

Feb 26, 2024 – 02:29 PM JST

PDB ID	:	8J7S
EMDB ID	:	EMD-36047
Title	:	Structure of the SPARTA complex
Authors	:	Guo, M.; Zhu, Y.; Lin, Z.; Huang, Z.
Deposited on	:	2023-04-28
Resolution	:	2.84 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.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.84 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	(#Entries)	(#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			
1	А	506	61%	27%	·	10%
1	Е	506	65%	23%		10%
1	Ι	506	5%	28%	·	10%
1	М	506	6 4%	23%	•	10%
2	В	418	69%	29%	,	·
2	F	418	68%	28%		•
2	J	418	<u>38%</u> 69%	26%		5%



Mol	Chain	Length		Quality of chain	
		44.0	31%		
2	N	418	(63% 33%	•
3	С	19	21%	68%	11%
3	G	19	16%	74%	11%
3	Κ	19	37%	47%	16%
3	0	19	21%	58%	21%
4	D	24	33%	50%	17%
4	Н	24	8% 50%	38%	12%
4	L	24	33%	58%	8%
4	Р	24	29% 33%	67%	



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 31812 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	454	Total	С	Ν	Ο	S	0	0
1	Π	404	3634	2362	604	657	11	0	0
1	F	454	Total	С	Ν	Ο	\mathbf{S}	0	0
1	Ľ	404	3636	2363	604	658	11	0	0
1	т	454	Total	С	Ν	Ο	\mathbf{S}	0	0
1	1	404	3633	2362	604	656	11	0	0
1	1 M	454	Total	С	Ν	0	S	0	0
	111	404	3629	2360	602	656	11	0	0

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	В	/18	Total	С	Ν	0	\mathbf{S}	0	0
	D	410	3479	2255	577	635	12	0	0
9	F	/18	Total	С	Ν	0	S	0	0
		410	3475	2250	577	636	12	0	0
0	т	110	Total	С	Ν	0	S	0	0
	J	410	3461	2242	573	634	12	0	0
0	N	/18	Total	С	Ν	0	S	0	0
	IN	410	3472	2251	575	634	12	U	0

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

Mol	Chain	Residues		At	oms			AltConf	Trace
2	C	10	Total	С	Ν	0	Р	0	0
0		19	399	179	66	135	19	0	0
2	C	10	Total	С	Ν	0	Р	0	0
3 G	19	399	179	66	135	19	0	0	
2	K	10	Total	С	Ν	0	Р	0	0
0	Γ	19	399	179	66	135	19	0	0
3	2 0	10	Total	С	Ν	0	Р	0	0
0	0	19	399	179	66	135	19	0	0



• Molecule 4 is a DNA chain called DNA (5'-D(P*TP*AP*AP*TP*AP*GP*AP*TP*TP*AP *GP*AP*GP*CP*CP*GP*TP*CP*AP*AP*TP*AP*GP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Л	20	Total	С	Ν	0	Р	0	0
4	D	20	413	197	79	117	20	0	0
4	Ц	91	Total	С	Ν	0	Р	0	0
4	11	21	433	207	81	124	21	0	0
4	т	<u> </u>	Total	С	Ν	Ο	Р	0	0
4			454	217	86	129	22	0	0
4	D	24	Total	С	Ν	Ο	Р	0	0
4	1	24	497	237	96	140	24	0	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: Piwi domain-containing protein



• Molecule 1: Piwi domain-containing protein







F30.4 F30.4 12 12 13 12 13

• Molecule 2: TIR domain-containing protein



Y416 N417 I418

• Molecule 2: TIR domain-containing protein



BANK





2404 N405 F409 F410 V414 Y415 Y415 Y415 N417

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

Chain C:	21%	68%	11%
0 8 2 8 8 7 9 7 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	010 411 412 013 015 416 416		
• Molecule P*UP*UP*	3: RNA (5'- A)-3')	R(P*UP*GP*AP*CP*GP*GP*CP*UP*CF	P*UP*AP*AP*UP*CP*UP*A
Chain G:	16%	74%	11%
U1 62 65 65 67 63 63 64	U10 A11 A12 U13 C14 U15 U15 U17 U17		
• Molecule P*UP*UP*	3: RNA (5'- A)-3')	R(P*UP*GP*AP*CP*GP*GP*CP*UP*CF	P*UP*AP*AP*UP*CP*UP*A
Chain K:	37%	47%	16%
01 43 05 04 05 04 01 0 01 0 01 0 01 0 01 0 0 0 0 0 0 0	A112 U13 U14 U17 U17 U18 A19		
• Molecule P*UP*UP*	3: RNA (5'- A)-3')	R(P*UP*GP*AP*CP*GP*GP*CP*UP*CI	P*UP*AP*AP*UP*CP*UP*A
Chain O:	% 21%	58%	21%



• Molecule 4: DNA (5'-D(P*TP*AP*AP*TP*AP*GP*AP*TP*TP*AP*GP*AP*GP*CP*CP*G P*TP*CP*AP*AP*TP*AP*GP*A)-3')

Chain D:	33%	50%	17%
18 49 412 412 414 414	115 116 116 221 223 223 223 224 224 224 224 224 225 7 225 7 225 7 225 7 225 7 225 7 225 7 225 7 227 7 227 7 227 7 227 7 227 7 7 7		

• Molecule 4: DNA (5'-D(P*TP*AP*AP*TP*AP*GP*AP*TP*TP*AP*GP*AP*GP*CP*CP*G P*TP*CP*AP*AP*TP*AP*GP*A)-3')

	8%		
Chain H:	50%	38%	12%





• Molecule 4: DNA (5'-D(P*TP*AP*AP*TP*AP*GP*AP*TP*TP*AP*GP*AP*GP*AP*GP*CP*CP*G P*TP*CP*AP*AP*TP*AP*GP*A)-3')

Chain L:	17% 33%		58%	8%
T8 A9 A10 A12 A12 G13 G13 A14	T15 T16 T16 C21 C21 C21 C25 C21 C25	A27 A27 T28 A27 DG DG		

• Molecule 4: DNA (5'-D(P*TP*AP*AP*TP*AP*GP*AP*TP*TP*AP*GP*AP*GP*AP*GP*CP*CP*G P*TP*CP*AP*AP*TP*AP*GP*A)-3')





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	832006	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 $(6k \ge 4k)$	Depositor
Maximum map value	1.551	Depositor
Minimum map value	-0.644	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.286	Depositor
Map size (Å)	430.91998, 430.91998, 430.91998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^{\circ}$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0773, 1.0773, 1.0773	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).

Mal	Mol Chain		Bond lengths		Bond angles	
	Ullaili	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.27	0/3727	0.52	0/5046	
1	Е	0.28	0/3729	0.51	0/5049	
1	Ι	0.26	0/3726	0.49	1/5045~(0.0%)	
1	М	0.28	0/3722	0.52	1/5040~(0.0%)	
2	В	0.26	0/3565	0.51	0/4807	
2	F	0.25	0/3560	0.50	1/4800~(0.0%)	
2	J	0.25	0/3546	0.51	1/4782~(0.0%)	
2	Ν	0.26	0/3558	0.50	0/4799	
3	С	0.28	0/444	0.88	0/688	
3	G	0.28	0/444	0.92	0/688	
3	Κ	0.26	0/444	0.85	0/688	
3	0	0.24	0/444	0.92	1/688~(0.1%)	
4	D	0.52	0/464	0.91	0/714	
4	Н	0.51	0/486	0.91	0/748	
4	L	0.52	0/510	0.91	0/785	
4	Р	0.49	0/559	0.88	0/861	
All	All	0.29	0/32928	0.57	5/45228~(0.0%)	

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	А	0	1
2	F	0	1
2	Ν	0	1
All	All	0	3

There are no bond length outliers.

All (5) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	М	378	PRO	CA-N-CD	-10.15	97.29	111.50
2	J	264	LEU	CA-CB-CG	6.38	129.98	115.30
2	F	264	LEU	CA-CB-CG	6.31	129.81	115.30
1	Ι	501	LEU	CA-CB-CG	6.07	129.25	115.30
3	0	15	U	C2-N1-C1'	5.07	123.78	117.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	307	ASN	Peptide
2	F	302	LYS	Peptide
2	Ν	302	LYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	3634	0	3626	101	0
1	Е	3636	0	3631	83	0
1	Ι	3633	0	3629	113	0
1	М	3629	0	3621	89	0
2	В	3479	0	3461	87	0
2	F	3475	0	3462	80	0
2	J	3461	0	3433	82	0
2	Ν	3472	0	3452	96	0
3	С	399	0	203	12	0
3	G	399	0	203	8	0
3	Κ	399	0	203	9	0
3	0	399	0	203	11	0
4	D	413	0	226	14	0
4	Н	433	0	238	11	0
4	L	454	0	249	19	0
4	Р	497	0	271	13	0
All	All	31812	0	30111	744	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 12.



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:J:187:PHE:O	2:J:238:THR:HA	1.76	0.85
2:N:310:LEU:HD23	2:N:311:VAL:HG13	1.64	0.78
1:M:350:ILE:HG22	1:M:352:GLU:H	1.49	0.75
2:F:260:GLU:O	2:F:264:LEU:HD12	1.88	0.74
2:J:310:LEU:HD23	2:J:311:VAL:HG23	1.68	0.73
2:B:189:GLU:HB2	2:B:237:LYS:HB3	1.70	0.73
1:E:99:GLU:OE1	1:E:99:GLU:N	2.22	0.73
2:B:320:HIS:HE2	2:B:344:THR:HG1	1.34	0.72
1:M:14:PHE:HZ	1:M:23:ALA:HA	1.54	0.72
2:F:280:LYS:HE2	2:F:384:LEU:HD13	1.70	0.72
2:F:112:ILE:HG22	2:F:115:LEU:HD12	1.71	0.72
1:M:303:MET:H	1:M:315:GLY:HA2	1.53	0.72
2:J:246:ILE:HD11	2:J:261:CYS:HB3	1.72	0.71
1:I:312:VAL:HG21	1:I:349:GLN:HE22	1.54	0.70
1:I:24:ARG:NH1	1:I:470:CYS:O	2.24	0.70
3:C:1:U:O2'	3:C:2:G:H5"	1.92	0.70
1:E:302:GLN:HA	1:E:315:GLY:HA2	1.74	0.69
1:I:322:ASN:ND2	1:I:329:HIS:O	2.26	0.69
1:M:399:THR:HA	2:N:374:ARG:HH12	1.56	0.69
2:B:42:GLY:H	2:F:116:ASN:HB3	1.58	0.69
1:A:99:GLU:O	1:A:103:LYS:HD2	1.93	0.69
1:A:307:ASN:OD1	1:A:308:GLY:N	2.26	0.69
2:J:42:GLY:H	2:N:116:ASN:HB3	1.57	0.69
2:F:100:ASP:OD1	2:F:102:GLN:N	2.26	0.68
1:A:504:LYS:NZ	1:E:134:GLU:O	2.26	0.68
1:I:307:ASN:HD22	1:I:310:GLY:H	1.40	0.68
2:J:261:CYS:O	2:J:265:ILE:HD12	1.93	0.68
2:F:108:ILE:HG23	2:F:113:VAL:HG22	1.74	0.68
2:B:181:PHE:HD1	2:B:182:PRO:HD2	1.59	0.68
1:E:343:LEU:HB3	1:E:353:TYR:HE1	1.60	0.67
1:I:78:PHE:HE1	1:I:84:CYS:HB2	1.58	0.67
1:A:54:ARG:NH1	1:A:88:SER:OG	2.26	0.67
2:B:307:LYS:HE2	2:B:307:LYS:HA	1.76	0.67
2:J:243:THR:HA	2:J:246:ILE:HG22	1.76	0.66
1:A:57:LEU:O	1:A:61:GLN:NE2	2.28	0.66
2:B:310:LEU:HD23	2:B:311:VAL:HG23	1.77	0.66
1:M:407:ARG:NE	1:M:422:THR:O	2.28	0.66
2:J:41:LYS:HD2	2:N:118:ILE:HG12	1.78	0.66
2:J:294:TRP:HB3	2:J:322:ALA:HB2	1.77	0.66
2:N:362:ARG:HH12	3:O:7:C:H1'	1.61	0.66

All (744) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



	lo de page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:N:280:LYS:HG2	2:N:384:LEU:HD21	1.78	0.66
2:J:263:ARG:NH2	4:L:12:DA:N3	2.44	0.66
1:M:399:THR:HA	2:N:374:ARG:NH1	2.11	0.66
1:A:222:GLN:NE2	3:C:1:U:O2	2.29	0.65
1:E:87:GLU:N	1:E:87:GLU:OE1	2.29	0.65
1:I:364:ARG:NH1	4:L:16:DT:OP2	2.30	0.65
1:A:51:LYS:HE2	1:A:51:LYS:HA	1.77	0.65
4:D:15:DT:H2"	4:D:16:DT:H5"	1.78	0.65
2:B:101:GLU:HG2	2:B:121:LYS:HB3	1.78	0.65
1:I:13:LEU:HD23	1:I:272:SER:HA	1.79	0.65
1:A:305:LEU:HD13	1:A:350:ILE:HD11	1.78	0.64
1:A:13:LEU:HD23	1:A:270:LYS:HE3	1.78	0.64
1:A:502:ALA:HB2	1:E:131:ASN:HA	1.79	0.64
1:E:5:ILE:HD12	1:E:453:LYS:HE2	1.80	0.64
1:I:420:LEU:HB2	1:I:456:LEU:HD22	1.80	0.64
1:E:107:ASN:OD1	1:E:108:SER:N	2.30	0.64
2:F:175:TRP:NE1	2:F:336:MET:SD	2.70	0.64
1:A:242:ILE:HD12	1:A:242:ILE:H	1.62	0.64
2:B:42:GLY:HA2	2:F:116:ASN:H	1.61	0.63
2:B:276:ARG:NH1	2:B:392:TYR:O	2.31	0.63
1:I:54:ARG:NE	1:I:88:SER:OG	2.28	0.63
2:B:257:ARG:NH1	2:B:257:ARG:HA	2.13	0.63
2:F:294:TRP:HB3	2:F:322:ALA:HB2	1.81	0.63
1:I:72:ARG:NH1	4:L:25:DC:OP1	2.31	0.63
1:A:210:PHE:HE1	1:A:221:THR:HG21	1.62	0.63
1:I:271:LEU:HD11	1:I:465:LEU:HD11	1.81	0.63
1:M:358:PHE:HZ	1:M:455:VAL:HG22	1.64	0.63
2:F:154:TYR:HA	2:F:158:PHE:HD2	1.64	0.63
1:I:502:ALA:HB2	1:M:131:ASN:HA	1.80	0.63
1:E:397:TYR:HE2	2:F:373:TRP:HB3	1.64	0.63
1:I:399:THR:HA	2:J:374:ARG:HH12	1.62	0.63
1:A:474:ASP:OD2	1:A:481:ARG:NH1	2.29	0.63
2:B:183:GLU:N	2:B:183:GLU:OE2	2.32	0.63
1:E:14:PHE:HZ	1:E:23:ALA:HA	1.64	0.63
2:B:201:ARG:HH12	4:D:11:DT:H4'	1.62	0.62
2:F:415:SER:OG	2:F:416:TYR:N	2.32	0.62
2:N:208:VAL:HB	2:N:215:CYS:HB3	1.80	0.62
1:I:109:SER:HB3	1:I:112:LYS:HG2	1.81	0.62
2:B:362:ARG:HD2	3:C:6:G:H21	1.63	0.62
1:A:33:LEU:HD11	1:A:270:LYS:HE2	1.81	0.62
1:I:414:ASN:ND2	2:J:330:TYR:OH	2.33	0.62



	lo uo puge	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:A:322:ASN:ND2	1:A:329:HIS:O	2.32	0.62
2:J:387:ASP:OD1	2:J:387:ASP:N	2.32	0.62
1:I:302:GLN:HA	1:I:315:GLY:HA2	1.81	0.62
1:A:449:GLU:N	1:A:449:GLU:OE1	2.33	0.61
2:J:198:PHE:O	2:J:209:ARG:NH2	2.33	0.61
2:J:246:ILE:O	2:J:262:LYS:NZ	2.33	0.61
2:B:165:ILE:HD12	2:B:416:TYR:HA	1.82	0.61
2:F:79:ALA:HB2	2:N:114:ARG:HH11	1.66	0.61
2:F:181:PHE:HZ	2:F:244:GLU:HG3	1.66	0.61
2:F:276:ARG:NH1	2:F:392:TYR:O	2.33	0.61
2:J:175:TRP:HB3	2:J:334:VAL:HG11	1.81	0.61
1:M:378:PRO:HA	1:M:379:LYS:HE2	1.83	0.61
4:P:28:DT:H2"	4:P:29:DA:C8	2.35	0.61
1:I:222:GLN:NE2	3:K:1:U:O2	2.34	0.61
1:A:496:ILE:C	1:A:497:LYS:HE2	2.21	0.61
2:B:201:ARG:NH2	4:D:12:DA:OP1	2.34	0.61
1:A:135:ASN:ND2	1:E:137:ASP:OD1	2.34	0.61
2:B:41:LYS:HD3	2:F:118:ILE:HG12	1.82	0.60
4:L:11:DT:H2"	4:L:12:DA:C8	2.36	0.60
2:B:400:LYS:HE3	2:B:400:LYS:HA	1.82	0.60
2:F:106:ASP:O	2:J:54:ARG:NH1	2.34	0.60
2:N:187:PHE:HB2	2:N:239:ILE:HG23	1.83	0.60
1:A:72:ARG:NH2	4:D:25:DC:OP1	2.34	0.60
2:J:129:LYS:HG3	2:J:158:PHE:HD1	1.67	0.60
1:E:476:GLU:OE2	1:E:481:ARG:NH2	2.35	0.60
1:M:476:GLU:OE1	1:M:481:ARG:NH2	2.35	0.60
1:M:469:ALA:HB2	3:O:3:A:H4'	1.84	0.60
1:E:305:LEU:HD23	1:E:305:LEU:H	1.67	0.60
1:A:137:ASP:OD1	1:E:135:ASN:ND2	2.35	0.59
2:N:188:HIS:O	2:N:213:TYR:HA	2.01	0.59
1:A:113:ARG:NH2	1:A:150:TYR:O	2.35	0.59
1:A:497:LYS:HE2	1:A:497:LYS:N	2.16	0.59
2:J:221:TYR:OH	2:J:233:TYR:O	2.17	0.59
2:N:194:LEU:HD13	2:N:195:PRO:HD2	1.84	0.59
1:A:44:ILE:HD11	1:A:139:TRP:HE3	1.67	0.59
2:J:261:CYS:HA	2:J:264:LEU:HD23	1.84	0.59
2:B:257:ARG:NH2	2:B:258:ASN:OD1	2.35	0.59
2:F:313:LYS:NZ	2:F:314:GLN:O	2.36	0.59
2:F:173:SER:OG	2:F:174:ASN:N	2.32	0.59
2:N:305:PHE:HE2	2:N:383:TYR:HD1	1.50	0.59
2:J:318:ASN:OD1	2:J:318:ASN:N	2.35	0.59



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:N:45:PHE:O	2:N:49:ILE:N	2.31	0.59
1:E:270:LYS:HB2	1:E:311:THR:HB	1.84	0.59
1:I:324:LYS:NZ	1:I:331:GLU:OE2	2.34	0.59
1:E:495:ASP:OD1	1:E:495:ASP:N	2.36	0.58
1:I:368:GLN:OE1	1:I:368:GLN:N	2.34	0.58
1:M:427:PRO:O	1:M:430:GLN:NE2	2.36	0.58
1:E:307:ASN:HB3	1:E:310:GLY:N	2.17	0.58
1:E:322:ASN:ND2	1:E:329:HIS:O	2.35	0.58
1:M:324:LYS:HD3	1:M:324:LYS:H	1.67	0.58
1:I:20:CYS:SG	1:I:21:THR:N	2.77	0.58
2:N:393:LEU:HB2	2:N:401:VAL:HG23	1.85	0.58
4:H:16:DT:H2'	4:H:17:DA:H8	1.69	0.58
1:E:9:GLU:OE2	1:E:407:ARG:NH1	2.34	0.58
1:E:6:TYR:HB2	2:F:414:VAL:HG21	1.86	0.58
4:D:11:DT:H2'	4:D:12:DA:C8	2.38	0.57
2:B:351:ILE:HB	2:B:357:GLN:HE21	1.70	0.57
1:M:317:VAL:HG22	1:M:318:GLY:H	1.70	0.57
2:N:323:ILE:HG23	2:N:337:ILE:HD11	1.86	0.57
1:I:231:TRP:NE1	1:I:249:GLU:OE1	2.37	0.57
1:A:34:ASN:HD21	1:A:266:GLY:HA2	1.70	0.57
1:A:420:LEU:HB2	1:A:456:LEU:HD22	1.87	0.57
1:E:463:THR:OG1	1:E:474:ASP:O	2.22	0.57
1:I:24:ARG:HH22	1:I:251:HIS:HD2	1.51	0.57
2:N:276:ARG:NH1	2:N:392:TYR:O	2.37	0.57
1:E:364:ARG:HH21	4:H:15:DT:H5"	1.70	0.57
2:B:186:ARG:NH1	2:B:217:PHE:O	2.38	0.56
2:B:193:MET:HG2	2:B:230:THR:HG22	1.86	0.56
1:I:14:PHE:CE2	1:I:26:GLY:HA3	2.40	0.56
1:I:118:VAL:O	1:I:122:ILE:HG12	2.05	0.56
1:M:464:LYS:NZ	1:M:472:PHE:O	2.31	0.56
1:I:307:ASN:HB3	1:I:310:GLY:N	2.20	0.56
2:N:318:ASN:OD1	2:N:320:HIS:CE1	2.58	0.56
2:J:281:GLU:OE2	2:J:383:TYR:OH	2.21	0.56
1:M:263:LYS:NZ	3:O:1:U:O4	2.36	0.56
2:B:174:ASN:ND2	2:B:337:ILE:O	2.34	0.56
2:B:199:ASP:OD1	2:B:200:VAL:N	2.39	0.56
2:F:181:PHE:HE2	2:F:243:THR:HB	1.70	0.56
2:J:271:LYS:HA	2:J:274:GLU:OE2	2.05	0.56
2:B:257:ARG:HA	2:B:257:ARG:HH11	1.69	0.56
1:E:110:THR:HA	1:E:113:ARG:HE	1.71	0.56
1:M:255:THR:HG22	1:M:470:CYS:H	1.70	0.56



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:I:121:PHE:HB3	1:I:210:PHE:HE1	1.71	0.56
2:N:314:GLN:NE2	2:N:317:LYS:H	2.03	0.56
2:B:198:PHE:O	2:B:209:ARG:NH1	2.37	0.56
1:A:222:GLN:OE1	1:A:263:LYS:NZ	2.30	0.55
2:B:187:PHE:O	2:B:238:THR:HA	2.06	0.55
2:B:393:LEU:HB2	2:B:401:VAL:HG23	1.87	0.55
2:J:277:MET:SD	2:J:277:MET:N	2.79	0.55
1:I:388:ILE:HG12	1:I:443:ILE:HG13	1.88	0.55
1:I:251:HIS:O	1:I:254:TRP:HB2	2.05	0.55
1:M:117:LEU:HA	1:M:120:LEU:HD23	1.88	0.55
1:A:15:ALA:O	1:A:16:HIS:ND1	2.39	0.55
2:N:256:ILE:HD11	2:N:260:GLU:HB3	1.88	0.55
1:E:117:LEU:HD21	1:E:147:ILE:HG12	1.88	0.55
1:I:317:VAL:HG13	1:I:486:ILE:HD12	1.89	0.55
3:K:12:A:H2'	3:K:13:U:C6	2.42	0.55
2:N:289:ASN:OD1	2:N:289:ASN:N	2.40	0.55
2:N:322:ALA:O	2:N:323:ILE:HD13	2.06	0.55
1:A:55:ASP:OD1	1:A:56:TYR:N	2.40	0.55
1:A:407:ARG:NE	1:A:422:THR:O	2.40	0.55
2:B:314:GLN:HE22	2:B:317:LYS:HG3	1.72	0.55
1:I:117:LEU:O	1:I:120:LEU:HD23	2.08	0.55
1:M:121:PHE:O	1:M:125:ILE:HG13	2.06	0.55
1:M:396:LEU:HD23	1:M:405:ILE:HD12	1.89	0.55
2:N:311:VAL:HG12	2:N:321:PHE:H	1.72	0.55
4:L:16:DT:H2'	4:L:17:DA:H8	1.70	0.54
1:E:4:LEU:N	2:F:411:LYS:O	2.38	0.54
1:M:9:GLU:OE2	1:M:407:ARG:NH1	2.32	0.54
2:N:385:SER:HA	2:N:391:PHE:HB3	1.90	0.54
3:O:12:A:H2'	3:O:13:U:C6	2.43	0.54
2:B:112:ILE:HG22	2:B:115:LEU:HD12	1.90	0.54
1:I:61:GLN:NE2	1:I:86:TRP:O	2.41	0.54
1:M:117:LEU:HD13	1:M:147:ILE:HG23	1.88	0.54
1:A:401:GLY:HA2	2:B:371:ASN:HB3	1.90	0.54
1:E:317:VAL:HG22	1:E:318:GLY:H	1.72	0.54
1:E:482:PHE:O	1:E:486:ILE:HG23	2.07	0.54
1:I:13:LEU:HD21	1:I:270:LYS:HE3	1.90	0.54
2:F:181:PHE:CZ	2:F:244:GLU:HG3	2.43	0.54
1:M:427:PRO:HG2	1:M:428:LYS:HE2	1.88	0.54
1:M:482:PHE:O	1:M:486:ILE:HG23	2.08	0.54
2:N:154:TYR:HA	2:N:158:PHE:HD2	1.72	0.54
2:B:262:LYS:O	2:B:266:VAL:HG23	2.08	0.53



	lous page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:F:170:ILE:O	2:F:170:ILE:HD12	2.08	0.53
2:N:167:LYS:HE2	2:N:415:SER:HB3	1.89	0.53
2:F:26:ILE:HD13	2:F:153:LEU:HD13	1.90	0.53
2:B:28:LEU:HD11	2:B:157:ILE:HD11	1.90	0.53
1:E:333:LYS:HE2	1:E:333:LYS:H	1.74	0.53
1:M:13:LEU:HD23	1:M:270:LYS:HE3	1.91	0.53
3:O:13:U:H2'	3:O:14:C:C6	2.43	0.53
1:I:275:ARG:NH1	1:I:458:ASP:OD1	2.41	0.53
1:I:307:ASN:ND2	1:I:309:ASP:H	2.07	0.53
1:I:398:LYS:O	2:J:374:ARG:NH2	2.41	0.53
1:M:110:THR:HG23	1:M:113:ARG:HH21	1.72	0.53
2:N:108:ILE:HG23	2:N:113:VAL:HG23	1.91	0.53
2:N:182:PRO:HG2	2:N:399:GLU:OE1	2.09	0.53
1:E:97:THR:HG23	1:E:100:ASP:H	1.74	0.53
2:F:328:LYS:O	2:F:333:PRO:HA	2.09	0.53
2:J:279:ASP:OD1	2:J:279:ASP:N	2.41	0.53
1:M:29:LEU:HD21	2:N:23:LEU:HD13	1.90	0.53
1:M:54:ARG:NH1	1:M:88:SER:O	2.41	0.53
2:N:221:TYR:OH	2:N:233:TYR:O	2.20	0.53
1:M:358:PHE:CZ	1:M:455:VAL:HG22	2.43	0.53
2:B:320:HIS:NE2	2:B:344:THR:OG1	2.34	0.53
1:E:469:ALA:HB2	3:G:3:A:H4'	1.89	0.53
1:E:307:ASN:OD1	1:E:308:GLY:N	2.42	0.53
1:I:476:GLU:OE2	1:I:481:ARG:NH2	2.40	0.53
2:J:217:PHE:HD2	2:J:395:MET:HE3	1.74	0.53
1:A:406:LEU:HA	1:A:425:TYR:HB3	1.90	0.52
1:E:373:PHE:O	1:E:377:THR:OG1	2.25	0.52
2:J:240:ARG:NH1	2:J:240:ARG:HB2	2.23	0.52
2:N:206:PRO:HG3	2:N:275:LEU:HD12	1.90	0.52
1:A:41:SER:OG	1:A:86:TRP:NE1	2.39	0.52
2:B:314:GLN:NE2	2:B:317:LYS:HG3	2.24	0.52
1:I:307:ASN:HB3	1:I:310:GLY:H	1.74	0.52
1:I:377:THR:OG1	1:I:381:THR:OG1	2.28	0.52
1:M:277:GLY:O	1:M:355:LYS:N	2.41	0.52
1:M:371:ASP:O	1:M:375:GLU:HG3	2.09	0.52
1:A:413:VAL:HG12	1:A:414:ASN:HD22	1.75	0.52
2:F:169:GLU:HG3	2:F:415:SER:HB2	1.91	0.52
2:F:178:ILE:HD11	2:F:401:VAL:HB	1.91	0.52
1:I:413:VAL:HG12	1:I:414:ASN:HD22	1.73	0.52
2:J:287:MET:HG3	2:J:290:LYS:HZ3	1.75	0.52
1:A:20:CYS:SG	1:A:21:THR:N	2.83	0.52



	bus page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:396:GLY:O	2:B:400:LYS:NZ	2.40	0.52
2:F:359:SER:OG	2:F:363:ARG:NH2	2.43	0.52
1:A:277:GLY:HA3	1:A:355:LYS:HE3	1.91	0.52
2:B:85:LYS:O	2:B:89:LYS:N	2.41	0.52
1:M:208:ASP:HB2	1:M:492:ALA:HB2	1.92	0.52
4:P:17:DA:H2'	4:P:18:DG:H8	1.75	0.52
3:C:12:A:H2'	3:C:13:U:C6	2.44	0.51
1:E:297:ALA:HB3	1:E:322:ASN:HB3	1.92	0.51
4:H:16:DT:H2'	4:H:17:DA:C8	2.45	0.51
1:I:275:ARG:NH2	1:I:458:ASP:OD2	2.42	0.51
1:E:54:ARG:HH11	1:E:88:SER:HG	1.56	0.51
1:I:353:TYR:HD1	1:I:354:PRO:HD2	1.76	0.51
2:B:172:ASP:OD1	2:B:172:ASP:N	2.40	0.51
2:F:198:PHE:CZ	2:F:203:LEU:HD11	2.45	0.51
1:I:402:ASP:HB2	2:J:369:TRP:CE3	2.45	0.51
2:J:200:VAL:HA	2:J:203:LEU:HD13	1.91	0.51
1:A:247:LYS:HE2	4:D:25:DC:H1'	1.92	0.51
2:N:307:LYS:HE2	2:N:307:LYS:HA	1.93	0.51
1:A:29:LEU:HD11	2:B:157:ILE:HG22	1.93	0.51
2:B:68:SER:OG	2:B:68:SER:O	2.29	0.51
2:F:155:GLN:HA	2:F:159:LEU:HD12	1.92	0.51
1:M:399:THR:OG1	2:N:170:ILE:O	2.26	0.51
1:I:277:GLY:HA3	1:I:355:LYS:HE3	1.91	0.51
1:E:56:TYR:O	1:E:60:ILE:HG23	2.11	0.51
4:H:12:DA:H2"	4:H:13:DG:C8	2.46	0.51
1:I:57:LEU:O	1:I:61:GLN:HG2	2.11	0.51
2:J:85:LYS:O	2:J:89:LYS:N	2.43	0.51
2:J:194:LEU:HD12	2:J:195:PRO:HD2	1.93	0.51
3:G:13:U:H2'	3:G:14:C:C6	2.46	0.51
2:F:339:SER:HB2	2:F:373:TRP:HE1	1.75	0.51
2:N:328:LYS:HG2	2:N:330:TYR:H	1.76	0.51
2:B:54:ARG:NH2	2:J:107:ASP:OD1	2.39	0.50
1:I:374:LEU:HA	1:I:377:THR:HG22	1.93	0.50
2:B:183:GLU:HG2	2:B:184:GLU:HG3	1.93	0.50
1:E:390:LYS:NZ	3:G:6:G:OP1	2.39	0.50
4:L:28:DT:H1'	4:L:29:DA:C4	2.47	0.50
4:D:12:DA:H2'	4:D:13:DG:C8	2.46	0.50
1:E:377:THR:HG21	1:E:383:LEU:HD12	1.94	0.50
4:P:9:DA:H2"	4:P:10:DA:C8	2.46	0.50
1:A:40:LYS:NZ	1:A:137:ASP:OD2	2.45	0.50
1:A:303:MET:H	1:A:315:GLY:HA2	1.77	0.50



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:F:181:PHE:CE2	2:F:243:THR:HB	2.46	0.50
1:A:107:ASN:HD21	1:A:113:ARG:HB3	1.77	0.50
1:A:303:MET:HE3	1:A:305:LEU:HD23	1.93	0.50
1:A:273:ASP:OD1	1:A:273:ASP:N	2.45	0.50
2:F:330:TYR:CD1	2:F:331:PRO:HA	2.47	0.50
4:L:12:DA:H2'	4:L:13:DG:C8	2.47	0.50
4:P:9:DA:H2"	4:P:10:DA:H8	1.76	0.50
2:F:341:ILE:HB	2:F:361:ARG:HD3	1.94	0.50
2:J:313:LYS:HD2	2:J:314:GLN:HG3	1.94	0.50
2:N:227:LEU:O	2:N:230:THR:OG1	2.29	0.50
2:B:187:PHE:HB2	2:B:239:ILE:HG13	1.95	0.49
2:B:216:THR:HG21	2:B:223:PHE:HZ	1.77	0.49
1:E:54:ARG:NH1	1:E:88:SER:OG	2.36	0.49
2:F:191:ASN:OD1	2:F:191:ASN:N	2.44	0.49
4:L:17:DA:H2'	4:L:18:DG:H8	1.77	0.49
1:A:109:SER:HB3	1:A:112:LYS:HG2	1.94	0.49
1:A:118:VAL:O	1:A:122:ILE:HG23	2.11	0.49
2:F:167:LYS:NZ	2:F:169:GLU:OE2	2.45	0.49
1:A:7:ILE:HD13	1:A:460:LEU:HD12	1.94	0.49
2:B:206:PRO:HB3	2:B:271:LYS:HG2	1.95	0.49
2:J:324:SER:HB2	2:J:340:HIS:CE1	2.47	0.49
1:A:54:ARG:NH1	1:A:88:SER:O	2.45	0.49
2:F:314:GLN:HG2	2:F:315:LYS:H	1.76	0.49
2:J:101:GLU:HG3	2:J:121:LYS:HB3	1.95	0.49
1:I:44:ILE:HD12	1:I:125:ILE:HG12	1.95	0.49
2:B:285:TYR:HB3	2:B:342:PHE:HE2	1.76	0.49
1:E:425:TYR:HA	1:E:432:ALA:HA	1.95	0.49
2:F:109:ASN:O	2:F:113:VAL:HG23	2.12	0.49
1:M:50:LEU:HD21	1:M:91:ILE:HG21	1.94	0.49
1:A:36:LEU:HB2	1:A:84:CYS:SG	2.53	0.49
1:A:41:SER:O	1:A:91:ILE:HA	2.12	0.49
2:F:201:ARG:NH1	4:H:12:DA:OP2	2.46	0.49
2:B:136:GLU:OE1	2:B:154:TYR:OH	2.30	0.49
3:G:12:A:H2'	3:G:13:U:C6	2.48	0.49
1:I:24:ARG:HH22	1:I:251:HIS:CD2	2.28	0.49
2:N:189:GLU:N	2:N:233:TYR:OH	2.42	0.49
1:A:317:VAL:HG12	1:A:318:GLY:N	2.28	0.48
2:B:49:ILE:HG13	2:B:50:GLU:N	2.28	0.48
2:B:176:LEU:HD11	2:B:381:ILE:HD11	1.94	0.48
2:B:201:ARG:NH1	4:D:11:DT:H4'	2.27	0.48
1:M:143:VAL:HB	1:M:147:ILE:HD12	1.95	0.48



	bus puge	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	(\dot{A})
1.M.319.PRO.HD3	1·M·490·LEU·HD13	1.95	0.48
1:A:148:TYB:O	1:A:152:ABG:NH1	2.46	0.48
1:E:55:ASP:OD1	1:E:56:TYB:N	2.45	0.48
1:A:317:VAL:HG12	1:A:318:GLY:H	1.77	0.48
1:A:346:TYR:CD1	1:A:350:ILE:HD13	2.48	0.48
1:M:363:THR:O	1:M:387:THR:OG1	2.25	0.48
1:A:263:LYS:HZ3	3:C:1:U:H3	1.61	0.48
1:A:306:ASP:O	1:A:307:ASN:HB2	2.13	0.48
3:G:4:C:H2'	3:G:5:G:C8	2.48	0.48
1:I:36:LEU:HB2	1:I:84:CYS:SG	2.54	0.48
1:I:122:ILE:HG22	1:I:214:LEU:HG	1.96	0.48
1:I:297:ALA:HB3	1:I:322:ASN:HB3	1.94	0.48
1:I:303:MET:H	1:I:315:GLY:HA2	1.79	0.48
1:M:144:PRO:HD2	1:M:147:ILE:HD11	1.93	0.48
2:N:4:LYS:HE2	2:N:4:LYS:HB2	1.56	0.48
2:N:341:ILE:HB	2:N:361:ARG:HD3	1.96	0.48
2:N:389:THR:O	2:N:389:THR:OG1	2.29	0.48
2:N:148:SER:O	2:N:152:LEU:HG	2.13	0.48
1:I:78:PHE:CE1	1:I:84:CYS:HB2	2.45	0.48
1:M:43:VAL:HG13	1:M:142:ILE:HD13	1.96	0.48
1:M:211:LYS:HB2	1:M:489:ILE:HD12	1.96	0.48
1:A:14:PHE:CE2	1:A:26:GLY:HA3	2.48	0.48
1:A:223:ILE:O	3:C:1:U:O2'	2.26	0.48
2:B:258:ASN:O	2:B:262:LYS:HG3	2.13	0.48
1:E:6:TYR:HE1	1:E:406:LEU:HD21	1.79	0.48
2:B:276:ARG:HB3	2:B:277:MET:HE2	1.96	0.48
1:E:96:VAL:HG22	1:E:124:LYS:HD2	1.95	0.48
1:I:131:ASN:HB3	1:M:501:LEU:HB2	1.96	0.48
1:I:317:VAL:HG21	1:I:501:LEU:HA	1.96	0.48
1:M:306:ASP:O	1:M:312:VAL:N	2.41	0.48
3:O:4:C:H2'	3:O:5:G:C8	2.49	0.47
1:A:97:THR:HB	1:A:99:GLU:HG2	1.96	0.47
1:A:384:VAL:HG21	1:A:450:ALA:HB2	1.96	0.47
3:C:13:U:H2'	3:C:14:C:C6	2.49	0.47
1:I:350:ILE:HG22	1:I:352:GLU:H	1.79	0.47
1:I:405:ILE:HD12	1:I:406:LEU:H	1.78	0.47
3:C:7:C:H2'	3:C:8:U:C6	2.50	0.47
1:E:29:LEU:HD11	2:F:23:LEU:HD13	1.95	0.47
2:F:92:LYS:HE2	2:F:92:LYS:HB2	1.75	0.47
1:I:22:ASP:OD1	1:I:23:ALA:N	2.45	0.47
2:N:59:LYS:HB2	2:N:59:LYS:HE2	1.67	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:343:LEU:HD12	1:A:353:TYR:CD2	2.50	0.47
2:B:193:MET:HA	2:B:229:LYS:HZ2	1.80	0.47
1:M:109:SER:HB3	1:M:112:LYS:HB2	1.96	0.47
1:E:306:ASP:O	1:E:307:ASN:HB2	2.14	0.47
1:M:500:PRO:O	1:M:501:LEU:HB2	2.15	0.47
2:N:221:TYR:HE2	2:N:235:LYS:HE2	1.79	0.47
4:H:17:DA:H2'	4:H:18:DG:H8	1.80	0.47
1:I:307:ASN:HB2	1:I:312:VAL:HG23	1.96	0.47
2:J:143:GLU:HG3	2:J:144:VAL:H	1.80	0.47
2:J:287:MET:HG3	2:J:290:LYS:NZ	2.30	0.47
1:A:112:LYS:NZ	1:A:116:ASP:OD2	2.48	0.47
1:A:495:ASP:OD1	1:A:495:ASP:N	2.47	0.47
1:E:15:ALA:O	1:E:16:HIS:ND1	2.48	0.47
2:F:413:ASN:OD1	2:F:413:ASN:N	2.48	0.47
2:N:2:ARG:NH2	2:N:54:ARG:O	2.48	0.47
4:D:10:DA:H2'	4:D:11:DT:H6	1.80	0.47
2:F:9:HIS:CG	2:F:18:THR:HG21	2.50	0.47
1:M:14:PHE:CE2	1:M:26:GLY:HA3	2.50	0.47
1:A:315:GLY:O	1:A:317:VAL:HG23	2.15	0.47
2:B:53:ILE:HA	2:B:57:THR:OG1	2.14	0.47
2:N:31:GLU:N	2:N:31:GLU:OE1	2.48	0.47
2:N:174:ASN:O	2:N:337:ILE:HG22	2.15	0.47
1:E:277:GLY:O	1:E:355:LYS:N	2.40	0.47
1:E:339:LEU:HD12	1:E:339:LEU:HA	1.81	0.47
1:E:379:LYS:HA	1:E:379:LYS:HD3	1.70	0.47
1:I:306:ASP:O	1:I:312:VAL:N	2.37	0.47
2:J:343:PHE:O	2:J:357:GLN:NE2	2.47	0.47
1:M:324:LYS:HE2	1:M:327:GLN:HG2	1.97	0.47
2:N:102:GLN:CD	2:N:102:GLN:H	2.17	0.47
1:I:210:PHE:HE2	1:I:221:THR:HG21	1.80	0.46
1:I:474:ASP:OD1	1:I:475:GLY:N	2.47	0.46
2:J:360:SER:O	2:J:364:GLN:HB2	2.15	0.46
4:L:9:DA:H8	4:L:9:DA:OP1	1.98	0.46
2:N:133:GLU:OE1	2:N:137:LYS:NZ	2.48	0.46
1:A:372:ALA:O	1:A:376:VAL:HG22	2.15	0.46
1:E:460:LEU:O	1:E:463:THR:HG22	2.15	0.46
3:G:17:U:H2'	3:G:18:U:C6	2.51	0.46
1:I:79:GLU:CD	1:I:79:GLU:H	2.19	0.46
1:I:288:VAL:HG22	1:I:296:ASN:HB3	1.96	0.46
2:J:172:ASP:OD1	2:J:172:ASP:N	2.46	0.46
2:N:76:LYS:O	2:N:80:VAL:HG23	2.15	0.46



	bus page	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:A:41:SER:HG	1:A:86:TRP:HE1	1.62	0.46
1:I:299:CYS:O	1:I:319:PRO:HA	2.15	0.46
2:N:185:LEU:HD21	2:N:215:CYS:SG	2.56	0.46
4:P:24:DT:OP1	4:P:26:DA:N6	2.49	0.46
1:A:8:GLU:CD	1:A:8:GLU:H	2.19	0.46
4:D:10:DA:H2'	4:D:11:DT:C6	2.51	0.46
2:F:277:MET:SD	2:F:277:MET:N	2.88	0.46
2:N:208:VAL:HG11	2:N:264:LEU:HD22	1.95	0.46
1:A:233:ASP:OD1	1:A:233:ASP:N	2.48	0.46
2:B:134:ALA:HA	2:B:137:LYS:HE2	1.97	0.46
1:I:402:ASP:HB2	2:J:369:TRP:HE3	1.81	0.46
3:O:7:C:H2'	3:O:8:U:C6	2.51	0.46
2:B:35:ASP:N	2:B:35:ASP:OD1	2.48	0.46
1:E:226:GLU:OE1	1:E:226:GLU:N	2.41	0.46
1:I:63:PRO:O	1:I:64:ILE:HD13	2.16	0.46
2:J:175:TRP:CD1	2:J:336:MET:HG3	2.51	0.46
2:F:315:LYS:HD2	2:F:315:LYS:HA	1.63	0.46
2:J:258:ASN:O	2:J:262:LYS:HG2	2.16	0.46
2:N:206:PRO:HB3	2:N:271:LYS:HB3	1.98	0.46
2:N:321:PHE:CE2	2:N:323:ILE:HD11	2.51	0.46
1:A:12:ILE:HG13	1:A:14:PHE:CE2	2.51	0.46
1:A:121:PHE:HB3	1:A:210:PHE:HE2	1.79	0.46
2:B:383:TYR:HD2	2:B:384:LEU:HD23	1.80	0.46
3:K:11:A:H2'	3:K:12:A:C8	2.51	0.46
2:N:267:GLN:HG2	4:P:13:DG:H5'	1.97	0.46
4:P:14:DA:H1'	4:P:15:DT:H5'	1.98	0.46
4:P:30:DG:H2"	4:P:31:DA:H5"	1.97	0.46
1:A:34:ASN:ND2	1:A:266:GLY:HA2	2.31	0.46
1:A:302:GLN:HA	1:A:315:GLY:HA2	1.98	0.46
2:B:139:LYS:HA	2:B:139:LYS:HD2	1.73	0.46
3:C:8:U:H2'	3:C:9:C:C6	2.51	0.46
1:I:423:VAL:HG13	1:I:433:LEU:HB2	1.98	0.46
2:N:36:ILE:HD12	2:N:39:LEU:HD13	1.98	0.45
2:N:283:GLN:OE1	2:N:296:GLU:HG2	2.16	0.45
2:B:305:PHE:O	2:B:306:GLU:HG2	2.16	0.45
1:I:122:ILE:HD11	1:I:213:ARG:NH2	2.31	0.45
2:J:112:ILE:HG22	2:J:115:LEU:HD12	1.98	0.45
4:P:26:DA:H2"	4:P:27:DA:C8	2.51	0.45
1:E:317:VAL:HG12	1:E:501:LEU:HD12	1.99	0.45
2:F:127:GLY:O	2:F:131:ILE:HG13	2.15	0.45
1:M:411:TYR:CG	2:N:410:PHE:HE2	2.34	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	(\dot{A})
2·N·26·ILE·HD11	2·N·32·VAL·H	1.82	0.45
2:N:285:TYB:HD2	2:N:350:LEU:HD13	1.82	0.45
1:E:330:LEU:HD23	1:E:330:LEU:HA	1.81	0.45
2·B·258·ASN·OD1	$2 \cdot B \cdot 258 \cdot ASN \cdot N$	2 49	0.45
2:B:390:SEB:OG	2:B:391:PHE:N	2.49	0.45
1:E:52:ILE:HG13	1:E:230:ALA:HB2	1.97	0.45
1:E:364:ABG:NH2	4:H:15:DT:OP1	2.50	0.45
3:0:12:A:H2'	3:0:13:U:H6	1.79	0.45
1:A:44:ILE:HD11	1:A:139:TRP:CE3	2.50	0.45
1:A:349:GLN:HB3	1:A:350:ILE:HD12	1.99	0.45
2:F:203:LEU:HD23	2:F:223:PHE:CE2	2.51	0.45
2:F:341:ILE:HD11	2:F:368:TRP:CZ3	2.52	0.45
1:I:267:LYS:HE2	1:I:267:LYS:HB3	1.75	0.45
1:I:363:THR:HG22	4:L:16:DT:H5'	1.99	0.45
2:J:181:PHE:HD1	2:J:182:PRO:HD2	1.82	0.45
1:M:302:GLN:HA	1:M:315:GLY:HA2	1.99	0.45
1:A:117:LEU:HD13	1:A:147:ILE:HG23	1.99	0.45
1:I:358:PHE:HB3	1:I:360:HIS:NE2	2.31	0.45
1:I:364:ARG:N	4:L:16:DT:OP1	2.35	0.45
2:N:273:PHE:CD2	2:N:335:LEU:HD21	2.50	0.45
2:N:305:PHE:CE2	2:N:383:TYR:HB2	2.52	0.45
2:N:313:LYS:HG3	2:N:313:LYS:O	2.17	0.45
2:N:374:ARG:HH11	2:N:374:ARG:HG3	1.81	0.45
1:E:394:LEU:HD13	2:F:175:TRP:CE2	2.52	0.45
2:F:194:LEU:HD22	2:F:214:LEU:HD21	1.99	0.45
2:J:61:LEU:HD23	2:J:95:ILE:HB	1.98	0.45
2:J:84:VAL:O	2:J:88:LEU:HD12	2.16	0.45
1:M:255:THR:HG21	3:O:2:G:H21	1.82	0.45
1:M:354:PRO:O	1:M:381:THR:HG22	2.16	0.45
2:N:395:MET:HB3	2:N:399:GLU:OE2	2.16	0.45
2:B:122:MET:HB2	2:B:126:ARG:HH12	1.81	0.45
4:D:9:DA:H2"	4:D:10:DA:H5"	1.98	0.45
4:D:21:DC:C2	4:D:22:DC:C5	3.05	0.45
2:F:5:ILE:HD12	2:F:30:TYR:HB3	1.99	0.45
1:I:44:ILE:HG12	1:I:94:LYS:HB2	1.98	0.45
1:M:54:ARG:HG2	1:M:91:ILE:HD12	1.99	0.45
2:F:282:VAL:HG11	2:F:293:TYR:HB3	1.99	0.45
2:J:274:GLU:HA	2:J:277:MET:HG2	1.99	0.45
4:D:22:DC:C2	4:D:23:DG:N7	2.85	0.44
1:E:119:SER:OG	1:E:213:ARG:NH2	2.43	0.44
2:F:9:HIS:NE2	2:F:35:ASP:OD1	2.50	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:F:134:ALA:HA	2:F:137:LYS:HE3	1.99	0.44
2:F:206:PRO:HG3	2:F:275:LEU:HD12	1.99	0.44
2:F:395:MET:HG2	2:F:401:VAL:HG22	2.00	0.44
2:N:382:LYS:NZ	2:N:405:ASN:O	2.50	0.44
1:A:307:ASN:HD22	1:A:310:GLY:C	2.18	0.44
2:B:343:PHE:O	2:B:357:GLN:NE2	2.47	0.44
2:J:130:ASP:O	2:J:133:GLU:HG2	2.17	0.44
1:M:453:LYS:HD3	1:M:453:LYS:HA	1.60	0.44
2:N:176:LEU:HD11	2:N:381:ILE:HD12	2.00	0.44
1:E:79:GLU:H	1:E:79:GLU:CD	2.19	0.44
1:E:407:ARG:HH22	1:E:463:THR:HG21	1.82	0.44
1:A:350:ILE:HD12	1:A:350:ILE:N	2.33	0.44
1:A:460:LEU:O	1:A:463:THR:HG22	2.17	0.44
3:C:9:C:H2'	3:C:10:U:C6	2.52	0.44
1:E:6:TYR:CE1	1:E:406:LEU:HD21	2.51	0.44
1:E:457:LYS:HB3	1:E:457:LYS:HE3	1.66	0.44
1:E:481:ARG:CZ	3:G:4:C:H5'	2.47	0.44
2:F:263:ARG:NH2	4:H:12:DA:H1'	2.32	0.44
1:I:223:ILE:O	3:K:1:U:O2'	2.25	0.44
2:B:184:GLU:OE1	2:B:240:ARG:HG2	2.17	0.44
2:B:284:GLU:N	2:B:284:GLU:OE1	2.51	0.44
1:I:421:TRP:CE2	1:I:440:PRO:HB3	2.53	0.44
3:K:13:U:H2'	3:K:14:C:C6	2.53	0.44
1:M:114:THR:HG22	1:M:151:CYS:SG	2.58	0.44
1:M:481:ARG:CZ	3:O:4:C:H5'	2.46	0.44
2:N:9:HIS:CG	2:N:18:THR:HG21	2.53	0.44
2:N:390:SER:OG	2:N:391:PHE:N	2.51	0.44
1:E:22:ASP:OD2	1:E:24:ARG:NH2	2.51	0.44
2:F:262:LYS:O	2:F:266:VAL:HG23	2.17	0.44
1:M:2:LYS:N	2:N:409:LYS:O	2.51	0.44
1:M:107:ASN:OD1	1:M:113:ARG:HB3	2.16	0.44
1:A:2:LYS:HB3	1:A:2:LYS:HE3	1.84	0.44
1:A:324:LYS:HE2	1:A:327:GLN:HG3	1.99	0.44
2:B:344:THR:HG22	2:B:350:LEU:HA	1.99	0.44
1:E:122:ILE:HG13	1:E:123:ASP:N	2.32	0.44
2:J:205:PHE:HB2	2:J:223:PHE:CZ	2.53	0.44
1:M:399:THR:HG22	2:N:374:ARG:HH22	1.83	0.44
1:E:371:ASP:N	1:E:371:ASP:OD1	2.51	0.44
2:J:272:ALA:HB2	2:J:395:MET:HB3	2.00	0.44
2:J:315:LYS:HE3	4:L:29:DA:H2"	1.98	0.44
1:M:490:LEU:HD23	1:M:490:LEU:HA	1.86	0.44



	lous page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:321:TYR:N	1:A:334:GLU:OE2	2.42	0.43
1:E:216:LYS:HG3	1:E:217:HIS:CE1	2.53	0.43
4:H:9:DA:H8	4:H:9:DA:OP1	2.01	0.43
1:M:495:ASP:OD1	1:M:495:ASP:N	2.51	0.43
1:A:25:ASP:OD2	1:A:428:LYS:NZ	2.50	0.43
1:A:97:THR:OG1	1:A:100:ASP:OD2	2.36	0.43
2:B:266:VAL:HG12	2:B:270:ASN:HD21	1.83	0.43
1:E:222:GLN:OE1	1:E:263:LYS:NZ	2.46	0.43
1:E:395:LYS:NZ	1:E:437:VAL:HG23	2.34	0.43
1:I:112:LYS:HE2	1:I:112:LYS:HB2	1.81	0.43
1:M:134:GLU:HA	1:M:134:GLU:OE1	2.17	0.43
2:N:4:LYS:HG2	2:N:33:TRP:HB2	1.98	0.43
2:N:271:LYS:HD3	2:N:271:LYS:HA	1.80	0.43
4:P:27:DA:H1'	4:P:28:DT:H5'	1.99	0.43
1:A:398:LYS:HE2	2:B:169:GLU:HG2	2.00	0.43
3:C:11:A:H2'	3:C:12:A:C8	2.53	0.43
1:E:2:LYS:HE2	2:F:332:PHE:CE2	2.53	0.43
2:F:279:ASP:OD1	2:F:279:ASP:N	2.47	0.43
1:I:125:ILE:HG22	1:I:219:ILE:HD13	2.00	0.43
1:I:405:ILE:HD12	1:I:406:LEU:N	2.33	0.43
2:J:271:LYS:HA	2:J:271:LYS:HD2	1.86	0.43
2:N:245:GLU:HA	2:N:248:SER:HB3	2.00	0.43
2:B:213:TYR:HE2	2:B:255:PHE:HE1	1.67	0.43
2:B:315:LYS:HD3	2:B:315:LYS:HA	1.70	0.43
1:I:53:PHE:HB2	1:I:142:ILE:HD11	1.99	0.43
2:J:390:SER:OG	2:J:391:PHE:N	2.51	0.43
2:B:300:LEU:HD13	2:B:304:LYS:H	1.82	0.43
2:J:172:ASP:HB3	2:J:409:LYS:HD3	2.00	0.43
2:N:178:ILE:HG12	2:N:403:VAL:HG22	2.01	0.43
4:P:16:DT:H2'	4:P:17:DA:H8	1.84	0.43
2:B:114:ARG:H	2:B:114:ARG:HG3	1.67	0.43
1:E:57:LEU:HD23	1:E:57:LEU:HA	1.75	0.43
2:F:200:VAL:HA	2:F:203:LEU:HD13	2.00	0.43
1:I:306:ASP:O	1:I:311:THR:N	2.52	0.43
2:J:287:MET:HE3	2:J:342:PHE:CZ	2.53	0.43
1:M:57:LEU:HD23	1:M:57:LEU:HA	1.86	0.43
2:N:63:VAL:HG13	2:N:99:ILE:HD13	1.99	0.43
1:A:474:ASP:OD1	1:A:481:ARG:NH2	2.47	0.43
2:B:282:VAL:HG23	2:B:295:LEU:HD22	2.00	0.43
1:E:303:MET:HE1	1:E:345:SER:HB3	2.00	0.43
1:I:48:GLN:HE21	1:I:48:GLN:HB3	1.64	0.43



	ous page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:I:397:TYR:CG	2:J:374:ARG:HB2	2.54	0.43
2:J:102:GLN:N	2:J:102:GLN:OE1	2.52	0.43
2:J:267:GLN:NE2	4:L:12:DA:H4'	2.34	0.43
1:M:63:PRO:HG3	2:N:124:TRP:NE1	2.33	0.43
1:A:303:MET:CE	1:A:305:LEU:HD23	2.48	0.43
1:A:317:VAL:CG1	1:A:318:GLY:H	2.32	0.43
1:E:134:GLU:HG3	1:E:136:VAL:HG23	2.00	0.43
2:F:54:ARG:NH2	2:N:106:ASP:O	2.41	0.43
1:M:215:LEU:HD12	1:M:215:LEU:HA	1.82	0.43
2:N:193:MET:HE3	2:N:229:LYS:O	2.18	0.43
2:N:279:ASP:OD1	2:N:279:ASP:N	2.50	0.43
2:N:305:PHE:HE2	2:N:383:TYR:CD1	2.33	0.43
2:F:332:PHE:O	2:F:334:VAL:HG13	2.19	0.43
1:I:368:GLN:HA	1:I:371:ASP:OD2	2.18	0.43
1:M:248:ILE:O	1:M:251:HIS:N	2.49	0.43
1:I:107:ASN:HD21	1:I:113:ARG:HB3	1.84	0.43
2:N:368:TRP:CH2	2:N:376:LYS:HE2	2.54	0.43
2:B:86:LYS:HB2	2:B:86:LYS:HE3	1.72	0.42
2:F:305:PHE:O	2:F:306:GLU:HG2	2.19	0.42
1:I:124:LYS:HE2	1:I:124:LYS:HB2	1.77	0.42
1:M:212:ALA:HA	1:M:215:LEU:HD22	2.00	0.42
1:A:112:LYS:HE2	1:A:112:LYS:HB2	1.79	0.42
1:E:208:ASP:N	1:E:208:ASP:OD1	2.51	0.42
1:E:222:GLN:NE2	3:G:1:U:O2	2.52	0.42
2:F:51:LYS:HB3	2:F:51:LYS:HE2	1.82	0.42
1:I:130:LYS:HB3	1:M:500:PRO:HA	2.00	0.42
2:J:42:GLY:O	2:N:92:LYS:HG3	2.19	0.42
2:J:314:GLN:HB2	2:J:315:LYS:HD2	2.00	0.42
2:B:189:GLU:HG2	2:B:213:TYR:CD1	2.54	0.42
2:B:217:PHE:HB2	2:B:395:MET:HB3	2.00	0.42
1:E:242:ILE:H	1:E:242:ILE:HD12	1.84	0.42
1:M:247:LYS:HG3	4:P:25:DC:H1'	2.02	0.42
2:B:276:ARG:HD2	2:B:276:ARG:HA	1.79	0.42
2:F:36:ILE:O	2:F:39:LEU:HG	2.20	0.42
1:I:364:ARG:NH1	4:L:15:DT:H3'	2.35	0.42
2:N:186:ARG:NH1	2:N:217:PHE:O	2.52	0.42
1:A:346:TYR:CD1	1:A:354:PRO:HD3	2.55	0.42
1:I:282:GLY:O	1:I:301:ALA:HA	2.19	0.42
1:I:501:LEU:O	1:I:501:LEU:HD23	2.19	0.42
2:J:46:TRP:HA	2:J:46:TRP:CE3	2.55	0.42
2:J:139:LYS:HD3	2:J:139:LYS:HA	1.89	0.42



	bus page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:F:205:PHE:HB2	2:F:223:PHE:HE1	1.84	0.42
1:M:460:LEU:HD12	1:M:460:LEU:HA	1.83	0.42
1:A:373:PHE:HB3	1:A:383:LEU:HD21	2.01	0.42
1:E:47:LYS:HD3	1:E:93:PHE:HE2	1.85	0.42
2:F:188:HIS:NE2	2:F:220:ALA:HA	2.35	0.42
1:I:268:PRO:HB2	1:I:269:TRP:CE3	2.54	0.42
1:I:307:ASN:ND2	1:I:310:GLY:H	2.11	0.42
1:I:482:PHE:O	1:I:486:ILE:HG23	2.19	0.42
1:M:378:PRO:O	1:M:378:PRO:HD2	2.18	0.42
1:A:68:ASN:OD1	1:A:68:ASN:N	2.51	0.42
2:F:188:HIS:CE1	2:F:220:ALA:HA	2.54	0.42
2:F:343:PHE:CZ	2:F:360:SER:HB2	2.55	0.42
1:I:32:PRO:HD3	1:I:81:VAL:O	2.18	0.42
1:M:502:ALA:HB3	1:M:505:TYR:CE2	2.55	0.42
2:N:37:LEU:HD22	2:N:153:LEU:HD21	2.02	0.42
2:N:280:LYS:HD2	2:N:280:LYS:HA	1.84	0.42
2:N:416:TYR:CE2	2:N:418:ILE:HG13	2.55	0.42
1:A:139:TRP:CD1	1:A:219:ILE:HG23	2.54	0.42
2:B:51:LYS:O	2:B:55:GLU:HB3	2.20	0.42
1:E:13:LEU:HD23	1:E:270:LYS:HE3	2.00	0.42
1:E:57:LEU:O	1:E:61:GLN:HG2	2.19	0.42
1:M:93:PHE:O	1:M:94:LYS:HD2	2.19	0.42
1:M:330:LEU:HD23	1:M:330:LEU:HA	1.86	0.42
2:N:28:LEU:HD13	2:N:132:LEU:HD21	2.01	0.42
2:F:263:ARG:HH22	4:H:12:DA:H1'	1.85	0.42
1:I:398:LYS:HD2	1:I:400:GLU:HB2	2.02	0.42
2:J:3:ASN:OD1	2:J:4:LYS:NZ	2.51	0.42
2:J:109:ASN:O	2:J:113:VAL:HG23	2.19	0.42
2:J:155:GLN:HE21	2:J:155:GLN:HB3	1.67	0.42
3:K:17:U:H2'	3:K:18:U:C6	2.54	0.42
1:A:398:LYS:HD3	2:B:171:TYR:CE1	2.55	0.41
1:E:407:ARG:NE	1:E:422:THR:O	2.53	0.41
1:I:149:LYS:HE3	1:I:149:LYS:HB3	1.73	0.41
1:M:206:PHE:CD1	1:M:206:PHE:C	2.93	0.41
2:N:188:HIS:HB3	2:N:233:TYR:HE2	1.85	0.41
1:A:7:ILE:HD12	1:A:7:ILE:O	2.19	0.41
2:B:114:ARG:HH11	2:B:115:LEU:HG	1.84	0.41
4:D:16:DT:H2'	4:D:17:DA:C8	2.54	0.41
1:E:428:LYS:HB3	1:E:428:LYS:HE3	1.86	0.41
2:F:189:GLU:N	2:F:233:TYR:OH	2.31	0.41
2:J:149:LYS:HD2	2:J:149:LYS:HA	1.79	0.41



	ouo puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:J:187:PHE:CE2	2:J:215:CYS:HB2	2.54	0.41
3:K:1:U:O2'	3:K:2:G:H5"	2.20	0.41
1:M:235:LYS:H	1:M:235:LYS:HG2	1.58	0.41
1:M:317:VAL:HG12	1:M:501:LEU:CD2	2.50	0.41
1:M:324:LYS:H	1:M:324:LYS:CD	2.33	0.41
1:M:339:LEU:HD22	1:M:339:LEU:HA	1.89	0.41
2:B:132:LEU:HD23	2:B:132:LEU:HA	1.91	0.41
2:F:83:LYS:HA	2:F:83:LYS:HD3	1.86	0.41
4:L:21:DC:C2	4:L:22:DC:C5	3.08	0.41
1:M:211:LYS:NZ	1:M:221:THR:O	2.53	0.41
1:A:382:ASN:OD1	1:A:383:LEU:N	2.53	0.41
1:A:411:TYR:HB3	1:A:419:PHE:HB2	2.02	0.41
1:I:67:SER:HB3	1:I:247:LYS:HB3	2.01	0.41
1:I:231:TRP:CE2	1:I:245:PHE:HB2	2.53	0.41
2:J:265:ILE:HD12	2:J:265:ILE:H	1.86	0.41
1:M:52:ILE:HA	1:M:55:ASP:OD2	2.19	0.41
1:M:122:ILE:HD12	1:M:126:ILE:HD12	2.02	0.41
1:M:236:ASN:OD1	1:M:240:LEU:N	2.51	0.41
1:A:307:ASN:ND2	1:A:312:VAL:HG23	2.35	0.41
1:A:469:ALA:HB2	3:C:3:A:H4'	2.02	0.41
2:B:411:LYS:HE3	2:B:411:LYS:HB3	1.87	0.41
1:E:395:LYS:HB2	2:F:174:ASN:ND2	2.35	0.41
1:I:317:VAL:HG23	1:I:501:LEU:HG	2.02	0.41
2:J:287:MET:HB2	2:J:290:LYS:O	2.20	0.41
2:N:362:ARG:NH1	3:O:7:C:H1'	2.31	0.41
1:A:322:ASN:OD1	1:A:331:GLU:HG2	2.20	0.41
1:A:394:LEU:HD12	1:A:395:LYS:H	1.85	0.41
2:B:276:ARG:HB3	2:B:277:MET:CE	2.50	0.41
2:F:325:GLY:HA2	2:F:336:MET:O	2.21	0.41
1:I:112:LYS:NZ	1:I:116:ASP:OD2	2.51	0.41
4:L:16:DT:H2'	4:L:17:DA:C8	2.52	0.41
1:A:396:LEU:HG	1:A:421:TRP:CZ2	2.55	0.41
2:F:20:TRP:CH2	2:F:124:TRP:HB3	2.54	0.41
1:I:247:LYS:HE3	4:L:25:DC:C6	2.55	0.41
4:L:12:DA:H2'	4:L:13:DG:H8	1.85	0.41
1:M:288:VAL:HG21	1:M:321:TYR:HE2	1.85	0.41
2:N:217:PHE:H	2:N:395:MET:HE1	1.86	0.41
1:E:401:GLY:O	2:F:370:ASN:ND2	2.50	0.41
1:I:50:LEU:HD11	1:I:54:ARG:HH11	1.86	0.41
1:I:253:ALA:O	1:I:257:SER:OG	2.36	0.41
1:I:392:LYS:HE2	1:I:442:PHE:CE2	2.55	0.41



	loue page	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:N:305:PHE:O	2:N:308:THR:HB	2.21	0.41	
2:B:316:ASP:OD2	2:B:317:LYS:HG2	2.21	0.41	
2:B:382:LYS:O	2:B:385:SER:OG	2.38	0.41	
1:I:37:TYR:CE2	1:M:40:LYS:HE3	2.56	0.41	
2:J:149:LYS:HB3	2:J:152:LEU:HG	2.02	0.41	
2:J:302:LYS:HE2	2:J:302:LYS:HB2	1.89	0.41	
1:M:55:ASP:OD1	1:M:56:TYR:N	2.54	0.41	
1:M:386:VAL:HG22	1:M:445:ILE:HA	2.03	0.41	
1:A:460:LEU:HD23	1:A:460:LEU:HA	1.80	0.41	
1:I:54:ARG:HE	1:I:88:SER:HG	1.62	0.41	
1:I:251:HIS:HE1	3:K:2:G:N2	2.19	0.41	
1:I:330:LEU:HD23	1:I:330:LEU:HA	1.88	0.41	
1:I:485:LYS:NZ	1:I:506:TYR:O	2.54	0.41	
2:J:157:ILE:HG22	2:J:158:PHE:H	1.86	0.41	
2:N:262:LYS:HB3	2:N:329:LEU:HD12	2.03	0.41	
2:N:385:SER:OG	2:N:405:ASN:ND2	2.53	0.41	
1:E:209:GLN:HE21	1:E:209:GLN:HB3	1.68	0.40	
1:I:394:LEU:HD13	2:J:175:TRP:NE1	2.36	0.40	
2:J:217:PHE:HB2	2:J:395:MET:HE1	2.02	0.40	
1:M:4:LEU:HD11	1:M:396:LEU:HD21	2.02	0.40	
4:P:17:DA:H2'	4:P:18:DG:C8	2.55	0.40	
2:F:418:ILE:HD12	2:F:418:ILE:HA	1.82	0.40	
1:I:423:VAL:HG22	1:I:475:GLY:HA2	2.02	0.40	
2:J:283:GLN:OE1	2:J:283:GLN:HA	2.21	0.40	
2:J:328:LYS:O	2:J:333:PRO:HA	2.21	0.40	
2:N:20:TRP:CH2	2:N:124:TRP:HB3	2.56	0.40	
1:A:58:ASP:HA	1:A:61:GLN:HG2	2.04	0.40	
2:B:85:LYS:HG3	2:B:90:ASP:O	2.21	0.40	
1:I:402:ASP:OD1	1:I:402:ASP:N	2.55	0.40	
2:J:415:SER:OG	2:J:416:TYR:N	2.52	0.40	
4:L:20:DG:C4	4:L:21:DC:C5	3.10	0.40	
2:B:13:ASP:OD1	2:B:71:ARG:NH2	2.45	0.40	
2:B:153:LEU:O	2:B:157:ILE:HG12	2.22	0.40	
1:E:144:PRO:HA	1:E:226:GLU:OE1	2.22	0.40	
2:F:387:ASP:OD1	2:F:390:SER:N	2.54	0.40	
4:H:10:DA:H2'	4:H:11:DT:C6	2.56	0.40	
1:I:14:PHE:N	1:I:18:GLN:O	2.46	0.40	
1:I:416:ARG:HH12	1:I:449:GLU:HG2	1.86	0.40	
2:J:317:LYS:HB3	2:J:344:THR:O	2.22	0.40	
3:K:4:C:H4'	3:K:5:G:OP1	2.22	0.40	
1:M:107:ASN:OD1	1:M:107:ASN:N	2.54	0.40	



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:267:LYS:H	1:M:267:LYS:HG2	1.78	0.40
2:N:169:GLU:HG3	2:N:415:SER:HB2	2.04	0.40
2:N:343:PHE:CE1	2:N:360:SER:HB2	2.56	0.40
2:J:232:THR:O	2:J:232:THR:OG1	2.34	0.40
2:J:325:GLY:HA2	2:J:336:MET:O	2.21	0.40
1:M:344:GLN:HA	1:M:347:LYS:HZ2	1.86	0.40
2:N:314:GLN:HE22	2:N:317:LYS:H	1.67	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	Perce	ntiles
1	А	450/506~(89%)	423 (94%)	27~(6%)	0	100	100
1	Е	450/506~(89%)	423 (94%)	27~(6%)	0	100	100
1	Ι	450/506~(89%)	422 (94%)	28 (6%)	0	100	100
1	М	450/506~(89%)	422 (94%)	28 (6%)	0	100	100
2	В	416/418 (100%)	375~(90%)	41 (10%)	0	100	100
2	F	416/418 (100%)	385 (92%)	31 (8%)	0	100	100
2	J	416/418 (100%)	384 (92%)	31 (8%)	1 (0%)	47	69
2	Ν	416/418 (100%)	390 (94%)	26 (6%)	0	100	100
All	All	3464/3696~(94%)	3224 (93%)	239 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	315	LYS



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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	А	388/445~(87%)	362~(93%)	26~(7%)	16	32
1	Ε	389/445~(87%)	361~(93%)	28 (7%)	14	29
1	Ι	388/445~(87%)	354 (91%)	34~(9%)	10	21
1	М	387/445~(87%)	356~(92%)	31 (8%)	12	25
2	В	381/384~(99%)	353~(93%)	28~(7%)	14	29
2	F	382/384~(100%)	343~(90%)	39 (10%)	7	15
2	J	378/384~(98%)	335~(89%)	43 (11%)	5	11
2	Ν	380/384~(99%)	345 (91%)	$35 \ (9\%)$	9	18
All	All	3073/3316~(93%)	2809 (91%)	264 (9%)	14	22

All (264) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	1	MET
1	А	11	LYS
1	А	59	HIS
1	А	72	ARG
1	А	83	ASP
1	А	112	LYS
1	А	131	ASN
1	А	207	HIS
1	А	208	ASP
1	А	216	LYS
1	А	232	ARG
1	А	233	ASP
1	А	279	CYS
1	А	296	ASN
1	А	305	LEU
1	А	333	LYS
1	А	364	ARG
1	А	379	LYS
1	А	391	THR



Mol	Chain	Res	Type
1	А	411	TYR
1	А	444	GLU
1	А	460	LEU
1	А	461	SER
1	А	470	CYS
1	А	478	VAL
1	А	495	ASP
2	В	1	MET
2	В	16	ASP
2	В	34	CYS
2	В	43	VAL
2	В	56	ASP
2	В	64	SER
2	В	68	SER
2	В	71	ARG
2	В	86	LYS
2	В	105	TYR
2	В	114	ARG
2	В	142	LYS
2	В	146	ASP
2	В	160	HIS
2	В	167	LYS
2	В	179	LEU
2	В	181	PHE
2	В	205	PHE
2	В	209	ARG
2	В	213	TYR
2	В	215	CYS
2	В	222	ASP
2	В	257	ARG
2	В	280	LYS
2	В	301	GLU
2	В	327	SER
2	В	380	PHE
2	B	401	VAL
1	E	12	ILE
1	Е	16	HIS
1	E	41	SER
1	E	44	ILE
1	E	52	ILE
1	Е	74	MET
1	Е	79	GLU



Mol	Chain	Res	Type
1	Е	120	LEU
1	Е	131	ASN
1	Е	137	ASP
1	Е	208	ASP
1	Е	232	ARG
1	Е	243	ARG
1	Е	298	CYS
1	Е	304	PHE
1	Е	324	LYS
1	Е	327	GLN
1	Е	333	LYS
1	Е	348	GLU
1	Е	364	ARG
1	Е	368	GLN
1	Е	371	ASP
1	Е	377	THR
1	Е	405	ILE
1	Е	435	MET
1	Е	444	GLU
1	Е	470	CYS
1	Ε	497	LYS
2	F	1	MET
2	F	11	THR
2	F	14	ASP
2	F	16	ASP
2	F	41	LYS
2	F	51	LYS
2	F	58	CYS
2	F	71	ARG
2	F	107	ASP
2	F	137	LYS
2	F	152	LEU
2	F	161	ASP
2	F	164	VAL
2	F	165	ILE
2	F	173	SER
2	F	181	PHE
2	F	191	ASN
2	F	193	MET
2	F	198	PHE
2	F	215	CYS
2	F	229	LYS



Mol	Chain	Res	Type
2	F	233	TYR
2	F	234	HIS
2	F	258	ASN
2	F	279	ASP
2	F	305	PHE
2	F	309	MET
2	F	310	LEU
2	F	318	ASN
2	F	327	SER
2	F	332	PHE
2	F	364	GLN
2	F	373	TRP
2	F	380	PHE
2	F	384	LEU
2	F	391	PHE
2	F	392	TYR
2	F	413	ASN
2	F	414	VAL
1	Ι	16	HIS
1	Ι	24	ARG
1	Ι	29	LEU
1	Ι	48	GLN
1	Ι	72	ARG
1	Ι	83	ASP
1	Ι	120	LEU
1	Ι	149	LYS
1	Ι	150	TYR
1	Ι	207	HIS
1	Ι	208	ASP
1	Ι	221	THR
1	Ι	224	PHE
1	Ι	229	LEU
1	Ι	232	ARG
1	Ι	251	HIS
1	Ι	255	THR
1	Ι	257	SER
1	Ι	274	VAL
1	Ι	275	ARG
1	I	303	MET
1	Ι	305	LEU
1	Ι	314	LYS
1	Ι	317	VAL



Mol	Chain	Res	Type
1	Ι	339	LEU
1	Ι	347	LYS
1	Ι	353	TYR
1	Ι	355	LYS
1	Ι	364	ARG
1	Ι	399	THR
1	Ι	415	GLU
1	Ι	470	CYS
1	Ι	479	THR
1	Ι	498	THR
2	J	1	MET
2	J	13	ASP
2	J	16	ASP
2	J	43	VAL
2	J	56	ASP
2	J	64	SER
2	J	87	GLN
2	J	101	GLU
2	J	122	MET
2	J	123	SER
2	J	130	ASP
2	J	137	LYS
2	J	139	LYS
2	J	146	ASP
2	J	151	ASN
2	J	154	TYR
2	J	155	GLN
2	J	164	VAL
2	J	173	SER
2	J	181	PHE
2	J	214	LEU
2	J	219	TRP
2	J	232	THR
2	J	234	HIS
2	J	245	GLU
2	J	274	GLU
2	J	283	GLN
2	J	310	LEU
2	J	313	LYS
2	J	318	ASN
2	J	321	PHE
2	J	324	SER



Mol	Chain	Res	Type
2	J	364	GLN
2	J	384	LEU
2	J	387	ASP
2	J	391	PHE
2	J	392	TYR
2	J	394	GLU
2	J	395	MET
2	J	402	PHE
2	J	406	GLU
2	J	415	SER
2	J	417	ASN
1	М	16	HIS
1	М	40	LYS
1	М	41	SER
1	М	50	LEU
1	М	64	ILE
1	М	72	ARG
1	М	95	GLU
1	М	103	LYS
1	М	104	PHE
1	М	120	LEU
1	М	150	TYR
1	М	206	PHE
1	М	208	ASP
1	М	215	LEU
1	М	216	LYS
1	М	221	THR
1	М	248	ILE
1	М	274	VAL
1	М	305	LEU
1	М	324	LYS
1	М	339	LEU
1	М	358	PHE
1	M	365	PHE
1	М	399	THR
1	М	423	VAL
1	М	430	GLN
1	М	437	VAL
1	М	470	CYS
1	М	486	ILE
1	М	488	GLU
1	М	498	THR



Mol	Chain	Res	Type
2	N	33	TRP
2	N	34	CYS
2	Ν	40	ASP
2	Ν	71	ARG
2	Ν	87	GLN
2	Ν	92	LYS
2	Ν	139	LYS
2	Ν	142	LYS
2	Ν	160	HIS
2	Ν	209	ARG
2	Ν	219	TRP
2	Ν	233	TYR
2	Ν	240	ARG
2	Ν	245	GLU
2	Ν	257	ARG
2	Ν	276	ARG
2	Ν	281	GLU
2	Ν	287	MET
2	Ν	305	PHE
2	Ν	309	MET
2	Ν	313	LYS
2	Ν	315	LYS
2	N	332	PHE
2	N	336	MET
2	Ν	357	GLN
2	N	374	ARG
2	N	380	PHE
2	N	382	LYS
2	Ν	383	TYR
2	N	389	THR
2	N	394	GLU
2	N	399	GLU
2	N	401	VAL
2	N	414	VAL
2	Ν	417	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	34	ASN
1	Ι	251	HIS
1	Ι	307	ASN



Continued from previous page...

Mol	Chain	Res	Type
1	Ι	349	GLN
1	Ι	414	ASN
2	J	160	HIS
2	J	340	HIS
2	Ν	314	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	С	18/19~(94%)	3~(16%)	2 (11%)
3	G	18/19~(94%)	6 (33%)	2 (11%)
3	K	18/19~(94%)	3~(16%)	2 (11%)
3	0	18/19~(94%)	6 (33%)	2 (11%)
All	All	72/76~(94%)	18~(25%)	8 (11%)

All (18) RNA backbone outliers are listed below:

Mol	Chain	Res Type	
3	С	5	G
3	С	10	U
3	С	16	А
3	G	2	G
3	G	5	G
3	G	8	U
3	G	10	U
3	G	15	U
3	G	16	А
3	Κ	2	G
3	Κ	5	G
3	Κ	10	U
3	0	2	G
3	0	5	G
3	0	10	U
3	0	15	U
3	0	16	А
3	0	19	А

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type	
3	С	4	С	
Continued on next page				



Continued from previous page...

Mol	Chain	Res	Type
3	С	9	С
3	G	4	С
3	G	9	С
3	Κ	4	С
3	Κ	9	С
3	0	4	С
3	0	9	С

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-36047. 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: 200



Y Index: 200



Z Index: 200

6.2.2 Raw map



X Index: 200

Y Index: 200

Z Index: 200

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: 197



Y Index: 181



Z Index: 248

6.3.2 Raw map



X Index: 197

Y Index: 181

Z Index: 248

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 0.286. 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 288 $\rm nm^3;$ this corresponds to an approximate mass of 260 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 0.352 ${\rm \AA^{-1}}$



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 0.352 $\mathrm{\AA^{-1}}$



8.2 Resolution estimates (i)

$\begin{bmatrix} Bosolution ostimato (Å) \end{bmatrix}$	Estimation criterion (FSC cut-off)		
Resolution estimate (A)	0.143	0.5	Half-bit
Reported by author	2.84	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.70	4.35	3.82

*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 3.70 differs from the reported value 2.84 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-36047 and PDB model 8J7S. 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 0.286 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 (0.286).



9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 77% 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 (0.286) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score	
All	0.7720	0.4160	
А	0.8930	0.4600	
В	0.7690	0.3980	— 10
С	0.9750	0.4330	
D	0.9520	0.4360	
Е	0.8910	0.4670	
F	0.7460	0.3920	
G	0.9770	0.4060	
Н	0.8520	0.4150	
Ι	0.8330	0.4370	
J	0.5340	0.3580	
K	0.9220	0.4250	0.0
L	0.7470	0.3940	<0.0
М	0.8330	0.4510	
N	0.5730	0.3690]
0	0.8920	0.3600	
Р	0.6480	0.3560	

