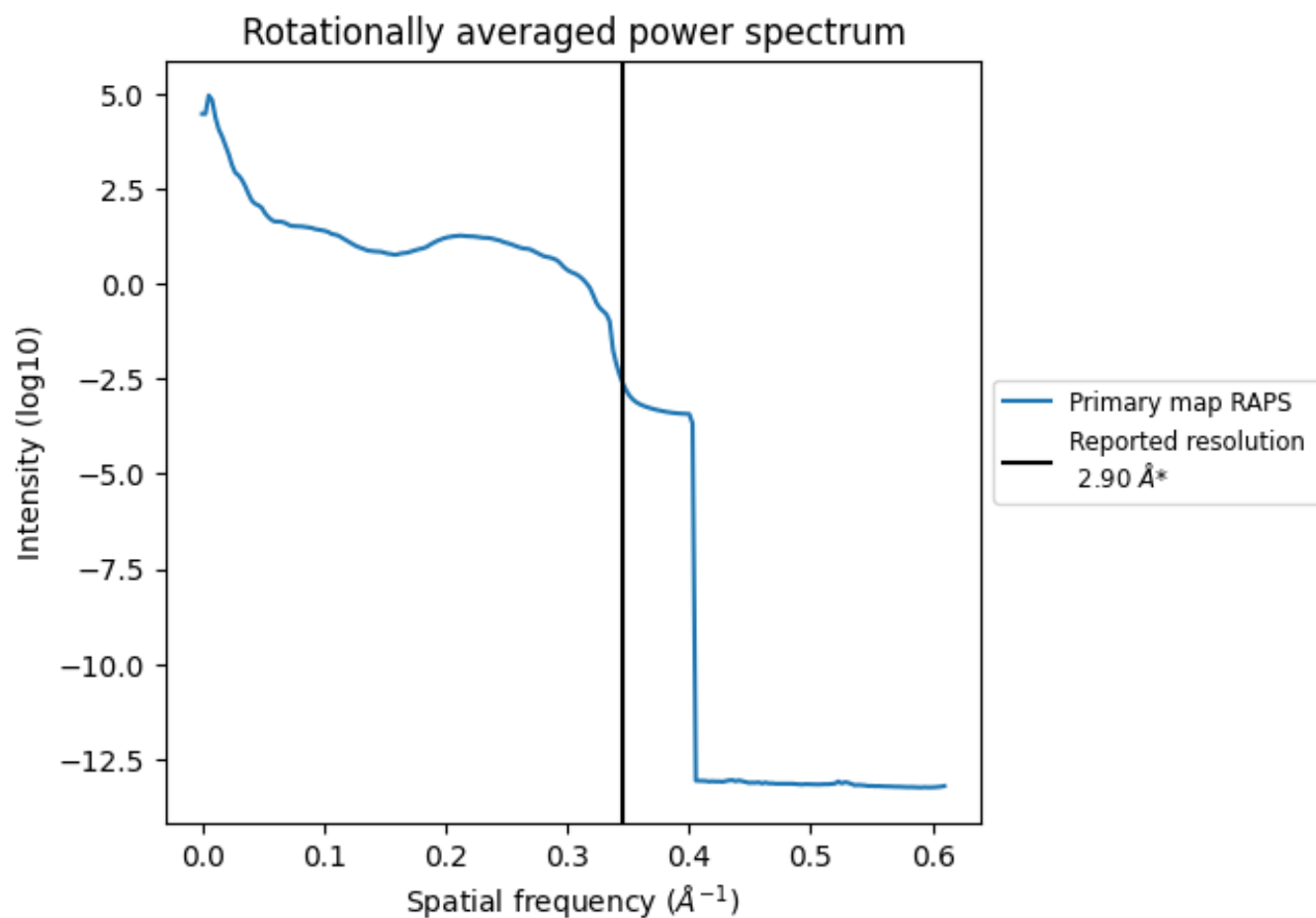
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 194 nm³; this corresponds to an approximate mass of 176 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 0.345 Å⁻¹

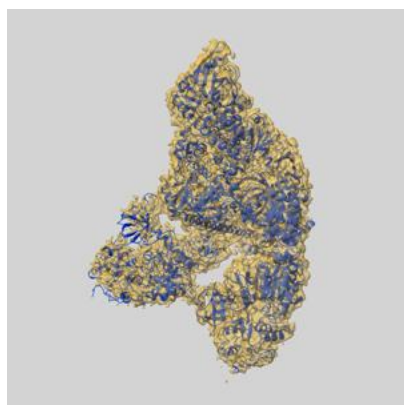
8 Fourier-Shell correlation

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

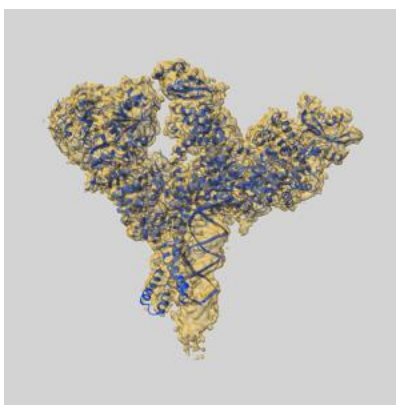
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30492 and PDB model 7CXM. Per-residue inclusion information can be found in section [3](#) on page [6](#).

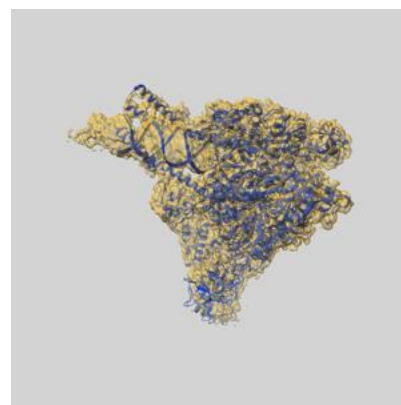
9.1 Map-model overlay [i](#)



X



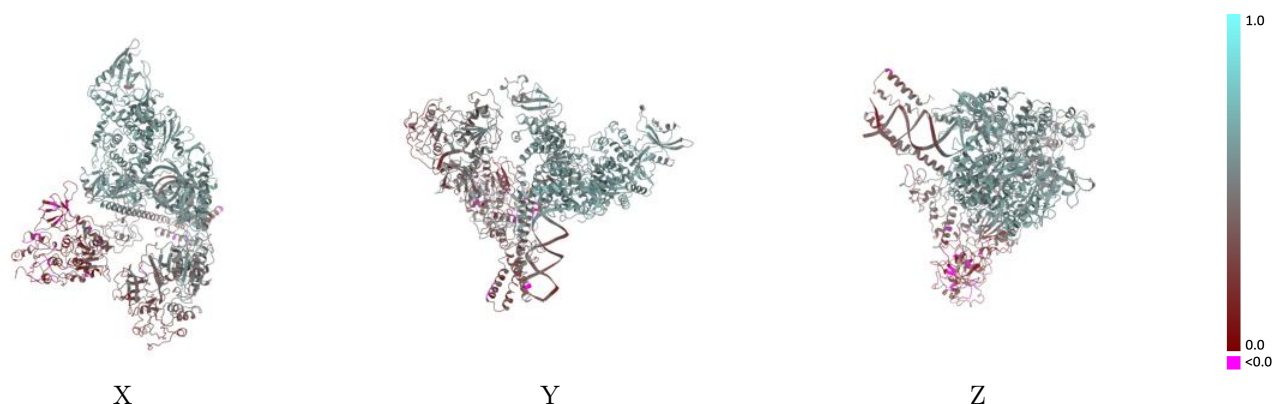
Y



Z

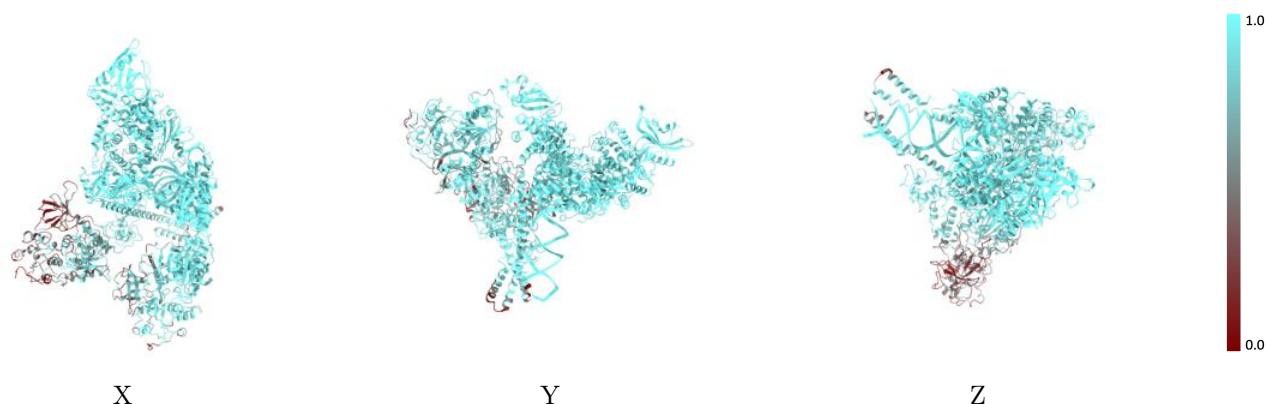
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



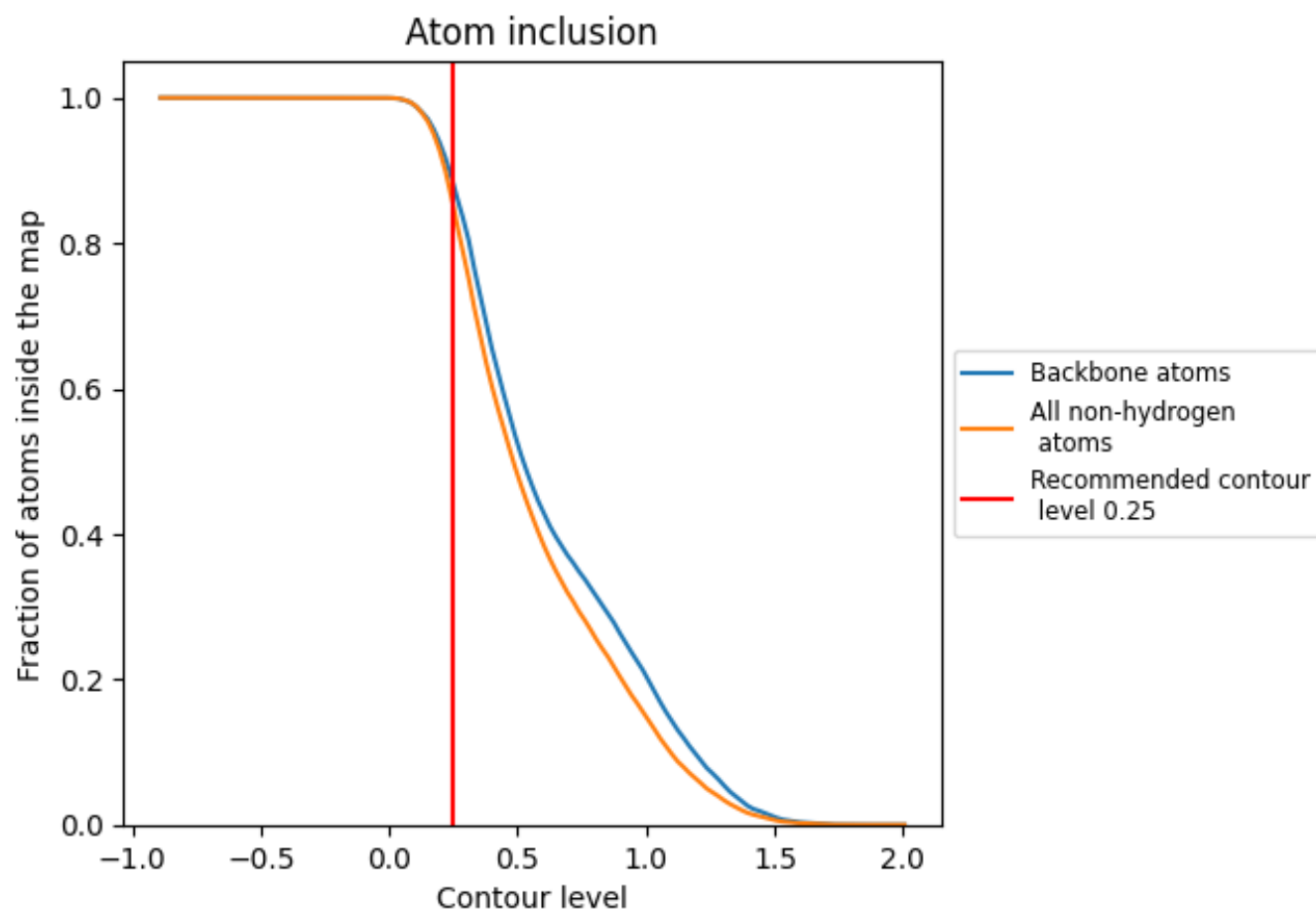
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 85% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8506	<div></div> 0.4610
A	<div></div> 0.9837	<div></div> 0.5870
B	<div></div> 0.9011	<div></div> 0.4860
C	<div></div> 0.9600	<div></div> 0.5650
D	<div></div> 0.9389	<div></div> 0.5040
E	<div></div> 0.8339	<div></div> 0.4250
F	<div></div> 0.5765	<div></div> 0.2670
I	<div></div> 0.9743	<div></div> 0.4270
J	<div></div> 0.9853	<div></div> 0.4670
L	<div></div> 0.4922	<div></div> 0.3520

1.0

0.0

<0.0