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PDB ID	:	6GEN
EMDB ID	:	EMD-4396
Title	:	Chromatin remodeller-nucleosome complex at 4.5 A resolution.
Authors	:	Willhoft, O.; Chua, E.Y.D.; Wilkinson, M.; Wigley, D.B.
Deposited on	:	2018-04-27
Resolution	:	3.60 Å(reported)
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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.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 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	$egin{array}{llllllllllllllllllllllllllllllllllll$	${f EM} {f structures} \ (\#{f Entries})$
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 c	hain	
1	Z	131	8%		
2	А	136	59%	12%	29%
2	В	136	• 60%	12%	29%
3	С	103	• 65%	14%	• 20%
3	D	103	• 66%	11%	• 22%
4	Е	132	69%	8%	• 22%
4	F	132	70%	6%	• 23%
5	G	131	● 61%	11% •	27%



Mol	Chain	Length	(Quality of cha	in	
5	Н	131	57%	1	1% •	31%
6	Ι	173	• •	91%		9%
7	J	173	9%	83%		17%
8	М	1514	35%	.0% •	55%	
9	R	438	•	9%		14% • 6%
10	S	280	62%		12%	26%
11	Т	463	13%	%		17% • •
11	V	463	77	%		15% • 6%
11	Х	463	24%	6		18% • 5%
12	U	471	• 69%		20%	% • 9%
12	W	471	69%		20%	% • 8%
12	Y	471	21%			20% • 5%



2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 44481 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

• Molecule 1 is a protein called Vacuolar protein sorting-associated protein 72.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	Ζ	131	Total 655	C 393	N 131	0 131	0	0

• Molecule 2 is a protein called Histone H3.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	Λ	07	Total	С	Ν	Ο	0	0
	91	796	506	152	138	0	0	
9	В	07	Total	С	Ν	Ο	0	0
	D	91	796	506	152	138	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	123	GLU	ASP	conflict	UNP P61830
В	123	GLU	ASP	conflict	UNP P61830

• Molecule 3 is a protein called Histone H4.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	С	82	Total 651	C 410	N 126	0 115	0	0
3	D	80	Total 638	C 401	N 124	0 113	0	0

• Molecule 4 is a protein called Histone H2A.1.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	Е	103	Total 795	C 499	N 156	O 140	0	0
4	F	101	Total 779	C 489	N 153	0 137	0	0



• Molecule 5 is a protein called Histone H2B.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	С	06	Total	С	Ν	0	\mathbf{S}	0	0
5 G	90	746	468	131	146	1	0	0	
5	и	01	Total	С	Ν	0	S	0	0
5	11	31	712	449	125	137	1		

• Molecule 6 is a DNA chain called DNA (173-MER).

Mol	Chain	Residues		А	AltConf	Trace			
6	Ι	173	$\begin{array}{c} \text{Total} \\ 3525 \end{array}$	C 1673	N 640	O 1039	Р 173	0	0

• Molecule 7 is a DNA chain called DNA (173-MER).

Mol	Chain	Residues		Α	toms			AltConf	Trace
7	J	173	Total 3568	C 1687	N 671	O 1037	Р 173	0	0

• Molecule 8 is a protein called Helicase SWR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	М	688	Total 5398	C 3438	N 960	0 974	S 26	0	0

• Molecule 9 is a protein called Actin-like protein ARP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	R	411	Total 3335	C 2156	N 544	O 619	S 16	0	0

• Molecule 10 is a protein called Vacuolar protein sorting-associated protein 71.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	S	208	Total 1695	C 1071	N 302	0 312	S 10	0	0

• Molecule 11 is a protein called RuvB-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Т	443	Total 3391	C 2140	N 584	O 657	S 10	0	0



• • • • • •			9						
Mol	Chain	Residues	Atoms					AltConf	Trace
11	V	424	Total	С	Ν	0	\mathbf{S}	0	0
	v	404	3336	2107	574	645	10	0	
11	v	449	Total	С	Ν	0	S	0	0
11	Λ	442	3397	2144	584	659	10	0	0

• Molecule 12 is a protein called RuvB-like protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	U	430	Total 3299	C 2063	N 570	O 655	S 11	0	0
12	W	433	Total 3325	C 2085	N 572	0 657	S 11	0	0
12	Y	447	Total 3410	C 2133	N 590	O 675	S 12	0	0

• Molecule 13 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues		Ate	oms			AltConf
12	М	1	Total	С	Ν	0	Р	0
10	IVI	L	27	10	5	10	2	0
12	D	1	Total	С	Ν	0	Р	0
10	n	L	27	10	5	10	2	0
12	Т	1	Total	С	Ν	0	Р	0
10	1	L	27	10	5	10	2	0
12	II	1	Total	С	Ν	Ο	Р	0
10	U	L	27	10	5	10	2	0



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Mol	Chain	Residues		Ate	oms			AltConf
12	V	1	Total	С	Ν	Ο	Р	0
10	v	L	27	10	5	10	2	0
12	W	1	Total	С	Ν	Ο	Р	0
10	vv	T	27	10	5	10	2	0
12	v	1	Total	С	Ν	Ο	Р	0
10	Λ	L	27	10	5	10	2	0
12	V	1	Total	С	Ν	Ο	Р	0
	I	L	27	10	5	10	2	U



Mol	Chain	Residues	Atoms	AltConf
14	М	1	Total Be F	0
14	111	1	4 1 3	0
14	D	1	Total Be F	0
14	n	I	4 1 3	0

• Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
15	М	1	Total Mg 1 1	0
15	R	1	Total Mg 1 1	0
15	U	2	Total Mg 2 2	0



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Mol	Chain	Residues	Atoms	AltConf
15	V	1	Total Mg 1 1	0
15	W	1	Total Mg 1 1	0
15	Y	2	Total Mg 2 2	0

• Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
16	S	2	Total Zn 2 2	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: Vacuolar protein sorting-associated protein 72





Chain D:	66	%	11% •	22%	
MET SER GLY GLY GLY GLY GLY CLYS GLY GLY	LEU CLY CLY CLY CLY CLY CLY ALA ALA ALA ALC TLSU LEU LEU	R23 R36 L37 L58 L62 L62 L62	A 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4	d102	
• Molecule 4:	Histone H2A.1				
Chain E:	6	9%	8% •	22%	
MET SER GLY GLY LYS GLY GLY ALA GLY GLY	SER ALA ALA ALA ALA SER SER 816 916 718 718 718 718 718 718 718 718	L34 Q42 V55 L86 L86 N90 N90	L98 V108 P118 LYS LYS SER ALA ALA	ALLA THR LYS ALA SER GLU GLU LEU	
• Molecule 4:	Histone H2A.1				
Chain F:	7	0%	6% •	23%	
MET SER GLY GLY CLY CLY GLY CLY ALA ALA GLY	SER ALA ALA LYS ALA ALA SER SER R30 R30 R30 L34	N39 179 186 188 188 188 188 198 198	L117 PRO LYS LYS SER ALA ALA THR THR THR ALA	SER GLU LEU LEU	
• Molecule 5:	Histone H2B.1				
Chain G:	61%		11% •	27%	
MET SER ALA LYS ALA GLU LYS LYS PRO PRO	SER LYS ALA PRO ALA CLV CVS PRO CLV PRO PRO LVS LVS LVS	THR THR THR SER SER ASP GLY LYS LYS LYS SAG SAG SAG	A35 D54 176 R95 A100 V101	L102 L103 L104 L105 P106 G107 L109 L119 A110 K111	A113 V114 T128
GLM ALA					
• Molecule 5:	Histone H2B.1				
Chain H:	57%		11% •	31%	
MET SER ALA LYS LYS GLU LYS LYS PRO ALA	SER LLYS ALA PRO ALA ALA GLU CLYS PRO PRO PRO FRO TLA	SER SER SER THR SER THR ASP LYS LYS LYS SER SER SER	A35 B38 D54 157 176	N95 A100 A101 L103 L103 L105 L105 C105 C107 C107	L109 A110 K111 H12
A113 V114 S125 SER SER SER THR GLN ALA					
• Molecule 6:	DNA (173-MER)				
Chain I:		91%		9%	
G-96 A-94 T-92 A-91 A-91 A-91	A-86 	C21 C22 A23 C48 C48 C48 C48 C72 T73 N76			
• Molecule 7:	DNA (173-MER)				















PROTEIN DATA BANK





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	98529	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 $(e^-/\text{\AA}^2)$	1.71794871794872	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.207	Depositor
Minimum map value	-0.092	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0359	Depositor
Map size (Å)	426.24, 426.24, 426.24	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.11, 1.11, 1.11	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: ADP, ZN, BEF, 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		
WIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
2	А	0.24	0/807	0.42	0/1081	
2	В	0.25	0/807	0.42	0/1081	
3	С	0.24	0/658	0.45	0/880	
3	D	0.24	0/645	0.45	0/862	
4	Е	0.24	0/806	0.42	0/1091	
4	F	0.24	0/789	0.42	0/1067	
5	G	0.25	0/756	0.41	0/1017	
5	Н	0.24	0/722	0.41	0/972	
6	Ι	0.58	0/3949	0.97	1/6087~(0.0%)	
7	J	0.56	0/4007	0.94	0/6188	
8	М	0.26	0/5495	0.48	3/7442~(0.0%)	
9	R	0.25	0/3429	0.43	2/4650~(0.0%)	
10	S	0.25	0/1722	0.42	0/2320	
11	Т	0.25	0/3433	0.47	0/4646	
11	V	0.25	0/3375	0.46	0/4565	
11	Х	0.25	0/3439	0.47	0/4652	
12	U	0.24	0/3333	0.45	0/4492	
12	W	0.25	0/3361	0.45	0/4530	
12	Y	0.25	0/3447	0.46	0/4649	
All	All	0.33	0/44980	0.59	6/62272~(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
8	М	0	2
11	Т	0	4
11	V	0	2
11	Х	0	5



Mol	Chain	#Chirality outliers	#Planarity outliers
12	U	0	1
12	W	0	3
12	Y	0	3
All	All	0	20

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
8	М	999	PHE	CB-CG-CD2	7.75	126.22	120.80
9	R	66	LEU	CA-CB-CG	6.60	130.49	115.30
9	R	63	LEU	CA-CB-CG	6.30	129.80	115.30
8	М	998	LEU	C-N-CA	5.59	135.68	121.70
6	Ι	48	DG	O4'-C4'-C3'	-5.39	102.34	104.50
8	М	999	PHE	CB-CG-CD1	-5.34	117.06	120.80

There are no chirality outliers.

Mol	Chain	Res	Type	Group
8	М	1067	CYS	Peptide
8	М	1344	ASN	Peptide
11	Т	152	ALA	Peptide
11	Т	160	GLY	Peptide
11	Т	161	LYS	Peptide
11	Т	162	THR	Peptide
12	U	222	VAL	Peptide
11	V	161	LYS	Peptide
11	V	162	THR	Peptide
12	W	205	SER	Mainchain
12	W	221	PHE	Peptide
12	W	222	VAL	Peptide
11	Х	151	ASP	Peptide
11	Х	152	ALA	Peptide
11	Х	160	GLY	Peptide
11	Х	161	LYS	Peptide
11	Х	162	THR	Peptide
12	Y	205	SER	Mainchain
12	Y	206	PHE	Peptide
12	Y	222	VAL	Peptide

All (20) planarity outliers are listed below:



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	Ζ	655	0	147	0	0
2	А	796	0	841	11	0
2	В	796	0	841	10	0
3	С	651	0	690	9	0
3	D	638	0	677	8	0
4	Е	795	0	834	9	0
4	F	779	0	819	6	0
5	G	746	0	771	12	0
5	Н	712	0	736	11	0
6	Ι	3525	0	1941	11	0
7	J	3568	0	1940	21	0
8	М	5398	0	5352	85	0
9	R	3335	0	3256	37	0
10	S	1695	0	1746	27	0
11	Т	3391	0	3513	47	0
11	V	3336	0	3475	38	0
11	Х	3397	0	3533	55	0
12	U	3299	0	3387	51	0
12	W	3325	0	3413	55	0
12	Y	3410	0	3466	57	0
13	М	27	0	12	3	0
13	R	27	0	12	0	0
13	Т	27	0	12	0	0
13	U	27	0	12	0	0
13	V	27	0	12	0	0
13	W	27	0	12	0	0
13	Х	27	0	12	2	0
13	Y	27	0	12	0	0
14	М	4	0	0	0	0
14	R	4	0	0	0	0
15	М	1	0	0	0	0
15	R	1	0	0	0	0
15	U	2	0	0	0	0
15	V	1	0	0	0	0
15	W	1	0	0	0	0
15	Y	2	0	0	0	0
16	S	2	0	0	0	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	44481	0	41474	479	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 6.

All (479) 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)
12:W:269:VAL:O	12:W:273:ILE:HB	1.65	0.97
12:U:269:VAL:O	12:U:273:ILE:HB	1.65	0.95
12:Y:269:VAL:O	12:Y:273:ILE:HB	1.65	0.93
3:C:62:LEU:O	3:C:66:ILE:HB	1.70	0.92
3:D:62:LEU:O	3:D:66:ILE:HB	1.70	0.92
10:S:176:GLN:O	10:S:180:LYS:HB2	1.70	0.90
9:R:116:ASP:O	9:R:120:PHE:HB2	1.73	0.87
9:R:77:ASP:O	9:R:81:PHE:HB2	1.74	0.86
8:M:1058:HIS:O	8:M:1062:ILE:HB	1.82	0.80
11:X:413:ARG:O	11:X:417:GLN:HB2	1.82	0.80
11:V:413:ARG:O	11:V:417:GLN:HB2	1.82	0.80
11:T:413:ARG:O	11:T:417:GLN:HB2	1.82	0.80
8:M:1089:PHE:O	8:M:1093:SER:HB3	1.85	0.77
12:W:175:MET:O	12:W:179:LEU:HB2	1.86	0.76
12:U:175:MET:O	12:U:179:LEU:HB2	1.86	0.74
9:R:118:VAL:O	9:R:122:GLU:HB2	1.88	0.74
12:Y:175:MET:O	12:Y:179:LEU:HB2	1.86	0.74
8:M:1133:ARG:HD2	12:Y:220:ARG:HB3	1.73	0.69
8:M:1057:TYR:O	8:M:1061:GLU:HB2	1.92	0.69
12:W:17:LEU:O	11:X:331:ASN:ND2	2.27	0.68
12:W:397:ARG:HG2	11:X:366:ARG:HA	1.79	0.64
11:T:286:GLN:O	11:T:290:LYS:HB2	1.98	0.64
5:G:110:ALA:O	5:G:114:VAL:HB	1.98	0.63
11:V:286:GLN:O	11:V:290:LYS:HB2	1.97	0.63
11:X:286:GLN:O	11:X:290:LYS:HB2	1.98	0.63
8:M:875:VAL:HG13	8:M:877:ASP:H	1.63	0.63
5:H:110:ALA:O	5:H:114:VAL:HB	1.98	0.62
11:T:413:ARG:HD3	12:U:350:ARG:HB3	1.81	0.62
11:V:119:GLU:O	11:V:123:GLU:HB2	1.99	0.62
12:W:327:ARG:HH22	11:X:353:VAL:HG13	1.65	0.62
5:H:108:GLU:HG2	10:S:44:ARG:HH11	1.64	0.62
11:T:119:GLU:O	11:T:123:GLU:HB2	1.99	0.62
11:V:127:ARG:NH2	12:W:267:SER:OG	2.32	0.62



A + a 1	A + ama - D	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
12:W:18:SER:HA	11:X:331:ASN:HD22	1.65	0.61	
11:X:119:GLU:O	11:X:123:GLU:HB2	1.99	0.61	
11:X:462:TYR:HD1	12:Y:327:ARG:HA	1.65	0.61	
12:W:126:GLY:HA2	12:W:240:SER:HA	1.83	0.61	
11:X:331:ASN:OD1	11:X:331:ASN:N	2.34	0.60	
12:U:126:GLY:HA2	12:U:240:SER:HA	1.83	0.60	
12:Y:126:GLY:HA2	12:Y:240:SER:HA	1.83	0.60	
8:M:806:VAL:O	8:M:810:GLN:HB3	2.02	0.60	
11:X:149:PRO:HB3	11:X:162:THR:HG21	1.84	0.60	
9:R:98:HIS:HD2	9:R:127:SER:HB2	1.67	0.60	
11:V:109:GLU:HG2	12:W:114:THR:HG21	1.84	0.59	
11:T:331:ASN:N	11:T:331:ASN:OD1	2.34	0.59	
6:I:-79:DG:N2	7:J:79:DC:C2	2.70	0.59	
11:T:313:VAL:HG21	11:T:338:LEU:HB3	1.85	0.59	
11:V:331:ASN:OD1	11:V:331:ASN:N	2.34	0.59	
9:R:228:LYS:HD2	9:R:239:MET:HA	1.84	0.59	
11:V:313:VAL:HG21	11:V:338:LEU:HB3	1.85	0.59	
11:X:453:THR:HG22	12:Y:341:HIS:HB2	1.85	0.59	
8:M:1023:ARG:HG2	8:M:1027:LYS:HE2	1.85	0.59	
11:T:54:ALA:O	11:T:58:CYS:HB2	2.03	0.58	
11:V:149:PRO:HB3	11:V:162:THR:HG21	1.85	0.58	
11:T:23:ARG:HH12	12:U:290:PRO:HB3	1.68	0.58	
11:X:54:ALA:O	11:X:58:CYS:HB2	2.03	0.58	
2:A:56:LYS:HG2	10:S:53:LEU:HD21	1.84	0.58	
11:V:54:ALA:O	11:V:58:CYS:HB2	2.03	0.58	
11:X:313:VAL:HG21	11:X:338:LEU:HB3	1.85	0.58	
10:S:100:ARG:HH12	10:S:132:GLU:HA	1.69	0.58	
12:U:127:ILE:HG12	12:U:288:ILE:HG22	1.86	0.58	
12:W:127:ILE:HG12	12:W:288:ILE:HG22	1.86	0.57	
9:R:5:PRO:HB3	9:R:98:HIS:HB2	1.86	0.57	
11:T:395:VAL:HG22	11:T:434:ILE:HD12	1.87	0.57	
11:T:445:LEU:HB3	12:U:53:ALA:HB2	1.87	0.56	
12:Y:127:ILE:HG12	12:Y:288:ILE:HG22	1.86	0.56	
8:M:778:GLY:HA3	8:M:782:GLN:HB2	1.88	0.56	
11:X:395:VAL:HG22	11:X:434:ILE:HD12	1.87	0.56	
10:S:256:CYS:SG	10:S:257:VAL:N	2.76	0.56	
11:X:42:LYS:O	11:X:55:ARG:NH2	2.39	0.56	
8:M:995:HIS:ND1	8:M:1245:CYS:SG	2.79	0.55	
9:R:228:LYS:O	9:R:232:SER:HB3	2.05	0.55	
11:T:42:LYS:O	11:T:55:ARG:NH2	2.39	0.55	
11:V:395:VAL:HG22	11:V:434:ILE:HD12	1.87	0.55	



A 4 1	A 4 D	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
9:R:58:ARG:HB3	10:S:166:VAL:HG13	1.88	0.55	
12:Y:128:LYS:HG2	12:Y:238:THR:HG22	1.88	0.55	
12:W:128:LYS:HG2	12:W:238:THR:HG22	1.88	0.55	
8:M:794:ASP:OD1	8:M:794:ASP:N	2.40	0.55	
9:R:323:SER:O	10:S:101:ARG:NH1	2.40	0.55	
12:U:128:LYS:HG2	12:U:238:THR:HG22	1.88	0.55	
8:M:822:VAL:HG12	8:M:849:LEU:HB3	1.88	0.54	
11:T:461:ASN:N	11:T:461:ASN:OD1	2.41	0.54	
11:V:42:LYS:O	11:V:55:ARG:NH2	2.39	0.54	
12:W:19:LEU:HD23	11:X:71:SER:HB2	1.88	0.54	
5:G:107:GLY:O	5:G:111:LYS:HB2	2.08	0.54	
11:V:380:ILE:HG13	11:V:412:LEU:HD13	1.88	0.54	
11:V:41:ALA:HB3	11:V:52:ILE:HG23	1.90	0.54	
12:W:115:GLU:OE2	12:W:270:ARG:NH2	2.41	0.54	
11:T:380:ILE:HG13	11:T:412:LEU:HD13	1.88	0.54	
11:V:461:ASN:N	11:V:461:ASN:OD1	2.40	0.54	
8:M:1062:ILE:HD11	12:Y:220:ARG:HH21	1.73	0.54	
12:U:38:ARG:O	12:U:51:ARG:NH2	2.40	0.54	
5:H:107:GLY:O	5:H:111:LYS:HB2	2.08	0.54	
8:M:695:ASN:O	13:M:1601:ADP:N6	2.41	0.54	
11:X:312:GLU:OE2	11:X:341:ASN:ND2	2.41	0.54	
11:X:380:ILE:HG13	11:X:412:LEU:HD13	1.88	0.54	
2:B:51:ILE:O	2:B:55:GLN:HB2	2.08	0.53	
8:M:1264:ARG:HB2	8:M:1333:ALA:HA	1.90	0.53	
12:U:115:GLU:OE2	12:U:270:ARG:NH2	2.41	0.53	
10:S:258:ASN:HD22	10:S:280:ARG:HA	1.73	0.53	
3:D:77:LYS:HZ3	5:G:95:ARG:HH22	1.56	0.53	
12:Y:157:LYS:HG2	12:Y:170:GLU:HG2	1.90	0.53	
2:A:51:ILE:O	2:A:55:GLN:HB2	2.08	0.53	
11:T:41:ALA:HB3	11:T:52:ILE:HG23	1.90	0.53	
12:W:157:LYS:HG2	12:W:170:GLU:HG2	1.90	0.53	
11:X:289:ASN:HA	11:X:292:VAL:HB	1.90	0.53	
8:M:1264:ARG:NH1	8:M:1314:ILE:O	2.42	0.53	
11:T:289:ASN:HA	11:T:292:VAL:HB	1.90	0.53	
11:X:461:ASN:OD1	11:X:461:ASN:N	2.40	0.53	
4:E:55:VAL:HG21	5:G:101:VAL:HG21	1.91	0.53	
9:R:198:THR:HB	HR:HB 9:R:216:LEU:HB2		0.53	
11:X:413:ARG:NH1	13:X:501:ADP:O3A	2.41	0.53	
9:R:197:CYS:SG	9:R:199:TRP:NE1	2.81	0.53	
11:X:41:ALA:HB3	11:X:52:ILE:HG23	1.90	0.53	
8:M:821:MET:HG2	8:M:845:THR:HG21	1.91	0.53	



Atom-1 Atom-2		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
10:S:264:CYS:SG	10:S:265:SER:N	2.82	0.53
11:V:289:ASN:HA	11:V:292:VAL:HB	1.90	0.53
12:W:401:ASN:HD22	11:X:368:LEU:HD21	1.74	0.53
12:U:157:LYS:HG2	12:U:170:GLU:HG2	1.90	0.53
11:X:117:LYS:HD2	11:X:320:ILE:HD11	1.91	0.53
12:Y:38:ARG:O	12:Y:51:ARG:NH2	2.40	0.53
8:M:1200:ASN:O	8:M:1210:ARG:NH1	2.42	0.52
7:J:-19:DG:H5"	8:M:1272:THR:HG23	1.91	0.52
9:R:58:ARG:NH1	10:S:112:ASP:OD1	2.43	0.52
11:V:312:GLU:OE2	11:V:341:ASN:ND2	2.41	0.52
8:M:957:GLN:HE21	8:M:996:PRO:HD3	1.74	0.52
8:M:1210:ARG:O	8:M:1214:MET:HB2	2.09	0.52
9:R:258:VAL:O	9:R:368:ARG:NH1	2.42	0.52
11:T:312:GLU:OE2	11:T:341:ASN:ND2	2.41	0.52
12:U:311:ARG:O	12:U:311:ARG:NH2	2.42	0.52
12:Y:115:GLU:OE2	12:Y:270:ARG:NH2	2.41	0.52
3:D:77:LYS:HG2	5:G:95:ARG:HH12	1.75	0.52
8:M:1156:SER:HB3	11:X:206:THR:HB	1.91	0.52
10:S:275:THR:O	10:S:278:ARG:NH1	2.42	0.52
12:W:38:ARG:O	12:W:51:ARG:NH2	2.40	0.52
2:B:116:ARG:NH2	2:B:123:GLU:OE2	2.43	0.52
11:T:117:LYS:HD2	11:T:320:ILE:HD11	1.91	0.52
8:M:957:GLN:O	8:M:961:TYR:HB2	2.09	0.51
3:C:40:ARG:HH21	4:E:108:VAL:HG13	1.76	0.51
11:X:114:GLU:OE2	12:Y:250:ARG:NH1	2.43	0.51
9:R:117:GLN:O	9:R:121:GLU:HB2	2.10	0.51
12:Y:61:VAL:HG22	12:Y:320:ILE:HG21	1.92	0.51
12:Y:204:ARG:H	12:Y:221:PHE:HA	1.75	0.51
12:W:139:GLU:N	12:W:161:LYS:O	2.44	0.51
2:A:116:ARG:NH2	2:A:123:GLU:OE2	2.43	0.51
8:M:1202:ASP:N	8:M:1202:ASP:OD1	2.43	0.51
2:B:68:GLN:HE21	2:B:72:ARG:HE	1.58	0.51
8:M:1336:VAL:HB	8:M:1366:ILE:HG23	1.92	0.51
11:T:278:THR:OG1	11:T:279:GLU:N	2.44	0.51
11:V:71:SER:O	11:V:73:ARG:NH1	2.44	0.51
11:V:117:LYS:HD2	11:V:320:ILE:HD11	1.91	0.51
8:M:1222:ASN:ND2	8:M:1228:GLN:OE1	2.44	0.51
9:R:339:SER:OG	10:S:233:ARG:NH2	2.43	0.51
6:I:-59:DT:H1'	8:M:815:ARG:HH21	1.76	0.51
8:M:778:GLY:HA3	8:M:782:GLN:HE21	1.74	0.51
11:T:71:SER:O	11:T:73:ARG:NH1	2.44	0.51



	1.0	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
11:T:286:GLN:HG2	12:Y:17:LEU:HB3	1.93	0.51	
12:U:27:THR:HA	12:U:90:GLN:HG2	1.93	0.51	
2:A:68:GLN:HE21	2:A:72:ARG:HE	1.58	0.51	
8:M:685:ASP:OD2	8:M:701:LYS:NZ	2.42	0.51	
8:M:1139:ASN:HB3	8:M:1143:LEU:HD13	1.93	0.51	
12:U:61:VAL:HG22	12:U:320:ILE:HG21	1.92	0.51	
12:U:122:ARG:HH12	12:U:274:ASN:HD21	1.59	0.51	
12:W:61:VAL:HG22	12:W:320:ILE:HG21	1.92	0.51	
2:B:100:LEU:HD23	3:C:37:LEU:HD13	1.93	0.50	
8:M:1209:THR:O	8:M:1213:VAL:HB	2.10	0.50	
8:M:1382:LYS:NZ	8:M:1393:VAL:O	2.44	0.50	
12:W:122:ARG:HH12	12:W:274:ASN:HD21	1.59	0.50	
4:F:30:ARG:HE	7:J:-45:DG:H5'	1.77	0.50	
4:F:79:ILE:HD12	5:H:57:ILE:HG12	1.93	0.50	
12:W:191:SER:HB3	12:W:202:LEU:HD11	1.94	0.50	
11:X:119:GLU:O	11:X:123:GLU:CB	2.59	0.50	
12:Y:122:ARG:HH12	12:Y:274:ASN:HD21	1.59	0.50	
8:M:1357:ARG:NH1	13:M:1601:ADP:O5'	2.45	0.50	
9:R:396:GLY:O	9:R:400:MET:HB2	2.11	0.50	
10:S:10:LYS:HE3	11:V:178:THR:HG21	1.93	0.50	
11:X:71:SER:O	11:X:73:ARG:NH1	2.44	0.50	
2:A:100:LEU:HD23	3:D:37:LEU:HD13	1.94	0.50	
12:U:436:SER:HB3	11:V:369:ILE:HD12	1.93	0.50	
11:V:119:GLU:O	11:V:123:GLU:CB	2.59	0.50	
12:W:311:ARG:O	12:W:311:ARG:NH2	2.42	0.50	
12:U:156:GLY:HA3	12:U:176:ILE:HD11	1.94	0.50	
12:Y:27:THR:HA	12:Y:90:GLN:HG2	1.93	0.50	
11:X:278:THR:OG1	11:X:279:GLU:N	2.44	0.50	
8:M:1045:LEU:O	11:T:256:ASN:ND2	2.45	0.50	
8:M:1085:LEU:HD11	8:M:1108:ASN:HB3	1.94	0.50	
8:M:1212:LYS:HD2	11:T:265:VAL:HG21	1.94	0.50	
9:R:414:VAL:HG22	9:R:431:ARG:HH11	1.76	0.50	
12:U:191:SER:HB3	12:U:202:LEU:HD11	1.93	0.50	
11:T:119:GLU:O	11:T:123:GLU:CB	2.59	0.50	
11:V:278:THR:OG1	11:V:279:GLU:N	2.44	0.50	
2:B:90:GLY:O	2:B:94:GLU:HB2	2.12	0.49	
8:M:750:ILE:HD11	8:M:800:ILE:HG23	1.94	0.49	
12:W:156:GLY:HA3	12:W:176:ILE:HD11	1.94	0.49	
12:Y:156:GLY:HA3	12:Y:176:ILE:HD11	1.94	0.49	
8:M:1025:LEU:HD11	12:U:239:VAL:HG11	1.93	0.49	
12:W:29:LEU:H	12:W:91:SER:HB3	1.77	0.49	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
5:G:101:VAL:HG13	5:G:105:LEU:HD12	1.95	0.49	
5:H:101:VAL:HG13	5:H:105:LEU:HD12	1.95	0.49	
7:J:-25:DC:H2"	7:J:-24:DT:H5"	1.93	0.49	
8:M:956:ARG:HD2	8:M:1002:ARG:HH21	1.78	0.49	
12:W:27:THR:HA	12:W:90:GLN:HG2	1.93	0.49	
8:M:772:LYS:H	8:M:797:HIS:HD2	1.59	0.49	
8:M:1162:LEU:O	11:X:256:ASN:ND2	2.45	0.49	
8:M:1226:GLN:O	8:M:1230:LYS:HB2	2.12	0.49	
12:Y:191:SER:HB3	12:Y:202:LEU:HD11	1.94	0.49	
12:Y:185:LEU:H	12:Y:188:ASP:HB2	1.78	0.49	
12:W:185:LEU:H	12:W:188:ASP:HB2	1.78	0.49	
12:U:29:LEU:H	12:U:91:SER:HB3	1.77	0.49	
12:W:149:ILE:HG13	12:W:150:THR:HG23	1.94	0.49	
2:A:90:GLY:O	2:A:94:GLU:HB2	2.12	0.49	
7:J:-46:DT:H2'	7:J:-45:DG:C8	2.48	0.49	
9:R:124:GLU:OE2	9:R:416:ARG:NH2	2.46	0.49	
11:V:65:ILE:HD13	11:V:96:LEU:HD11	1.94	0.49	
11:X:65:ILE:HD13	11:X:96:LEU:HD11	1.94	0.48	
11:T:65:ILE:HD13	11:T:96:LEU:HD11	1.94	0.48	
12:Y:29:LEU:H	12:Y:91:SER:HB3	1.77	0.48	
8:M:1214:MET:O	8:M:1218:PHE:HB2	2.13	0.48	
4:F:86:LEU:O	4:F:90:ASN:HB2	2.13	0.48	
11:T:428:THR:HG21	12:U:35:LEU:HD22	1.94	0.48	
8:M:1061:GLU:HB3	12:Y:202:LEU:HD23	1.94	0.48	
9:R:196:ASN:OD1	9:R:221:ARG:NH1	2.47	0.48	
3:C:30:THR:HG21	7:J:-13:DA:H5"	1.96	0.48	
12:Y:139:GLU:N	12:Y:161:LYS:O	2.44	0.48	
12:Y:311:ARG:O	12:Y:311:ARG:NH2	2.42	0.48	
12:U:185:LEU:H	12:U:188:ASP:HB2	1.78	0.48	
4:E:86:LEU:O	4:E:90:ASN:HB2	2.13	0.48	
9:R:435:GLN:NE2	10:S:221:ASP:OD2	2.47	0.48	
12:Y:223:GLN:HG2	12:Y:225:PRO:HD3	1.96	0.48	
5:H:100:ALA:HA	5:H:103:LEU:HD23	1.96	0.47	
8:M:1209:THR:HG23	11:T:191:ARG:HH12	1.78	0.47	
12:U:139:GLU:N	12:U:161:LYS:O	2.44	0.47	
12:W:429:LEU:HB3	11:X:57:ALA:HB2	1.96	0.47	
9:R:434:TYR:OH	10:S:221:ASP:OD1	2.32	0.47	
12:W:204:ARG:H	12:W:221:PHE:HA	1.79	0.47	
12:Y:20:ILE:HG21	12:Y:375:GLU:HG2	1.96	0.47	
8:M:759:ASN:O	8:M:763:GLU:HB2	2.14	0.47	
12:U:20:ILE:HG21	12:U:375:GLU:HG2	1.96	0.47	



A + a 1	A 4 a	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
12:Y:310:ASN:O	12:Y:350:ARG:NH1	2.47	0.47	
7:J:-19:DG:H2'	7:J:-18:DG:C8	2.50	0.47	
7:J:11:DC:H2'	7:J:12:DG:C8	2.49	0.47	
8:M:1086:GLN:O	8:M:1090:GLY:HA3	2.14	0.47	
12:U:162:THR:OG1	12:U:163:THR:N	2.47	0.47	
12:Y:185:LEU:HG	12:Y:208:ARG:HB2	1.96	0.47	
5:G:100:ALA:HA	5:G:103:LEU:HD23	1.96	0.47	
6:I:-58:DG:O4'	8:M:815:ARG:NH2	2.48	0.47	
8:M:991:LYS:HG2	8:M:997:ASN:HB2	1.97	0.47	
8:M:1045:LEU:HD21	11:T:291:VAL:HG21	1.97	0.47	
12:U:310:ASN:O	12:U:350:ARG:NH1	2.47	0.47	
12:W:310:ASN:O	12:W:350:ARG:NH1	2.47	0.47	
8:M:1165:PRO:HB3	11:X:259:PRO:HD3	1.97	0.47	
8:M:1340:ASP:OD1	8:M:1340:ASP:N	2.46	0.47	
2:A:62:ILE:O	2:A:93:GLN:NE2	2.49	0.47	
12:Y:402:LEU:HA	12:Y:405:VAL:HG22	1.97	0.47	
2:A:96:VAL:HG13	3:D:58:LEU:HD21	1.96	0.46	
11:T:80:GLY:HA2	12:Y:448:ILE:HD11	1.97	0.46	
11:X:453:THR:HB	12:Y:340:PRO:HB2	1.97	0.46	
12:Y:262:THR:OG1	12:Y:263:GLY:N	2.48	0.46	
8:M:1065:LEU:HD22	12:Y:202:LEU:HB2	1.97	0.46	
9:R:70:GLU:H	9:R:70:GLU:HG2	1.51	0.46	
12:U:262:THR:OG1	12:U:263:GLY:N	2.48	0.46	
12:W:145:ILE:HA	12:W:156:GLY:HA2	1.97	0.46	
11:X:151:ASP:OD1	11:X:151:ASP:N	2.48	0.46	
6:I:-59:DT:O2	8:M:815:ARG:NH2	2.49	0.46	
12:W:20:ILE:HG21	12:W:375:GLU:HG2	1.96	0.46	
12:W:162:THR:OG1	12:W:163:THR:N	2.47	0.46	
12:W:262:THR:OG1	12:W:263:GLY:N	2.48	0.46	
9:R:27:ARG:HE	9:R:394:LEU:HD21	1.80	0.46	
12:W:402:LEU:HA	12:W:405:VAL:HG22	1.97	0.46	
12:Y:145:ILE:HA	12:Y:156:GLY:HA2	1.97	0.46	
12:Y:162:THR:OG1	12:Y:163:THR:N	2.47	0.46	
7:J:25:DT:H2"	7:J:26:DA:C8	2.51	0.46	
11:T:83:THR:O	11:T:375:TYR:OH	2.34	0.46	
12:W:329:VAL:HG22	12:W:341:HIS:H	1.81	0.46	
9:R:65:GLN:HE21	9:R:107:THR:HA	1.80	0.46	
2:B:96:VAL:HG13	3:C:58:LEU:HD21	1.96	0.46	
12:W:17:LEU:HD11	11:X:332:ILE:HD13	1.97	0.46	
12:Y:329:VAL:HG22	12:Y:341:HIS:H	1.81	0.46	
9:R:339:SER:O	9:R:346:ARG:NH2	2.49	0.45	



Atom 1	Atom 2	Interatomic	Clash overlap (Å)	
Atom-1	Atom-2	distance (\AA)		
11:T:33:LEU:O	11:T:55:ARG:NH1	2.50	0.45	
11:X:33:LEU:O	11:X:55:ARG:NH1	2.50	0.45	
2:B:62:ILE:O	2:B:93:GLN:NE2	2.49	0.45	
5:H:76:ILE:HG12	5:H:104:ILE:HD11	1.99	0.45	
5:H:107:GLY:O	5:H:111:LYS:CB	2.65	0.45	
4:E:42:GLN:OE1	4:F:39:ASN:ND2	2.49	0.45	
11:T:158:GLY:HA2	12:Y:145:ILE:HB	1.99	0.45	
12:W:14:LEU:HD12	12:W:15:LYS:HB2	1.98	0.45	
4:F:89:ARG:NH1	4:F:98:LEU:O	2.49	0.45	
5:G:76:ILE:HG12	5:G:104:ILE:HD11	1.99	0.45	
12:U:145:ILE:HA	12:U:156:GLY:HA2	1.97	0.45	
11:V:33:LEU:O	11:V:55:ARG:NH1	2.50	0.45	
12:U:402:LEU:HA	12:U:405:VAL:HG22	1.97	0.45	
10:S:257:VAL:HG21	12:U:166:GLU:HG2	1.99	0.45	
12:U:28:GLY:H	12:U:90:GLN:HB3	1.82	0.45	
12:U:189:VAL:HG11	12:U:223:GLN:HG2	1.99	0.45	
12:U:243:GLU:HA	12:U:257:LEU:HD11	1.99	0.45	
8:M:990:ARG:NH1	8:M:1376:GLU:OE2	2.50	0.45	
8:M:1264:ARG:NH2	8:M:1312:SER:O	2.48	0.45	
9:R:121:GLU:HB3	10:S:198:LEU:HD11	1.99	0.45	
12:U:329:VAL:HG22	12:U:341:HIS:H	1.81	0.45	
12:W:243:GLU:HA	12:W:257:LEU:HD11	1.99	0.45	
11:X:72:GLY:N	11:X:333:ALA:O	2.45	0.45	
12:Y:28:GLY:H	12:Y:90:GLN:HB3	1.82	0.45	
4:E:89:ARG:NH1	4:E:98:LEU:O	2.49	0.44	
12:Y:243:GLU:HA	12:Y:257:LEU:HD11	1.99	0.44	
3:C:93:GLN:OE1	3:C:95:ARG:NH2	2.51	0.44	
8:M:942:PRO:HB2	8:M:1363:ASP:HA	1.99	0.44	
8:M:1300:ASP:O	8:M:1304:LEU:HB2	2.17	0.44	
12:U:26:ILE:HG22	12:U:44:MET:HG2	1.99	0.44	
12:W:26:ILE:HG22	12:W:44:MET:HG2	1.99	0.44	
12:W:28:GLY:H	12:W:90:GLN:HB3	1.82	0.44	
12:W:158:LEU:HD23	12:W:171:LEU:HD21	2.00	0.44	
4:F:30:ARG:O	4:F:34:LEU:HB2	2.17	0.44	
11:X:127:ARG:HH22	12:Y:271:ASP:HB2	1.81	0.44	
8:M:1150:VAL:HG12	8:M:1152:TYR:H	1.83	0.44	
12:W:402:LEU:HD22	12:W:426:ALA:HB1	1.99	0.44	
5:G:107:GLY:O	5:G:111:LYS:CB	2.65	0.44	
9:R:58:ARG:HD2	10:S:166:VAL:HG22	1.98	0.44	
12:U:332:THR:OG1	12:U:335:THR:OG1	2.36	0.44	
9:R:69:TRP:O	9:R:73:SER:CB	2.66	0.44	



Atom-1	Atom-2	Interatomic	Clash	
		distance (A)	overlap (A)	
11:'T:72:GLY:N	11:T:333:ALA:O	2.45	0.44	
11:V:188:SER:HA	11:V:191:ARG:HD2	2.00	0.44	
12:Y:26:ILE:HG22	12:Y:44:MET:HG2	1.99	0.44	
12:Y:332:THR:OG1	12:Y:335:THR:OG1	2.36	0.44	
4:E:30:ARG:O	4:E:34:LEU:HB2	2.17	0.44	
7:J:15:DT:H6	7:J:15:DT:H2'	1.69	0.44	
8:M:778:GLY:O	8:M:783:ARG:N	2.43	0.44	
9:R:69:TRP:O	9:R:73:SER:HB2	2.17	0.44	
12:W:201:LYS:HB2	12:W:201:LYS:HE2	1.72	0.44	
11:X:188:SER:HA	11:X:191:ARG:HD2	2.00	0.44	
6:I:22:DC:H2"	6:I:23:DA:H5"	2.00	0.44	
7:J:-74:DC:H2"	7:J:-73:DA:C8	2.53	0.44	
12:U:158:LEU:HD23	12:U:171:LEU:HD21	2.00	0.44	
2:A:65:LEU:HB2	7:J:17:DA:H5"	2.00	0.43	
5:G:34:LYS:HE2	5:G:34:LYS:HB2	1.88	0.43	
10:S:54:ALA:O	10:S:58:ALA:HB2	2.18	0.43	
10:S:261:ASN:HD22	10:S:272:HIS:HE1	1.66	0.43	
12:U:114:THR:O	12:U:118:THR:OG1	2.36	0.43	
7:J:23:DG:H2"	7:J:24:DC:H5"	2.01	0.43	
11:T:71:SER:OG	11:T:331:ASN:O	2.36	0.43	
12:U:137:GLU:HG2	12:U:191:SER:HB2	2.00	0.43	
12:Y:402:LEU:HD22	:402:LEU:HD22 12:Y:426:ALA:HB1		0.43	
3:D:93:GLN:OE1	3:D:95:ARG:NH2	2.51	0.43	
11:T:188:SER:HA	11:T:191:ARG:HD2	2.00	0.43	
8:M:967:ARG:O	8:M:970:THR:OG1	2.32	0.43	
11:T:286:GLN:HA	12:Y:17:LEU:HD22	1.99	0.43	
8:M:1200:ASN:OD1	8:M:1200:ASN:N	2.51	0.43	
12:U:402:LEU:HD22	12:U:426:ALA:HB1	1.99	0.43	
12:U:407:GLN:HE21	12:U:407:GLN:HB3	1.58	0.43	
12:W:32:ASP:OD1	12:W:32:ASP:N	2.51	0.43	
12:W:332:THR:OG1	12:W:335:THR:OG1	2.36	0.43	
11:X:151:ASP:HA	11:X:161:LYS:HD3	2.00	0.43	
12:Y:114:THR:O	12:Y:118:THR:OG1	2.36	0.43	
2:A:61:LEU:HD13	3:D:36:ARG:HB3	2.01	0.43	
11:V:72:GLY:N	11:V:333:ALA:O	2.45	0.43	
2:B:95:SER:O	2:B:99:TYR:HB3	2.19	0.43	
6:I:-68:DG:N2	7:J:68:DC:C2	2.84	0.43	
7:J:4:DG:H2"	7:J:5:DT:C5	2.53	0.43	
11:X:71:SER:OG	11:X:333:ALA:O	2.37	0.43	
5:G:54:ASP:OD1	5:G:54:ASP:N	2.50	0.43	
10:S:268:CYS:O	10:S:272:HIS:HB2	2.18	0.43	



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
11:T:362:ASP:OD1	11:T:362:ASP:N	362:ASP:N 2.45		
11:V:54:ALA:O	11:V:58:CYS:CB	2.67	0.43	
12:Y:158:LEU:HD23	12:Y:171:LEU:HD21	2.00	0.42	
11:T:381:ARG:O	11:T:385:GLU:HB2	2.19	0.42	
12:U:32:ASP:OD1	12:U:32:ASP:N	2.51	0.42	
11:V:25:ALA:HB1	12:W:68:GLY:HA3	2.01	0.42	
11:V:381:ARG:O	11:V:385:GLU:HB2	2.19	0.42	
12:W:114:THR:O	12:W:118:THR:OG1	2.36	0.42	
4:E:29:GLY:HA3	6:I:-44:DA:H3'	2.01	0.42	
8:M:992:VAL:HG23	8:M:998:LEU:HD13	2.02	0.42	
8:M:1144:LEU:HD22	12:Y:254:PHE:HZ	1.84	0.42	
9:R:425:ASP:N	9:R:425:ASP:OD1	2.53	0.42	
8:M:1030:LYS:HD2	8:M:1030:LYS:HA	1.80	0.42	
8:M:1225:HIS:O	8:M:1229:THR:OG1	2.33	0.42	
8:M:1386:LYS:HE3	8:M:1386:LYS:HB3	1.88	0.42	
11:V:71:SER:OG	11:V:333:ALA:O	2.37	0.42	
12:Y:455:GLN:OE1	12:Y:457:SER:OG	2.37	0.42	
8:M:1004:ILE:H	8:M:1004:ILE:HG12	1.66	0.42	
8:M:1276:ASP:OD1	8:M:1276:ASP:N	2.44	0.42	
11:X:381:ARG:O	11:X:385:GLU:HB2	2.19	0.42	
8:M:860:LEU:H	8:M:860:LEU:HG	1.69	0.42	
9:R:227:LEU:HD13	9:R:313:ILE:HG13	2.01	0.42	
11:X:54:ALA:O	11:X:58:CYS:CB	2.67	0.42	
12:Y:103:GLY:N	12:Y:296:ASP:O	2.53	0.42	
2:A:95:SER:O	2:A:99:TYR:HB3	2.19	0.42	
8:M:1350:GLN:HE21	8:M:1354:ARG:HH12	1.68	0.42	
8:M:1357:ARG:NH2	13:M:1601:ADP:O1B	2.41	0.42	
12:W:103:GLY:N	12:W:296:ASP:O	2.53	0.42	
11:X:76:LEU:HD21	11:X:369:ILE:HG12	2.02	0.42	
11:X:225:GLU:HG3	11:X:227:GLU:H	1.85	0.42	
2:B:61:LEU:HD13	3:C:36:ARG:HB3	2.02	0.42	
5:G:109:LEU:O	5:G:113:ALA:CB	2.68	0.42	
6:I:21:DC:OP2	8:M:831:ASN:ND2	2.52	0.42	
8:M:1200:ASN:ND2	8:M:1202:ASP:O	2.53	0.42	
11:T:106:VAL:HB	11:T:109:GLU:HG3	2.01	0.42	
7:J:3:DC:H2"	7:J:4:DG:C8	2.55	0.42	
8:M:1142:ASP:HA	8:M:1145:THR:HG22	2.02	0.42	
11:T:225:GLU:HG3	11:T:227:GLU:H	1.85	0.42	
12:U:102:ALA:HB3	12:U:105:GLU:HB2	2.02	0.42	
12:U:103:GLY:N	12:U:296:ASP:O	2.53	0.42	
12:U:134:GLU:OE2	12:U:232:ARG:NH2	2.43	0.42	



A 4 1		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
11:V:106:VAL:HB	11:V:109:GLU:HG3	2.01	0.42	
11:V:225:GLU:HG3	11:V:227:GLU:H	1.85	0.42	
7:J:36:DA:H1'	7:J:37:DC:H5'	2.01	0.42	
8:M:723:MET:H	8:M:723:MET:HG2	1.65	0.42	
8:M:953:LEU:HD12	8:M:953:LEU:HA	1.95	0.42	
11:T:54:ALA:O	11:T:58:CYS:CB	2.67	0.42	
11:T:76:LEU:HD21	11:T:369:ILE:HG12	2.02	0.42	
11:V:325:ASN:ND2	11:V:362:ASP:OD2	2.53	0.42	
12:Y:32:ASP:OD1	12:Y:32:ASP:N	2.51	0.42	
12:Y:102:ALA:HB3	12:Y:105:GLU:HB2	2.02	0.42	
9:R:191:ILE:HG12	9:R:200:ILE:HG23	2.02	0.41	
11:X:277:LYS:HE2	11:X:277:LYS:HB2	1.85	0.41	
11:X:325:ASN:ND2	11:X:362:ASP:OD2	2.53	0.41	
12:Y:407:GLN:HE21	12:Y:407:GLN:HB3	1.58	0.41	
11:T:326:LYS:HE3	11:T:326:LYS:HB3	1.92	0.41	
12:U:455:GLN:OE1	12:U:457:SER:OG	2.37	0.41	
11:V:212:VAL:HG12	11:V:230:VAL:HG11	2.02	0.41	
12:W:361:GLU:HG3	12:W:392:VAL:HG21	2.02	0.41	
5:H:109:LEU:O	5:H:113:ALA:CB	2.68	0.41	
9:R:13:TYR:HA	9:R:59:ARG:HH22	1.85	0.41	
12:U:361:GLU:HG3	12:U:392:VAL:HG21	2.02	0.41	
7:J:-76:DT:H2"	7:J:-75:DG:C8	2.55	0.41	
12:W:102:ALA:HB3	12:W:105:GLU:HB2	2.02	0.41	
12:Y:159:THR:HA	12:Y:168:ILE:HA	2.03	0.41	
6:I:72:DG:H1'	6:I:73:DT:H5'	2.02	0.41	
9:R:8:ILE:HG12	9:R:17:PHE:HB2	2.03	0.41	
9:R:233:PHE:HB3	10:S:276:ARG:HH11	1.85	0.41	
11:T:51:GLN:HG3	11:T:54:ALA:HB3	2.03	0.41	
3:D:85:ASP:O	3:D:89:ALA:HB2	2.20	0.41	
8:M:1069:LYS:HE2	8:M:1069:LYS:HB2	1.86	0.41	
11:T:325:ASN:ND2	11:T:362:ASP:OD2	2.53	0.41	
12:U:159:THR:HA	12:U:168:ILE:HA	2.03	0.41	
11:V:76:LEU:HD21	11:V:369:ILE:HG12	2.02	0.41	
11:V:277:LYS:HB2	11:V:277:LYS:HE2	1.85	0.41	
12:W:159:THR:HA	12:W:168:ILE:HA	2.03	0.41	
7:J:-24:DT:H2"	7:J:-23:DT:H5'	2.02	0.41	
8:M:987:MET:O	8:M:991:LYS:HB2	2.20	0.41	
12:U:146:ASP:O	12:U:155:GLN:N	2.51	0.41	
12:W:19:LEU:H	11:X:331:ASN:HB3	1.85	0.41	
11:X:51:GLN:HG3	11:X:54:ALA:HB3	2.03	0.41	
11:X:106:VAL:HB	11:X:109:GLU:HG3	2.01	0.41	



	1.5	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
3:C:85:ASP:O	3:C:89:ALA:HB2	2.20	0.41	
8:M:1241:LEU:HD11	1241:LEU:HD11 8:M:1277:VAL:HG13		0.41	
11:T:117:LYS:HE3	11:T:117:LYS:HB2	1.92	0.41	
12:U:21:ALA:HB3	12:U:24:SER:HB2	2.03	0.41	
3:C:77:LYS:HG2	5:H:95:ARG:HH12	1.85	0.41	
10:S:128:ARG:O	10:S:132:GLU:HB2	2.21	0.41	
11:V:51:GLN:HG3	11:V:54:ALA:HB3	2.03	0.41	
12:W:146:ASP:O	12:W:155:GLN:N	2.51	0.41	
12:Y:146:ASP:O	12:Y:155:GLN:N	2.51	0.41	
2:B:101:VAL:HG11	4:E:108:VAL:HG11	2.03	0.41	
6:I:-70:DG:H2"	6:I:-69:DA:C8	2.57	0.41	
9:R:229:GLU:OE1	10:S:101:ARG:NH2	2.55	0.41	
9:R:237:ASN:N	9:R:237:ASN:OD1	2.49	0.41	
11:T:212:VAL:HG12	11:T:230:VAL:HG11	2.02	0.41	
11:T:456:LEU:HD23	12:U:329:VAL:HG23	2.03	0.41	
12:W:455:GLN:OE1	12:W:457:SER:OG	2.37	0.41	
11:X:48:PHE:HA	13:X:501:ADP:HN62	1.85	0.41	
12:Y:361:GLU:HG3	12:Y:392:VAL:HG21	2.02	0.41	
4:E:78:ARG:HH11	7:J:58:DC:H5'	1.85	0.40	
8:M:722:GLU:HB2	8:M:933:LEU:HA	2.04	0.40	
8:M:836:ARG:HA	8:M:839:ALA:HB3	2.03	0.40	
8:M:1068:VAL:HG13	8:M:1126:ASN:HD21	1.86	0.40	
11:X:326:LYS:HE3	11:X:326:LYS:HB3	1.92	0.40	
5:H:54:ASP:OD1	5:H:54:ASP:N	2.50	0.40	
11:V:405:THR:O	11:V:409:GLU:HB2	2.21	0.40	
11:X:212:VAL:HG12	11:X:230:VAL:HG11	2.02	0.40	
6:I:-86:DA:H2"	6:I:-85:DT:C6	2.56	0.40	
8:M:1055:THR:HA	8:M:1141:ILE:H	1.86	0.40	
7:J:88:DC:H2"	7:J:89:DA:C8	2.57	0.40	
10:S:54:ALA:O	10:S:58:ALA:CB	2.69	0.40	
10:S:258:ASN:OD1	10:S:258:ASN:N	2.55	0.40	
12:W:21:ALA:HB3	12:W:24:SER:HB2	2.03	0.40	
11:X:462:TYR:HB2	12:Y:327:ARG:HD3	2.02	0.40	
8:M:1045:LEU:HD23	8:M:1045:LEU:HA	1.84	0.40	
8:M:1331:THR:HG22	8:M:1357:ARG:HB2	2.03	0.40	
10:S:246:ILE:HG13	10:S:268:CYS:HB3	2.04	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
2	А	95/136~(70%)	93~(98%)	2(2%)	0	100	100
2	В	95/136~(70%)	93~(98%)	2 (2%)	0	100	100
3	С	80/103~(78%)	78~(98%)	2 (2%)	0	100	100
3	D	78/103~(76%)	76 (97%)	2 (3%)	0	100	100
4	Ε	101/132~(76%)	101 (100%)	0	0	100	100
4	F	99/132~(75%)	99 (100%)	0	0	100	100
5	G	94/131~(72%)	90 (96%)	4 (4%)	0	100	100
5	Н	89/131~(68%)	87 (98%)	2 (2%)	0	100	100
8	М	684/1514 ($45%$)	627 (92%)	56 (8%)	1 (0%)	51	83
9	R	407/438 (93%)	401 (98%)	6 (2%)	0	100	100
10	S	200/280~(71%)	199 (100%)	1 (0%)	0	100	100
11	Т	441/463~(95%)	417 (95%)	23~(5%)	1 (0%)	47	79
11	V	430/463~(93%)	411 (96%)	19 (4%)	0	100	100
11	Х	440/463~(95%)	420 (96%)	20 (4%)	0	100	100
12	U	426/471~(90%)	414 (97%)	12 (3%)	0	100	100
12	W	429/471 (91%)	415 (97%)	14 (3%)	0	100	100
12	Y	445/471 (94%)	427 (96%)	18 (4%)	0	100	100
All	All	4633/6038 (77%)	4448 (96%)	183 (4%)	2(0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	М	1345	PRO
11	Т	161	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
2	А	84/113~(74%)	84 (100%)	0	100	100
2	В	84/113~(74%)	84 (100%)	0	100	100
3	С	68/81~(84%)	64 (94%)	4 (6%)	19	55
3	D	67/81~(83%)	64 (96%)	3 (4%)	27	62
4	Е	82/99~(83%)	80 (98%)	2 (2%)	49	75
4	F	80/99~(81%)	78~(98%)	2(2%)	47	75
5	G	83/109~(76%)	80 (96%)	3 (4%)	35	67
5	Н	78/109~(72%)	76~(97%)	2(3%)	46	74
8	М	574/1376~(42%)	518 (90%)	56 (10%)	8	36
9	R	372/396~(94%)	359~(96%)	13 (4%)	36	68
10	S	199/261~(76%)	193~(97%)	6 (3%)	41	71
11	Т	371/391~(95%)	343 (92%)	28 (8%)	13	45
11	V	368/391~(94%)	340 (92%)	28 (8%)	13	45
11	Х	374/391~(96%)	343 (92%)	31 (8%)	11	42
12	U	367/403~(91%)	335 (91%)	32 (9%)	10	41
12	W	369/403~(92%)	339 (92%)	30 (8%)	11	43
12	Y	372/403~(92%)	339 (91%)	33 (9%)	9	40
All	All	3992/5219~(76%)	3719 (93%)	273 (7%)	19	50

All (273) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	С	22	LEU
3	С	58	LEU
3	С	92	ARG
3	С	97	LEU
3	D	58	LEU
3	D	92	ARG
3	D	97	LEU



Mol	Chain	Res	Type
4	Е	18	ARG
4	Е	34	LEU
4	F	18	ARG
4	F	34	LEU
5	G	103	LEU
5	G	114	VAL
5	G	128	THR
5	Н	103	LEU
5	Н	114	VAL
8	М	686	VAL
8	М	693	ARG
8	М	696	LEU
8	М	756	VAL
8	М	757	LEU
8	М	764	PHE
8	М	806	VAL
8	М	833	ARG
8	М	836	ARG
8	М	845	THR
8	М	854	THR
8	М	860	LEU
8	М	867	LEU
8	М	932	ARG
8	М	934	LYS
8	М	937	VAL
8	М	971	LYS
8	М	999	PHE
8	М	1001	VAL
8	М	1004	ILE
8	М	1018	TYR
8	М	1040	LEU
8	М	1052	LYS
8	М	1054	LEU
8	М	1055	THR
8	М	1058	HIS
8	М	1066	THR
8	М	1068	VAL
8	М	1082	ASN
8	М	1085	LEU
8	М	1135	ILE
8	M	1138	LYS
8	М	1143	LEU



Mol	Chain	Res	Type
8	М	1158	ILE
8	М	1166	LEU
8	М	1188	VAL
8	М	1195	LEU
8	М	1199	LEU
8	М	1205	VAL
8	М	1209	THR
8	М	1229	THR
8	М	1238	LYS
8	М	1239	SER
8	М	1274	VAL
8	М	1278	LEU
8	М	1280	GLN
8	М	1282	LEU
8	М	1298	ILE
8	М	1313	ARG
8	М	1322	ARG
8	М	1328	ILE
8	М	1352	GLN
8	М	1358	ILE
8	М	1384	ASN
8	М	1386	LYS
8	М	1392	VAL
9	R	3	THR
9	R	15	ILE
9	R	63	LEU
9	R	66	LEU
9	R	70	GLU
9	R	120	PHE
9	R	128	LEU
9	R	149	THR
9	R	189	LEU
9	R	204	LEU
9	R	266	THR
9	R	345	VAL
9	R	406	THR
10	S	8	ILE
10	S	107	THR
10	S	126	VAL
10	S	182	THR
10	S	192	THR
10	S	254	SER



Mol	Chain	Res	Type
11	Т	42	LYS
11	Т	49	VAL
11	Т	70	MET
11	Т	115	VAL
11	Т	133	ILE
11	Т	148	THR
11	Т	159	TYR
11	Т	182	ASP
11	Т	186	TYR
11	Т	202	ILE
11	Т	241	LYS
11	Т	243	ILE
11	Т	244	VAL
11	Т	268	MET
11	Т	273	LEU
11	Т	274	LYS
11	Т	277	LYS
11	Т	278	THR
11	Т	312	GLU
11	Т	322	THR
11	Т	331	ASN
11	Т	336	VAL
11	Т	337	VAL
11	Т	364	ILE
11	Т	417	GLN
11	Т	435	VAL
11	Т	456	LEU
11	Т	461	ASN
12	U	15	LYS
12	U	29	LEU
12	U	69	ARG
12	U	111	LEU
12	U	115	GLU
12	U	118	THR
12	U	135	LEU
12	U	147	ARG
12	U	149	ILE
12	U	150	THR
12	U	153	HIS
12	U	154	LYS
12	U	158	LEU
12	U	183	LYS



Mol	Chain	Res	Type
12	U	191	SER
12	U	198	LYS
12	U	202	LEU
12	U	234	THR
12	U	236	VAL
12	U	252	GLN
12	U	257	LEU
12	U	266	ARG
12	U	273	ILE
12	U	296	ASP
12	U	298	VAL
12	U	320	ILE
12	U	339	SER
12	U	352	ILE
12	U	396	LEU
12	U	397	ARG
12	U	407	GLN
12	U	456	ILE
11	V	42	LYS
11	V	49	VAL
11	V	70	MET
11	V	115	VAL
11	V	133	ILE
11	V	148	THR
11	V	162	THR
11	V	182	ASP
11	V	186	TYR
11	V	202	ILE
11	V	241	LYS
11	V	243	ILE
11	V	244	VAL
11	V	268	MET
11	V	273	LEU
11	V	274	LYS
11	V	277	LYS
11	V	278	THR
11	V	312	GLU
11	V	322	THR
11	V	331	ASN
11	V	336	VAL
11	V	337	VAL
11	V	364	ILE



Mol	Chain	Res	Type
11	V	417	GLN
11	V	435	VAL
11	V	456	LEU
11	V	461	ASN
12	W	15	LYS
12	W	29	LEU
12	W	69	ARG
12	W	111	LEU
12	W	115	GLU
12	W	118	THR
12	W	135	LEU
12	W	147	ARG
12	W	158	LEU
12	W	183	LYS
12	W	191	SER
12	W	198	LYS
12	W	201	LYS
12	W	202	LEU
12	W	206	PHE
12	W	234	THR
12	W	236	VAL
12	W	252	GLN
12	W	257	LEU
12	W	266	ARG
12	W	273	ILE
12	W	296	ASP
12	W	298	VAL
12	W	320	ILE
12	W	339	SER
12	W	352	ILE
12	W	396	LEU
12	W	397	ARG
12	W	407	GLN
12	W	456	ILE
11	Х	42	LYS
11	Х	49	VAL
11	Х	70	MET
11	Х	115	VAL
11	Х	133	ILE
11	Х	148	THR
11	Х	153	GLU
11	Х	161	LYS



Mol	Chain	Res	Type
11	Х	162	THR
11	Х	163	ILE
11	Х	182	ASP
11	Х	186	TYR
11	Х	202	ILE
11	Х	241	LYS
11	Х	243	ILE
11	Х	244	VAL
11	Х	268	MET
11	Х	273	LEU
11	Х	274	LYS
11	Х	277	LYS
11	Х	278	THR
11	Х	312	GLU
11	Х	322	THR
11	Х	331	ASN
11	Х	336	VAL
11	Х	337	VAL
11	Х	364	ILE
11	Х	417	GLN
11	Х	435	VAL
11	Х	456	LEU
11	Х	461	ASN
12	Y	14	LEU
12	Y	15	LYS
12	Y	29	LEU
12	Y	69	ARG
12	Y	111	LEU
12	Y	115	GLU
12	Y	118	THR
12	Y	135	LEU
12	Y	158	LEU
12	Y	183	LYS
12	Y	191	SER
12	Y	198	LYS
12	Y	202	LEU
12	Y	213	ASP
12	Y	219	THR
12	Y	220	ARG
12	Y	221	PHE
12	Y	223	GLN
12	Y	234	THR



Mol	Chain	Res	Type
12	Y	236	VAL
12	Y	252	GLN
12	Y	257	LEU
12	Y	266	ARG
12	Y	273	ILE
12	Y	296	ASP
12	Y	298	VAL
12	Y	320	ILE
12	Y	339	SER
12	Y	352	ILE
12	Y	396	LEU
12	Ý	397	ARG
12	Y	407	GLN
12	Y	456	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
4	Е	42	GLN
4	F	39	ASN
4	F	42	GLN
4	F	115	ASN
5	G	52	HIS
5	Н	52	HIS
8	М	782	GLN
8	М	797	HIS
8	М	857	GLN
8	М	1126	ASN
8	М	1283	ASN
9	R	45	HIS
9	R	98	HIS
9	R	251	GLN
9	R	289	ASN
10	S	261	ASN
11	Т	124	ASN
11	Т	263	GLN
11	Т	271	GLN
11	Т	357	HIS
12	U	63	ASN
12	U	252	GLN
12	U	407	GLN
12	U	408	GLN



Mol	Chain	Res	Type
11	V	124	ASN
11	V	263	GLN
11	V	271	GLN
11	V	357	HIS
12	W	63	ASN
12	W	401	ASN
12	W	407	GLN
12	W	408	GLN
11	Х	124	ASN
11	Х	256	ASN
11	Х	263	GLN
11	Х	271	GLN
11	Х	357	HIS
12	Y	63	ASN
12	Y	252	GLN
12	Y	407	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).



Mal	Turne	Chain	Dec	Tinle	Bo	ond leng	ths	Bond angles		
IVIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
13	ADP	М	1601	14	24,29,29	0.96	1 (4%)	29,45,45	1.36	3 (10%)
13	ADP	Y	502	15	$24,\!29,\!29$	0.94	1 (4%)	29,45,45	1.39	4 (13%)
14	BEF	R	502	-	0,3,3	-	-	-		
14	BEF	М	1602	13	0,3,3	-	-	-		
13	ADP	U	502	15	$24,\!29,\!29$	0.98	1 (4%)	$29,\!45,\!45$	1.53	4 (13%)
13	ADP	Х	501	15	$24,\!29,\!29$	0.96	1 (4%)	29,45,45	1.47	4 (13%)
13	ADP	W	501	15	24,29,29	0.99	1 (4%)	29,45,45	1.46	4 (13%)
13	ADP	Т	501	15	24,29,29	0.96	1 (4%)	29,45,45	1.44	4 (13%)
13	ADP	V	501	15	24,29,29	0.96	1 (4%)	29,45,45	1.44	4 (13%)
13	ADP	R	501	15	24,29,29	0.96	1 (4%)	29,45,45	1.37	3 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	ADP	М	1601	14	-	6/12/32/32	0/3/3/3
13	ADP	Y	502	15	-	1/12/32/32	0/3/3/3
13	ADP	U	502	15	-	2/12/32/32	0/3/3/3
13	ADP	Х	501	15	-	2/12/32/32	0/3/3/3
13	ADP	W	501	15	-	0/12/32/32	0/3/3/3
13	ADP	Т	501	15	-	3/12/32/32	0/3/3/3
13	ADP	V	501	15	-	3/12/32/32	0/3/3/3
13	ADP	R	501	15	-	4/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms		Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
13	W	501	ADP	C5-C4	2.59	1.47	1.40
13	U	502	ADP	C5-C4	2.56	1.47	1.40
13	R	501	ADP	C5-C4	2.50	1.47	1.40
13	Х	501	ADP	C5-C4	2.50	1.47	1.40
13	М	1601	ADP	C5-C4	2.49	1.47	1.40
13	Y	502	ADP	C5-C4	2.48	1.47	1.40
13	V	501	ADP	C5-C4	2.45	1.47	1.40
13	Т	501	ADP	C5-C4	2.44	1.47	1.40

All (30) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
13	U	502	ADP	PA-O3A-PB	-3.78	119.84	132.83
13	Y	502	ADP	PA-O3A-PB	-3.73	120.02	132.83
13	W	501	ADP	PA-O3A-PB	-3.64	120.33	132.83
13	Y	502	ADP	N3-C2-N1	-3.39	123.38	128.68
13	Х	501	ADP	PA-O3A-PB	-3.37	121.25	132.83
13	М	1601	ADP	C3'-C2'-C1'	3.36	106.04	100.98
13	V	501	ADP	PA-O3A-PB	-3.34	121.35	132.83
13	R	501	ADP	C3'-C2'-C1'	3.34	106.01	100.98
13	Т	501	ADP	PA-O3A-PB	-3.31	121.48	132.83
13	U	502	ADP	C3'-C2'-C1'	3.29	105.93	100.98
13	Х	501	ADP	C3'-C2'-C1'	3.29	105.93	100.98
13	М	1601	ADP	N3-C2-N1	-3.25	123.60	128.68
13	Х	501	ADP	N3-C2-N1	-3.23	123.64	128.68
13	V	501	ADP	N3-C2-N1	-3.22	123.65	128.68
13	R	501	ADP	N3-C2-N1	-3.21	123.66	128.68
13	W	501	ADP	C3'-C2'-C1'	3.20	105.80	100.98
13	Т	501	ADP	C3'-C2'-C1'	3.16	105.73	100.98
13	U	502	ADP	N3-C2-N1	-3.15	123.75	128.68
13	W	501	ADP	N3-C2-N1	-3.14	123.77	128.68
13	Т	501	ADP	N3-C2-N1	-3.09	123.85	128.68
13	V	501	ADP	C3'-C2'-C1'	3.08	105.61	100.98
13	Т	501	ADP	C4-C5-N7	-2.90	106.37	109.40
13	V	501	ADP	C4-C5-N7	-2.70	106.58	109.40
13	U	502	ADP	C4-C5-N7	-2.68	106.61	109.40
13	R	501	ADP	C4-C5-N7	-2.65	106.63	109.40
13	Х	501	ADP	C4-C5-N7	-2.64	106.64	109.40
13	М	1601	ADP	C4-C5-N7	-2.58	106.71	109.40
13	Y	502	ADP	C3'-C2'-C1'	2.52	104.77	100.98
13	W	501	ADP	C4-C5-N7	-2.49	106.80	109.40
13	Y	502	ADP	C4-C5-N7	-2.43	106.87	109.40

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms
13	М	1601	ADP	PA-O3A-PB-O2B
13	М	1601	ADP	C5'-O5'-PA-O1A
13	М	1601	ADP	C5'-O5'-PA-O2A
13	R	501	ADP	C5'-O5'-PA-O1A
13	R	501	ADP	C5'-O5'-PA-O2A
13	R	501	ADP	C5'-O5'-PA-O3A
13	Т	501	ADP	C5'-O5'-PA-O1A
13	Т	501	ADP	C5'-O5'-PA-O2A



Mol	Chain	Res	Type	Atoms
13	V	501	ADP	C5'-O5'-PA-O1A
13	V	501	ADP	C5'-O5'-PA-O2A
13	Х	501	ADP	C5'-O5'-PA-O3A
13	Y	502	ADP	C5'-O5'-PA-O1A
13	U	502	ADP	O4'-C4'-C5'-O5'
13	U	502	ADP	C3'-C4'-C5'-O5'
13	Т	501	ADP	C5'-O5'-PA-O3A
13	Х	501	ADP	C5'-O5'-PA-O1A
13	М	1601	ADP	PA-O3A-PB-O1B
13	R	501	ADP	C3'-C4'-C5'-O5'
13	М	1601	ADP	C5'-O5'-PA-O3A
13	V	501	ADP	C5'-O5'-PA-O3A
13	М	1601	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	М	1601	ADP	3	0
13	Х	501	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

















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-4396. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections (i)

6.1.1 Primary map



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

6.2 Central slices (i)

6.2.1 Primary map



X Index: 192

Y Index: 192



Z Index: 192

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: 207

Z Index: 154

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0359. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



6.5 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 773 $\rm nm^3;$ this corresponds to an approximate mass of 699 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 0.278 $\mathrm{\AA^{-1}}$



8 Fourier-Shell correlation (i)

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



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4396 and PDB model 6GEN. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.0359 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 (0.0359).



9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.



1.0

0.0 <0.0

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0359) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8229	0.1950
А	0.8403	0.2140
В	0.8506	0.2570
С	0.8368	0.2540
D	0.8219	0.2200
E	0.8627	0.2360
F	0.8399	0.2110
G	0.8468	0.2050
Н	0.8407	0.2100
Ι	0.8933	0.1780
J	0.8688	0.1740
М	0.8823	0.2540
R	0.8887	0.2410
S	0.8513	0.2350
Т	0.7376	0.1230
U	0.8177	0.2130
V	0.8578	0.2770
W	0.8711	0.2680
Х	0.6409	0.0630
Y	0.6728	0.0610
Z	0.8855	0.1990

