

Sep 4, 2023 – 02:24 PM JST

PDB ID	:	8187
EMDB ID	:	EMD-35240
Title	:	Cryo-EM structure of TIR-APAZ/Ago-gRNA-DNA complex
Authors	:	Zhang, H.; Deng, Z.Q.; Yu, G.M.; Li, X.Z.; Wang, X.S.
Deposited on	:	2023-02-03
Resolution	:	3.10 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 (i) 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 (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1. dev 50
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)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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	EM structures
	$(\# { m Entries})$	$(\# { m Entries})$
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 $\geq=3, 2, 1$ 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			
		170	6%			
1	A	452	69%	19%	•	9%
	~		8%		_	
1	С	452	69%	21%	•	8%
			13%			
1	G	452	63%	24%	•	10%
	_		7%			
1	0	452	71%	18%	•	8%
			<u>-</u>			
2	В	507	66%	24%	•	8%
2	D	507	73%	19%		• 7%
2	F	507	68%	24%		• 8%



Mol	Chain	Length	Quality of	of chain	
2	Т	507	• 73%	18%	• 7%
3	Е	19	5% 5% 9!	5%	
3	J	19	42%	53%	5%
3	Κ	19	47%	42%	11%
3	U	19	5%	37%	11%
4	Н	19	32%	58%	5% 5%
4	Ι	19	53%	37%	5% 5%
4	L	19	63%	26%	5% 5%
4	S	19	5%	42%	5%



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 31066 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.

Mol	Chain	Residues		At	oms		AltConf	Trace		
1	Δ	413	Total	С	Ν	Ο	S	0	0	
	410	3264	2128	550	576	10	0			
1 C	414	Total	С	Ν	0	S	0	0		
	414	3306	2151	555	590	10	0	0		
1	C	406	Total	С	Ν	0	S	0	0	
I G	400	3203	2089	540	564	10	0	0		
1	0	414	Total	С	Ν	0	S	0	0	
	0	414	3292	2141	555	586	10	0	0	

• Molecule 1 is a protein called TIR domain-containing protein.

• Molecule 2 is a protein called Piwi domain-containing protein.

Mol	Chain	Residues		At	oms		AltConf	Trace		
2	В	467	Total	С	Ν	0	\mathbf{S}	0	0	
2		407	3758	2435	623	690	10	0	0	
2	2 D	460	Total	С	Ν	Ο	\mathbf{S}	0	0	
		409	3782	2453	625	692	12	0		
0	Б	467	Total	С	Ν	0	S	0	0	
2 Г	407	3762	2438	624	690	10	0	U		
0	Т	460	Total	С	Ν	0	S	0	0	
	L	409	3782	2453	625	692	12	0	0	

• Molecule 3 is a DNA chain called DNA (5'-D(P*TP*AP*TP*AP*CP*AP*AP*CP*CP*TP *AP*CP*TP*AP*CP*CP*TP*CP*A)-3').

Mol	Chain	Residues		At	\mathbf{oms}		AltConf	Trace	
2 E		10	Total	С	Ν	Ο	Р	0	0
5 Е	19	362	173	61	109	19	0	0	
3	2 I	18	Total	С	Ν	0	Р	0	0
9 1	10	343	163	59	103	18	0		
		17	Total	С	Ν	Ο	Р	0	0
A C	17	324	154	56	97	17	0	0	
3	T	17	Total	С	Ν	0	Р	0	0
	U	17	324	154	56	97	17	0	U



• Molecule 4 is a RNA chain called RNA (5'-R(P*UP*GP*AP*GP*GP*UP*AP*GP*UP*AP *GP*UP*UP*GP*UP*AP*UP*A)-3').

Mol	Chain	Residues		At	\mathbf{oms}		AltConf	Trace		
4	Ц	18	Total	С	Ν	0	Р	0	0	
4	4 11	10	390	173	69	130	18	0	0	
4	Т	18	Total	С	Ν	0	Р	0	0	
4	4 1	10	390	173	69	130	18	0	0	
4	т	18	Total	С	Ν	0	Р	0	0	
	10	390	173	69	130	18	0	0		
4	C	19	Total	С	Ν	0	Р	0	0	
4	G	10	390	173	69	130	18	U	0	

• Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
5	В	1	Total Mg 1 1	0
5	D	1	Total Mg 1 1	0
5	F	1	Total Mg 1 1	0
5	Н	1	Total Mg 1 1	0



3 Residue-property plots (i)

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: TIR domain-containing protein







• Molecule 2: Piwi domain-containing protein



• Molecule 2: Piwi domain-containing protein



Chain T:	73%		18% •	7%	
M1 K2 F10 F14 F14 T21 A23 A23 A23 A23 A23 A23 A23 A23 A23 A23	841 144 146 160 173 872 872 872 872 833 189 189	K94 N98 N107 K103 K112 R113 R113 S119 S119	A128 E132 V141 V143	7144 1147 1148 1149 1150 1157	
B160 M161 V162 V162 V162 V162 V162 V162 LV8 MET LV8 SER LV8 SER LV8 AL8	LYS SER PHE ARC TYR ARC CLU PERO PRO PRO PRO PRO ASP ASP	LEU LEU GLU GLU GLU GLU ALLA ALLA ALLA ALLA AL	4209 (1209 (13) (13) (13) (13) (13) (13) (13) (13)	D233 S246 K247 1248 H251	
T255 K267 P268 W269 W269 W269 K270 G277 K287 K287 K287	N296 A297 A297 B316 P319 V324 K324 K333 K333	K336 L339 S349 S349 C348 L350 L350 C351 L350 C351 L350 R364 R364	E380 L383 L383 T387 T387 S389	6401 0402 R407 R416	
1422 V423 V428 8434 8434 8434 8434 1435 1443 1443 1443 1459	L460 2461 2461 1463 1463 1465 1465 1470 1470 1470 1472 1472 1472 1472 1472 1478 1478 1478	L490			
• Molecule 3: DNA P*TP*CP*A)-3')	(5'-D(P*TP*AP*TP*	*AP*CP*AP*AP*(CP*CP*TI	P*AP*CP*1	CP*AP*CP*C
Chain E: 5%		95%		_	
11 42 44 45 45 46 47 41 110 411 113 113 113 113 113 113	C16 C117 C118 A19				
• Molecule 3: DNA P*TP*CP*A)-3')	(5'-D(P*TP*AP*TP*	*AP*CP*AP*AP*(CP*CP*TI	P*AP*CP*J	P*AP*CP*C
Chain J:	42%	53%		5%	
DT 73 75 75 75 71 71 71 71 71 71 71 71 71 71 71 71 71					
• Molecule 3: DNA P*TP*CP*A)-3')	(5'-D(P*TP*AP*TP*	*AP*CP*AP*AP*(CP*CP*TI	P*AP*CP*7	P*AP*CP*C
Chain K:	47%	42%	12	L%	
DT A2 A2 A7 C12 C12 C12 C13 C15 C15 D1 D1 D1					
• Molecule 3: DNA P*TP*CP*A)-3')	(5'-D(P*TP*AP*TP*	*AP*CP*AP*AP*(CP*CP*TI	P*AP*CP*J	CP*AP*CP*C
Chain U:	53%	37%	1	1%	
DT A2 C5 A7 A7 A11 A11 C18 DA					



U1

• Molecule 4: RNA (5'-R(P*UP*GP*AP*GP*GP*UP*AP*GP*UP*AP*GP*GP*UP*AP*GP*UP*AP*GP*UP*A)-3')

Chain	F	ł: '							32	%		58%	5%	5%
U1 G2 G4	A7	<u>68</u>	<u>م</u>	G12	U13	U14	G15	U16	A17	U18	А			

• Molecule 4: RNA (5'-R(P*UP*GP*AP*GP*GP*UP*AP*GP*UP*AP*GP*GP*UP*AP*GP*UP*AP*GP*UP*A)-3')

Chain I:	53%	37%	5% 5%
U1 62 62 612 013 014 016 015 016 016 016 018 018			

• Molecule 4: RNA (5'-R(P*UP*GP*AP*GP*GP*UP*AP*GP*UP*AP*GP*GP*UP*UP*GP*UP*AP*GP*UP*A)-3')

Chain L:	63%	26%	5%	5%
U1 G2 A3 U14 G15 U16 U18 A17 A17 A17 A17				

• Molecule 4: RNA (5'-R(P*UP*GP*AP*GP*GP*UP*AP*GP*UP*AP*GP*GP*UP*AP*GP*UP*CP*UP*GP*UP*A)-3')

a a	5%		
Chain S:	53%	42%	5%
	•		
_			



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	257382	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 $(6k \ge 4k)$	Depositor
Maximum map value	1.707	Depositor
Minimum map value	-1.150	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	285.0, 285.0, 285.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	Depositor



5 Model quality (i)

5.1 Standard geometry (i)

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

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).

Mal	Chain	Bond lengths		Bond angles	
	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.24	0/3342	0.47	1/4524~(0.0%)
1	С	0.24	0/3385	0.48	1/4578~(0.0%)
1	G	0.24	0/3277	0.49	2/4433~(0.0%)
1	0	0.27	0/3370	0.52	4/4558~(0.1%)
2	В	0.26	0/3854	0.47	0/5221
2	D	0.25	0/3879	0.45	0/5253
2	F	0.25	0/3858	0.46	0/5225
2	Т	0.26	0/3879	0.47	2/5253~(0.0%)
3	Е	0.53	0/403	0.94	0/616
3	J	0.57	0/382	0.92	0/585
3	K	0.52	0/361	0.88	0/553
3	U	0.50	0/361	0.89	0/553
4	Н	0.56	1/436~(0.2%)	0.73	0/677
4	Ι	0.55	1/436~(0.2%)	0.77	0/677
4	L	0.55	1/436~(0.2%)	0.74	0/677
4	S	0.55	1/436~(0.2%)	0.76	0/677
All	All	0.30	4/32095~(0.0%)	0.53	10/44060~(0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
4	Н	1	U	OP3-P	-10.87	1.48	1.61
4	L	1	U	OP3-P	-10.84	1.48	1.61
4	S	1	U	OP3-P	-10.69	1.48	1.61
4	Ι	1	U	OP3-P	-10.67	1.48	1.61

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	0	242	PRO	CA-N-CD	-12.03	94.67	111.50



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	195	PRO	N-CA-CB	7.01	111.72	103.30
1	0	242	PRO	N-CD-CG	-7.01	92.68	103.20
1	С	195	PRO	N-CA-CB	6.94	111.63	103.30
1	0	195	PRO	N-CA-CB	6.88	111.56	103.30
1	G	195	PRO	N-CA-CB	6.54	111.15	103.30
2	Т	83	ASP	CB-CG-OD1	6.29	123.97	118.30
1	G	269	LEU	CA-CB-CG	6.09	129.30	115.30
2	Т	484	ASP	CB-CG-OD1	5.96	123.67	118.30
1	0	242	PRO	CA-CB-CG	-5.12	94.27	104.00

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	А	3264	0	3165	56	0
1	С	3306	0	3228	56	0
1	G	3203	0	3108	71	0
1	0	3292	0	3210	60	0
2	В	3758	0	3746	71	0
2	D	3782	0	3778	53	0
2	F	3762	0	3757	69	0
2	Т	3782	0	3778	53	0
3	Е	362	0	203	16	0
3	J	343	0	191	12	0
3	Κ	324	0	180	8	0
3	U	324	0	180	6	0
4	Н	390	0	192	10	0
4	Ι	390	0	192	6	0
4	L	390	0	192	5	0
4	S	390	0	192	4	0
5	В	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
5	Н	1	0	0	0	0



Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	31066	0	29292	515	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (515) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:D:201:ASN:N	2:D:201:ASN:HD22	1.57	0.98
3:K:13:DT:H2'	3:K:14:DA:H8	1.41	0.85
3:J:3:DT:H2'	3:J:4:DA:H8	1.48	0.77
2:B:390:LYS:HG3	2:B:441:LEU:HD23	1.67	0.77
1:G:300:LEU:HD21	1:G:305:PHE:HB2	1.68	0.76
2:D:201:ASN:N	2:D:201:ASN:ND2	2.31	0.76
3:J:5:DC:H2'	3:J:6:DA:C8	2.21	0.75
3:E:13:DT:H2'	3:E:14:DA:H8	1.52	0.73
2:D:297:ALA:HB1	2:D:319:PRO:HB2	1.69	0.73
1:O:260:GLU:OE1	4:H:15:G:N2	2.23	0.71
1:0:242:PRO:HD2	1:0:242:PRO:0	1.89	0.71
3:E:13:DT:H2'	3:E:14:DA:C8	2.25	0.71
1:A:80:VAL:HG21	1:O:110:ILE:HG12	1.73	0.71
3:J:13:DT:H2'	3:J:14:DA:C8	2.27	0.70
1:G:112:ILE:HA	1:G:115:LEU:HD12	1.74	0.70
2:B:21:THR:O	2:B:464:LYS:NZ	2.25	0.69
1:G:110:ILE:HD12	1:G:110:ILE:H	1.56	0.69
1:G:265:ILE:O	1:G:269:LEU:HD22	1.93	0.68
2:D:296:ASN:ND2	2:D:327:GLN:O	2.26	0.68
1:C:263:ARG:NH2	3:K:5:DC:O2	2.25	0.68
3:K:13:DT:H2'	3:K:14:DA:C8	2.26	0.68
3:J:5:DC:H2'	3:J:6:DA:H8	1.57	0.67
2:T:297:ALA:HB1	2:T:319:PRO:HB2	1.77	0.67
2:D:122:ILE:HG12	2:D:214:LEU:HD13	1.76	0.66
2:T:21:THR:O	2:T:464:LYS:NZ	2.28	0.66
2:B:423:VAL:HG13	2:B:433:LEU:HB2	1.78	0.66
2:D:368:GLN:OE1	2:D:368:GLN:N	2.22	0.66
3:E:7:DA:H2"	3:E:8:DC:H5"	1.79	0.65
2:B:94:LYS:HE3	2:B:128:ALA:HB2	1.78	0.65
1:A:276:ARG:NH2	1:A:386:ASP:OD2	2.29	0.65
4:I:16:U:O4	4:I:17:A:N6	2.30	0.65
2:F:469:ALA:HB2	4:S:3:A:H4'	1.77	0.65
1:G:361:ARG:HH12	1:G:373:TRP:HH2	1.44	0.64



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	lo uo puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:D:22:ASP:HB2	2:D:428:LYS:HE3	1.79	0.64
2:D:44:ILE:HD12	2:D:141:VAL:HG22	1.78	0.64
3:J:3:DT:H2'	3:J:4:DA:C8	2.33	0.63
2:D:416:ARG:NH2	2:D:448:GLY:O	2.32	0.63
2:B:9:GLU:OE2	2:B:407:ARG:NH1	2.31	0.63
3:E:3:DT:H2'	3:E:4:DA:C8	2.33	0.63
2:F:274:VAL:HB	2:F:305:LEU:HD13	1.81	0.63
1:A:173:SER:OG	1:A:408:VAL:O	2.17	0.63
2:B:380:GLU:OE1	2:B:380:GLU:N	2.30	0.63
1:O:296:GLU:HB3	1:O:299:LYS:HE3	1.81	0.63
2:F:24:ARG:NH1	3:E:19:DA:O5'	2.32	0.62
4:L:14:U:H2'	4:L:15:G:H8	1.63	0.62
3:J:13:DT:H2'	3:J:14:DA:H8	1.63	0.62
2:D:459:ILE:HG23	2:D:477:PRO:HG3	1.81	0.62
3:J:7:DA:H2"	3:J:8:DC:H5"	1.81	0.62
2:F:99:GLU:OE2	2:F:99:GLU:N	2.31	0.62
2:T:416:ARG:NH2	2:T:448:GLY:O	2.33	0.62
2:B:322:ASN:ND2	2:B:329:HIS:O	2.32	0.62
2:F:297:ALA:HB1	2:F:319:PRO:HB2	1.82	0.61
1:C:161:ASP:OD1	1:C:162:LYS:NZ	2.33	0.61
1:G:314:GLN:OE1	1:G:364:GLN:NE2	2.34	0.61
3:K:5:DC:H2'	3:K:6:DA:C8	2.35	0.61
2:D:113:ARG:NH1	2:D:150:TYR:O	2.33	0.61
2:F:144:PRO:HD2	2:F:147:ILE:HD12	1.82	0.61
2:T:319:PRO:HD3	2:T:490:LEU:HD13	1.83	0.61
2:T:469:ALA:HB2	4:H:3:A:H4'	1.83	0.61
1:G:343:PHE:O	1:G:357:GLN:NE2	2.34	0.61
1:C:80:VAL:O	1:C:84:VAL:HG23	2.01	0.61
2:F:21:THR:O	2:F:464:LYS:NZ	2.25	0.61
1:A:241:ILE:HD12	1:A:241:ILE:H	1.65	0.60
1:C:186:ARG:HG3	1:C:240:ARG:HG2	1.81	0.60
3:J:12:DC:H2'	3:J:13:DT:H71	1.82	0.60
1:C:294:TRP:HB3	1:C:322:ALA:HB2	1.84	0.60
2:B:72:ARG:HH12	2:B:248:ILE:HG22	1.66	0.60
1:G:41:LYS:HD2	1:O:118:ILE:HG12	1.84	0.60
1:G:211:LYS:NZ	1:G:255:PHE:O	2.35	0.60
1:O:408:VAL:HG21	2:T:2:LYS:HE2	1.84	0.60
1:C:199:ASP:O	1:C:201:ARG:N	2.33	0.60
1:G:129:LYS:HD2	1:G:158:PHE:HA	1.84	0.59
2:B:297:ALA:HB1	2:B:319:PRO:HB2	1.83	0.59
2:B:469:ALA:HB2	4:I:3:A:H4'	1.85	0.59



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		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:G:395:MET:O	1:G:398:GLU:N	2.36	0.59
2:D:21:THR:O	2:D:464:LYS:NZ	2.33	0.59
1:G:302:LYS:H	1:G:304:LYS:HE3	1.67	0.59
1:A:116:ASN:OD1	1:A:116:ASN:N	2.30	0.59
1:G:176:LEU:HD11	1:G:381:ILE:HD11	1.85	0.58
2:T:13:LEU:HD22	2:T:270:LYS:HE2	1.84	0.58
1:G:294:TRP:HB3	1:G:322:ALA:HB2	1.84	0.58
4:L:14:U:H2'	4:L:15:G:C8	2.39	0.58
2:B:319:PRO:HD3	2:B:490:LEU:HD13	1.85	0.58
3:U:7:DA:H2"	3:U:8:DC:H5"	1.86	0.58
1:A:263:ARG:NH1	3:J:5:DC:O2	2.37	0.58
2:D:122:ILE:O	2:D:126:ILE:HG12	2.03	0.58
1:A:41:LYS:HD2	1:C:118:ILE:HG12	1.85	0.58
1:C:206:PRO:HG3	1:C:272:ALA:HB2	1.86	0.58
3:K:7:DA:H2"	3:K:8:DC:H5"	1.84	0.58
1:G:186:ARG:HB2	1:G:216:THR:O	2.04	0.57
2:D:493:SER:OG	2:D:495:ASP:OD1	2.22	0.57
2:D:275:ARG:HG3	2:D:278:VAL:HG11	1.85	0.57
1:G:283:GLN:NE2	1:G:294:TRP:O	2.37	0.57
2:B:61:GLN:NE2	2:B:86:TRP:O	2.38	0.57
1:C:385:SER:HA	1:C:391:PHE:HB3	1.86	0.57
2:D:240:LEU:HD22	2:D:241:PRO:HD2	1.85	0.57
2:F:95:GLU:O	2:F:124:LYS:NZ	2.37	0.57
2:B:300:ALA:HB3	2:B:316:GLU:HB2	1.86	0.57
2:D:322:ASN:ND2	2:D:329:HIS:O	2.37	0.57
1:G:274:GLU:O	1:G:278:LYS:HB2	2.05	0.57
2:F:336:LYS:O	2:F:340:SER:OG	2.22	0.57
1:G:203:LEU:H	1:G:203:LEU:HD12	1.69	0.57
2:F:97:THR:HG23	2:F:100:ASP:H	1.70	0.57
2:D:25:ASP:O	2:D:29:LEU:HD12	2.04	0.56
1:A:246:ILE:HD11	1:A:261:CYS:HB3	1.86	0.56
1:G:198:PHE:HA	1:G:209:ARG:HH22	1.71	0.56
1:O:23:LEU:HD13	2:T:29:LEU:HD21	1.87	0.56
2:T:434:SER:OG	2:T:435:MET:N	2.39	0.56
4:L:17:A:O2'	4:L:18:U:OP2	2.23	0.56
3:U:5:DC:H2'	3:U:6:DA:C8	2.40	0.56
1:A:357:GLN:HE21	1:A:357:GLN:CA	2.17	0.56
2:F:101:ILE:HD13	2:F:147:ILE:HD11	1.87	0.56
1:G:186:ARG:NH1	1:G:217:PHE:O	2.38	0.56
1:C:159:LEU:HD21	2:D:428:LYS:HD2	1.88	0.56
1:0:14:ASP:0	1:O:18:THR:OG1	2.18	0.56



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Interstomic Clash				
Atom-1	Atom-2	distance $(Å)$	overlap (Å)	
2:T:10:PRO:HG3	2:T:461:SER:HA	1.86	0.56	
1:A:393:LEU:HB2	1:A:401:VAL:HG22	1.87	0.56	
1:G:116:ASN:OD1	1:G:116:ASN:N	2.32	0.56	
2:B:296:ASN:ND2	2:B:327:GLN:O	2.38	0.56	
2:D:300:ALA:HB3	2:D:316:GLU:HB3	1.88	0.56	
3:E:5:DC:H2"	3:E:6:DA:C8	2.41	0.56	
2:F:22:ASP:HB2	2:F:428:LYS:HE2	1.88	0.55	
2:T:339:LEU:HD11	2:T:383:LEU:HD11	1.88	0.55	
1:A:217:PHE:HB2	1:A:395:MET:HB3	1.88	0.55	
2:D:282:GLY:O	2:D:300:ALA:HA	2.06	0.55	
1:O:295:LEU:O	1:O:320:HIS:ND1	2.38	0.55	
1:0:370:ASN:OD1	1:O:371:ASN:N	2.40	0.55	
1:O:294:TRP:HB3	1:O:322:ALA:HB2	1.88	0.55	
3:E:5:DC:H2"	3:E:6:DA:H8	1.72	0.55	
2:B:245:PHE:HD1	2:B:248:ILE:HD11	1.72	0.55	
1:O:34:CYS:HB3	1:O:37:LEU:HG	1.89	0.55	
1:A:50:GLU:HB2	1:O:110:ILE:HG13	1.89	0.55	
2:F:322:ASN:ND2	2:F:329:HIS:O	2.40	0.55	
1:O:371:ASN:ND2	2:T:401:GLY:O	2.40	0.55	
1:G:328:LYS:NZ	3:E:7:DA:OP2	2.39	0.55	
1:A:260:GLU:O	1:A:264:LEU:HD23	2.07	0.55	
1:O:85:LYS:HB2	1:O:93:PHE:HB3	1.88	0.55	
4:H:7:A:H2'	4:H:8:G:C8	2.41	0.55	
3:J:14:DA:H2"	3:J:15:DC:H5"	1.89	0.55	
1:A:182:PRO:HD3	1:A:401:VAL:HG12	1.88	0.54	
1:A:230:THR:O	1:A:235:LYS:NZ	2.40	0.54	
1:C:59:LYS:NZ	1:C:92:LYS:O	2.38	0.54	
2:D:8:GLU:OE1	2:D:457:LYS:NZ	2.40	0.54	
1:G:2:ARG:NH2	1:G:54:ARG:O	2.38	0.54	
3:J:4:DA:H2'	3:J:5:DC:C6	2.43	0.54	
2:D:10:PRO:HD3	2:D:460:LEU:HD23	1.87	0.54	
1:O:153:LEU:HG	1:O:157:ILE:HD12	1.88	0.54	
1:A:2:ARG:NH2	1:A:54:ARG:O	2.37	0.54	
1:A:193:MET:HA	1:A:229:LYS:HG2	1.90	0.54	
2:T:350:ILE:HG22	2:T:352:GLU:H	1.71	0.54	
2:B:14:PHE:HZ	2:B:23:ALA:HA	1.73	0.54	
2:D:5:ILE:HG23	2:D:410:ALA:HB3	1.90	0.54	
1:A:344:THR:HG22	1:A:350:LEU:HD23	1.88	0.54	
2:T:471:ILE:HG13	2:T:472:PHE:O	2.08	0.54	
1:A:236:SER:O	1:A:240:ARG:NH2	2.40	0.54	
1:G:239:ILE:HG22	1:G:241:ILE:HG23	1.90	0.54	



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Interstomic Clash				
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:G:261:CYS:O	1:G:265:ILE:HG23	2.08	0.53	
2:B:128:ALA:HA	2:B:132:GLU:HG3	1.88	0.53	
1:G:168:GLU:HA	1:G:412:GLY:O	2.08	0.53	
1:0:199:ASP:0	1:O:201:ARG:N	2.41	0.53	
4:S:14:U:H2'	4:S:15:G:C8	2.43	0.53	
2:B:379:LYS:O	2:B:379:LYS:NZ	2.35	0.53	
2:B:5:ILE:HD12	2:B:453:LYS:HD3	1.88	0.53	
1:O:187:PHE:HB2	1:O:239:ILE:HB	1.90	0.53	
2:T:247:LYS:NZ	3:U:18:DC:OP2	2.37	0.53	
1:C:175:TRP:NE1	1:C:336:MET:SD	2.82	0.53	
1:G:241:ILE:HD12	1:G:246:ILE:HD13	1.90	0.53	
1:G:252:ASP:O	1:G:253:SER:HB3	2.09	0.52	
1:A:14:ASP:O	1:A:18:THR:OG1	2.21	0.52	
1:C:6:PHE:HB2	1:C:57:THR:HG21	1.91	0.52	
2:F:94:LYS:HE3	2:F:128:ALA:HB2	1.91	0.52	
3:K:5:DC:H2'	3:K:6:DA:H8	1.74	0.52	
1:A:44:ASP:OD2	1:C:114:ARG:NH2	2.38	0.52	
2:D:118:VAL:HG13	2:D:122:ILE:HD12	1.91	0.52	
2:T:113:ARG:NH1	2:T:150:TYR:O	2.41	0.52	
2:D:268:PRO:HB2	2:D:269:TRP:CE3	2.45	0.52	
2:F:459:ILE:HG23	2:F:477:PRO:HG3	1.92	0.52	
2:B:72:ARG:NH1	2:B:248:ILE:HG22	2.25	0.52	
2:T:423:VAL:HG12	2:T:438:PRO:HB3	1.91	0.52	
2:F:339:LEU:HD22	2:F:373:PHE:CD1	2.45	0.52	
1:O:168:GLU:OE1	1:0:411:LYS:NZ	2.33	0.52	
3:E:16:DC:H2'	3:E:17:DT:H71	1.90	0.52	
3:J:4:DA:H2'	3:J:5:DC:H6	1.75	0.52	
2:B:426:VAL:HB	2:B:429:ILE:HG12	1.92	0.52	
1:C:23:LEU:HD13	2:D:29:LEU:HD21	1.91	0.52	
1:C:14:ASP:OD2	1:C:65:SER:OG	2.25	0.52	
2:B:44:ILE:HD12	2:B:125:ILE:HG13	1.92	0.51	
1:A:227:LEU:O	1:A:230:THR:OG1	2.23	0.51	
1:G:385:SER:HA	1:G:391:PHE:HB3	1.92	0.51	
2:B:278:VAL:HA	2:B:356:GLU:O	2.11	0.51	
2:F:44:ILE:HD12	2:F:141:VAL:HG22	1.91	0.51	
3:K:12:DC:H2'	3:K:13:DT:H71	1.92	0.51	
2:B:228:THR:OG1	2:B:243:ARG:NH2	2.43	0.51	
1:C:362:ARG:NH2	2:D:436:GLU:OE2	2.43	0.51	
3:E:1:DT:H2"	3:E:2:DA:C8	2.46	0.51	
1:0:371:ASN:OD1	1:O:374:ARG:NH2	2.43	0.51	
2:D:286:LYS:NZ	2:D:484:ASP:OD2	2.41	0.51	



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		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:D:469:ALA:HB2	4:L:3:A:H4'	1.93	0.51
2:F:490:LEU:HD23	2:F:496:ILE:HD13	1.93	0.51
1:0:173:SER:OG	1:O:408:VAL:O	2.28	0.51
2:T:363:THR:HG22	3:U:9:DC:H5'	1.92	0.51
2:B:121:PHE:HB3	2:B:210:PHE:HE2	1.76	0.50
4:I:13:U:H2'	4:I:14:U:C6	2.46	0.50
2:T:422:THR:HG22	2:T:460:LEU:HD12	1.93	0.50
3:E:2:DA:H2'	3:E:3:DT:C6	2.46	0.50
2:B:245:PHE:CD1	2:B:248:ILE:HD11	2.46	0.50
2:F:152:ARG:HG3	2:F:152:ARG:HH11	1.75	0.50
2:B:301:ALA:HA	2:B:315:GLY:HA2	1.93	0.50
1:C:393:LEU:HB2	1:C:401:VAL:HG13	1.93	0.50
2:B:44:ILE:HG12	2:B:94:LYS:HB2	1.93	0.50
2:B:104:PHE:HE2	2:B:120:LEU:HD13	1.77	0.50
2:F:50:LEU:HD22	2:F:93:PHE:CG	2.47	0.50
1:C:185:LEU:HB3	1:C:241:ILE:HD11	1.93	0.50
2:F:363:THR:HG22	3:E:9:DC:H5'	1.94	0.50
2:B:231:TRP:CE2	2:B:245:PHE:HB2	2.47	0.50
2:B:268:PRO:HB2	2:B:269:TRP:CE3	2.47	0.50
2:B:96:VAL:HG22	2:B:124:LYS:HE2	1.94	0.49
2:D:464:LYS:HD3	2:D:473:ALA:HB2	1.94	0.49
1:G:83:LYS:O	1:G:87:GLN:HG3	2.12	0.49
1:O:272:ALA:HA	1:O:275:LEU:HD12	1.94	0.49
1:0:14:ASP:OD2	1:0:65:SER:OG	2.29	0.49
2:D:210:PHE:HE1	2:D:221:THR:HG21	1.77	0.49
2:F:300:ALA:HB3	2:F:316:GLU:HB2	1.94	0.49
1:G:385:SER:OG	1:G:390:SER:O	2.30	0.49
1:A:230:THR:HA	1:A:233:TYR:HB3	1.94	0.49
2:F:14:PHE:CE2	2:F:26:GLY:HA3	2.48	0.49
1:G:308:THR:HG21	1:G:379:ALA:HB2	1.93	0.49
2:T:34:ASN:HB2	2:T:267:LYS:H	1.78	0.48
2:T:141:VAL:HG12	2:T:143:VAL:HG23	1.95	0.48
1:O:301:GLU:HA	1:O:302:LYS:HA	1.63	0.48
1:O:227:LEU:O	1:O:230:THR:OG1	2.24	0.48
1:O:303:ASP:O	1:O:309:MET:HA	2.13	0.48
2:T:255:THR:HG22	2:T:470:CYS:H	1.78	0.48
2:T:443:ILE:HG12	2:T:459:ILE:HD13	1.95	0.48
2:B:459:ILE:HG23	2:B:477:PRO:HG3	1.94	0.48
1:C:72:GLU:H	1:C:72:GLU:CD	2.17	0.48
2:F:423:VAL:HG23	2:F:433:LEU:HB2	1.94	0.48
1:G:260:GLU:OE1	1:G:263:ARG:NH1	2.46	0.48



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		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:G:313:LYS:NZ	1:G:315:LYS:O	2.32	0.48
1:G:351:ILE:HG22	1:G:353:SER:H	1.78	0.48
1:C:198:PHE:HA	1:C:209:ARG:HH22	1.78	0.48
2:F:111:HIS:CE1	2:F:204:ALA:HB2	2.49	0.48
2:F:139:TRP:HB2	2:F:221:THR:HG22	1.94	0.48
2:F:251:HIS:ND1	3:E:18:DC:O2	2.45	0.48
1:G:300:LEU:HD23	1:G:303:ASP:HA	1.95	0.48
1:O:211:LYS:HG2	4:H:17:A:H3'	1.95	0.48
1:C:249:GLY:HA2	1:C:258:ASN:HD21	1.78	0.48
2:T:276:ASN:OD1	2:T:277:GLY:N	2.47	0.48
4:S:13:U:H2'	4:S:14:U:C6	2.49	0.47
2:D:306:ASP:HA	2:D:350:ILE:HD11	1.96	0.47
2:F:339:LEU:HD12	2:F:339:LEU:HA	1.68	0.47
1:A:385:SER:HA	1:A:391:PHE:HB3	1.96	0.47
1:A:110:ILE:HB	1:G:50:GLU:HG3	1.96	0.47
2:F:398:LYS:HB2	1:G:370:ASN:HD21	1.79	0.47
2:D:13:LEU:HD21	2:D:17:GLY:HA2	1.97	0.47
2:F:336:LYS:HG3	2:F:372:ALA:HB1	1.95	0.47
1:G:73:GLY:O	1:G:77:GLU:HG3	2.13	0.47
1:O:263:ARG:NH2	3:U:5:DC:O2	2.30	0.47
2:T:268:PRO:HB2	2:T:269:TRP:CE3	2.50	0.47
1:A:247:LEU:HD11	1:A:329:LEU:HD22	1.97	0.47
1:C:185:LEU:HD11	1:C:215:CYS:SG	2.54	0.47
2:D:10:PRO:HG3	2:D:461:SER:HA	1.96	0.47
1:G:185:LEU:HB3	1:G:241:ILE:HG13	1.97	0.47
1:G:371:ASN:O	1:G:375:THR:OG1	2.28	0.47
2:B:202:TYR:HB2	2:B:209:GLN:HE21	1.80	0.47
1:A:188:HIS:O	1:A:213:TYR:HA	2.15	0.47
2:F:493:SER:OG	2:F:495:ASP:OD2	2.32	0.47
2:F:248:ILE:O	2:F:251:HIS:N	2.47	0.47
1:G:28:LEU:HD13	1:G:132:LEU:HD21	1.96	0.47
1:O:277:MET:HG2	1:0:293:TYR:CG	2.50	0.47
2:F:287:LYS:NZ	2:F:328:TYR:OH	2.34	0.46
1:O:341:ILE:HB	1:O:361:ARG:HD3	1.96	0.46
1:A:242:PRO:O	1:A:246:ILE:HG22	2.14	0.46
2:B:248:ILE:HD12	2:B:248:ILE:O	2.15	0.46
2:F:203:ASP:O	2:F:209:GLN:NE2	2.48	0.46
2:D:459:ILE:O	2:D:463:THR:HG23	2.16	0.46
2:F:282:GLY:O	2:F:300:ALA:HA	2.15	0.46
1:A:303:ASP:O	1:A:309:MET:HA	2.15	0.46
1:A:411:LYS:NZ	2:B:3:GLU:OE1	2.47	0.46



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		Interatomic	Clash	
Atom-1	Atom-2	distance $(Å)$	overlap (Å)	
1:C:175:TRP:CE2	2:D:394:LEU:HD13	2.50	0.46	
1:C:187:PHE:CE2	1:C:215:CYS:HB2	2.50	0.46	
1:A:108:ILE:O	1:G:54:ARG:NH2	2.49	0.46	
1:A:370:ASN:OD1	1:A:371:ASN:N	2.49	0.46	
1:G:9:HIS:CD2	1:G:18:THR:HG21	2.51	0.46	
2:F:231:TRP:CE2	2:F:245:PHE:HB2	2.51	0.46	
2:T:14:PHE:HZ	2:T:23:ALA:HA	1.81	0.46	
3:E:14:DA:H2"	3:E:15:DC:H5'	1.98	0.46	
2:B:50:LEU:HD22	2:B:93:PHE:CG	2.51	0.46	
2:B:236:ASN:OD1	2:B:236:ASN:N	2.49	0.46	
2:T:119:SER:HB2	2:T:213:ARG:HH22	1.79	0.46	
2:B:151:CYS:HB3	2:B:206:PHE:HB2	1.98	0.46	
1:O:272:ALA:HB1	1:O:393:LEU:HD13	1.97	0.46	
2:T:300:ALA:HB3	2:T:316:GLU:HB3	1.98	0.46	
1:A:149:LYS:HB2	1:A:149:LYS:HE2	1.75	0.46	
1:G:285:TYR:N	1:G:292:ALA:O	2.39	0.46	
1:A:417:ASN:N	1:A:417:ASN:OD1	2.49	0.45	
2:F:278:VAL:HA	2:F:356:GLU:O	2.16	0.45	
1:O:176:LEU:HD21	1:O:381:ILE:HD13	1.98	0.45	
1:O:181:PHE:CD1	1:0:182:PRO:HD2	2.51	0.45	
1:A:9:HIS:CD2	1:A:9:HIS:CD2 1:A:18:THR:HG21		0.45	
1:A:177:SER:HA	1:A:177:SER:HA 1:A:334:VAL:HG12		0.45	
1:C:106:ASP:O	1:O:54:ARG:NH1	2.50	0.45	
1:A:86:LYS:HB2	1:A:86:LYS:HE3	1.75	0.45	
2:F:268:PRO:HB2	2:F:269:TRP:CE3	2.51	0.45	
4:H:8:G:H2'	4:H:9:U:C6	2.51	0.45	
2:B:335:ALA:HB1	2:B:373:PHE:CE1	2.51	0.45	
2:B:416:ARG:NH1	2:B:449:GLU:OE2	2.50	0.45	
1:C:195:PRO:O	1:C:209:ARG:NH1	2.50	0.45	
2:F:427:PRO:HG2	1:G:164:VAL:HG12	1.98	0.45	
1:C:230:THR:HA	1:C:233:TYR:HB3	1.98	0.45	
1:G:182:PRO:HD3	1:G:401:VAL:HG22	1.98	0.45	
2:T:333:LYS:HB2	2:T:333:LYS:HB2 2:T:333:LYS:HE2		0.45	
2:B:144:PRO:HD2	2:B:147:ILE:HG21	1.99	0.45	
1:C:52:VAL:O	1:C:57:THR:HG23	2.16	0.45	
1:0:253:SER:OG	1:O:254:ASN:N	2.50	0.45	
2:T:21:THR:HB	2:T:428:LYS:NZ	2.31	0.45	
2:T:407:ARG:NH1	2:T:422:THR:O	2.47	0.45	
2:F:383:LEU:HD12	2:F:383:LEU:HA	1.86	0.45	
1:G:276:ARG:HD2	1:G:393:LEU:HA	1.99	0.45	
1:O:99:ILE:HG22	1:O:120:PHE:HB2	1.98	0.45	



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		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:F:270:LYS:HB2	2:F:311:THR:HG22	1.99	0.44	
2:F:423:VAL:HG13	2:F:438:PRO:HB2	1.99	0.44	
2:B:57:LEU:HD12	2:B:57:LEU:HA	1.81	0.44	
2:F:104:PHE:O	2:F:107:ASN:ND2	2.50	0.44	
4:H:7:A:H2'	4:H:8:G:H8	1.81	0.44	
1:A:357:GLN:HE21	1:A:357:GLN:HA	1.83	0.44	
1:0:109:ASN:OD1	1:O:109:ASN:N	2.50	0.44	
1:0:331:PRO:HG2	1:O:332:PHE:CD2	2.53	0.44	
1:A:221:TYR:HA	1:A:224:THR:HG23	1.99	0.44	
2:F:5:ILE:HG13	2:F:410:ALA:HB3	1.99	0.44	
1:G:395:MET:N	1:G:395:MET:HE2	2.32	0.44	
2:D:286:LYS:HZ2	2:D:488:GLU:HG2	1.83	0.44	
1:0:174:ASN:HB2	1:O:337:ILE:HD12	1.99	0.44	
1:A:76:LYS:HB3	1:O:110:ILE:HG23	1.99	0.44	
2:B:40:LYS:HE3	2:B:40:LYS:HB2	1.89	0.44	
1:C:243:THR:O	1:C:247:LEU:HG	2.18	0.44	
1:O:283:GLN:HB2	1:O:294:TRP:CE2	2.53	0.44	
2:T:324:LYS:HZ2	2:T:327:GLN:HB2	1.82	0.44	
4:H:12:G:H2'	4:H:13:U:C6	2.52	0.44	
1:C:282:VAL:HG21	1:C:293:TYR:HB3	2.00	0.44	
1:A:175:TRP:NE1	1:A:336:MET:HG3	2.33	0.44	
2:B:4:LEU:HD22	2:B:411:TYR:HB2	1.99	0.44	
2:B:41:SER:O 2:B:91:ILE:HA		2.17	0.44	
2:D:231:TRP:CE2	:D:231:TRP:CE2 2:D:245:PHE:HB2		0.44	
1:G:52:VAL:O	1:G:57:THR:HG23	2.18	0.44	
1:0:91:ASP:OD1	1:O:91:ASP:N	2.46	0.44	
1:O:167:LYS:HE3	1:O:415:SER:HB3	2.00	0.44	
1:C:318:ASN:HB3	1:C:320:HIS:CE1	2.52	0.44	
2:T:336:LYS:O	2:T:340:SER:OG	2.23	0.44	
1:A:52:VAL:O	1:A:57:THR:HG23	2.18	0.43	
1:A:358:HIS:CE1	1:A:362:ARG:HG3	2.53	0.43	
2:D:10:PRO:HG2	2:D:464:LYS:HG3	2.00	0.43	
2:F:231:TRP:CG	2:F:245:PHE:HD2	2.36	0.43	
2:F:346:TYR:CE1	2:F:350:ILE:HG13	2.53	0.43	
1:0:86:LYS:HB2 1:0:86:LYS:HE3		1.77	0.43	
2:T:107:ASN:HD21	2:T:112:LYS:HE3	1.83	0.43	
2:B:117:LEU:CD2	2:B:147:ILE:HD12	2.48	0.43	
2:B:459:ILE:O	2:B:463:THR:HG23	2.18	0.43	
1:O:296:GLU:HB3	1:O:299:LYS:HG2	2.00	0.43	
2:T:50:LEU:HB2	2:T:93:PHE:CE1	2.53 0.43		
2:T:209:GLN:HE21	2:T:213:ARG:HH11	1.67	0.43	



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		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:T:287:LYS:HE2	3:U:11:DA:H5'	2.00	0.43	
2:B:244:ASP:OD1	2:B:246:SER:OG	2.36	0.43	
2:B:465:LEU:HB2	2:B:478:VAL:HG11	2.00	0.43	
1:C:41:LYS:HG3	1:C:45:PHE:CG	2.52	0.43	
2:F:288:VAL:O	2:F:289:GLU:HG2	2.18	0.43	
2:B:303:MET:HE2	2:B:311:THR:HG23	2.00	0.43	
1:C:328:LYS:O	1:C:333:PRO:HA	2.19	0.43	
1:G:4:LYS:HG3	1:G:56:ASP:HB3	1.99	0.43	
1:G:276:ARG:HD2	1:G:393:LEU:HG	2.00	0.43	
2:T:72:ARG:HE	2:T:248:ILE:HG22	1.84	0.43	
3:E:9:DC:H2'	3:E:10:DT:C6	2.53	0.43	
2:B:339:LEU:HD21	2:B:383:LEU:HD21	2.00	0.43	
1:C:211:LYS:HG3	4:L:17:A:H5"	2.01	0.43	
1:C:350:LEU:HD23	1:C:350:LEU:HA	1.80	0.43	
2:F:485:LYS:O	2:F:488:GLU:HG3	2.18	0.43	
1:C:233:TYR:OH	1:C:237:LYS:O	2.26	0.43	
2:F:40:LYS:HE3	2:F:40:LYS:HB2	1.87	0.43	
1:O:299:LYS:N	1:O:299:LYS:HE2	2.34	0.43	
2:T:103:LYS:HB3	2:T:103:LYS:HE2	1.69	0.43	
2:T:233:ASP:OD1	2:T:233:ASP:N	2.51	0.43	
4:I:12:G:H2'	4:I:13:U:C6	2.54	0.43	
2:B:232:ARG:NH2	2:B:249:GLU:OE2	2.50	0.43	
2:B:271:LEU:HB3 2:B:274:VAL:HG23		2.00	0.43	
1:A:304:LYS:HG2	1:A:307:LYS:HA	2.01	0.43	
2:B:242:ILE:HD12	2:B:242:ILE:H	1.84	0.43	
1:C:28:LEU:HD13	1:C:132:LEU:HD21	2.01	0.43	
2:D:121:PHE:O	2:D:125:ILE:HG13	2.18	0.43	
2:D:206:PHE:O	2:D:210:PHE:HB2	2.19	0.43	
1:O:395:MET:HB2	1:O:400:LYS:HA	2.01	0.43	
2:D:12:ILE:H	2:D:12:ILE:HG12	1.69	0.43	
1:O:112:ILE:HG22	1:O:115:LEU:HD12	2.01	0.43	
2:T:128:ALA:HA	2:T:132:GLU:HG3	2.01	0.43	
1:A:174:ASN:OD1	1:A:174:ASN:N	2.52	0.43	
1:A:415:SER:OG	1:A:416:TYR:N	2.51	0.43	
2:B:329:HIS:NE2 2:B:364:ARG:O		2.49	0.43	
2:T:460:LEU:O	2:T:463:THR:OG1	2.31	0.42	
1:C:387:ASP:OD1	1:C:390:SER:N	2.51	0.42	
2:D:14:PHE:HZ	2:D:23:ALA:HA	1.84	0.42	
2:F:392:LYS:HD2	2:F:392:LYS:HA	1.77	0.42	
1:G:301:GLU:HA	1:G:302:LYS:HA	1.74 0.42		
1:C:106:ASP:HA 1:O:83:LYS:HG2		2.00	0.42	



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		Interatomic	Clash overlap (Å)	
Atom-1	Atom-2	distance (Å)		
2:T:118:VAL:HG11	2:T:209:GLN:HG2	2.01	0.42	
2:B:413:VAL:HG12	2:B:414:ASN:HD22	1.83	0.42	
1:C:101:GLU:HG2	1:C:121:LYS:HB3	2.01	0.42	
2:D:157:LEU:HD23	2:D:162:VAL:HG22	2.01	0.42	
2:F:112:LYS:HB3	2:F:112:LYS:HE2	1.93	0.42	
2:F:397:TYR:CE2	2:F:437:VAL:HG21	2.54	0.42	
2:T:94:LYS:HB3	2:T:94:LYS:HE3	1.77	0.42	
2:B:14:PHE:CZ	2:B:23:ALA:HA	2.52	0.42	
1:C:304:LYS:HG2	1:C:307:LYS:HA	2.01	0.42	
2:D:57:LEU:HD23	2:D:57:LEU:HA	1.87	0.42	
1:A:315:LYS:HD2	1:A:315:LYS:HA	1.82	0.42	
2:D:112:LYS:HB2	2:D:112:LYS:HE3	1.89	0.42	
1:G:190:TYR:C	1:G:192:TRP:H	2.23	0.42	
2:T:157:LEU:HD23	2:T:162:VAL:HG22	2.01	0.42	
4:H:17:A:O2'	4:H:18:U:OP2	2.38	0.42	
2:D:227:SER:OG	2:D:243:ARG:NH1	2.49	0.42	
1:O:187:PHE:CE1	1:O:215:CYS:HB2	2.55	0.42	
1:O:208:VAL:HG22	1:O:215:CYS:HB3	2.02	0.42	
3:E:12:DC:C6	3:E:13:DT:H72	2.54	0.42	
2:B:355:LYS:HB3	2:B:355:LYS:NZ	2.35	0.42	
2:F:51:LYS:HA	2:F:51:LYS:HD3	1.69	0.42	
2:B:231:TRP:CD2	2:B:245:PHE:HB2	2.54	0.41	
2:F:110:THR:HG23 2:F:113:ARG:HH21		1.85	0.41	
2:F:364:ARG:NH1	2:F:444:GLU:OE1	2.52	0.41	
1:G:179:LEU:HD21	1:G:404:SER:HB2	2.02	0.41	
2:B:22:ASP:HB3	2:B:25:ASP:HB2	2.03	0.41	
2:B:231:TRP:CG	2:B:245:PHE:HD2	2.38	0.41	
1:C:418:ILE:HD13	1:C:418:ILE:HA	1.93	0.41	
2:F:296:ASN:ND2	2:F:327:GLN:O	2.51	0.41	
1:G:6:PHE:HB2	1:G:57:THR:HG21	2.02	0.41	
1:G:198:PHE:HA	1:G:209:ARG:NH2	2.34	0.41	
1:A:8:SER:OG	1:A:77:GLU:OE1	2.29	0.41	
1:A:246:ILE:CD1	1:A:261:CYS:HB3	2.50	0.41	
1:A:248:SER:O	1:A:248:SER:OG	2.36	0.41	
2:F:148:TYR:O 2:F:152:ARG:HD3		2.20	0.41	
4:S:5:G:H2'	4:S:6:U:C6	2.55	0.41	
1:A:283:GLN:HB2	1:A:294:TRP:O	2.20	0.41	
2:B:33:LEU:HD23	2:B:33:LEU:HA	1.92	0.41	
2:B:141:VAL:HG21	2:B:210:PHE:CZ	2.55	0.41	
2:D:362:LYS:HG3	2:D:480:LEU:HD22	22 2.02 0.41		
1:G:262:LYS:HZ2 1:G:329:LEU:HD23		1.85	0.41	



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		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:O:51:LYS:HE3	1:O:51:LYS:HB3	1.90	0.41	
1:O:179:LEU:HD23	1:O:179:LEU:H	1.85	0.41	
2:T:149:LYS:HB2	2:T:149:LYS:HE2	1.89	0.41	
2:T:363:THR:O	2:T:387:THR:OG1	2.30	0.41	
4:H:3:A:H2'	4:H:4:G:C8	2.55	0.41	
4:H:13:U:H2'	4:H:14:U:C6	2.55	0.41	
1:C:99:ILE:HG22	1:C:120:PHE:HB2	2.02	0.41	
1:C:331:PRO:HG2	1:C:332:PHE:CE2	2.56	0.41	
1:G:40:ASP:HB3	1:O:92:LYS:HD3	2.02	0.41	
1:O:227:LEU:HD23	1:O:227:LEU:HA	1.91	0.41	
4:I:17:A:H2'	4:I:18:U:C6	2.56	0.41	
1:C:303:ASP:O	1:C:309:MET:HA	2.21	0.41	
1:G:132:LEU:HD23	1:G:132:LEU:HA	1.90	0.41	
1:G:185:LEU:HD23	1:G:241:ILE:HD11	2.02	0.41	
1:0:271:LYS:0	1:O:275:LEU:HG	2.20	0.41	
2:T:251:HIS:NE2	2:T:471:ILE:HG22	2.36	0.41	
2:T:295:ARG:HG2	2:T:323:PRO:HA	2.03	0.41	
2:T:468:ASN:HD22	2:T:485:LYS:HE3	1.86	0.41	
1:A:301:GLU:HA	1:A:302:LYS:HA	1.60	0.41	
1:A:336:MET:SD	1:A:336:MET:N	2.93	0.41	
1:C:152:LEU:HD12 1:C:152:LEU:HA		1.82	0.41	
2:F:152:ARG:HG3 2:F:152:ARG:N		2.34	0.41	
2:F:406:LEU:HD21	06:LEU:HD21 1:G:164:VAL:HG11		0.41	
2:F:422:THR:HG22	2:F:460:LEU:HD12	2.02	0.41	
1:C:332:PHE:O	1:C:332:PHE:O 1:C:334:VAL:HG22		0.41	
2:D:292:LYS:H	2:D:292:LYS:HG2	1.69	0.41	
2:F:15:ALA:HB2	2:F:32:PRO:O	2.20	0.41	
2:F:299:CYS:SG	2:F:319:PRO:HB3	2.61	0.41	
1:G:300:LEU:HB3	1:G:303:ASP:H	1.86	0.41	
2:B:422:THR:HG22	2:B:460:LEU:HD12	2.03	0.41	
1:C:341:ILE:HB	1:C:361:ARG:HD3	2.03	0.41	
2:D:235:LYS:HE3	2:D:235:LYS:HB2	1.89	0.41	
2:F:57:LEU:HA	2:F:57:LEU:HD23	1.85	0.41	
2:F:214:LEU:HD11	2:F:219:ILE:HD12	2.03	0.41	
1:O:277:MET:HG2	1:O:293:TYR:CD2	2.56	0.41	
1:C:129:LYS:HA	1:C:129:LYS:HD3	1.79	0.41	
2:F:347:LYS:NZ	2:F:351:GLY:O	2.54	0.41	
2:F:459:ILE:O	2:F:463:THR:HG23	2.20	0.41	
1:G:3:ASN:OD1	1:G:3:ASN:N	2.53	0.41	
1:O:216:THR:HG21	1:O:223:PHE:CE2	2.56 0.41		
2:T:247:LYS:HB2	2:T:247:LYS:HE3	1.75	0.41	



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		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:211:LYS:HD3	4:I:17:A:H4'	2.02	0.40	
2:B:148:TYR:CG	2:B:225:ARG:HD3	2.56	0.40	
2:D:149:LYS:HE3	2:D:149:LYS:HB3	1.66	0.40	
2:D:398:LYS:HB3	2:D:398:LYS:HE2	1.81	0.40	
2:F:214:LEU:HD12	2:F:214:LEU:HA	1.92	0.40	
2:F:406:LEU:HD13	1:G:416:TYR:CD1	2.56	0.40	
1:G:265:ILE:HD11	1:G:329:LEU:HD21	2.02	0.40	
1:G:317:LYS:HE3	1:G:317:LYS:HB2	1.79	0.40	
2:T:144:PRO:HD2	2:T:147:ILE:HD12	2.03	0.40	
1:A:385:SER:OG	1:A:405:ASN:ND2	2.47	0.40	
2:B:364:ARG:NH2	2:B:444:GLU:OE1	2.54	0.40	
1:C:9:HIS:CE1	1:C:18:THR:HG21	2.57	0.40	
1:G:65:SER:HB2	1:G:100:ASP:HB2	2.03	0.40	
1:C:49:ILE:O	1:C:52:VAL:HG12	2.21	0.40	
1:C:272:ALA:HA	1:C:275:LEU:HD12	2.02	0.40	
1:G:36:ILE:HG13	1:G:37:LEU:HG	2.02	0.40	
1:G:178:ILE:HG21	1:G:181:PHE:CE2	2.56	0.40	
2:B:15:ALA:HB2	2:B:32:PRO:O	2.21	0.40	
2:B:317:VAL:HG12	2:B:490:LEU:HD11	2.03	0.40	
1:O:266:VAL:HG23	1:O:329:LEU:HD23	2.03	0.40	
3:K:14:DA:H2"	3:K:15:DC:H6	1.86	0.40	
1:A:384:LEU:HD23	1:A:384:LEU:HA	1.85	0.40	
2:B:10:PRO:HD3	2:B:460:LEU:HD23	2.03	0.40	
2:B:13:LEU:HD23	2:B:270:LYS:HE2	2.04	0.40	
1:C:34:CYS:HB3	1:C:37:LEU:HG	2.02	0.40	
1:C:46:TRP:CH2	1:C:76:LYS:HG2	2.56	0.40	
1:C:159:LEU:HA	1:C:159:LEU:HD23	1.83	0.40	
2:F:474:ASP:OD1	2:F:474:ASP:N	2.55	0.40	
1:G:321:PHE:CZ	1:G:339:SER:HB3	2.56	0.40	
1:O:283:GLN:HB2	1:0:294:TRP:NE1	2.36	0.40	
2:T:383:LEU:HD23	2:T:383:LEU:HA	1.87	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.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	А	407/452~(90%)	384 (94%)	20~(5%)	3~(1%)	22 57
1	С	410/452~(91%)	387 (94%)	21 (5%)	2~(0%)	29 64
1	G	398/452~(88%)	376 (94%)	19 (5%)	3~(1%)	19 54
1	Ο	410/452~(91%)	391~(95%)	17 (4%)	2~(0%)	29 64
2	В	463/507~(91%)	447 (96%)	16 (4%)	0	100 100
2	D	465/507~(92%)	455~(98%)	10 (2%)	0	100 100
2	F	463/507~(91%)	443 (96%)	20 (4%)	0	100 100
2	Т	465/507~(92%)	449 (97%)	16 (3%)	0	100 100
All	All	3481/3836~(91%)	3332 (96%)	139 (4%)	10 (0%)	44 73

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

All (10) Ramachandran outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	195	PRO
1	С	195	PRO
1	G	195	PRO
1	0	195	PRO
1	G	200	VAL
1	А	309	MET
1	С	309	MET
1	0	309	MET
1	А	200	VAL
1	G	239	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	А	334/414~(81%)	304 (91%)	30~(9%)	9 34
1	\mathbf{C}	344/414~(83%)	323 (94%)	21~(6%)	18 49

Continued on next page...



Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	G	327/414~(79%)	298~(91%)	29 (9%)	9	34
1	Ο	340/414~(82%)	325~(96%)	15 (4%)	28	61
2	В	406/446~(91%)	375~(92%)	31 (8%)	13	41
2	D	410/446~(92%)	386~(94%)	24 (6%)	19	50
2	F	407/446~(91%)	383~(94%)	24~(6%)	19	50
2	Т	410/446~(92%)	389~(95%)	21 (5%)	24	56
All	All	2978/3440 (87%)	2783~(94%)	195 (6%)	21	47

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	16	ASP
1	А	43	VAL
1	А	47	SER
1	А	68	SER
1	А	71	ARG
1	А	87	GLN
1	А	105	TYR
1	А	116	ASN
1	А	160	HIS
1	А	181	PHE
1	А	213	TYR
1	А	215	CYS
1	А	226	HIS
1	А	232	THR
1	А	233	TYR
1	А	236	SER
1	А	247	LEU
1	А	248	SER
1	А	253	SER
1	А	258	ASN
1	А	303	ASP
1	А	309	MET
1	А	327	SER
1	А	336	MET
1	А	355	SER
1	А	357	GLN
1	А	362	ARG
1	А	392	TYR
1	А	403	VAL



Mol	Chain	Res	Type
1	А	417	ASN
2	В	12	ILE
2	В	25	ASP
2	В	35	ASN
2	В	36	LEU
2	В	41	SER
2	В	44	ILE
2	В	60	ILE
2	В	72	ARG
2	В	84	CYS
2	В	88	SER
2	В	119	SER
2	В	145	ASP
2	В	152	ARG
2	В	203	ASP
2	В	205	GLN
2	В	222	GLN
2	В	227	SER
2	В	272	SER
2	В	278	VAL
2	В	279	CYS
2	В	298	CYS
2	В	303	MET
2	В	309	ASP
2	В	347	LYS
2	В	399	THR
2	В	407	ARG
2	В	437	VAL
2	В	461	SER
2	В	478	VAL
2	В	481	ARG
2	В	495	ASP
1	C	8	SER
1	C	68	SER
1	С	78	LEU
1	С	108	ILE
1	С	142	LYS
1	С	143	GLU
1	С	144	VAL
1	С	150	SER
1	С	180	SER
1	С	181	PHE



Mol	Chain	Res	Type
1	С	186	ARG
1	С	215	CYS
1	С	251	TYR
1	С	277	MET
1	С	304	LYS
1	С	313	LYS
1	С	354	SER
1	С	356	VAL
1	С	401	VAL
1	С	408	VAL
1	С	415	SER
2	D	12	ILE
2	D	34	ASN
2	D	41	SER
2	D	85	LYS
2	D	88	SER
2	D	97	THR
2	D	112	LYS
2	D	133	ASP
2	D	152	ARG
2	D	155	SER
2	D	161	MET
2	D	201	ASN
2	D	203	ASP
2	D	205	GLN
2	D	222	GLN
2	D	235	LYS
2	D	305	LEU
2	D	314	LYS
2	D	340	SER
2	D	379	LYS
2	D	383	LEU
2	D	402	ASP
2	D	422	THR
2	D	423	VAL
2	F	13	LEU
2	F	41	SER
2	F	69	SER
2	F	74	MET
2	F	84	CYS
2	F	88	SER
2	F	104	PHE



Mol	Chain	Res	Type
2	F	107	ASN
2	F	111	HIS
2	F	137	ASP
2	F	145	ASP
2	F	216	LYS
2	F	275	ARG
2	F	279	CYS
2	F	295	ARG
2	F	298	CYS
2	F	340	SER
2	F	353	TYR
2	F	355	LYS
2	F	399	THR
2	F	405	ILE
2	F	411	TYR
2	F	439	ASN
2	F	481	ARG
1	G	71	ARG
1	G	116	ASN
1	G	138	GLN
1	G	149	LYS
1	G	151	ASN
1	G	159	LEU
1	G	160	HIS
1	G	168	GLU
1	G	184	GLU
1	G	203	LEU
1	G	209	ARG
1	G	267	GLN
1	G	277	MET
1	G	282	VAL
1	G	283	GLN
1	G	288	SER
1	G	291	THR
1	G	293	TYR
1	G	303	ASP
1	G	304	LYS
1	G	313	LYS
1	G	327	SER
1	G	329	LEU
1	G	335	LEU
1	G	336	MET



Mol	Chain	Res	Type
1	G	354	SER
1	G	391	PHE
1	G	395	MET
1	G	408	VAL
1	0	28	LEU
1	0	66	SER
1	0	91	ASP
1	0	104	SER
1	0	179	LEU
1	0	181	PHE
1	0	210	TYR
1	0	229	LYS
1	0	240	ARG
1	0	251	TYR
1	0	278	LYS
1	0	313	LYS
1	0	371	ASN
1	0	391	PHE
1	0	395	MET
2	Т	1	MET
2	Т	2	LYS
2	Т	13	LEU
2	Т	41	SER
2	Т	44	ILE
2	Т	74	MET
2	Т	89	THR
2	Т	98	ASN
2	Т	149	LYS
2	Т	161	MET
2	Т	205	GLN
2	Т	222	GLN
2	Т	233	ASP
2	Т	246	SER
2	Т	333	LYS
2	Т	339	LEU
2	Т	348	GLU
2	Т	364	ARG
2	Т	389	SER
2	Т	402	ASP
2	Т	478	VAL

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. There are no such side chains identified.



5.3.3	\mathbf{RNA}	í
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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	Н	17/19~(89%)	1 (5%)	0
4	Ι	17/19~(89%)	1 (5%)	0
4	L	17/19~(89%)	1 (5%)	0
4	S	17/19~(89%)	1 (5%)	0
All	All	68/76~(89%)	4(5%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	Н	18	U
4	Ι	18	U
4	L	18	U
4	S	2	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 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 (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-35240. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map



6.1.2 Raw map



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



6.2 Central slices (i)

6.2.1 Primary map



X Index: 150



Y Index: 150



Z Index: 150

6.2.2 Raw map



X Index: 150

Y Index: 150

Z Index: 150

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: 144



Y Index: 171



Z Index: 104

6.3.2 Raw map



X Index: 144

Y Index: 172



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



6.4.2 Raw map



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



6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

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



7 Map analysis (i)

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

7.1 Map-value distribution (i)



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



7.2 Volume estimate (i)



The volume at the recommended contour level is 235 nm^3 ; this corresponds to an approximate mass of 213 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.323 ${\rm \AA^{-1}}$



8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.323 ${\rm \AA}^{-1}$



8.2 Resolution estimates (i)

$\begin{bmatrix} Bosolution ostimato (Å) \end{bmatrix}$	Estim	Estimation criterion (FSC cut-off)		
resolution estimate (A)	0.143	0.5	Half-bit	
Reported by author	3.10	-	-	
Author-provided FSC curve	2.95	3.40	3.03	
Unmasked-calculated*	3.60	4.09	3.70	

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.60 differs from the reported value 3.1 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-35240 and PDB model 8187. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.



9.2 Q-score mapped to coordinate model (i)



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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.16).



9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.



9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score	
All	0.8680	0.5300	
А	0.8300	0.5050	
В	0.9100	0.5620	10
С	0.8170	0.5030	
D	0.9230	0.5690	
Е	0.8430	0.4690	
F	0.8960	0.5540	
G	0.7500	0.4810	
Н	0.8870	0.4850	
Ι	0.9150	0.5210	
J	0.9300	0.5220	
K	0.9260	0.5310	0.0
L	0.9150	0.4760	<0.0
0	0.8270	0.4990	
S	0.8490	0.4800]
Т	0.9320	0.5740	
U	0.9100	0.5130	

