



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 12:00 AM UTC

PDB ID : 6X0M / pdb_00006x0m
EMDB ID : EMD-21979
Title : Bridging of double-strand DNA break activates PARP2/HPF1 to modify chromatin
Authors : Halic, M.; Bilokapic, S.
Deposited on : 2020-05-16
Resolution : 6.30 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

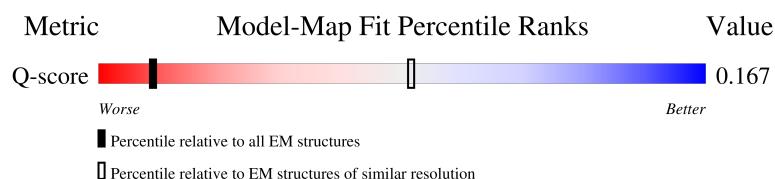
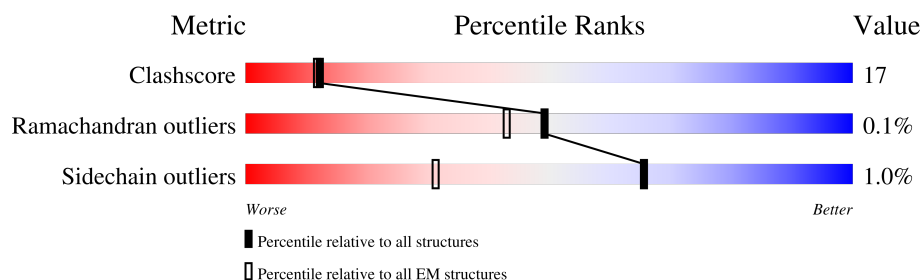
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 6.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	550 (5.80 - 6.80)

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	O	356	
1	o	356	
2	P	590	
2	p	590	

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Mol	Chain	Length	Quality of chain
3	I	167	 93%
3	i	167	 93%
4	J	167	 93%
4	j	167	 93%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12421 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 Histone PARylation factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	O	246	Total	C	N	O	S	0	0
			1995	1280	338	367	10		
1	o	242	Total	C	N	O	S	0	0
			1967	1264	332	361	10		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	-9	MET	-	initiating methionine	UNP Q9NWX4
O	-8	GLY	-	expression tag	UNP Q9NWX4
O	-7	HIS	-	expression tag	UNP Q9NWX4
O	-6	HIS	-	expression tag	UNP Q9NWX4
O	-5	HIS	-	expression tag	UNP Q9NWX4
O	-4	HIS	-	expression tag	UNP Q9NWX4
O	-3	HIS	-	expression tag	UNP Q9NWX4
O	-2	HIS	-	expression tag	UNP Q9NWX4
O	-1	GLY	-	expression tag	UNP Q9NWX4
O	0	GLY	-	expression tag	UNP Q9NWX4
O	174	LYS	ARG	variant	UNP Q9NWX4
o	-9	MET	-	initiating methionine	UNP Q9NWX4
o	-8	GLY	-	expression tag	UNP Q9NWX4
o	-7	HIS	-	expression tag	UNP Q9NWX4
o	-6	HIS	-	expression tag	UNP Q9NWX4
o	-5	HIS	-	expression tag	UNP Q9NWX4
o	-4	HIS	-	expression tag	UNP Q9NWX4
o	-3	HIS	-	expression tag	UNP Q9NWX4
o	-2	HIS	-	expression tag	UNP Q9NWX4
o	-1	GLY	-	expression tag	UNP Q9NWX4
o	0	GLY	-	expression tag	UNP Q9NWX4
o	174	LYS	ARG	variant	UNP Q9NWX4

- Molecule 2 is a protein called Poly [ADP-ribose] polymerase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	470	Total	C	N	O	S	0	0
			3761	2388	649	697	27		
2	p	468	Total	C	N	O	S	0	0
			3754	2386	646	695	27		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	-19	MET	-	initiating methionine	UNP Q9UGN5
P	-18	GLY	-	expression tag	UNP Q9UGN5
P	-17	SER	-	expression tag	UNP Q9UGN5
P	-16	SER	-	expression tag	UNP Q9UGN5
P	-15	HIS	-	expression tag	UNP Q9UGN5
P	-14	HIS	-	expression tag	UNP Q9UGN5
P	-13	HIS	-	expression tag	UNP Q9UGN5
P	-12	HIS	-	expression tag	UNP Q9UGN5
P	-11	HIS	-	expression tag	UNP Q9UGN5
P	-10	HIS	-	expression tag	UNP Q9UGN5
P	-9	SER	-	expression tag	UNP Q9UGN5
P	-8	SER	-	expression tag	UNP Q9UGN5
P	-7	GLY	-	expression tag	UNP Q9UGN5
P	-6	LEU	-	expression tag	UNP Q9UGN5
P	-5	VAL	-	expression tag	UNP Q9UGN5
P	-4	PRO	-	expression tag	UNP Q9UGN5
P	-3	ARG	-	expression tag	UNP Q9UGN5
P	-2	GLY	-	expression tag	UNP Q9UGN5
P	-1	SER	-	expression tag	UNP Q9UGN5
P	0	HIS	-	expression tag	UNP Q9UGN5
p	-19	MET	-	initiating methionine	UNP Q9UGN5
p	-18	GLY	-	expression tag	UNP Q9UGN5
p	-17	SER	-	expression tag	UNP Q9UGN5
p	-16	SER	-	expression tag	UNP Q9UGN5
p	-15	HIS	-	expression tag	UNP Q9UGN5
p	-14	HIS	-	expression tag	UNP Q9UGN5
p	-13	HIS	-	expression tag	UNP Q9UGN5
p	-12	HIS	-	expression tag	UNP Q9UGN5
p	-11	HIS	-	expression tag	UNP Q9UGN5
p	-10	HIS	-	expression tag	UNP Q9UGN5
p	-9	SER	-	expression tag	UNP Q9UGN5
p	-8	SER	-	expression tag	UNP Q9UGN5
p	-7	GLY	-	expression tag	UNP Q9UGN5
p	-6	LEU	-	expression tag	UNP Q9UGN5
p	-5	VAL	-	expression tag	UNP Q9UGN5

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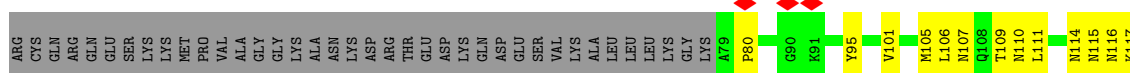
Chain	Residue	Modelled	Actual	Comment	Reference
p	-4	PRO	-	expression tag	UNP Q9UGN5
p	-3	ARG	-	expression tag	UNP Q9UGN5
p	-2	GLY	-	expression tag	UNP Q9UGN5
p	-1	SER	-	expression tag	UNP Q9UGN5
p	0	HIS	-	expression tag	UNP Q9UGN5

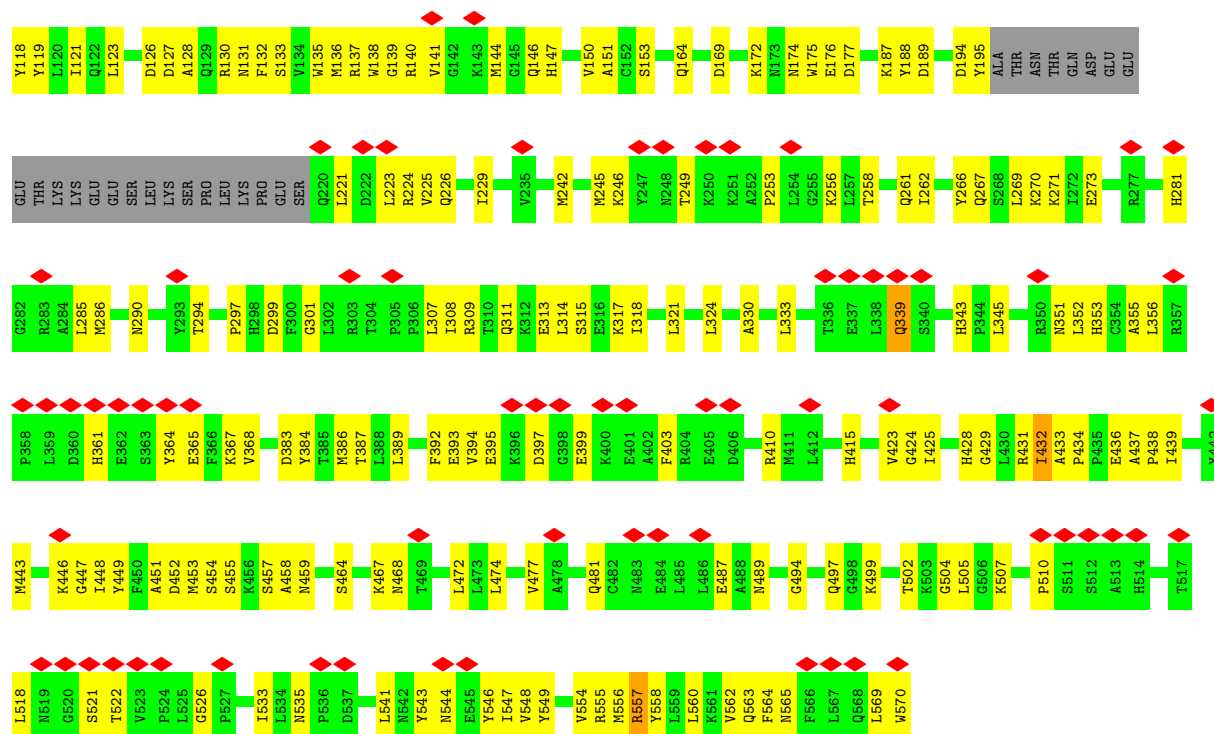
- Molecule 3 is a DNA chain called DNA (167-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	12	Total	C	N	O	P	0	0
			243	116	46	69	12		
3	i	11	Total	C	N	O	P	0	0
			229	108	45	65	11		

- Molecule 4 is a DNA chain called DNA (167-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	12	Total	C	N	O	P	0	0
			249	119	43	75	12		
4	j	11	Total	C	N	O	P	0	0
			223	106	38	68	11		





• Molecule 3: DNA (167-MER)

Chain I: 93%



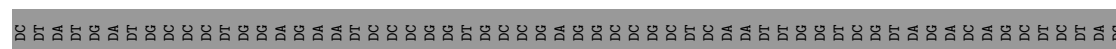
• Molecule 3: DNA (167-MER)

Chain i: 93%



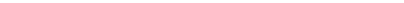
• Molecule 4: DNA (167-MER)

Chain J: 93%



DC	DT	DA	DG	DT	DC	DT	DC	DC	DA	DG	DG	DC	DA	DC	DG	DT	DG	DT	DC	DA	DG	DA	DT	DA	DT	DT	DA	DC	DC	DA	DT	DT	DC	DC	DT	G72	T73	G74	G75	A76	T77	G78	T79	A80	T81	T82	G83
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- Molecule 4: DNA (167-MER)

Chain j:  5% 93%

DC	DT	DA	DG	DT	DC	DT	DC	DC	DA	DG	DG	DC	DC	DA	DA	DT	DT	DT	DT	DC	DC	DC	DT	DG	DT	DG	DC	DA	DT	DT	DT	DG	DT	DT	DG
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	16000	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 ($e^-/\text{\AA}^2$)	80, 80	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k), GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.299	Depositor
Minimum map value	-0.102	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	508.8, 508.8, 508.8	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.12, 2.12, 2.12	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	O	0.37	0/2038	0.72	0/2746
1	o	0.33	0/2010	0.69	0/2710
2	P	0.39	0/3842	0.75	0/5182
2	p	0.37	0/3836	0.74	0/5176
3	I	0.35	0/272	0.70	0/416
3	i	0.40	0/257	0.56	0/395
4	J	0.39	0/278	0.73	0/428
4	j	0.38	0/248	0.58	0/378
All	All	0.37	0/12781	0.72	0/17431

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	1995	0	1970	47	0
1	o	1967	0	1938	37	0
2	P	3761	0	3740	144	0
2	p	3754	0	3728	157	0
3	I	243	0	135	7	0
3	i	229	0	124	16	0
4	J	249	0	138	13	0
4	j	223	0	125	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12421	0	11898	415	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 17.

All (415) 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:P:432:ILE:CG2	2:P:447:GLY:HA2	1.49	1.42
2:P:432:ILE:HG23	2:P:447:GLY:CA	1.55	1.36
2:P:432:ILE:CG2	2:P:447:GLY:CA	2.15	1.17
2:P:432:ILE:HD11	2:P:551:PRO:HD3	1.28	1.14
2:p:432:ILE:HG23	2:p:447:GLY:HA2	1.25	1.12
2:P:433:ALA:HB3	2:P:446:LYS:CD	1.91	1.01
2:P:433:ALA:HB3	2:P:446:LYS:CG	1.90	1.00
2:P:432:ILE:HG23	2:P:447:GLY:C	1.85	0.99
2:p:433:ALA:CB	2:p:446:LYS:HD3	1.93	0.99
2:P:433:ALA:HB3	2:P:446:LYS:HD3	1.43	0.99
2:P:432:ILE:HG23	2:P:447:GLY:HA2	1.06	0.97
2:P:432:ILE:HG21	2:P:447:GLY:HA2	1.45	0.96
2:P:433:ALA:CB	2:P:446:LYS:HG2	1.95	0.95
2:p:433:ALA:HB3	2:p:446:LYS:CG	1.96	0.95
2:P:140:ARG:HG2	4:J:83:DG:H5"	1.49	0.95
2:p:433:ALA:HB3	2:p:446:LYS:HD3	1.48	0.94
2:p:433:ALA:HB3	2:p:446:LYS:CD	2.01	0.91
2:p:266:TYR:HE2	2:p:434:PRO:CG	1.84	0.90
2:p:432:ILE:CG2	2:p:447:GLY:HA2	2.04	0.88
2:P:242:MET:HE2	2:P:246:LYS:HE3	1.57	0.87
2:P:437:ALA:O	2:P:446:LYS:NZ	2.09	0.86
2:p:433:ALA:CB	2:p:446:LYS:CG	2.55	0.85
2:p:270:LYS:HE2	2:p:436:GLU:O	1.76	0.84
2:P:246:LYS:HG3	2:P:252:ALA:O	1.77	0.83
2:p:433:ALA:CB	2:p:446:LYS:HG2	2.10	0.82
2:P:270:LYS:HE2	2:P:436:GLU:O	1.80	0.81
2:P:432:ILE:HG22	2:P:447:GLY:H	1.46	0.80
2:P:400:LYS:HG2	2:P:555:ARG:HH21	1.47	0.80
2:p:433:ALA:HB3	2:p:446:LYS:HB3	1.64	0.80
2:p:432:ILE:HG23	2:p:447:GLY:CA	2.11	0.80
2:p:266:TYR:HE2	2:p:434:PRO:HG3	1.46	0.79
2:p:433:ALA:CB	2:p:446:LYS:CD	2.57	0.78
2:P:433:ALA:HB3	2:P:446:LYS:HG2	1.58	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:p:433:ALA:HB3	2:p:446:LYS:CB	2.14	0.77
2:P:432:ILE:CG2	2:P:447:GLY:N	2.47	0.77
2:P:433:ALA:CB	2:P:446:LYS:CG	2.60	0.77
2:P:266:TYR:CD1	2:P:437:ALA:HB2	2.21	0.76
2:P:138:TRP:O	2:P:145:GLY:HA3	1.86	0.76
2:p:80:PRO:CG	2:p:195:TYR:CD1	2.69	0.75
2:p:80:PRO:HG2	2:p:195:TYR:CD1	2.21	0.75
2:P:270:LYS:HA	2:P:438:PRO:HG3	1.69	0.74
2:P:246:LYS:HE2	2:P:255:GLY:HA2	1.68	0.74
2:P:432:ILE:HG22	2:P:447:GLY:N	2.03	0.74
2:P:433:ALA:CB	2:P:446:LYS:HD3	2.19	0.73
2:P:433:ALA:CB	2:P:446:LYS:CD	2.67	0.72
1:o:154:ILE:HG22	1:o:223:HIS:HB2	1.72	0.72
2:P:138:TRP:NE1	2:P:146:GLN:HB2	2.03	0.72
3:I:-80:DT:H2'	3:I:-79:DA:C8	2.25	0.72
2:P:356:LEU:HA	2:P:393:GLU:O	1.90	0.72
2:p:116:ASN:N	3:i:83:DG:OP1	2.23	0.71
2:P:221:LEU:HB2	2:P:226:GLN:HE21	1.56	0.71
2:p:356:LEU:HA	2:p:393:GLU:O	1.92	0.70
2:p:432:ILE:HD13	2:p:448:ILE:HG13	1.73	0.70
2:p:307:LEU:HB2	2:p:309:ARG:HE	1.55	0.70
4:J:77:DT:H2''	4:J:78:DG:C8	2.26	0.70
2:p:281:HIS:HA	2:p:285:LEU:HD13	1.74	0.70
3:i:81:DT:H2''	3:i:82:DA:H8	1.57	0.69
2:P:138:TRP:NE1	4:j:-83:DC:H2''	2.08	0.69
2:P:453:MET:HB2	2:P:456:LYS:HE2	1.74	0.68
2:p:266:TYR:CE2	2:p:434:PRO:HG3	2.28	0.68
2:P:266:TYR:CE1	2:P:437:ALA:HB2	2.30	0.67
2:P:307:LEU:HD22	2:P:309:ARG:HH21	1.59	0.66
2:p:111:LEU:H	2:p:290:ASN:HD21	1.44	0.66
2:P:138:TRP:CE2	4:j:-83:DC:H2''	2.30	0.66
2:P:242:MET:HE2	2:P:246:LYS:CE	2.27	0.65
2:p:80:PRO:HG3	2:p:195:TYR:CD1	2.31	0.65
1:o:221:THR:HG22	1:o:292:GLU:HG3	1.79	0.65
2:P:111:LEU:H	2:P:290:ASN:HD21	1.44	0.65
2:p:266:TYR:HE2	2:p:434:PRO:HG2	1.59	0.65
2:P:355:ALA:HB3	2:P:395:GLU:HB2	1.77	0.65
2:p:270:LYS:CE	2:p:436:GLU:O	2.45	0.65
1:O:307:LYS:O	1:O:311:GLN:N	2.30	0.64
2:p:429:GLY:O	2:p:431:ARG:NH1	2.31	0.64
1:O:107:ARG:NH1	1:O:112:PRO:O	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:81:VAL:HG22	2:P:94:VAL:HG23	1.81	0.63
1:O:316:ALA:O	1:O:320:LEU:N	2.32	0.63
1:o:82:GLY:O	1:o:85:ASP:HB2	1.99	0.62
2:p:80:PRO:CG	2:p:195:TYR:HD1	2.11	0.62
1:O:127:TYR:OH	1:O:171:LYS:NZ	2.33	0.62
1:o:45:TYR:HB3	1:o:47:LEU:HG	1.81	0.62
2:p:315:SER:HA	2:p:318:ILE:HD12	1.82	0.62
2:P:266:TYR:CZ	2:P:434:PRO:HG2	2.35	0.62
2:p:433:ALA:HB1	2:p:446:LYS:HD3	1.78	0.61
2:P:219:SER:N	2:P:342:GLU:OE1	2.33	0.61
1:O:154:ILE:HG22	1:O:223:HIS:HB2	1.82	0.61
2:P:169:ASP:O	2:P:187:LYS:NZ	2.33	0.61
2:p:437:ALA:O	2:p:446:LYS:NZ	2.29	0.61
2:p:355:ALA:HB3	2:p:395:GLU:HB3	1.82	0.61
1:o:102:PHE:HA	1:o:105:HIS:HB2	1.84	0.60
2:P:377:HIS:HD2	2:P:386:MET:HG2	1.66	0.60
2:p:169:ASP:O	2:p:187:LYS:NZ	2.34	0.60
2:p:123:LEU:HD21	2:p:132:PHE:HB3	1.82	0.60
2:p:133:SER:HA	2:p:150:VAL:O	2.01	0.60
2:p:140:ARG:NH1	2:p:301:GLY:O	2.35	0.60
2:P:140:ARG:CG	4:J:83:DG:H5''	2.28	0.60
2:p:136:MET:O	2:p:147:HIS:HA	2.01	0.60
2:p:266:TYR:CE2	2:p:437:ALA:HB2	2.36	0.59
2:p:116:ASN:H	3:i:83:DG:P	2.25	0.59
2:p:164:GLN:HG2	2:p:175:TRP:HB3	1.84	0.59
3:i:76:DC:H2''	3:i:77:DA:C8	2.36	0.59
3:i:81:DT:H2''	3:i:82:DA:C8	2.37	0.59
1:o:118:ILE:HG12	1:o:130:GLY:HA2	1.85	0.59
2:p:121:ILE:HA	2:p:135:TRP:O	2.03	0.59
2:p:447:GLY:HA3	2:p:548:VAL:O	2.03	0.59
2:P:136:MET:O	2:P:147:HIS:HA	2.02	0.59
2:p:245:MET:HA	2:p:249:THR:OG1	2.02	0.59
4:j:-79:DG:H2''	4:j:-78:DA:C8	2.37	0.59
1:O:85:ASP:OD2	1:O:106:TRP:NE1	2.35	0.58
1:o:119:ILE:HD12	1:o:129:MET:HE3	1.85	0.58
2:P:193:MET:SD	2:P:193:MET:N	2.75	0.58
2:p:118:TYR:HB3	2:p:141:VAL:HG22	1.85	0.58
2:p:439:ILE:HA	2:p:446:LYS:HE3	1.86	0.58
2:P:324:LEU:HA	2:P:327:ILE:HD12	1.85	0.58
2:p:518:LEU:O	2:p:521:SER:OG	2.21	0.58
2:p:311:GLN:HA	2:p:314:LEU:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:o:316:ALA:O	1:o:320:LEU:N	2.36	0.58
2:p:110:ASN:O	2:p:114:ASN:N	2.37	0.58
2:p:273:GLU:HG3	2:p:438:PRO:HB3	1.85	0.58
2:P:436:GLU:H	2:P:436:GLU:CD	2.10	0.58
2:p:140:ARG:HG2	3:i:83:DG:H5''	1.85	0.57
2:P:272:ILE:HD11	2:P:292:PHE:HB2	1.86	0.57
2:p:109:THR:HG22	2:p:294:THR:HG23	1.86	0.57
2:p:80:PRO:HG3	2:p:195:TYR:HD1	1.66	0.57
2:P:143:LYS:NZ	2:P:299:ASP:OD1	2.37	0.57
1:o:107:ARG:NH1	1:o:112:PRO:O	2.37	0.57
2:p:95:TYR:HB3	2:p:123:LEU:HB3	1.86	0.56
3:I:-81:DA:C8	3:I:-80:DT:H72	2.40	0.56
2:p:139:GLY:C	3:i:83:DG:H4'	2.30	0.56
2:p:433:ALA:HB1	2:p:446:LYS:CD	2.32	0.56
2:p:308:ILE:HG23	2:p:313:GLU:HB2	1.86	0.56
2:p:510:PRO:HB3	2:p:526:GLY:HA2	1.86	0.56
4:J:80:DA:H2''	4:J:81:DT:H71	1.88	0.56
2:P:138:TRP:CE2	2:P:146:GLN:HB2	2.41	0.56
2:P:392:PHE:HE1	2:P:561:LYS:HB2	1.70	0.56
1:o:125:THR:HG22	1:o:147:GLU:HB3	1.87	0.56
2:P:251:LYS:HB3	2:P:320:LEU:HD11	1.89	0.55
2:p:258:THR:HG23	2:p:261:GLN:H	1.71	0.55
2:p:504:GLY:O	2:p:544:ASN:HA	2.07	0.55
2:p:109:THR:HG23	2:p:290:ASN:HD22	1.71	0.55
1:o:258:ALA:HB3	1:o:264:ARG:HG3	1.88	0.54
2:p:472:LEU:HD12	2:p:562:VAL:HG21	1.88	0.54
1:o:103:ASN:HB3	1:o:328:ILE:HG12	1.89	0.54
2:P:109:THR:HG22	2:P:294:THR:HG23	1.89	0.54
1:o:84:TYR:O	1:o:88:ALA:N	2.37	0.54
2:p:266:TYR:HA	2:p:269:LEU:HD12	1.90	0.54
1:o:107:ARG:NH1	1:o:115:PHE:O	2.41	0.54
1:O:281:ALA:O	1:O:286:ASP:N	2.40	0.53
2:p:138:TRP:NE1	2:p:146:GLN:OE1	2.41	0.53
2:p:472:LEU:HB2	2:p:560:LEU:HB2	1.89	0.53
4:J:73:DT:H2''	4:J:74:DG:C8	2.43	0.53
1:O:235:ASP:O	2:P:312:LYS:NZ	2.42	0.53
2:P:112:GLN:HG3	2:P:286:MET:HE2	1.91	0.53
2:P:138:TRP:CD1	4:j:-83:DC:O4'	2.62	0.53
2:P:253:PRO:HD2	2:P:297:PRO:HB2	1.89	0.53
2:p:131:ASN:HD21	2:p:151:ALA:HB1	1.74	0.53
1:O:107:ARG:HG3	1:O:111:ASP:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:p:172:LYS:HG2	2:p:187:LYS:HE3	1.90	0.53
2:P:140:ARG:HD2	4:J:83:DG:OP1	2.09	0.53
2:p:140:ARG:NH2	2:p:299:ASP:OD1	2.41	0.53
1:o:111:ASP:OD2	1:o:117:THR:OG1	2.27	0.53
1:O:217:VAL:HG22	1:O:226:GLY:HA3	1.90	0.53
2:p:311:GLN:HG2	2:p:443:MET:HE1	1.91	0.53
2:P:472:LEU:HB3	2:P:560:LEU:HB2	1.91	0.53
2:p:518:LEU:HD21	2:p:558:TYR:HE2	1.74	0.53
2:P:456:LYS:NZ	2:P:544:ASN:O	2.42	0.52
1:O:83:PRO:HD2	1:O:118:ILE:HG13	1.90	0.52
2:P:309:ARG:N	2:P:313:GLU:OE1	2.36	0.52
1:O:129:MET:HE3	1:O:157:ASN:HD21	1.75	0.52
4:J:78:DG:C8	4:J:79:DT:H72	2.43	0.52
2:P:416:GLY:N	2:P:457:SER:OG	2.40	0.52
2:p:174:ASN:HD21	2:p:176:GLU:HB3	1.73	0.52
2:P:399:GLU:O	2:P:403:PHE:N	2.41	0.52
1:o:41:VAL:HG13	1:o:86:ILE:HD12	1.90	0.52
2:p:266:TYR:CE2	2:p:434:PRO:CG	2.77	0.52
1:O:118:ILE:HG23	1:O:119:ILE:HG13	1.90	0.52
3:i:74:DG:H2''	3:i:75:DG:OP2	2.08	0.52
2:P:270:LYS:CA	2:P:438:PRO:HG3	2.40	0.52
2:P:140:ARG:NH1	2:P:301:GLY:O	2.29	0.52
2:P:315:SER:HA	2:P:318:ILE:HD12	1.91	0.52
1:O:314:PRO:O	1:O:318:ASN:N	2.37	0.51
2:P:137:ARG:HH11	2:P:144:MET:HG2	1.73	0.51
2:P:439:ILE:HA	2:P:446:LYS:HE3	1.91	0.51
2:P:510:PRO:HB3	2:P:526:GLY:HA2	1.92	0.51
2:P:385:THR:HG23	2:P:565:ASN:HD22	1.75	0.51
2:p:352:LEU:HD21	2:p:423:VAL:HG23	1.93	0.51
1:o:48:SER:O	1:o:133:ARG:NH2	2.33	0.51
1:o:268:PHE:HZ	1:o:304:TYR:HB3	1.76	0.51
2:p:138:TRP:CG	3:I:-83:DC:H4'	2.45	0.51
2:p:253:PRO:HD2	2:p:297:PRO:HB2	1.93	0.51
2:P:128:ALA:O	2:P:130:ARG:NH1	2.43	0.51
2:P:429:GLY:HA2	2:P:556:MET:HE1	1.93	0.51
2:P:518:LEU:O	2:P:521:SER:OG	2.28	0.51
2:P:140:ARG:HG2	4:J:83:DG:C5'	2.32	0.50
3:i:77:DA:H2''	3:i:78:DT:H72	1.91	0.50
2:P:466:LEU:HD23	2:P:467:LYS:HG2	1.93	0.50
2:p:361:HIS:NE2	2:p:389:LEU:O	2.44	0.50
2:p:266:TYR:CE2	2:p:434:PRO:HG2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:315:LEU:O	1:O:318:ASN:HB3	2.10	0.50
2:p:137:ARG:HA	2:p:146:GLN:O	2.11	0.50
1:O:315:LEU:O	1:O:319:LEU:N	2.36	0.50
1:o:311:GLN:HB3	2:p:383:ASP:HB3	1.93	0.50
2:p:477:VAL:HG22	2:p:554:VAL:HG22	1.93	0.50
1:O:317:TYR:HA	1:O:320:LEU:HB2	1.93	0.49
2:p:106:LEU:HB3	2:p:188:TYR:HB3	1.94	0.49
2:P:146:GLN:NE2	3:I:-82:DA:O4'	2.45	0.49
2:p:286:MET:HE1	2:p:307:LEU:HD21	1.94	0.49
2:p:563:GLN:HE21	2:p:565:ASN:HB2	1.77	0.49
2:P:121:ILE:HA	2:P:135:TRP:O	2.12	0.49
2:p:281:HIS:HE1	2:p:309:ARG:HA	1.78	0.49
1:O:86:ILE:HG13	1:O:91:HIS:HB3	1.94	0.49
2:P:443:MET:O	2:P:489:ASN:N	2.46	0.49
2:p:137:ARG:HH11	2:p:144:MET:HG2	1.78	0.49
2:p:194:ASP:HB2	2:p:256:LYS:HE3	1.94	0.49
2:P:241:MET:HE3	2:P:245:MET:HE3	1.94	0.49
2:p:399:GLU:O	2:p:403:PHE:N	2.45	0.49
1:O:158:GLY:HA2	1:O:205:GLN:HA	1.94	0.48
1:O:156:PRO:O	1:O:205:GLN:NE2	2.40	0.48
2:P:265:GLY:HA2	2:P:296:ILE:HD11	1.95	0.48
2:p:221:LEU:O	2:p:226:GLN:NE2	2.46	0.48
2:p:225:VAL:HG12	2:p:392:PHE:HE2	1.77	0.48
2:P:164:GLN:HG2	2:P:175:TRP:HB3	1.94	0.48
3:I:-82:DA:C6	3:I:-81:DA:C6	3.01	0.48
4:j:-78:DA:H1'	4:j:-77:DT:H5'	1.95	0.48
2:P:188:TYR:OH	4:j:-83:DC:OP1	2.30	0.48
3:i:82:DA:H2''	3:i:83:DG:H8	1.77	0.48
2:P:135:TRP:HA	2:P:148:SER:O	2.14	0.48
4:J:74:DG:C5	4:J:75:DC:C4	3.02	0.48
2:p:494:GLY:O	2:p:497:GLN:NE2	2.47	0.48
1:o:231:VAL:HG12	1:o:237:GLY:HA3	1.96	0.48
2:P:174:ASN:HD21	2:P:176:GLU:HB3	1.78	0.48
1:o:38:ARG:HH22	1:o:51:GLU:HA	1.77	0.48
2:p:434:PRO:O	2:p:446:LYS:NZ	2.34	0.48
1:o:158:GLY:HA2	1:o:205:GLN:HA	1.94	0.47
2:P:192:GLN:HG3	2:P:258:THR:HG21	1.96	0.47
3:i:81:DT:H2'	3:i:81:DT:OP2	2.14	0.47
2:P:85:CYS:O	2:P:89:VAL:N	2.48	0.47
1:O:317:TYR:HE1	1:O:322:ARG:HH11	1.63	0.47
4:j:-77:DT:H2''	4:j:-76:DG:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:104:VAL:HG23	2:P:190:MET:HE3	1.97	0.47
2:p:464:SER:HB3	2:p:467:LYS:HB3	1.96	0.47
2:p:474:LEU:HD12	2:p:557:ARG:HB3	1.96	0.47
1:O:328:ILE:O	1:O:332:HIS:HB2	2.14	0.47
2:P:96:CYS:HB3	2:P:101:VAL:HG22	1.97	0.47
2:P:389:LEU:HB2	2:P:561:LYS:HD3	1.96	0.47
2:p:221:LEU:HB2	2:p:226:GLN:HE21	1.79	0.47
2:P:471:LEU:HD13	2:P:559:LEU:HD21	1.96	0.47
2:p:451:ALA:HB3	2:p:457:SER:HB3	1.97	0.47
3:I:-83:DC:H2'	3:I:-82:DA:C8	2.50	0.47
1:o:50:PRO:HD3	1:o:140:PRO:HD2	1.96	0.47
2:p:434:PRO:HG2	2:p:437:ALA:HB2	1.97	0.47
2:P:482:CYS:O	2:P:499:LYS:NZ	2.42	0.47
3:i:80:DA:H2''	3:i:81:DT:H71	1.96	0.47
2:P:373:LEU:HD22	2:P:388:LEU:HB2	1.97	0.46
2:p:343:HIS:CE1	2:p:345:LEU:HB2	2.51	0.46
2:p:434:PRO:HG2	2:p:437:ALA:CB	2.45	0.46
1:O:114:GLU:OE2	1:O:317:TYR:OH	2.18	0.46
2:p:140:ARG:CG	3:i:83:DG:H5''	2.45	0.46
4:j:-83:DC:H3'	4:j:-82:DT:C7	2.45	0.46
4:j:-82:DT:H73	4:j:-82:DT:OP2	2.16	0.46
1:o:297:LEU:HD13	1:o:297:LEU:HA	1.75	0.46
1:o:315:LEU:O	1:o:318:ASN:HB3	2.15	0.46
1:O:205:GLN:HG2	1:O:206:ARG:HD3	1.98	0.46
2:p:424:GLY:O	2:p:428:HIS:N	2.49	0.46
2:p:502:THR:HG23	2:p:547:ILE:HB	1.97	0.46
2:p:330:ALA:HA	2:p:333:LEU:HG	1.97	0.46
2:p:333:LEU:O	2:p:351:ASN:ND2	2.50	0.46
2:P:383:ASP:OD1	2:P:383:ASP:N	2.43	0.45
1:O:221:THR:OG1	1:O:223:HIS:NE2	2.49	0.45
2:P:83:PRO:HA	2:P:89:VAL:HG21	1.98	0.45
2:p:453:MET:HG3	2:p:543:TYR:HB3	1.99	0.45
2:P:320:LEU:HD12	2:P:320:LEU:HA	1.77	0.45
4:j:-81:DA:H2''	4:j:-80:DT:C6	2.52	0.45
1:O:135:SER:OG	1:O:137:ASP:OD1	2.28	0.45
1:O:220:LYS:HB3	1:O:224:GLY:HA2	1.97	0.45
2:p:321:LEU:HA	2:p:324:LEU:HD12	1.97	0.45
4:j:-82:DT:C2	4:j:-81:DA:C8	3.04	0.45
2:P:436:GLU:OE1	2:P:436:GLU:N	2.44	0.45
1:O:123:ASN:OD1	1:O:123:ASN:N	2.45	0.45
2:P:133:SER:HA	2:P:150:VAL:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:433:ALA:HB1	2:P:446:LYS:HE2	1.99	0.45
2:P:556:MET:HE2	2:P:556:MET:HB3	1.91	0.45
2:p:474:LEU:CD1	2:p:557:ARG:HB3	2.47	0.45
2:P:433:ALA:HB2	2:P:446:LYS:HG2	1.90	0.45
2:P:483:ASN:HB2	2:P:502:THR:HG22	1.99	0.45
2:p:226:GLN:HA	2:p:229:ILE:HG12	1.98	0.45
4:J:82:DT:H2''	4:J:83:DG:H8	1.82	0.45
1:O:126:GLN:HB3	1:O:148:ALA:HB3	1.99	0.44
2:p:126:ASP:O	2:p:130:ARG:NH2	2.49	0.44
2:p:223:LEU:HD12	2:p:224:ARG:HG3	1.99	0.44
1:O:275:MET:HE3	1:O:312:LEU:HD11	1.98	0.44
2:p:474:LEU:HD11	2:p:558:TYR:HD2	1.81	0.44
2:P:369:ILE:HG21	2:P:391:LEU:HD22	1.99	0.44
2:p:138:TRP:CD1	3:I:-83:DC:H4'	2.53	0.44
2:P:474:LEU:HD23	2:P:560:LEU:HD11	1.98	0.44
2:p:454:SER:O	2:p:458:ALA:HB2	2.18	0.44
4:j:-83:DC:H3'	4:j:-82:DT:H73	1.99	0.44
2:P:177:ASP:OD1	2:P:177:ASP:N	2.46	0.44
2:P:425:ILE:HG12	2:P:430:LEU:HD12	2.00	0.44
1:o:278:VAL:HG11	1:o:312:LEU:HD13	2.00	0.44
2:P:399:GLU:HG3	2:P:555:ARG:HG3	2.00	0.44
2:P:424:GLY:O	2:P:427:SER:OG	2.35	0.44
4:J:83:DG:C4	4:j:-83:DC:C5	3.06	0.44
2:P:474:LEU:HD11	2:P:558:TYR:HD2	1.83	0.43
2:p:242:MET:HG3	2:p:246:LYS:HE2	2.00	0.43
2:p:386:MET:HE1	2:p:455:SER:HA	2.00	0.43
2:p:397:ASP:OD1	2:p:397:ASP:N	2.51	0.43
2:p:569:LEU:HB3	2:p:570:TRP:CE3	2.53	0.43
2:P:138:TRP:NE1	4:j:-83:DC:C2'	2.80	0.43
2:p:415:HIS:ND1	2:p:449:TYR:O	2.49	0.43
2:p:505:LEU:HB3	2:p:533:ILE:HD12	1.99	0.43
2:p:177:ASP:OD1	2:p:177:ASP:N	2.44	0.43
2:P:359:LEU:HD22	2:P:391:LEU:HD23	2.00	0.43
2:p:127:ASP:OD1	2:p:128:ALA:N	2.52	0.43
2:p:256:LYS:HE3	2:p:256:LYS:HB2	1.87	0.43
2:p:365:GLU:HA	2:p:368:VAL:HG22	2.00	0.43
2:p:131:ASN:OD1	2:p:153:SER:N	2.39	0.43
2:p:557:ARG:HD2	2:p:557:ARG:HA	1.65	0.43
2:P:452:ASP:OD1	2:P:452:ASP:N	2.38	0.43
2:p:262:ILE:HG23	2:p:321:LEU:HD12	1.99	0.43
2:p:443:MET:O	2:p:489:ASN:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:127:ASP:OD1	2:P:128:ALA:N	2.52	0.43
2:P:244:GLU:O	2:P:248:ASN:HB2	2.19	0.43
2:p:140:ARG:HD2	3:i:83:DG:H5''	1.99	0.43
2:P:244:GLU:HA	2:P:248:ASN:OD1	2.19	0.43
1:o:82:GLY:N	1:o:85:ASP:OD2	2.52	0.43
1:o:317:TYR:HA	1:o:320:LEU:HB2	2.01	0.43
4:j:-81:DA:C2'	4:j:-80:DT:H71	2.49	0.43
2:P:416:GLY:H	2:P:457:SER:HG	1.66	0.43
2:p:403:PHE:CD1	2:p:555:ARG:HB2	2.54	0.43
1:O:275:MET:HG2	1:O:312:LEU:HD11	2.01	0.43
2:p:432:ILE:HD12	2:p:549:TYR:O	2.19	0.43
1:O:272:GLN:HE22	2:P:465:ARG:H	1.65	0.42
2:p:458:ALA:HA	2:p:472:LEU:HD21	2.01	0.42
3:i:76:DC:C2	3:i:77:DA:C5	3.06	0.42
1:O:258:ALA:HB3	1:O:264:ARG:HG3	2.00	0.42
2:P:433:ALA:HB3	2:P:446:LYS:CB	2.48	0.42
1:O:157:ASN:HA	1:O:167:LEU:HD13	2.01	0.42
2:P:477:VAL:HG22	2:P:554:VAL:HG22	2.02	0.42
1:O:239:ARG:HH22	1:O:284:GLU:HB2	1.84	0.42
1:O:242:PRO:HD3	1:O:289:MET:HE3	2.01	0.42
2:P:400:LYS:H	2:P:400:LYS:HG3	1.50	0.42
2:P:506:GLY:HA2	2:P:541:LEU:HB2	2.00	0.42
2:P:454:SER:O	2:P:458:ALA:HB2	2.20	0.42
2:p:128:ALA:O	2:p:130:ARG:NH1	2.51	0.42
2:p:383:ASP:OD1	2:p:383:ASP:N	2.44	0.42
4:j:-75:DC:OP2	4:j:-75:DC:H2'	2.19	0.42
1:o:216:LYS:HB3	1:o:228:VAL:HG13	2.02	0.42
4:J:75:DC:H2''	4:J:76:DA:C8	2.55	0.42
1:O:111:ASP:OD2	1:O:117:THR:OG1	2.31	0.42
2:P:409:ASN:ND2	2:P:482:CYS:SG	2.93	0.42
1:o:81:VAL:HB	1:o:106:TRP:NE1	2.34	0.42
1:O:244:THR:HG23	1:O:247:ASP:H	1.84	0.42
2:P:138:TRP:CD1	4:j:-83:DC:C1'	3.03	0.42
2:P:544:ASN:OD1	2:P:545:GLU:N	2.53	0.42
2:p:109:THR:HA	2:p:115:ASN:O	2.20	0.42
1:O:221:THR:HG22	1:O:292:GLU:HG3	2.02	0.41
2:p:353:HIS:ND1	2:p:397:ASP:OD2	2.49	0.41
2:P:403:PHE:CD1	2:P:555:ARG:HB2	2.55	0.41
2:P:506:GLY:HA3	2:P:543:TYR:C	2.45	0.41
2:p:452:ASP:HB3	2:p:546:TYR:HE2	1.84	0.41
1:O:141:VAL:HG23	1:O:142:TYR:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:p:115:ASN:HB3	2:p:117:LYS:HE2	2.02	0.41
1:O:80:LEU:HB3	1:O:84:TYR:CG	2.56	0.41
2:P:270:LYS:NZ	2:P:438:PRO:HA	2.35	0.41
2:P:110:ASN:O	2:P:114:ASN:N	2.53	0.41
2:P:119:TYR:HD2	2:P:121:ILE:HD11	1.86	0.41
2:P:361:HIS:HA	2:P:366:PHE:CG	2.56	0.41
1:o:216:LYS:HA	1:o:216:LYS:HD2	1.85	0.41
1:O:341:ILE:HG23	1:O:344:LEU:HA	2.03	0.41
2:P:476:GLU:HG2	2:P:555:ARG:O	2.21	0.41
1:o:39:LYS:HE2	1:o:39:LYS:HB2	1.91	0.41
2:p:119:TYR:CD1	2:p:138:TRP:HB3	2.56	0.41
2:p:468:ASN:O	2:p:564:PHE:N	2.54	0.41
2:p:487:GLU:OE2	2:p:535:ASN:ND2	2.53	0.41
4:J:79:DT:C2	4:J:80:DA:C5	3.09	0.41
2:p:313:GLU:O	2:p:317:LYS:HG2	2.21	0.41
2:p:364:TYR:HA	2:p:367:LYS:HE3	2.03	0.41
2:p:507:LYS:N	2:p:541:LEU:O	2.45	0.41
1:O:116:GLN:OE1	1:O:133:ARG:NH1	2.53	0.41
2:P:384:TYR:HB3	2:P:566:PHE:CD1	2.56	0.41
2:P:417:SER:HB2	2:P:421:ASN:HD21	1.86	0.41
2:P:482:CYS:HB3	2:P:503:LYS:HG2	2.02	0.41
1:o:156:PRO:HB3	1:o:210:MET:HE1	2.03	0.41
1:o:285:CYS:HA	1:o:287:TYR:CZ	2.56	0.41
1:o:329:ILE:HD12	1:o:329:ILE:HA	1.98	0.41
2:p:105:MET:HE1	2:p:107:ASN:HB2	2.03	0.41
2:p:139:GLY:HA2	3:i:83:DG:H4'	2.03	0.41
2:P:396:LYS:NZ	2:P:427:SER:O	2.47	0.41
2:P:472:LEU:HD23	2:P:560:LEU:HD22	2.03	0.41
2:p:356:LEU:HD23	2:p:394:VAL:HA	2.01	0.41
4:j:-82:DT:N3	4:j:-81:DA:C5	2.89	0.41
2:P:429:GLY:O	2:P:431:ARG:NH2	2.54	0.40
1:O:48:SER:O	1:O:133:ARG:NH2	2.48	0.40
1:O:313:LEU:HD23	1:O:329:ILE:HD12	2.04	0.40
2:p:106:LEU:HA	2:p:189:ASP:O	2.22	0.40
2:p:410:ARG:O	2:p:522:THR:OG1	2.31	0.40
2:p:425:ILE:O	2:p:429:GLY:N	2.33	0.40
2:P:410:ARG:HA	2:P:478:ALA:HA	2.04	0.40
2:p:221:LEU:HB2	2:p:226:GLN:HG3	2.04	0.40
2:p:458:ALA:HB1	2:p:564:PHE:HE2	1.86	0.40
1:O:112:PRO:HB3	1:O:295:MET:HE1	2.02	0.40
2:P:152:CYS:SG	2:P:155:ASN:N	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:326:ASP:HA	2:P:329:ILE:HG12	2.04	0.40
2:P:483:ASN:HD21	2:P:496:LEU:HA	1.86	0.40
1:o:92:LYS:HD2	1:o:92:LYS:HA	1.88	0.40
1:o:251:ILE:HD13	1:o:251:ILE:HA	1.95	0.40
2:p:123:LEU:HA	2:p:133:SER:O	2.20	0.40
2:p:339:GLN:O	2:p:339:GLN:CG	2.70	0.40
2:p:481:GLN:HG2	2:p:499:LYS:HE3	2.03	0.40
1:O:102:PHE:HD1	1:O:102:PHE:HA	1.77	0.40
2:P:541:LEU:H	2:P:541:LEU:HG	1.60	0.40
2:p:267:GLN:HE21	2:p:271:LYS:HG3	1.86	0.40
2:p:384:TYR:OH	2:p:459:ASN:OD1	2.29	0.40
2:p:389:LEU:HD11	2:p:563:GLN:HB2	2.04	0.40
2:p:448:ILE:HB	2:p:548:VAL:HG12	2.02	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	O	238/356 (67%)	233 (98%)	5 (2%)	0	100	100
1	o	234/356 (66%)	230 (98%)	4 (2%)	0	100	100
2	P	466/590 (79%)	443 (95%)	22 (5%)	1 (0%)	43	77
2	p	464/590 (79%)	448 (97%)	16 (3%)	0	100	100
All	All	1402/1892 (74%)	1354 (97%)	47 (3%)	1 (0%)	49	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	P	246	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	215/308 (70%)	213 (99%)	2 (1%)	70	79
1	o	212/308 (69%)	212 (100%)	0	100	100
2	P	409/511 (80%)	405 (99%)	4 (1%)	68	78
2	p	408/511 (80%)	402 (98%)	6 (2%)	57	72
All	All	1244/1638 (76%)	1232 (99%)	12 (1%)	65	78

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	45	TYR
1	O	228	VAL
2	P	338	LEU
2	P	432	ILE
2	P	495	LEU
2	P	565	ASN
2	p	101	VAL
2	p	339	GLN
2	p	387	THR
2	p	432	ILE
2	p	556	MET
2	p	557	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	272	GLN
1	O	323	ASN
1	O	340	ASN
2	P	174	ASN
2	P	192	GLN
2	P	226	GLN
2	P	261	GLN

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Mol	Chain	Res	Type
2	P	311	GLN
2	P	319	GLN
2	P	343	HIS
2	P	351	ASN
2	P	409	ASN
2	P	500	HIS
2	P	514	HIS
2	P	563	GLN
2	P	565	ASN
1	o	44	HIS
1	o	272	GLN
2	p	108	GLN
2	p	122	GLN
2	p	174	ASN
2	p	226	GLN
2	p	234	ASN
2	p	267	GLN
2	p	280	GLN
2	p	281	HIS
2	p	290	ASN
2	p	339	GLN
2	p	468	ASN
2	p	497	GLN
2	p	519	ASN
2	p	553	GLN
2	p	563	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

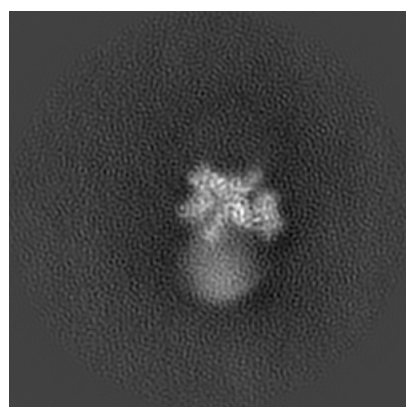
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21979. These allow visual inspection of the internal detail of the map and identification of artifacts.

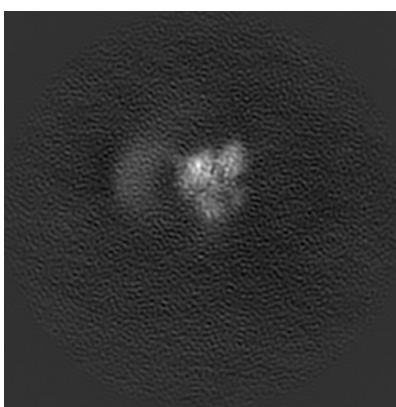
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

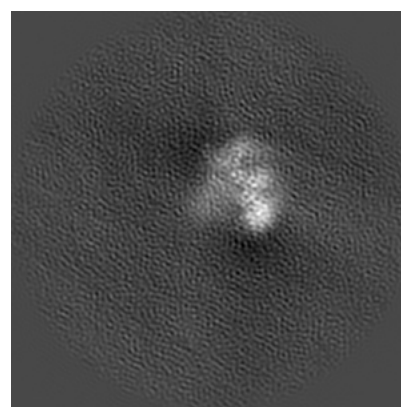
6.1.1 Primary map



X



Y

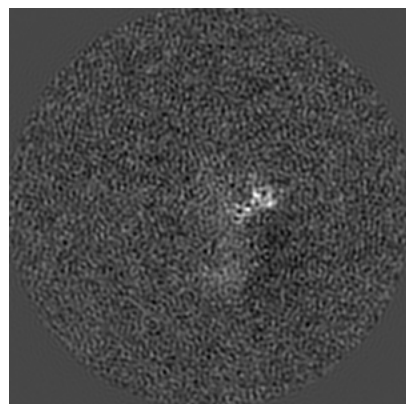


Z

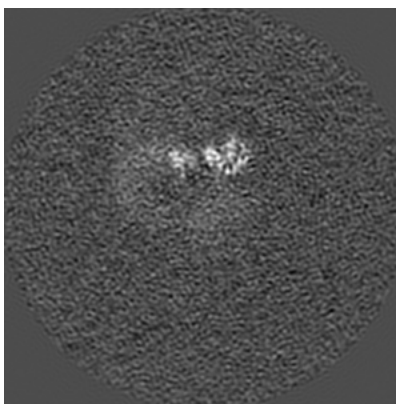
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

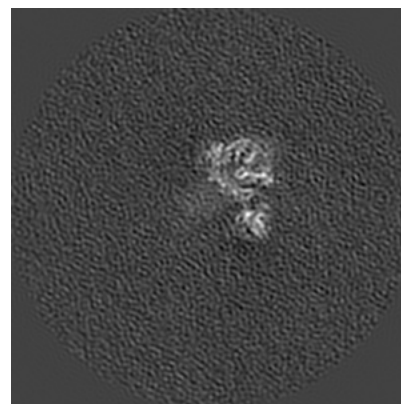
6.2.1 Primary map



X Index: 120



Y Index: 120

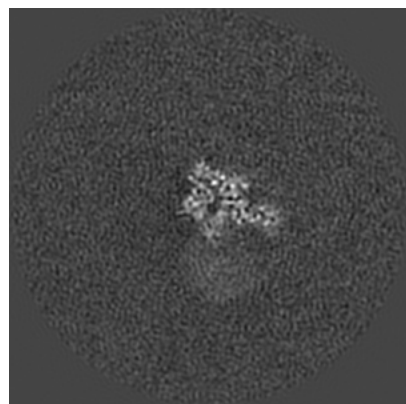


Z Index: 120

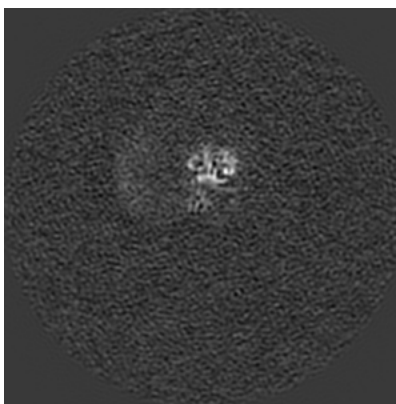
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 145



Y Index: 138

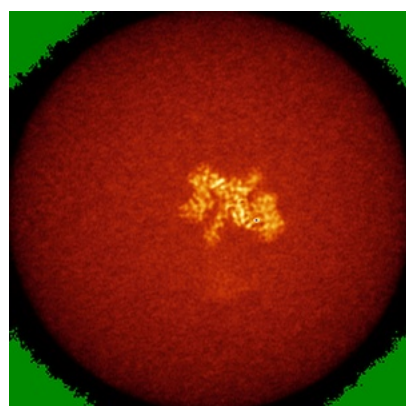


Z Index: 123

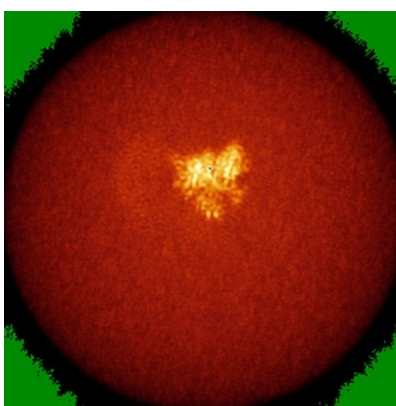
The images above show the largest variance slices of the map in three orthogonal directions.

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

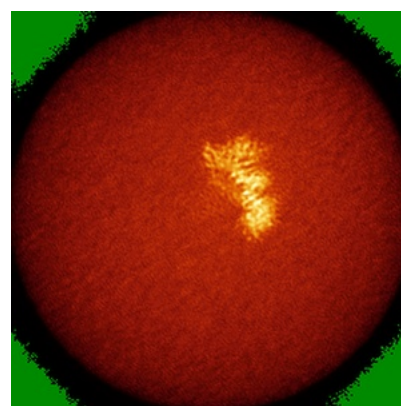
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

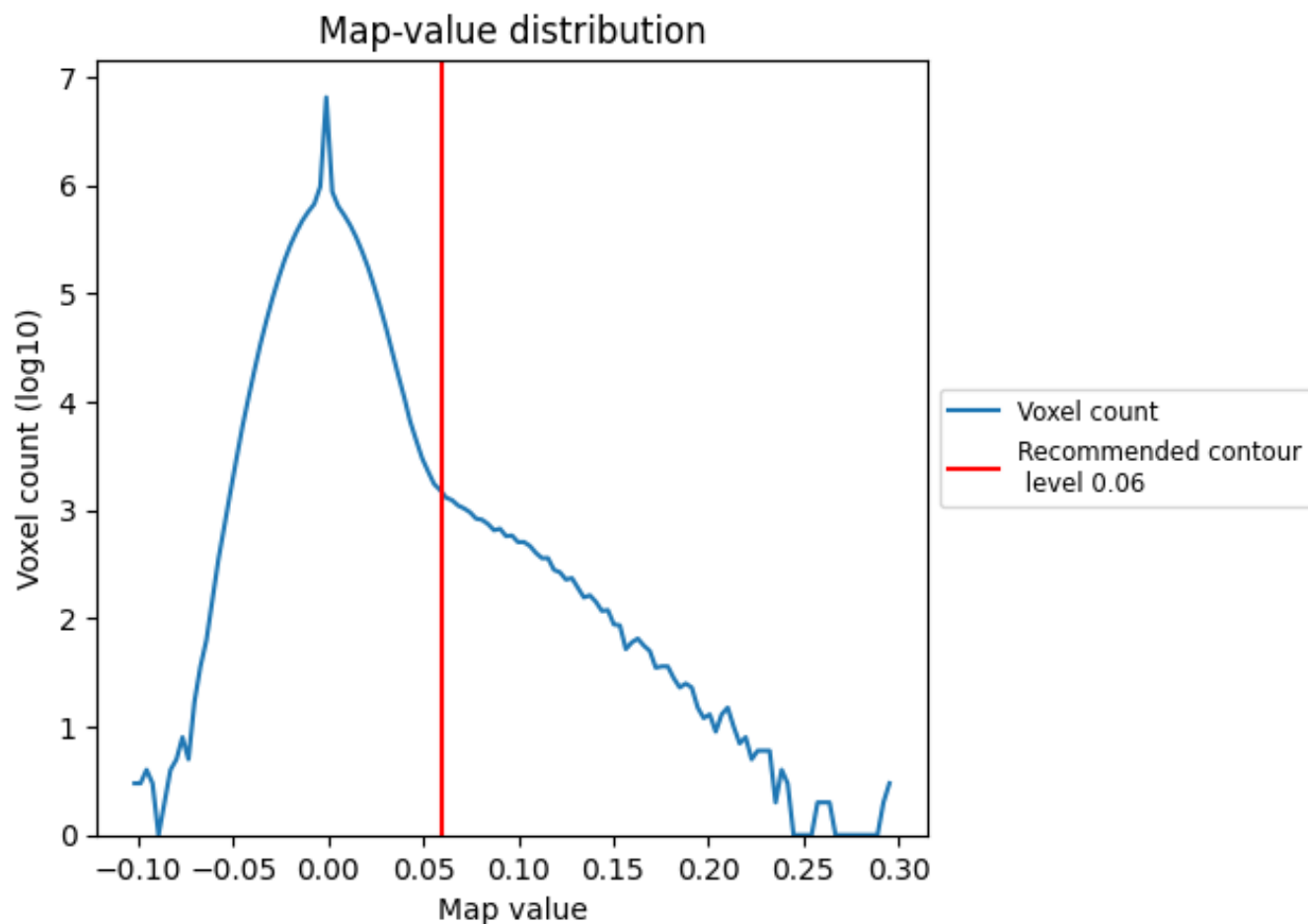
6.6 Mask visualisation

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

7 Map analysis [i](#)

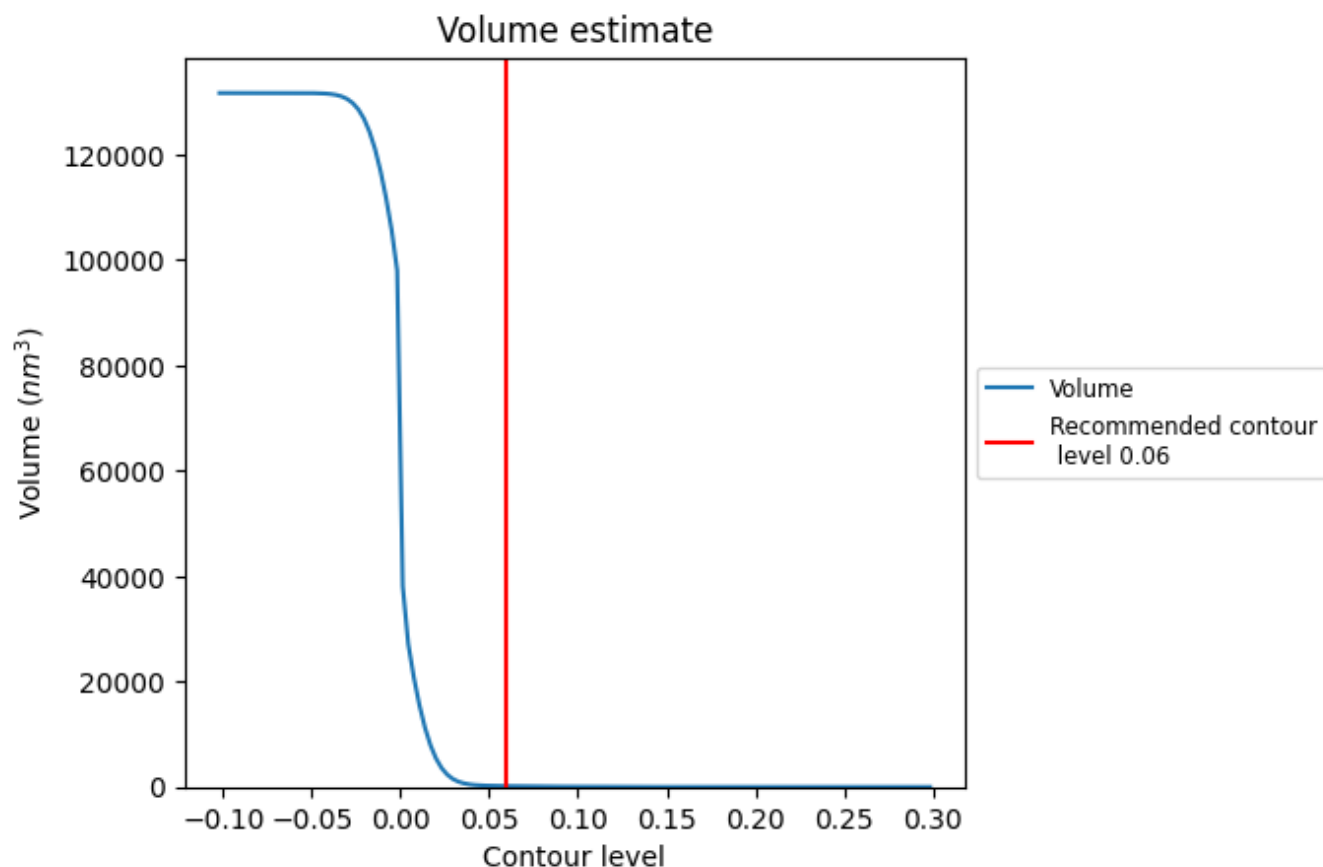
This section contains the results of statistical analysis of the map.

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.

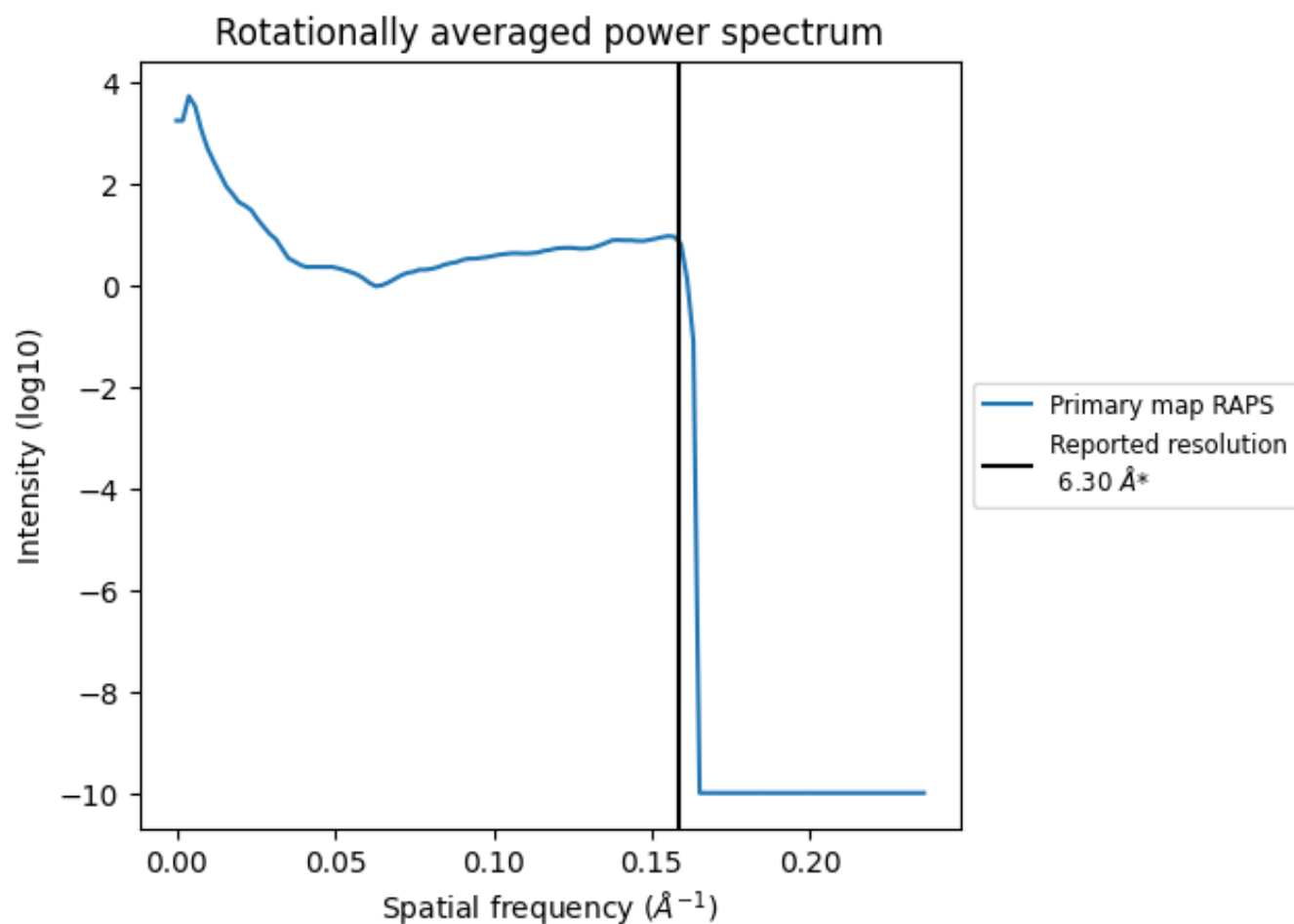
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 159 nm³; this corresponds to an approximate mass of 144 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 0.159 $\text{\AA}^{-1}$

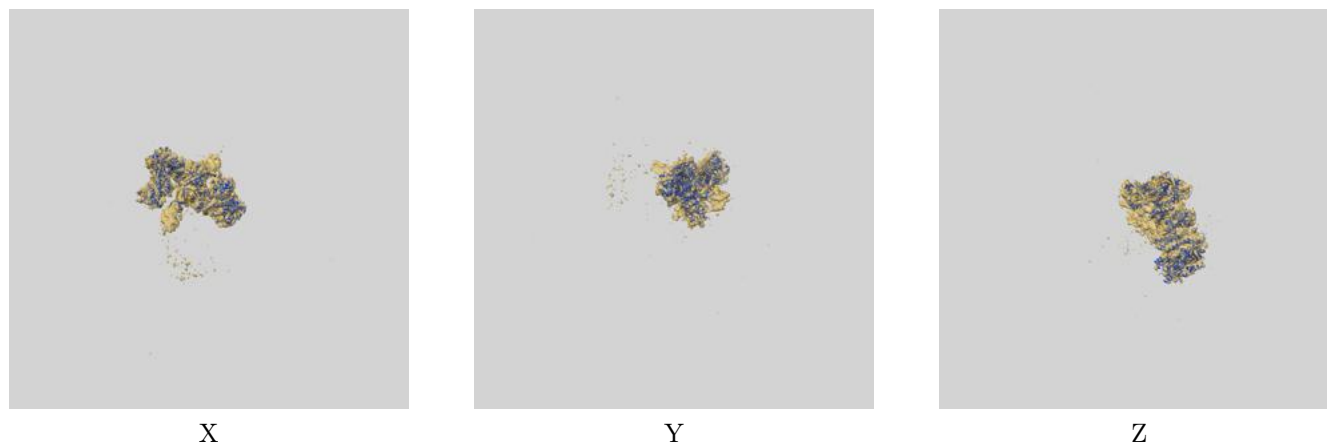
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21979 and PDB model 6X0M. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



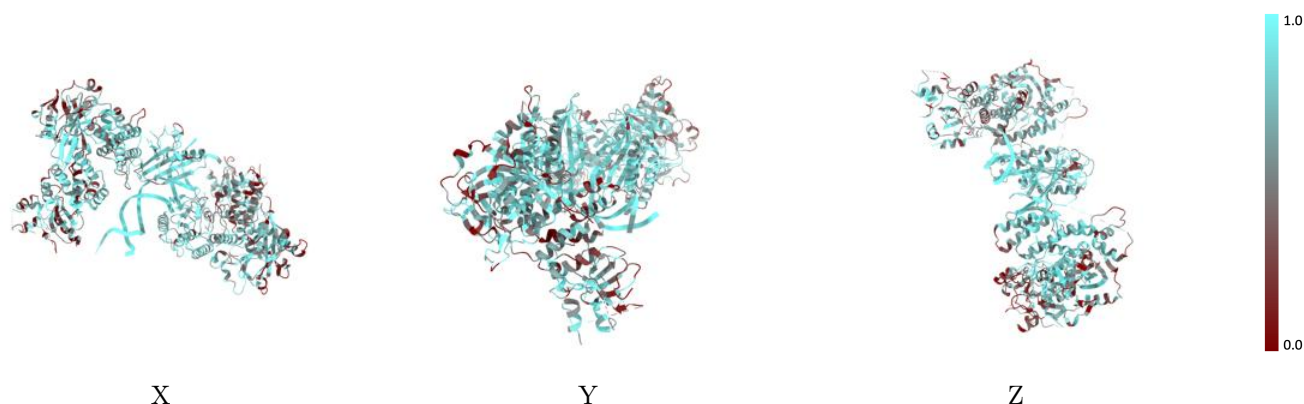
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



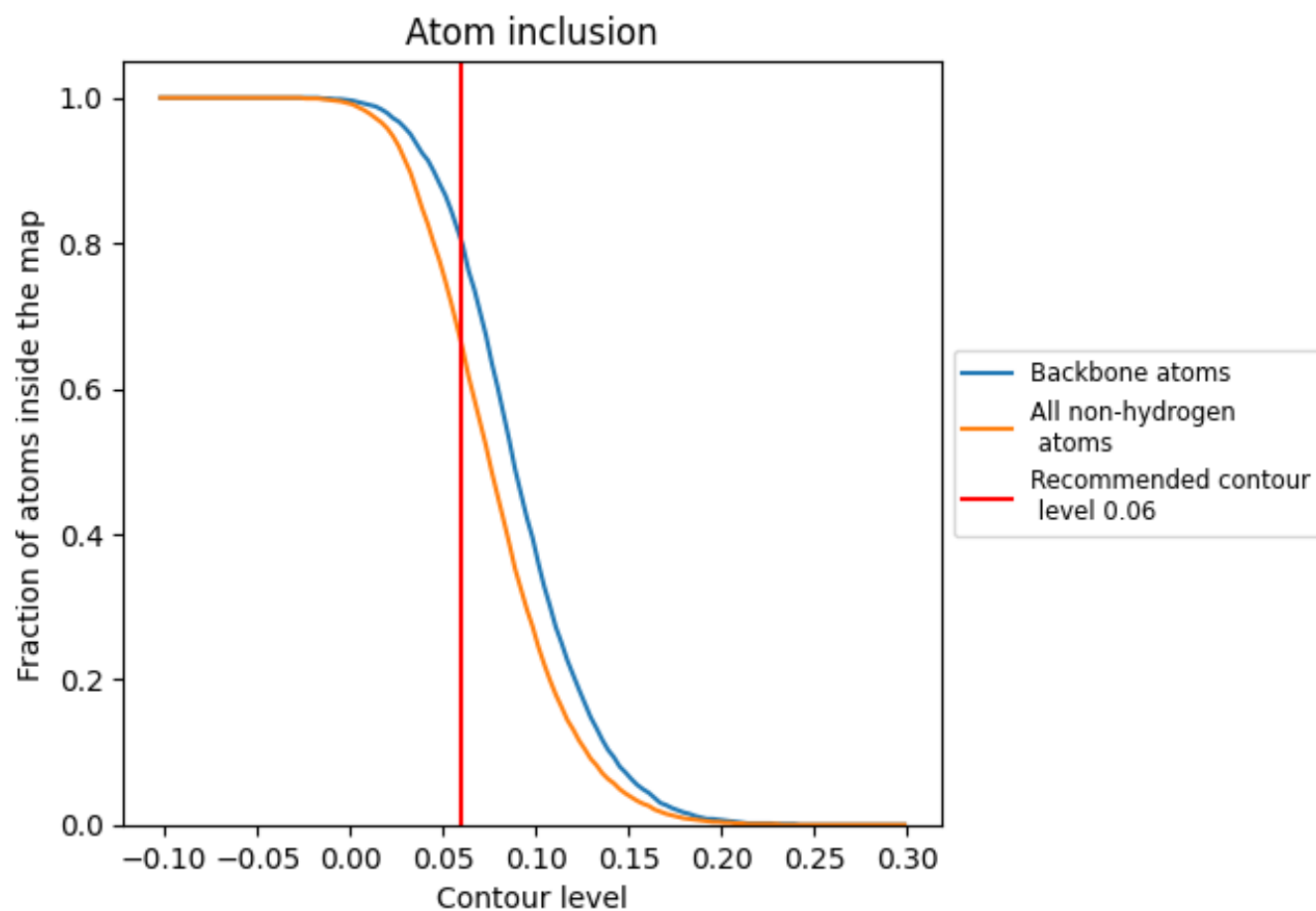
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

9.4 Atom inclusion ⓘ



At the recommended contour level, 80% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6610	0.1670
I	0.9420	0.2600
J	0.9120	0.2290
O	0.5970	0.1620
P	0.6800	0.1660
i	0.9260	0.2570
j	0.9150	0.2210
o	0.5650	0.1510
p	0.6600	0.1610

1.0

0.0

<0.0