



Full wwPDB EM Validation Report ⓘ

Nov 12, 2022 – 07:43 PM EST

PDB ID : 6V5C
EMDB ID : EMD-21052
Title : Human Drosha and DGCR8 in complex with Primary MicroRNA (MP/RNA complex) - partially docked state
Authors : Partin, A.; Zhang, K.; Jeong, B.; Herrell, E.; Li, S.; Chiu, W.; Nam, Y.
Deposited on : 2019-12-04
Resolution : 4.40 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

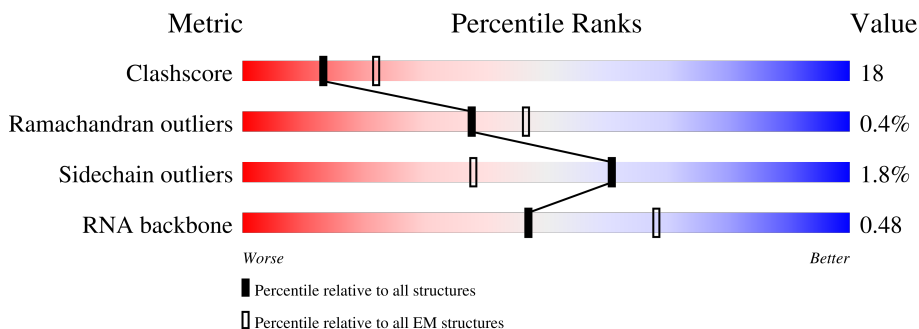
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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
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	1016	
2	B	532	
2	C	532	
3	D	105	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12251 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 Ribonuclease 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	903	7371	4696	1301	1325	49	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	350	GLY	-	expression tag	UNP Q9NRR4
A	351	SER	-	expression tag	UNP Q9NRR4
A	352	GLY	-	expression tag	UNP Q9NRR4
A	1045	GLN	GLU	engineered mutation	UNP Q9NRR4
A	1222	GLN	GLU	engineered mutation	UNP Q9NRR4

- Molecule 2 is a protein called Microprocessor complex subunit DGCR8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	217	1747	1104	312	321	10	0	0
2	B	216	1739	1099	308	322	10	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	220	GLY	-	expression tag	UNP Q8WYQ5
C	221	SER	-	expression tag	UNP Q8WYQ5
C	222	GLY	-	expression tag	UNP Q8WYQ5
B	220	GLY	-	expression tag	UNP Q8WYQ5
B	221	SER	-	expression tag	UNP Q8WYQ5
B	222	GLY	-	expression tag	UNP Q8WYQ5

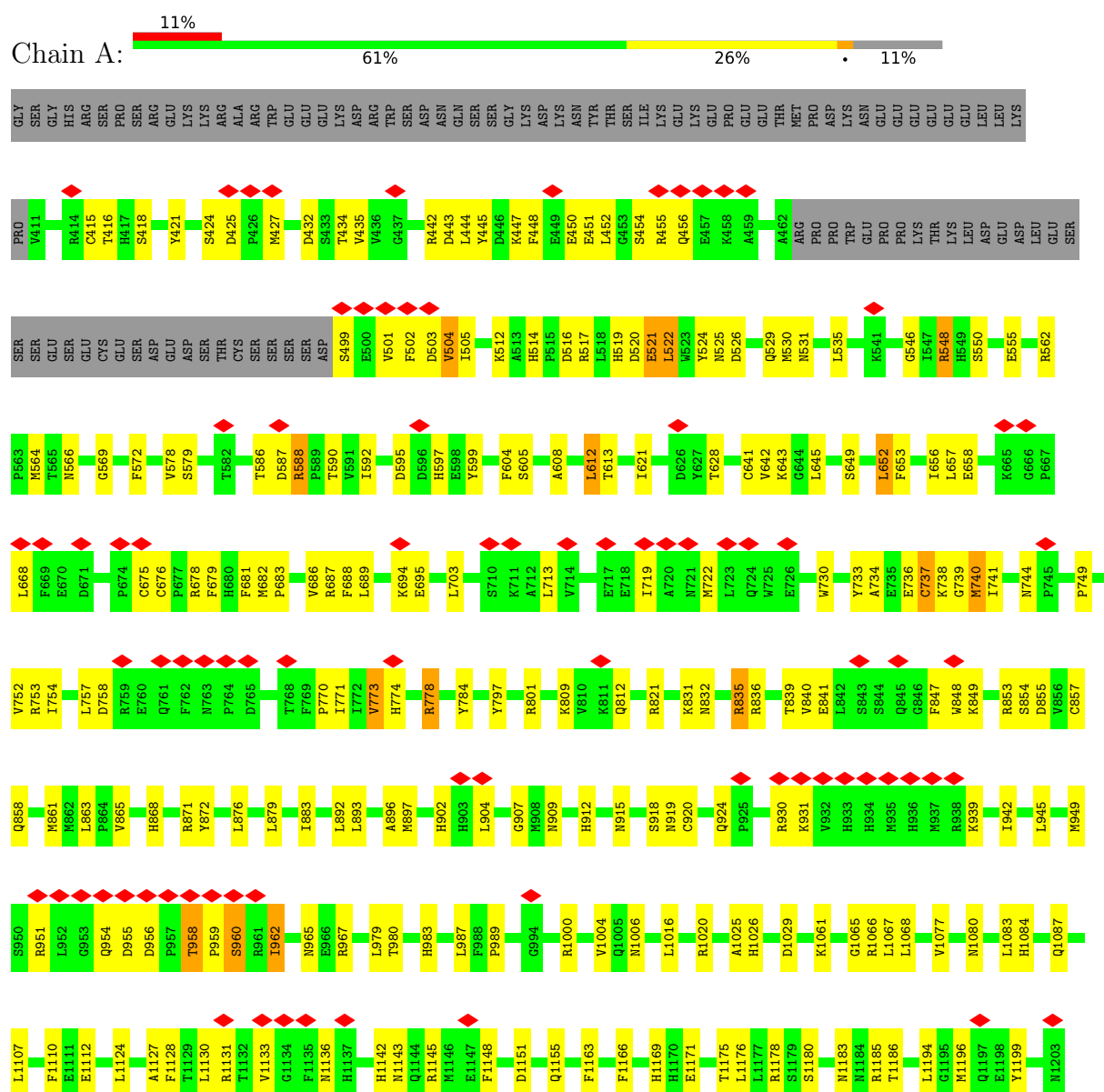
- Molecule 3 is a RNA chain called Pri-miR-16-2 (66-MER).

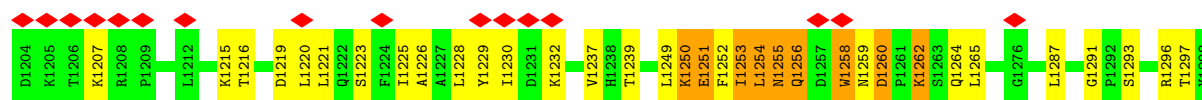
Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	66	Total	C	N	O	P	0	0
			1394	624	237	467	66		

3 Residue-property plots

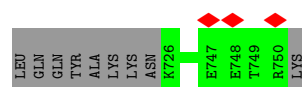
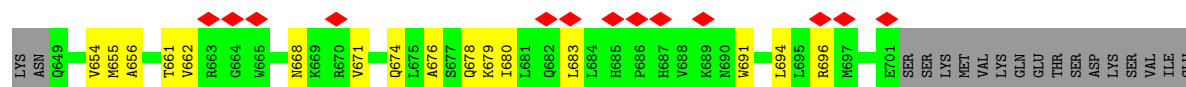
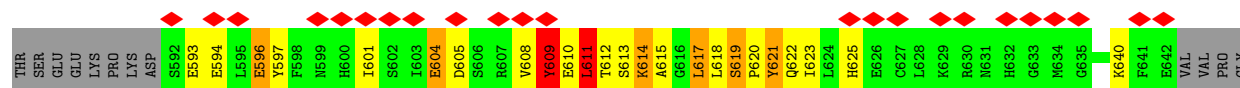
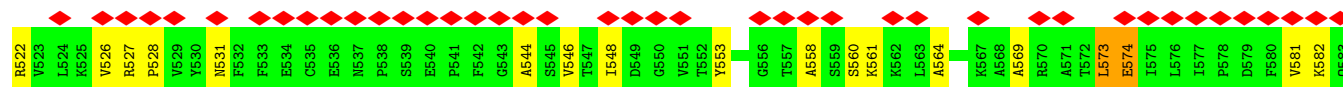
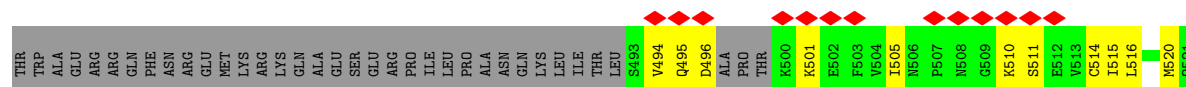
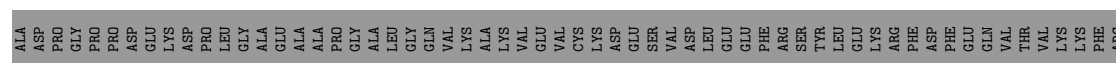
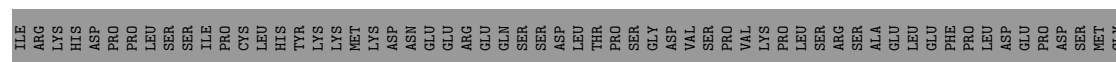
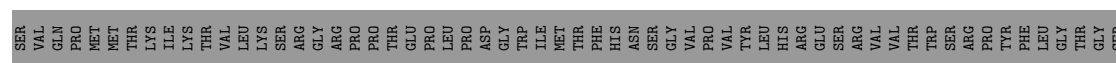
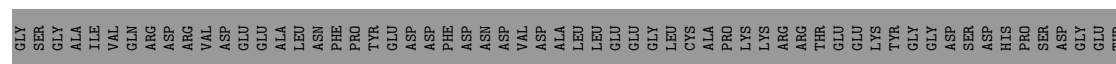
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Ribonuclease 3

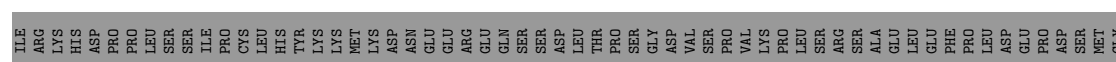
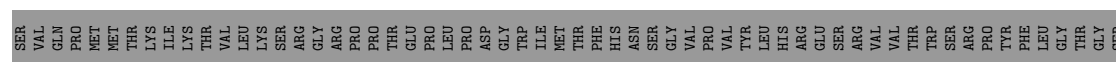
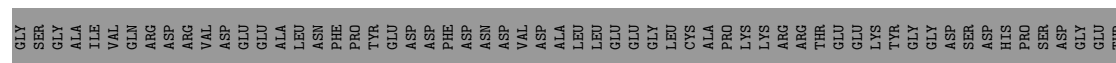




• Molecule 2: Microprocessor complex subunit DGCR8



• Molecule 2: Microprocessor complex subunit DGCR8



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	381468	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 ($e^-/\text{\AA}^2$)	46.8	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3600	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.361	Depositor
Minimum map value	-1.169	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.091	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	271.36, 271.36, 271.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality i

5.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.40	0/7555	0.68	15/10217 (0.1%)
2	B	0.30	0/1769	0.58	0/2369
2	C	0.40	0/1777	0.70	7/2379 (0.3%)
3	D	0.58	0/1554	1.27	15/2414 (0.6%)
All	All	0.41	0/12655	0.78	37/17379 (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	A	0	5
2	B	0	2
2	C	0	2
All	All	0	9

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	904	LEU	CA-CB-CG	8.18	134.12	115.30
1	A	1124	LEU	CA-CB-CG	7.78	133.18	115.30
1	A	736	GLU	O-C-N	7.61	134.87	122.70
2	C	608	VAL	N-CA-C	7.34	130.83	111.00
1	A	736	GLU	C-N-CA	7.15	139.56	121.70
3	D	78	C	C2-N1-C1'	6.84	126.32	118.80
1	A	855	ASP	CB-CG-OD1	6.84	124.45	118.30
1	A	736	GLU	CA-C-N	-6.45	103.02	117.20
3	D	82	U	N1-C2-O2	6.37	127.26	122.80
2	C	573	LEU	CA-CB-CG	6.30	129.79	115.30
3	D	29	C	C2-N1-C1'	6.16	125.57	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1258	TRP	N-CA-CB	6.15	121.66	110.60
3	D	9	C	N1-C2-O2	6.06	122.53	118.90
2	C	611	LEU	CB-CG-CD2	5.94	121.09	111.00
1	A	958	THR	C-N-CD	5.92	140.83	128.40
1	A	652	LEU	CA-CB-CG	5.90	128.87	115.30
2	C	609	TYR	N-CA-C	5.90	126.93	111.00
2	C	621	TYR	CA-CB-CG	-5.85	102.28	113.40
3	D	82	U	N3-C2-O2	-5.79	118.15	122.20
3	D	93	A	C2-N3-C4	5.72	113.46	110.60
3	D	78	C	C6-N1-C2	-5.57	118.07	120.30
3	D	74	U	N1-C2-O2	5.53	126.67	122.80
2	C	611	LEU	CA-CB-CG	5.49	127.92	115.30
1	A	740	MET	CB-CG-SD	5.43	128.70	112.40
3	D	82	U	C2-N1-C1'	5.42	124.20	117.70
3	D	37	U	N1-C2-O2	5.41	126.59	122.80
3	D	64	C	N1-C2-O2	5.41	122.14	118.90
3	D	90	G	N3-C4-N9	5.36	129.22	126.00
2	C	604	GLU	N-CA-C	5.34	125.43	111.00
3	D	37	U	N3-C2-O2	-5.25	118.52	122.20
3	D	78	C	N1-C2-O2	5.15	121.99	118.90
1	A	1124	LEU	CB-CG-CD2	-5.13	102.27	111.00
1	A	955	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	1258	TRP	N-CA-C	-5.09	97.25	111.00
1	A	854	SER	C-N-CA	5.09	134.42	121.70
3	D	64	C	C2-N1-C1'	5.05	124.36	118.80
1	A	737	CYS	N-CA-C	5.01	124.53	111.00

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	521	GLU	Peptide
1	A	522	LEU	Peptide
1	A	773	VAL	Peptide
1	A	778	ARG	Peptide
1	A	983	HIS	Peptide
2	B	640	LYS	Peptide
2	B	668	ASN	Peptide
2	C	574	GLU	Peptide
2	C	596	GLU	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	7371	0	7304	259	0
2	B	1739	0	1753	36	0
2	C	1747	0	1764	123	0
3	D	1394	0	707	25	0
All	All	12251	0	11528	431	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 18.

All (431) 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)
2:C:495:GLN:HB2	2:C:582:LYS:CG	1.39	1.50
2:C:495:GLN:CB	2:C:582:LYS:HG2	1.36	1.49
1:A:740:MET:HE1	1:A:920:CYS:CB	1.52	1.37
1:A:740:MET:CE	1:A:920:CYS:HB3	1.52	1.36
1:A:738:LYS:HA	1:A:754:ILE:CD1	1.56	1.35
1:A:738:LYS:CA	1:A:754:ILE:HD11	1.58	1.32
1:A:1254:LEU:HD23	1:A:1343:PHE:CD1	1.63	1.31
2:C:593:GLU:HB3	2:C:596:GLU:CG	1.61	1.28
1:A:740:MET:CE	1:A:920:CYS:CB	2.11	1.26
1:A:733:TYR:O	1:A:737:CYS:HB2	1.35	1.23
2:C:597:TYR:CE1	2:C:601:ILE:HD11	1.77	1.20
2:C:619:SER:HB2	2:C:620:PRO:CD	1.74	1.17
2:C:613:SER:OG	2:C:619:SER:HB2	1.43	1.15
2:C:495:GLN:H	2:C:582:LYS:HB2	1.11	1.14
2:C:582:LYS:HE2	2:C:582:LYS:HA	1.28	1.14
1:A:1254:LEU:CD2	1:A:1343:PHE:HD1	1.62	1.12
1:A:740:MET:O	1:A:847:PHE:CZ	2.02	1.12
1:A:1083:LEU:CD2	1:A:1230:ILE:HD13	1.80	1.10
2:B:605:ASP:HB3	2:B:608:VAL:HG21	1.32	1.09
2:C:619:SER:CB	2:C:620:PRO:HD2	1.83	1.08
1:A:1343:PHE:CD2	1:A:1344:ILE:HG23	1.88	1.08
2:C:593:GLU:CG	2:C:596:GLU:HG3	1.84	1.08
2:C:495:GLN:N	2:C:582:LYS:HB2	1.70	1.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:593:GLU:HB3	2:C:596:GLU:HG3	1.37	1.06
2:C:613:SER:CB	2:C:620:PRO:HD3	1.86	1.05
2:C:593:GLU:HB3	2:C:596:GLU:HG2	1.35	1.04
2:C:593:GLU:CB	2:C:596:GLU:HG3	1.85	1.04
2:C:619:SER:HB2	2:C:620:PRO:HD2	1.38	1.03
2:C:495:GLN:H	2:C:582:LYS:CB	1.75	1.00
2:C:593:GLU:HG2	2:C:596:GLU:HG3	1.41	1.00
2:C:619:SER:CB	2:C:620:PRO:CD	2.35	1.00
2:C:593:GLU:CB	2:C:596:GLU:CG	2.39	0.99
1:A:1083:LEU:HD23	1:A:1230:ILE:HD13	1.44	0.99
2:C:597:TYR:HE1	2:C:601:ILE:HD11	1.14	0.97
1:A:754:ILE:HD13	1:A:757:LEU:HD11	1.46	0.96
1:A:1343:PHE:HD2	1:A:1344:ILE:HG12	1.30	0.96
2:C:613:SER:OG	2:C:620:PRO:HD3	1.66	0.95
1:A:737:CYS:SG	1:A:757:LEU:HD22	2.06	0.95
1:A:740:MET:CE	1:A:920:CYS:HB2	1.95	0.94
1:A:740:MET:HE1	1:A:920:CYS:HB3	0.95	0.93
1:A:1254:LEU:HD23	1:A:1343:PHE:HD1	0.76	0.92
2:C:613:SER:HB2	2:C:620:PRO:HD3	1.51	0.92
1:A:740:MET:HE3	1:A:920:CYS:CB	2.00	0.92
1:A:1343:PHE:CE2	1:A:1344:ILE:HG23	2.04	0.92
2:C:619:SER:HB2	2:C:620:PRO:HD3	1.50	0.91
2:C:613:SER:OG	2:C:619:SER:CB	2.19	0.91
1:A:1252:PHE:O	1:A:1255:ASN:ND2	2.04	0.90
1:A:1259:ASN:O	1:A:1260:ASP:HB2	1.73	0.89
1:A:1254:LEU:CD2	1:A:1343:PHE:CD1	2.46	0.87
1:A:740:MET:HE1	1:A:920:CYS:HB2	1.55	0.87
2:C:612:THR:HG21	2:C:678:GLN:HE22	1.42	0.84
2:B:605:ASP:HB3	2:B:608:VAL:CG2	2.07	0.84
1:A:733:TYR:O	1:A:737:CYS:CB	2.24	0.83
2:C:597:TYR:CE1	2:C:601:ILE:CD1	2.58	0.83
1:A:754:ILE:CD1	1:A:757:LEU:HD11	2.09	0.82
2:C:614:LYS:HE2	2:C:615:ALA:HA	1.59	0.82
1:A:1343:PHE:HD2	1:A:1344:ILE:CG1	1.93	0.81
1:A:958:THR:OG1	1:A:962:ILE:HD11	1.81	0.81
1:A:1249:LEU:O	1:A:1253:ILE:HG12	1.82	0.80
1:A:1343:PHE:CD2	1:A:1344:ILE:CG2	2.64	0.80
1:A:1083:LEU:HD21	1:A:1230:ILE:HD13	1.63	0.80
1:A:1343:PHE:CE2	1:A:1344:ILE:CG2	2.65	0.79
1:A:740:MET:O	1:A:847:PHE:CE2	2.37	0.77
2:C:619:SER:OG	2:C:620:PRO:HD2	1.84	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:601:ILE:HG23	2:C:609:TYR:CE2	2.20	0.77
1:A:1083:LEU:HD23	1:A:1230:ILE:CD1	2.15	0.76
2:C:582:LYS:HA	2:C:582:LYS:CE	2.13	0.76
3:D:10:U:C4	3:D:94:G:C6	2.73	0.76
2:C:495:GLN:HB3	2:C:582:LYS:HG2	1.62	0.76
1:A:740:MET:HE3	1:A:920:CYS:HB3	1.56	0.74
3:D:10:U:N3	3:D:94:G:C6	2.55	0.73
2:C:617:LEU:N	2:C:617:LEU:HD12	2.03	0.73
1:A:1258:TRP:HH2	1:A:1264:GLN:HE21	1.35	0.73
1:A:738:LYS:HA	1:A:754:ILE:HD11	0.76	0.72
2:C:597:TYR:CZ	2:C:601:ILE:HD11	2.24	0.72
2:C:494:VAL:CG2	2:C:505:ILE:HB	2.19	0.72
3:D:10:U:C2	3:D:94:G:N1	2.58	0.72
2:C:495:GLN:HB2	2:C:582:LYS:HG3	1.65	0.72
1:A:1258:TRP:CH2	1:A:1264:GLN:NE2	2.57	0.72
1:A:962:ILE:HD12	1:A:962:ILE:N	2.06	0.71
3:D:30:G:H1	3:D:74:U:H3	1.37	0.71
1:A:1249:LEU:O	1:A:1253:ILE:CG1	2.40	0.70
2:C:614:LYS:HD2	2:C:614:LYS:O	1.91	0.70
2:C:594:GLU:OE1	2:C:696:ARG:NH2	2.24	0.70
2:B:620:PRO:O	2:B:624:LEU:HB2	1.91	0.70
2:C:573:LEU:O	2:C:581:VAL:CG2	2.40	0.70
1:A:1250:LYS:HE3	1:A:1343:PHE:CZ	2.27	0.69
1:A:621:ILE:HG21	1:A:960:SER:HB3	1.73	0.69
2:C:495:GLN:HB3	2:C:582:LYS:H	1.56	0.69
2:C:582:LYS:HE2	2:C:582:LYS:CA	2.15	0.69
1:A:1343:PHE:CD2	1:A:1344:ILE:HG12	2.21	0.69
1:A:1253:ILE:HD13	1:A:1253:ILE:N	2.07	0.68
2:B:610:GLU:O	2:B:612:THR:N	2.27	0.68
1:A:1254:LEU:HD13	1:A:1254:LEU:O	1.95	0.67
2:C:622:GLN:O	2:C:625:HIS:N	2.26	0.67
2:C:601:ILE:CG2	2:C:609:TYR:CE2	2.77	0.67
1:A:435:VAL:H	1:A:566:ASN:HD21	1.43	0.66
1:A:734:ALA:O	1:A:737:CYS:HB3	1.96	0.66
1:A:1250:LYS:HE3	1:A:1343:PHE:HZ	1.59	0.66
3:D:10:U:C4	3:D:94:G:O6	2.48	0.66
1:A:517:ARG:NH1	1:A:519:HIS:O	2.28	0.66
1:A:1194:LEU:HB3	1:A:1196:MET:HG2	1.77	0.66
2:C:511:SER:HG	2:C:514:CYS:HG	1.40	0.65
2:B:572:THR:O	2:B:576:LEU:HB2	1.96	0.65
1:A:579:SER:HB2	1:A:628:THR:H	1.60	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1249:LEU:O	1:A:1253:ILE:CD1	2.44	0.65
2:C:496:ASP:CB	2:C:501:LYS:HZ3	2.10	0.65
2:C:615:ALA:HB3	2:C:617:LEU:HD11	1.78	0.64
2:C:546:VAL:HG23	2:C:553:TYR:HB2	1.79	0.64
1:A:1252:PHE:C	1:A:1255:ASN:HD22	2.00	0.64
1:A:590:THR:HG22	1:A:853:ARG:HB2	1.80	0.64
1:A:1186:THR:OG1	1:A:1252:PHE:CE2	2.50	0.64
1:A:1254:LEU:HD21	1:A:1343:PHE:HB2	1.80	0.63
1:A:424:SER:HB3	1:A:435:VAL:HA	1.81	0.63
1:A:734:ALA:C	1:A:737:CYS:HB3	2.19	0.63
1:A:1249:LEU:O	1:A:1253:ILE:HD11	1.98	0.63
1:A:1259:ASN:O	1:A:1260:ASP:CB	2.44	0.63
2:C:612:THR:HG21	2:C:678:GLN:NE2	2.12	0.63
1:A:1258:TRP:C	1:A:1260:ASP:H	2.01	0.63
2:C:495:GLN:N	2:C:582:LYS:CB	2.48	0.62
1:A:809:LYS:HE3	1:A:1004:VAL:HG13	1.82	0.62
2:C:597:TYR:CZ	2:C:601:ILE:CD1	2.82	0.62
1:A:512:LYS:NZ	1:A:530:MET:SD	2.71	0.62
1:A:962:ILE:HD13	1:A:962:ILE:O	2.00	0.62
2:C:597:TYR:OH	2:C:601:ILE:HD13	2.00	0.62
1:A:1083:LEU:CD2	1:A:1230:ILE:CD1	2.69	0.61
1:A:448:PHE:HB3	1:A:452:LEU:HD13	1.83	0.61
2:C:622:GLN:O	2:C:623:ILE:C	2.39	0.61
2:C:495:GLN:HB3	2:C:582:LYS:N	2.14	0.61
2:B:610:GLU:C	2:B:612:THR:H	2.02	0.61
1:A:1287:LEU:HD12	1:A:1301:ALA:HB3	1.82	0.61
2:C:597:TYR:OH	2:C:601:ILE:CD1	2.49	0.61
1:A:649:SER:O	1:A:653:PHE:HB2	2.00	0.61
1:A:962:ILE:HD12	1:A:962:ILE:H	1.65	0.61
1:A:434:THR:OG1	1:A:566:ASN:ND2	2.34	0.61
1:A:504:VAL:HG23	1:A:505:ILE:HD12	1.83	0.61
1:A:737:CYS:SG	1:A:757:LEU:CD2	2.85	0.60
1:A:1133:VAL:HG13	1:A:1136:ASN:HB2	1.82	0.60
1:A:738:LYS:CB	1:A:754:ILE:HD11	2.29	0.60
1:A:555:GLU:OE2	1:A:678:ARG:NH1	2.34	0.60
1:A:1291:GLY:O	1:A:1296:ARG:NH2	2.34	0.60
2:B:521:GLN:NE2	2:B:526:VAL:O	2.34	0.60
1:A:1065:GLY:HA2	1:A:1068:LEU:HB3	1.84	0.60
1:A:979:LEU:HD21	1:A:1061:LYS:HA	1.84	0.59
1:A:1258:TRP:C	1:A:1260:ASP:N	2.53	0.59
2:B:552:THR:HG22	2:B:554:GLY:H	1.68	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:SER:H	1:A:435:VAL:HG12	1.67	0.59
1:A:744:ASN:OD1	1:A:744:ASN:N	2.35	0.58
2:B:637:THR:HG21	2:B:656:ALA:H	1.67	0.58
1:A:1239:THR:HG21	2:B:742:LEU:HD13	1.86	0.58
1:A:1258:TRP:HH2	1:A:1264:GLN:NE2	1.99	0.58
2:C:544:ALA:HB3	2:C:564:ALA:HB3	1.86	0.58
1:A:689:LEU:HD23	1:A:695:GLU:HB2	1.85	0.58
1:A:989:PRO:O	1:A:1145:ARG:NH1	2.35	0.58
1:A:675:CYS:SG	1:A:676:CYS:N	2.77	0.57
1:A:612:LEU:HD12	1:A:613:THR:H	1.69	0.57
1:A:774:HIS:ND1	1:A:918:SER:O	2.37	0.57
1:A:1186:THR:OG1	1:A:1252:PHE:CZ	2.58	0.57
2:B:572:THR:O	2:B:576:LEU:CB	2.53	0.57
1:A:514:HIS:ND1	1:A:516:ASP:OD1	2.38	0.57
2:C:494:VAL:HG22	2:C:505:ILE:HB	1.87	0.56
1:A:442:ARG:HH21	1:A:643:LYS:HB2	1.69	0.56
1:A:548:ARG:HH21	1:A:1026:HIS:CG	2.23	0.56
1:A:770:PRO:HB3	1:A:840:VAL:HG23	1.87	0.56
1:A:857:CYS:SG	1:A:858:GLN:N	2.77	0.56
1:A:753:ARG:HH22	1:A:924:GLN:HE21	1.54	0.56
1:A:967:ARG:NH2	1:A:1166:PHE:O	2.33	0.56
2:C:613:SER:OG	2:C:620:PRO:CD	2.48	0.56
1:A:876:LEU:HD12	1:A:893:LEU:HD21	1.87	0.56
1:A:713:LEU:HD22	1:A:847:PHE:H	1.69	0.56
1:A:1301:ALA:HA	1:A:1311:CYS:HA	1.88	0.56
2:C:618:LEU:HB3	2:C:622:GLN:HB2	1.88	0.56
1:A:450:GLU:OE2	1:A:455:ARG:NH1	2.39	0.56
2:B:575:ILE:HG12	2:B:696:ARG:HB3	1.86	0.56
1:A:512:LYS:NZ	1:A:531:ASN:OD1	2.40	0.55
1:A:1253:ILE:HD13	1:A:1253:ILE:H	1.69	0.55
1:A:442:ARG:NH2	1:A:641:CYS:SG	2.79	0.55
1:A:1066:ARG:O	1:A:1066:ARG:NH1	2.40	0.55
1:A:1338:ALA:HA	1:A:1341:LYS:HB2	1.87	0.55
2:C:610:GLU:O	2:C:612:THR:HG23	2.07	0.55
1:A:525:ASN:ND2	1:A:658:GLU:O	2.40	0.55
2:C:495:GLN:CB	2:C:582:LYS:H	2.20	0.55
2:C:611:LEU:HG	2:C:614:LYS:HB3	1.89	0.55
2:B:660:HIS:HB3	2:B:679:LYS:HE2	1.88	0.55
1:A:448:PHE:HA	1:A:451:GLU:HB2	1.87	0.55
2:C:601:ILE:HG23	2:C:609:TYR:HE2	1.72	0.55
2:C:668:ASN:HB3	2:C:671:VAL:HG12	1.87	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1020:ARG:O	1:A:1020:ARG:HG3	2.06	0.54
1:A:1155:GLN:OE1	1:A:1178:ARG:NH1	2.36	0.54
2:C:601:ILE:CG2	2:C:609:TYR:HE2	2.21	0.54
1:A:740:MET:SD	1:A:920:CYS:HB2	2.46	0.54
2:C:495:GLN:CB	2:C:582:LYS:CG	2.28	0.54
1:A:1131:ARG:NH1	3:D:75:G:O2'	2.41	0.54
1:A:1316:SER:OG	1:A:1319:GLN:OE1	2.24	0.54
1:A:519:HIS:ND1	1:A:520:ASP:OD1	2.38	0.54
2:C:494:VAL:HG12	2:C:582:LYS:O	2.07	0.54
2:B:610:GLU:C	2:B:612:THR:N	2.61	0.54
1:A:1133:VAL:O	1:A:1142:HIS:NE2	2.39	0.53
1:A:1343:PHE:CD2	1:A:1344:ILE:CG1	2.84	0.53
1:A:958:THR:HG1	1:A:962:ILE:HD11	1.72	0.53
2:C:620:PRO:HB3	2:C:678:GLN:HB2	1.91	0.53
1:A:915:ASN:O	1:A:919:ASN:ND2	2.42	0.53
1:A:415:CYS:SG	1:A:416:THR:N	2.82	0.53
1:A:739:GLY:O	1:A:754:ILE:HG12	2.09	0.53
1:A:949:MET:O	1:A:954:GLN:NE2	2.41	0.53
1:A:687:ARG:HH21	1:A:689:LEU:HB3	1.74	0.53
1:A:967:ARG:NH1	1:A:1169:HIS:O	2.41	0.53
1:A:713:LEU:HD13	1:A:847:PHE:HB3	1.91	0.52
1:A:1253:ILE:CD1	1:A:1253:ILE:H	2.22	0.52
1:A:1265:LEU:HD21	1:A:1325:ALA:HA	1.90	0.52
2:C:617:LEU:HD12	2:C:617:LEU:H	1.72	0.52
1:A:771:ILE:O	1:A:839:THR:OG1	2.25	0.52
1:A:1311:CYS:N	1:A:1327:ASP:OD2	2.42	0.52
2:C:495:GLN:H	2:C:582:LYS:CA	2.23	0.52
2:C:560:SER:OG	2:C:561:LYS:N	2.41	0.52
1:A:942:ILE:HA	1:A:945:LEU:HB2	1.92	0.52
2:C:527:ARG:NH2	3:D:70:U:OP1	2.42	0.52
1:A:535:LEU:HD22	1:A:548:ARG:HD2	1.92	0.52
2:C:495:GLN:HB2	2:C:582:LYS:HG2	0.58	0.52
1:A:686:VAL:HG21	1:A:694:LYS:HD3	1.91	0.51
2:B:631:ASN:HD21	2:B:684:LEU:HD22	1.74	0.51
1:A:740:MET:HE3	1:A:920:CYS:CA	2.40	0.51
1:A:1251:GLU:O	1:A:1255:ASN:HB3	2.10	0.51
2:C:593:GLU:CB	2:C:596:GLU:CB	2.89	0.51
1:A:572:PHE:HB2	1:A:608:ALA:HB3	1.92	0.51
2:C:522:ARG:NH2	3:D:36:A:O3'	2.43	0.51
2:B:555:SER:OG	2:B:556:GLY:N	2.44	0.51
1:A:1171:GLU:OE2	1:A:1175:THR:OG1	2.28	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:527:ARG:HH12	3:D:66:A:H4'	1.76	0.51
1:A:1143:ASN:ND2	1:A:1216:THR:OG1	2.44	0.51
1:A:657:LEU:HD13	1:A:920:CYS:SG	2.51	0.50
1:A:741:ILE:HB	1:A:752:VAL:HB	1.92	0.50
1:A:1112:GLU:O	2:B:736:GLN:NE2	2.45	0.50
1:A:1293:SER:OG	3:D:77:G:N2	2.41	0.50
2:C:516:LEU:HD11	2:C:569:ALA:HB2	1.92	0.50
2:B:517:HIS:HA	2:B:520:MET:HE1	1.93	0.50
1:A:1251:GLU:OE2	1:A:1251:GLU:HA	2.11	0.50
1:A:1343:PHE:CE2	1:A:1344:ILE:HG21	2.45	0.50
1:A:897:MET:HA	1:A:965:ASN:HD21	1.77	0.49
1:A:512:LYS:O	1:A:524:TYR:OH	2.29	0.49
1:A:868:HIS:HB3	1:A:872:TYR:CZ	2.47	0.49
1:A:1346:ARG:HG2	1:A:1347:LYS:HG3	1.94	0.49
2:C:495:GLN:N	2:C:582:LYS:H	2.10	0.49
2:B:511:SER:OG	2:B:512:GLU:N	2.45	0.49
1:A:892:LEU:O	1:A:896:ALA:HB2	2.11	0.49
2:C:655:MET:O	2:C:662:VAL:N	2.44	0.49
3:D:14:U:H3	3:D:90:G:H1	1.60	0.49
1:A:1326:MET:O	1:A:1330:GLU:HB2	2.12	0.49
2:C:527:ARG:HD3	2:B:509:GLY:HA2	1.93	0.49
1:A:1262:LYS:HA	1:A:1265:LEU:HD12	1.94	0.49
1:A:652:LEU:HA	1:A:656:ILE:HG12	1.94	0.49
1:A:939:LYS:H	1:A:951:ARG:HH12	1.60	0.49
1:A:1107:LEU:HA	1:A:1110:PHE:HB3	1.95	0.49
2:B:651:SER:OG	2:B:652:GLU:N	2.45	0.49
2:C:621:TYR:CD2	2:C:621:TYR:C	2.85	0.49
1:A:418:SER:HB2	1:A:421:TYR:HB2	1.95	0.49
1:A:1220:LEU:HD23	1:A:1221:LEU:HD22	1.95	0.49
2:B:495:GLN:NE2	2:B:583:GLN:O	2.43	0.48
1:A:604:PHE:HA	1:A:683:PRO:HA	1.95	0.48
2:B:531:ASN:O	2:B:545:SER:OG	2.32	0.48
2:C:573:LEU:O	2:C:581:VAL:HG21	2.11	0.48
1:A:688:PHE:HD1	1:A:694:LYS:HB3	1.78	0.48
1:A:967:ARG:HH12	1:A:1169:HIS:H	1.61	0.48
1:A:1319:GLN:HA	1:A:1322:MET:HB3	1.96	0.48
2:C:495:GLN:H	2:C:582:LYS:H	1.60	0.48
1:A:587:ASP:OD1	1:A:587:ASP:N	2.47	0.48
1:A:522:LEU:HB3	1:A:778:ARG:HH21	1.79	0.48
1:A:1258:TRP:HZ3	1:A:1264:GLN:HB2	1.77	0.48
1:A:499:SER:N	1:A:503:ASP:O	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:740:MET:HE3	1:A:920:CYS:HA	1.96	0.48
2:C:495:GLN:H	2:C:582:LYS:N	2.11	0.47
1:A:784:TYR:OH	1:A:832:ASN:O	2.31	0.47
1:A:930:ARG:HE	1:A:931:LYS:HG2	1.79	0.47
2:C:527:ARG:HD2	2:C:528:PRO:HD2	1.96	0.47
2:C:593:GLU:HB2	2:C:596:GLU:HB2	1.95	0.47
1:A:425:ASP:HB3	1:A:427:MET:HG2	1.95	0.47
1:A:595:ASP:O	1:A:597:HIS:ND1	2.48	0.47
1:A:1252:PHE:HB2	1:A:1253:ILE:HD13	1.95	0.47
1:A:524:TYR:HB3	1:A:749:PRO:HA	1.95	0.47
1:A:1006:ASN:N	1:A:1006:ASN:OD1	2.46	0.47
1:A:1151:ASP:HB3	1:A:1215:LYS:HZ1	1.79	0.47
2:C:511:SER:O	2:C:515:ILE:N	2.47	0.47
2:C:611:LEU:C	2:C:611:LEU:CD2	2.83	0.47
2:B:620:PRO:HB2	2:B:673:LYS:HB3	1.97	0.47
1:A:548:ARG:HE	1:A:1026:HIS:HB2	1.80	0.47
2:C:605:ASP:N	2:C:605:ASP:OD1	2.48	0.47
1:A:980:THR:OG1	1:A:1000:ARG:NH2	2.47	0.47
1:A:1183:ASN:OD1	1:A:1186:THR:N	2.44	0.47
2:C:610:GLU:OE2	2:C:612:THR:CG2	2.62	0.47
1:A:1219:ASP:O	1:A:1223:SER:OG	2.28	0.47
1:A:1219:ASP:O	1:A:1223:SER:CB	2.62	0.46
1:A:1228:LEU:HB3	1:A:1232:LYS:HB2	1.97	0.46
2:C:593:GLU:CB	2:C:596:GLU:HB2	2.45	0.46
1:A:753:ARG:HD3	1:A:774:HIS:CD2	2.50	0.46
1:A:831:LYS:HG3	1:A:832:ASN:H	1.80	0.46
1:A:1299:THR:O	1:A:1299:THR:OG1	2.32	0.46
2:B:695:LEU:HD12	2:B:699:GLY:HA3	1.96	0.46
1:A:1254:LEU:CD1	1:A:1254:LEU:C	2.84	0.46
3:D:87:U:H2'	3:D:88:G:C8	2.50	0.46
1:A:517:ARG:NH2	1:A:520:ASP:O	2.34	0.46
1:A:550:SER:HB3	1:A:668:LEU:HD11	1.97	0.46
1:A:1127:ALA:HA	1:A:1143:ASN:HB3	1.98	0.46
2:C:548:ILE:H	2:C:553:TYR:HE2	1.64	0.46
1:A:432:ASP:HB3	1:A:569:GLY:H	1.80	0.46
1:A:588:ARG:CZ	1:A:853:ARG:NH1	2.79	0.46
2:C:593:GLU:HB3	2:C:596:GLU:CB	2.37	0.46
1:A:456:GLN:HG2	1:A:516:ASP:HB3	1.96	0.46
2:C:614:LYS:HD2	2:C:614:LYS:C	2.36	0.46
1:A:730:TRP:NE1	1:A:758:ASP:OD2	2.35	0.45
1:A:1130:LEU:HG	1:A:1131:ARG:HG2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:618:LEU:HD22	2:C:622:GLN:OE1	2.17	0.45
1:A:657:LEU:CD1	1:A:920:CYS:SG	3.05	0.45
1:A:592:ILE:HG23	1:A:599:TYR:HB2	1.98	0.45
2:C:610:GLU:OE2	2:C:612:THR:HG21	2.15	0.45
1:A:546:GLY:HA2	1:A:1020:ARG:HA	1.99	0.45
2:C:614:LYS:C	2:C:614:LYS:CD	2.85	0.45
3:D:10:U:C2	3:D:94:G:C2	3.05	0.45
1:A:821:ARG:HA	1:A:821:ARG:HD3	1.83	0.45
2:C:613:SER:HB2	2:C:620:PRO:CD	2.33	0.45
2:C:620:PRO:HG2	2:C:674:GLN:HB3	1.99	0.45
1:A:681:PHE:HE2	1:A:863:LEU:HD22	1.82	0.44
1:A:835:ARG:O	1:A:836:ARG:NH1	2.49	0.44
2:C:656:ALA:HA	2:C:661:THR:HA	1.99	0.44
3:D:89:U:H2'	3:D:90:G:H8	1.82	0.44
3:D:10:U:N3	3:D:94:G:N1	2.63	0.44
1:A:526:ASP:OD2	1:A:529:GLN:N	2.50	0.44
1:A:548:ARG:HH21	1:A:1026:HIS:CD2	2.36	0.44
1:A:1219:ASP:OD1	1:A:1223:SER:OG	2.34	0.44
2:B:617:LEU:HG	2:B:691:TRP:HD1	1.83	0.44
1:A:443:ASP:N	1:A:443:ASP:OD1	2.44	0.44
1:A:1293:SER:HB2	1:A:1296:ARG:HH11	1.83	0.44
2:C:680:ILE:HA	2:C:683:LEU:HB2	1.99	0.44
1:A:586:THR:OG1	1:A:587:ASP:N	2.51	0.44
1:A:861:MET:SD	1:A:861:MET:N	2.91	0.44
1:A:516:ASP:OD1	1:A:516:ASP:N	2.38	0.44
1:A:1297:THR:HG21	2:B:538:PRO:HA	1.99	0.44
1:A:562:ARG:HG3	1:A:564:MET:H	1.83	0.43
1:A:737:CYS:SG	1:A:737:CYS:O	2.75	0.43
2:B:531:ASN:N	2:B:531:ASN:OD1	2.51	0.43
2:C:582:LYS:CE	2:C:582:LYS:CA	2.85	0.43
1:A:734:ALA:HA	1:A:737:CYS:CB	2.49	0.43
2:C:604:GLU:O	2:C:604:GLU:HG2	2.18	0.43
2:C:613:SER:CB	2:C:620:PRO:CD	2.77	0.43
1:A:1225:ILE:HG13	1:A:1237:VAL:HB	1.99	0.43
2:C:526:VAL:HG12	2:B:506:ASN:HD21	1.82	0.43
1:A:865:VAL:HG12	1:A:907:GLY:H	1.84	0.43
1:A:1336:GLN:HG2	1:A:1338:ALA:H	1.83	0.43
2:C:610:GLU:O	2:C:612:THR:CG2	2.66	0.43
1:A:642:VAL:HG13	1:A:645:LEU:HD12	1.99	0.43
2:C:610:GLU:HA	2:C:610:GLU:OE1	2.19	0.43
1:A:679:PHE:HE2	1:A:871:ARG:HD2	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1254:LEU:HD13	1:A:1254:LEU:C	2.38	0.43
1:A:797:TYR:OH	1:A:801:ARG:NH1	2.52	0.43
3:D:33:A:H2'	3:D:34:A:H8	1.83	0.43
1:A:1253:ILE:N	1:A:1253:ILE:CD1	2.73	0.42
1:A:1000:ARG:HD2	1:A:1148:PHE:HZ	1.85	0.42
1:A:1077:VAL:HA	1:A:1080:ASN:HB2	2.01	0.42
2:B:640:LYS:N	2:B:668:ASN:O	2.52	0.42
1:A:1084:HIS:HB3	1:A:1087:GLN:HB2	2.01	0.42
2:C:528:PRO:HA	2:C:548:ILE:HG12	2.02	0.42
2:B:610:GLU:O	2:B:613:SER:OG	2.35	0.42
2:B:620:PRO:HA	2:B:623:ILE:HG22	2.01	0.42
1:A:753:ARG:HH11	1:A:774:HIS:CD2	2.37	0.42
2:C:676:ALA:HA	2:C:679:LYS:HE2	2.00	0.42
1:A:744:ASN:HD21	1:A:848:TRP:HB2	1.85	0.42
2:C:531:ASN:OD1	2:C:531:ASN:N	2.52	0.42
2:C:640:LYS:N	2:C:656:ALA:O	2.48	0.42
1:A:1304:PHE:HB3	1:A:1309:ILE:HB	2.02	0.42
2:C:510:LYS:NZ	3:D:35:U:O2'	2.42	0.42
3:D:41:C:O2'	3:D:64:C:N3	2.52	0.42
1:A:879:LEU:HG	1:A:883:ILE:HG12	2.01	0.42
1:A:909:ASN:OD1	1:A:912:HIS:N	2.47	0.42
1:A:1300:VAL:HG12	1:A:1302:VAL:HG13	2.02	0.42
1:A:605:SER:N	1:A:682:MET:O	2.49	0.41
1:A:967:ARG:HG2	1:A:1163:PHE:HE1	1.85	0.41
2:C:618:LEU:HD23	2:C:618:LEU:HA	1.80	0.41
2:B:598:PHE:HA	2:B:601:ILE:HB	2.02	0.41
3:D:10:U:O2	3:D:94:G:C2	2.73	0.41
3:D:76:U:H2'	3:D:77:G:C8	2.55	0.41
1:A:770:PRO:HA	1:A:841:GLU:H	1.85	0.41
2:C:597:TYR:OH	2:C:601:ILE:HD11	2.18	0.41
1:A:1207:LYS:HD3	1:A:1207:LYS:HA	1.92	0.41
2:C:494:VAL:CG2	2:C:505:ILE:CB	2.95	0.41
2:C:594:GLU:OE2	2:C:594:GLU:HA	2.20	0.41
2:C:601:ILE:HG21	2:C:609:TYR:CD2	2.55	0.41
1:A:612:LEU:H	1:A:612:LEU:HG	1.76	0.41
1:A:752:VAL:HG13	1:A:773:VAL:HG22	2.02	0.41
1:A:1110:PHE:HB2	1:A:1199:TYR:CZ	2.56	0.41
1:A:1260:ASP:HB3	1:A:1262:LYS:HG3	2.02	0.41
1:A:1342:ARG:NE	3:D:89:U:OP1	2.53	0.41
3:D:63:A:H4'	3:D:64:C:C5	2.55	0.41
1:A:445:TYR:HA	1:A:448:PHE:CD2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:719:ILE:HA	1:A:722:MET:HB3	2.03	0.41
1:A:987:LEU:HD23	1:A:987:LEU:HA	1.89	0.41
1:A:450:GLU:HA	1:A:454:SER:H	1.85	0.41
2:C:494:VAL:HG21	2:C:505:ILE:CG2	2.51	0.41
2:B:671:VAL:HA	2:B:674:GLN:HB2	2.02	0.41
3:D:29:C:H2'	3:D:30:G:H8	1.86	0.41
3:D:92:C:H2'	3:D:93:A:H8	1.85	0.41
1:A:741:ILE:HG12	1:A:847:PHE:CD2	2.56	0.41
1:A:1221:LEU:HD13	1:A:1221:LEU:HA	1.92	0.41
1:A:1228:LEU:HD22	1:A:1232:LYS:HD2	2.03	0.41
2:C:520:MET:HE1	2:C:548:ILE:HG21	2.02	0.41
1:A:902:HIS:ND1	1:A:1025:ALA:HB2	2.36	0.41
1:A:501:VAL:HG13	1:A:502:PHE:HD1	1.86	0.41
1:A:1176:LEU:O	1:A:1180:SER:OG	2.35	0.41
1:A:1256:GLN:CA	1:A:1256:GLN:HE21	2.33	0.41
2:C:558:ALA:HB2	2:C:564:ALA:HB2	2.02	0.41
2:C:573:LEU:HD12	2:C:574:GLU:HG2	2.02	0.41
2:C:610:GLU:O	2:C:610:GLU:CG	2.68	0.41
2:C:691:TRP:HA	2:C:694:LEU:HD22	2.02	0.41
3:D:27:C:H2'	3:D:28:A:C8	2.56	0.41
1:A:444:LEU:HD22	1:A:703:LEU:HD12	2.03	0.41
1:A:962:ILE:N	1:A:962:ILE:CD1	2.72	0.41
1:A:1128:PHE:HD1	1:A:1128:PHE:HA	1.78	0.41
1:A:1251:GLU:O	1:A:1255:ASN:N	2.39	0.41
1:A:517:ARG:NH1	1:A:521:GLU:OE2	2.53	0.40
1:A:713:LEU:H	1:A:849:LYS:H	1.68	0.40
2:B:623:ILE:HA	2:B:626:GLU:HB2	2.03	0.40
2:C:494:VAL:HA	2:C:582:LYS:HB2	2.04	0.40
1:A:444:LEU:O	1:A:447:LYS:NZ	2.53	0.40
1:A:566:ASN:N	1:A:566:ASN:OD1	2.54	0.40
1:A:713:LEU:HB2	1:A:848:TRP:H	1.86	0.40
1:A:809:LYS:O	1:A:812:GLN:NE2	2.45	0.40
1:A:1016:LEU:HD22	1:A:1067:LEU:HD21	2.02	0.40
1:A:1133:VAL:HA	1:A:1136:ASN:HD22	1.87	0.40
1:A:1185:ARG:NH2	1:A:1256:GLN:HA	2.37	0.40
1:A:1225:ILE:HG21	1:A:1237:VAL:HB	2.03	0.40
1:A:930:ARG:HH22	1:A:956:ASP:HB3	1.86	0.40
1:A:1226:ALA:HA	1:A:1229:TYR:HB2	2.03	0.40
2:C:604:GLU:O	2:C:604:GLU:CG	2.70	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	A	899/1016 (88%)	753 (84%)	144 (16%)	2 (0%)	47	81
2	B	206/532 (39%)	192 (93%)	13 (6%)	1 (0%)	29	68
2	C	207/532 (39%)	182 (88%)	23 (11%)	2 (1%)	15	54
All	All	1312/2080 (63%)	1127 (86%)	180 (14%)	5 (0%)	38	72

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1260	ASP
2	B	611	LEU
2	C	609	TYR
2	C	619	SER
1	A	959	PRO

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	807/916 (88%)	790 (98%)	17 (2%)	53	72
2	B	193/475 (41%)	193 (100%)	0	100	100
2	C	193/475 (41%)	188 (97%)	5 (3%)	46	67
All	All	1193/1866 (64%)	1171 (98%)	22 (2%)	61	77

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	504	VAL
1	A	548	ARG
1	A	578	VAL
1	A	588	ARG
1	A	612	LEU
1	A	835	ARG
1	A	960	SER
1	A	962	ILE
1	A	1029	ASP
1	A	1250	LYS
1	A	1251	GLU
1	A	1253	ILE
1	A	1254	LEU
1	A	1255	ASN
1	A	1256	GLN
1	A	1262	LYS
1	A	1346	ARG
2	C	609	TYR
2	C	611	LEU
2	C	614	LYS
2	C	617	LEU
2	C	654	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	429	GLN
1	A	549	HIS
1	A	680	HIS
1	A	826	GLN
1	A	873	HIS
1	A	894	GLN
1	A	924	GLN
1	A	954	GLN
1	A	964	HIS
1	A	1080	ASN
1	A	1136	ASN
1	A	1255	ASN
1	A	1256	GLN
1	A	1294	HIS
2	C	632	HIS
2	C	736	GLN
2	B	521	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	678	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	D	64/105 (60%)	20 (31%)	0

All (20) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	D	11	U
3	D	17	A
3	D	18	C
3	D	21	U
3	D	25	A
3	D	26	G
3	D	32	A
3	D	33	A
3	D	37	U
3	D	41	C
3	D	64	C
3	D	65	C
3	D	70	U
3	D	78	C
3	D	80	G
3	D	82	U
3	D	89	U
3	D	91	A
3	D	92	C
3	D	93	A

There are no RNA pucker outliers to report.

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

There are no ligands in this entry.

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.

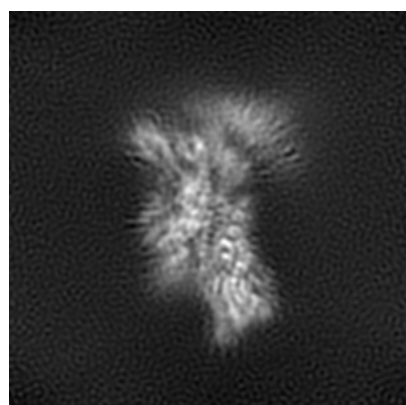
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21052. These allow visual inspection of the internal detail of the map and identification of artifacts.

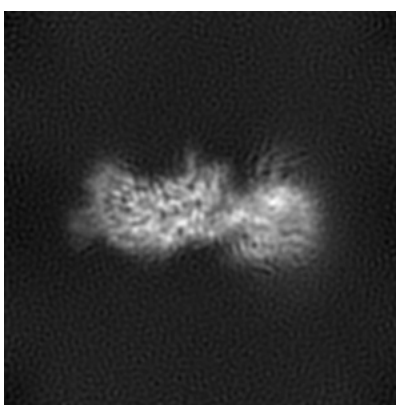
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

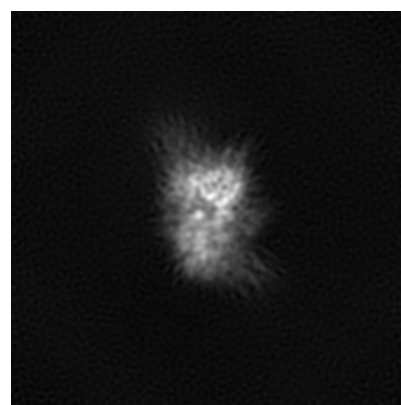
6.1.1 Primary map



X



Y

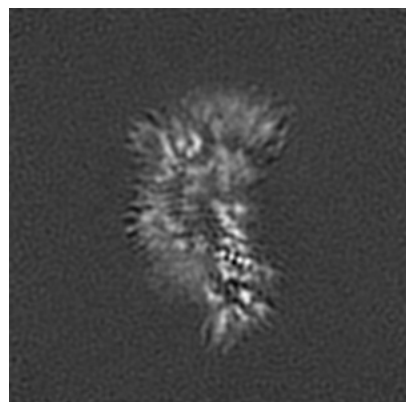


Z

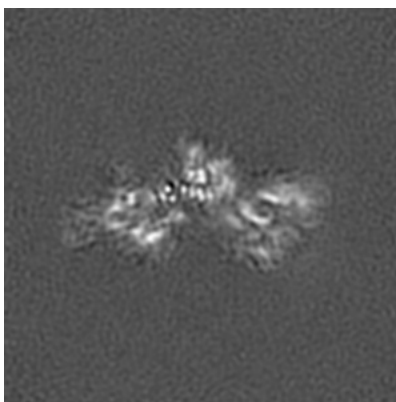
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

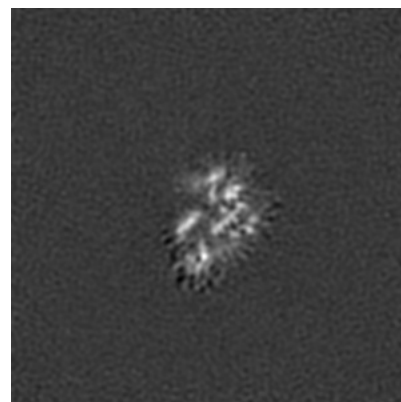
6.2.1 Primary map



X Index: 128



Y Index: 128

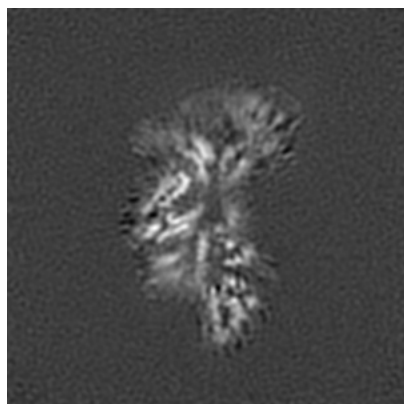


Z Index: 128

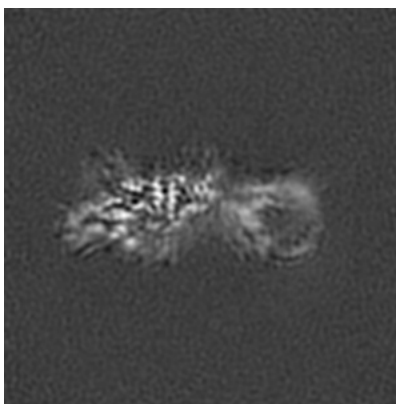
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

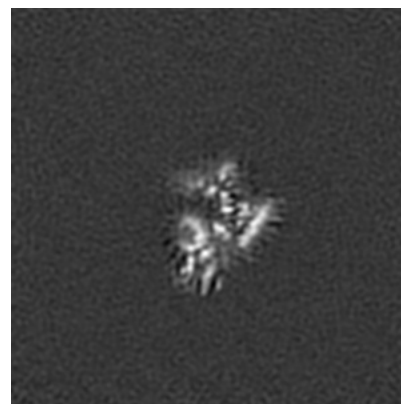
6.3.1 Primary map



X Index: 120



Y Index: 138



Z Index: 120

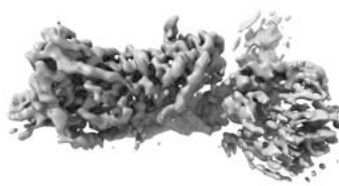
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

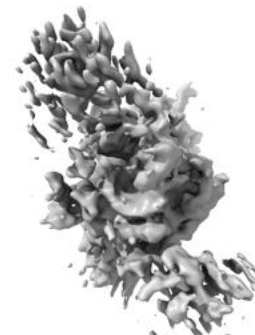
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

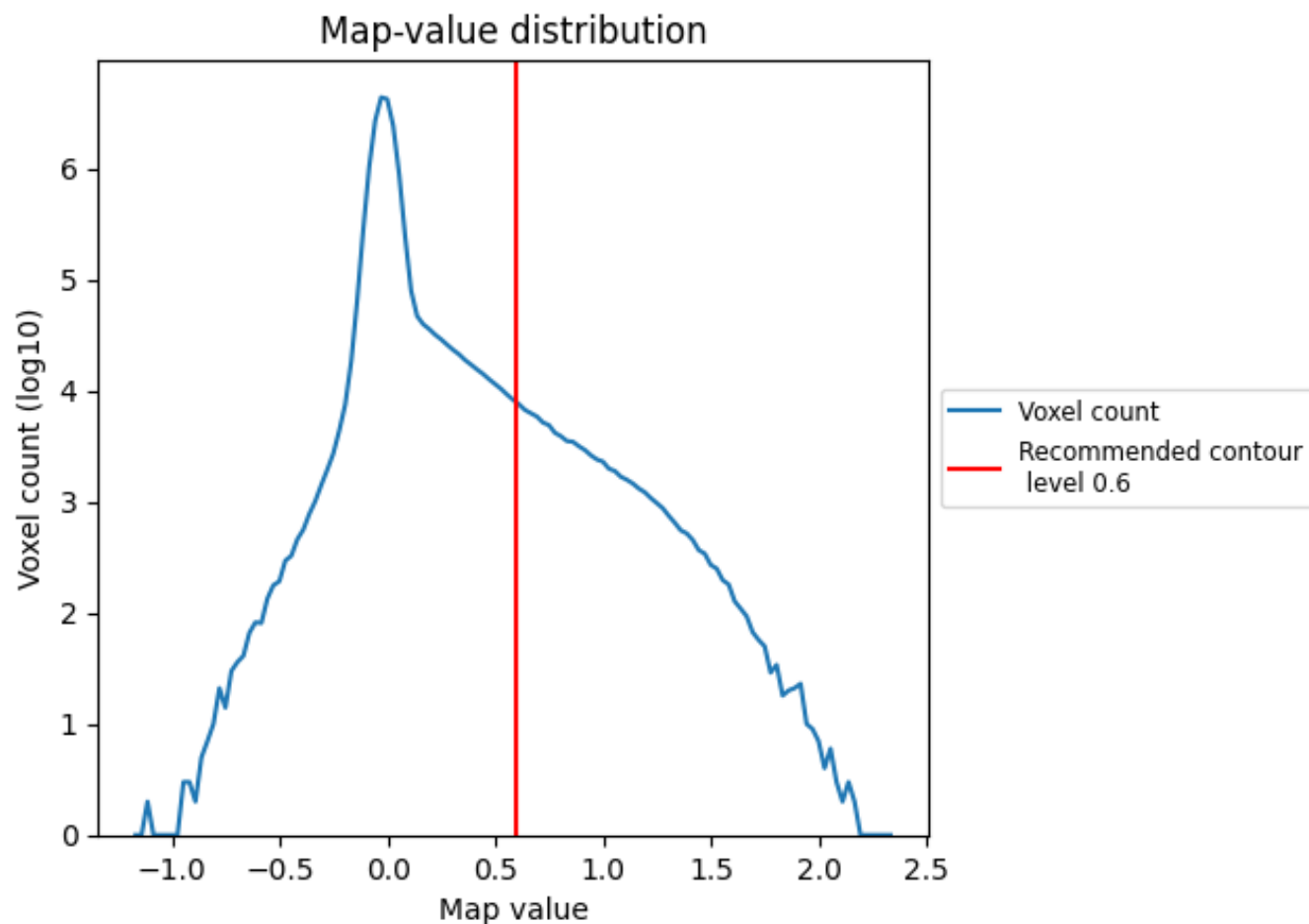
6.5 Mask visualisation

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

7 Map analysis [i](#)

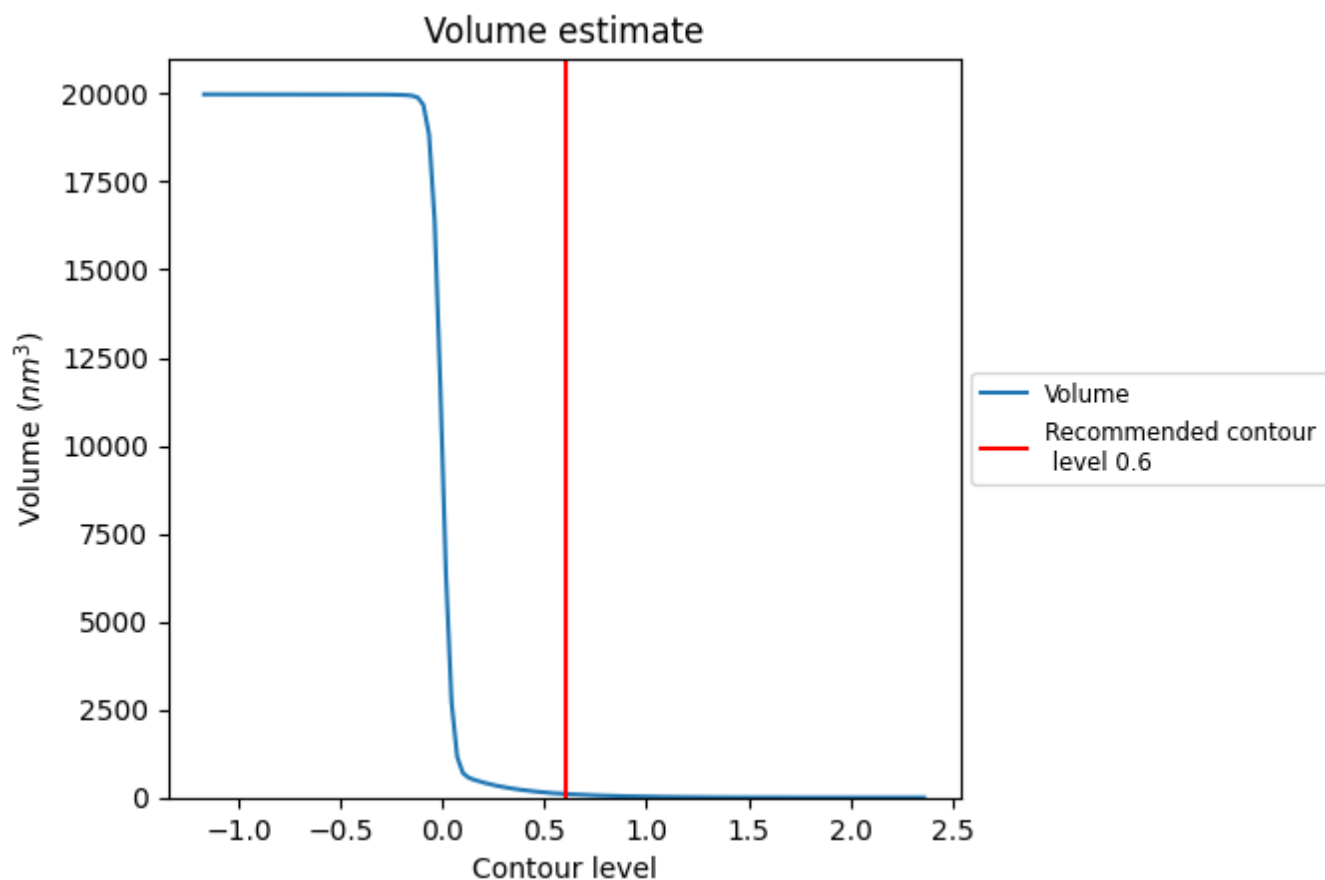
This section contains the results of statistical analysis of the map.

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.

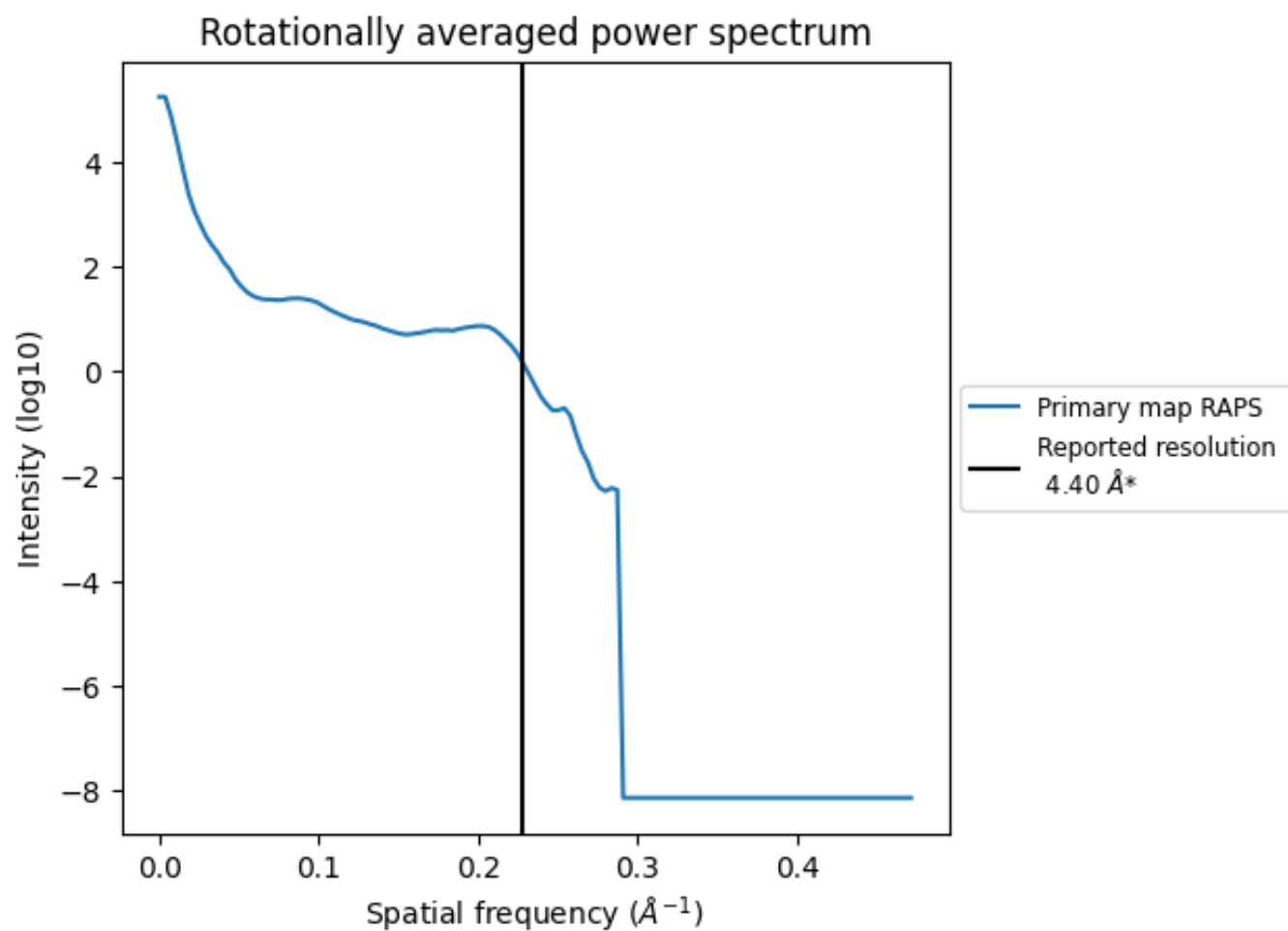
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 104 nm³; this corresponds to an approximate mass of 94 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 0.227 Å⁻¹

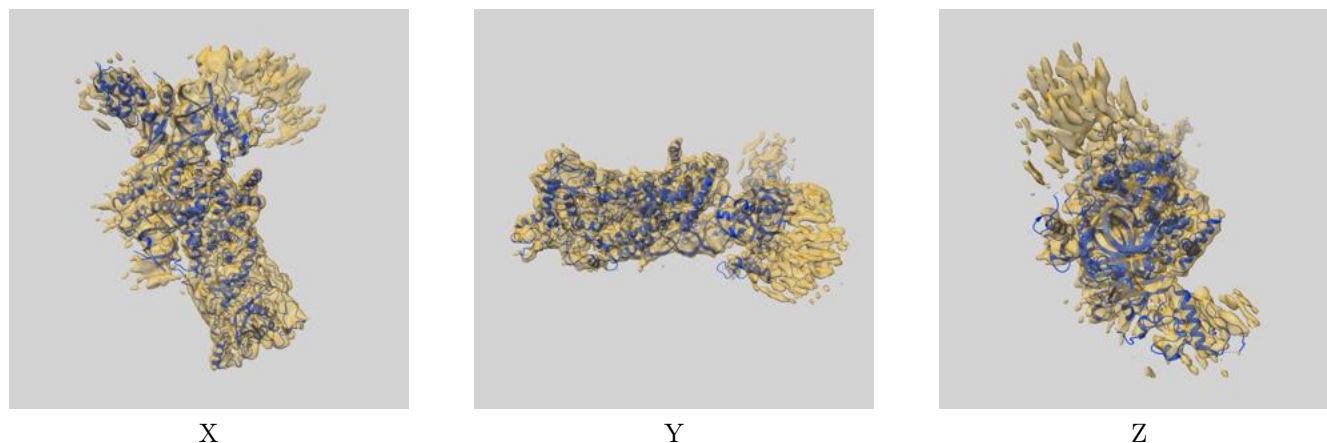
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

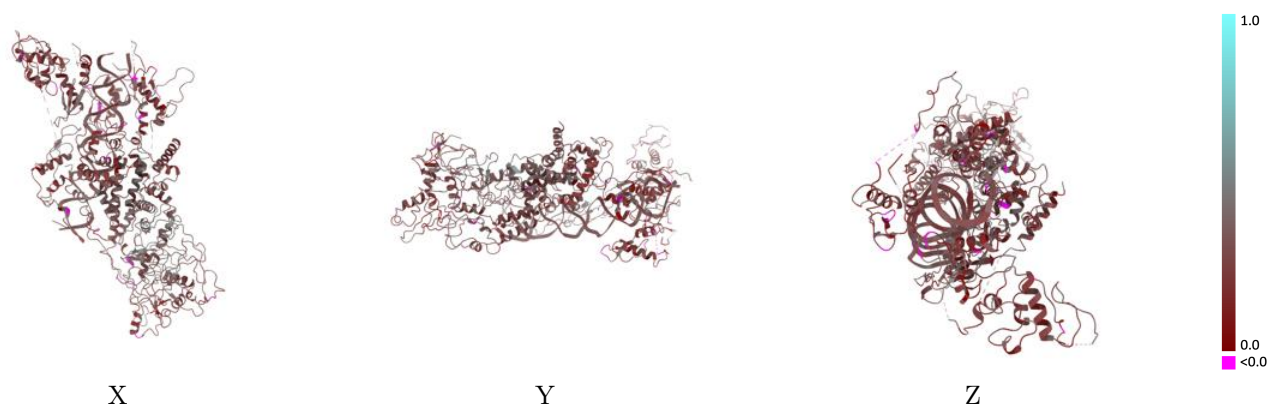
This section contains information regarding the fit between EMDB map EMD-21052 and PDB model 6V5C. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



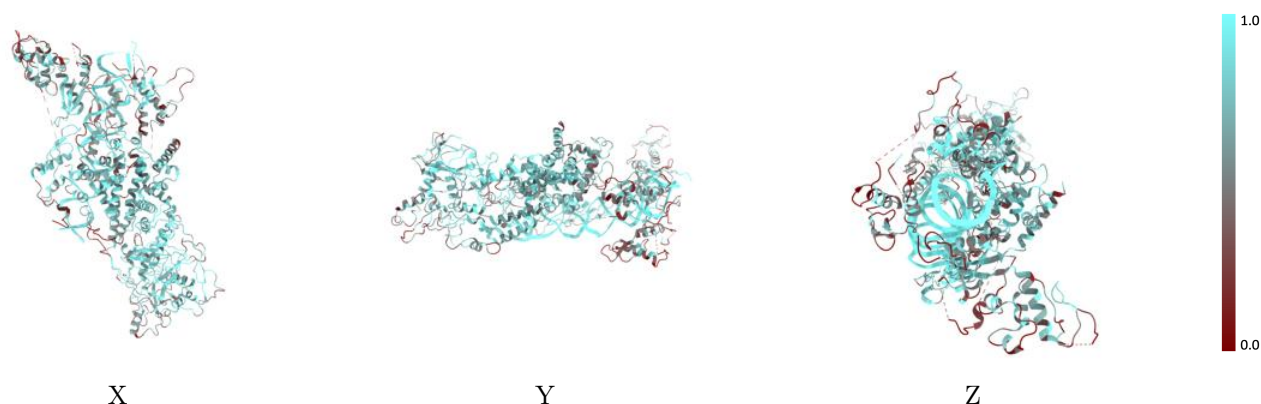
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



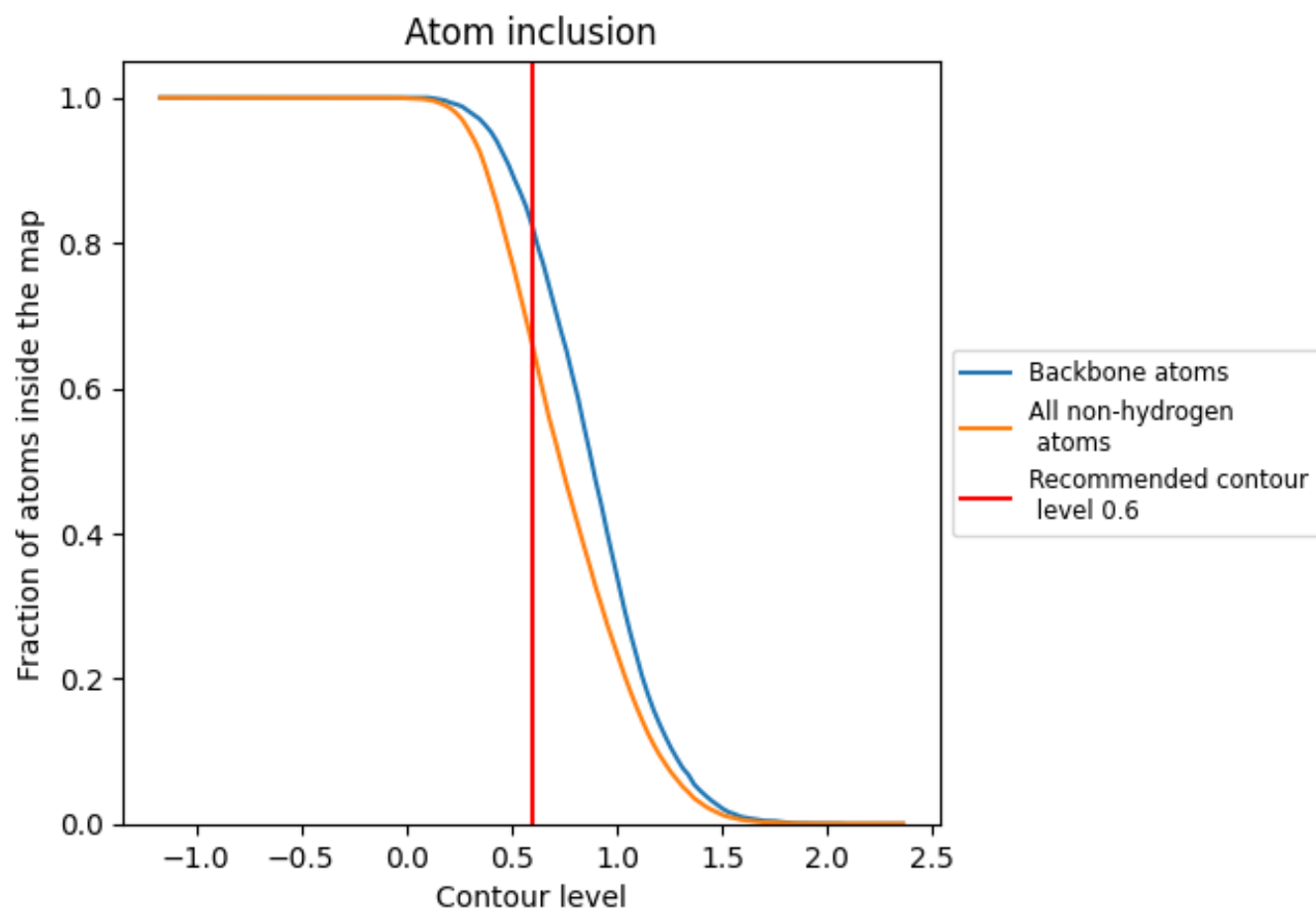
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 66% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6585	<div></div> 0.2940
A	<div></div> 0.6873	<div></div> 0.3130
B	<div></div> 0.5067	<div></div> 0.2630
C	<div></div> 0.4495	<div></div> 0.2320
D	<div></div> 0.9519	<div></div> 0.3090

