

Feb 11, 2023 – 02:30 PM EST

PDB I	D	: 8E5O
EMDB I	D	: EMD-27916
Tit	le	: Escherichia coli Rho-dependent transcription pre-termination complex con-
		taining 24 nt long RNA spacer, Mg-ADP-BeF3, and NusG; TEC part
Author	\mathbf{rs}	: Molodtsov, V.; Wang, C.
Deposited of	n	: 2022-08-22
Resolutio	n	: $4.40 \text{ Å}(\text{reported})$
This	s is a	a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/EMValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1. dev 43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 4.40 Å.

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



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM} {f structures} \ (\#{f Entries})$
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		Qua	lity of chain		
1	5	60	18%	28%	8%	45%	
2	6	60	23%	33%	5%	38%	
3	7	41	27%	15%		59%	
4	А	1342	•	81%			17% •
5	В	1407	•	67%		25%	• 5%
6	С	329		62%	59	% 339	%
6	D	329		54%	12%	34%	, 0



Mol	Chain	Length	Quality of ch	ain	
7	Е	91	67%	14%	• 18%
8	F	181	• 59%	22%	7% • 11%



2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 39229 atoms, of which 11229 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 DNA chain called NT DNA.

Mol	Chain	Residues			AltConf	Trace				
1	5	33	Total 913	C 322	Н 237	N 125	0 196	Р 33	0	0

• Molecule 2 is a DNA chain called T DNA.

Mol	Chain	Residues			AltConf	Trace				
2	6	37	Total 1031	C 357	Н 283	N 126	0 228	Р 37	0	0

• Molecule 3 is a RNA chain called RNA with 24 nt long spacer.

Mol	Chain	Residues		L	AltConf	Trace				
3	7	17	Total 464	C 163	Н 97	N 64	0 123	Р 17	0	0

• Molecule 4 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues		Α	AltConf	Trace			
4	А	1340	Total	С	N	0	S	0	0
	_		10567	6631	1841	2052	43		

• Molecule 5 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues			AltConf	Trace				
5	В	1335	Total 21000	C 6526	Н 10612	N 1854	O 1958	S 50	0	0

• Molecule 6 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues		Ate	AltConf	Trace			
6	С	221	Total 1698	C 1060	N 299	O 333	S 6	0	0



Mol	Chain	Residues		At	AltConf	Trace			
6	D	218	Total 1677	C 1048	N 297	O 326	S 6	0	0

• Molecule 7 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Е	75	Total 600	$\begin{array}{c} \mathrm{C} \\ 365 \end{array}$	N 114	O 120	S 1	0	0

• Molecule 8 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	161	Total 1276	C 813	N 221	0 235	${f S}{7}$	0	0

• Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
9	В	1	Total Mg 1 1	0

• Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
10	В	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.

- Chain 5: 18% 28% 8% 45% 5555 • Molecule 2: T DNA Chain 6: 23% 33% 5% 38% 33 33 637 138 05 05 05 05 07 07 • Molecule 3: RNA with 24 nt long spacer Chain 7: 27% 15% 59% U U U26 U26 • Molecule 4: DNA-directed RNA polymerase subunit beta Chain A: 81% 17%
- Molecule 1: NT DNA





• Molecule 5: DNA-directed RNA polymerase subunit beta'



MET SER GLU ALA

E1.2.93 E1.2.93 E1.158 R.1306 G1161 1.1306 G1166 1.1306 G1166 1.1306 G1166 R.1310 G1166 R.1311 E1188 R.1311 E1168 R.1312 E1168 R.1317 E1168 R.1324 E1175 R.1324 E1175 R.1324 E1176 R.1324 E1176 R.1324 E1176 R.1332 P1190 V1337 R1173 V1337 R1176 V1337 R1126 V1337 R1190 V1337 R1190 V1337 R1190 V1337 R1190 V1358 H1224 R1369 H1224 R1360 R1220 R1361 R1223 R1360 R1224 R1373 R1220 R1360 R1224 R1373 R1224</

ALA SER ALA SER ALA CLEU ALA CLEU CLEU CLY GLY SER ASP ASP ASP ASP CLU

• Molecule 6: DNA-directed RNA polymerase subunit alpha



• Molecule 6: DNA-directed RNA polymerase subunit alpha







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	270373	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)	1250	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.026	Depositor
Minimum map value	-0.005	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0041	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles $(^{\circ})$	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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: ZN, 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	Bo	ond lengths	B	ond angles
WIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	5	1.12	8/757~(1.1%)	0.95	1/1163~(0.1%)
2	6	1.12	5/834~(0.6%)	1.44	7/1283~(0.5%)
3	7	0.63	1/410~(0.2%)	0.80	0/638
4	А	0.43	1/10736~(0.0%)	0.61	2/14487~(0.0%)
5	В	0.52	3/10545~(0.0%)	0.66	5/14236~(0.0%)
6	С	0.41	0/1718	0.62	0/2328
6	D	0.36	0/1696	0.62	0/2298
7	Ε	0.34	0/602	0.58	0/810
8	F	0.36	0/1304	0.54	1/1759~(0.1%)
All	All	0.52	18/28602~(0.1%)	0.68	16/39002~(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
5	В	0	5
6	С	0	1
6	D	0	1
All	All	0	7

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
5	В	88	CYS	CB-SG	-10.14	1.65	1.82
1	5	109	DT	O3'-P	8.72	1.71	1.61
4	А	920	VAL	C-N	8.41	1.50	1.34
2	6	10	DG	C1'-N9	-8.14	1.35	1.47
1	5	121	DG	C1'-N9	-7.24	1.37	1.47
3	7	40	G	C1'-N9	-7.15	1.36	1.46



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	6	26	DT	O3'-P	6.91	1.69	1.61
1	5	112	DG	C1'-N9	-6.68	1.37	1.47
1	5	100	DA	C1'-N9	-6.46	1.38	1.47
2	6	21	DA	C1'-N9	-6.45	1.38	1.47
1	5	95	DA	C1'-N9	-6.44	1.38	1.47
5	В	93	THR	CA-C	6.24	1.69	1.52
1	5	116	DG	C1'-N9	-6.19	1.38	1.47
1	5	115	DA	C1'-N9	-6.03	1.38	1.47
5	В	70	CYS	CA-CB	-5.91	1.41	1.53
1	5	89	DG	C1'-N9	-5.58	1.39	1.47
2	6	29	DT	C1'-N1	5.26	1.56	1.49
2	6	24	DT	C1'-N1	5.25	1.56	1.49

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	6	27	DG	O3'-P-O5'	23.18	148.03	104.00
2	6	27	DG	OP1-P-O3'	-20.70	59.66	105.20
2	6	28	DA	P-O3'-C3'	13.78	136.23	119.70
2	6	28	DA	O3'-P-O5'	11.60	126.05	104.00
5	В	271	ARG	NE-CZ-NH2	-9.31	115.64	120.30
2	6	28	DA	OP1-P-O3'	-6.75	90.35	105.20
2	6	26	DT	P-O3'-C3'	6.52	127.52	119.70
1	5	109	DT	P-O3'-C3'	6.39	127.37	119.70
2	6	27	DG	P-O3'-C3'	6.15	127.08	119.70
8	F	122	PRO	N-CA-CB	5.90	110.38	103.30
5	В	903	LEU	C-N-CA	5.75	136.09	121.70
5	В	363	LEU	CA-CB-CG	5.59	128.17	115.30
4	А	920	VAL	C-N-CD	-5.55	108.39	120.60
4	А	516	ASP	CB-CG-OD2	5.27	123.05	118.30
5	В	807	LEU	CB-CG-CD2	-5.10	102.33	111.00
5	В	73	GLY	N-CA-C	5.06	125.74	113.10

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	В	1184	ASP	Peptide
5	В	1326	GLN	Peptide
5	В	313	GLY	Peptide
5	В	416	ILE	Peptide
5	В	804	ALA	Peptide



Continued from previous page...

Mol	Chain	Res	Type	Group
6	С	192	VAL	Peptide
6	D	20	SER	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	5	676	237	372	42	0
2	6	748	283	419	36	0
3	7	367	97	180	45	0
4	А	10567	0	10584	241	0
5	В	10388	10612	10611	369	0
6	С	1698	0	1718	10	0
6	D	1677	0	1713	23	0
7	Е	600	0	607	12	0
8	F	1276	0	1247	68	0
9	В	1	0	0	0	0
10	В	2	0	0	0	0
All	All	28000	11229	27451	733	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 13.

All (733) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:123:ARG:HB2	8:F:124:PRO:CD	1.45	1.46
8:F:129:GLU:HB3	8:F:130:PRO:CD	1.45	1.42
4:A:920:VAL:HG22	4:A:921:PRO:CD	1.51	1.37
4:A:854:ILE:CG2	4:A:917:SER:HB3	1.52	1.36
4:A:857:VAL:CG1	4:A:919:ARG:HH21	1.39	1.34
4:A:888:THR:O	4:A:890:LYS:HD2	1.17	1.23
4:A:880:GLY:HA2	4:A:921:PRO:O	1.37	1.21
8:F:129:GLU:CB	8:F:130:PRO:HD3	1.71	1.20
8:F:47:GLU:HG3	8:F:64:PHE:CE1	1.80	1.16
4:A:845:LEU:HD11	4:A:909:LYS:HZ3	1.10	1.15



	in a second	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:A:895:LEU:HD21	5:B:69:GLU:OE2	1.45	1.15
4:A:857:VAL:HG12	4:A:919:ARG:HH21	1.08	1.12
4:A:856:ASN:ND2	4:A:915:ASP:O	1.82	1.12
8:F:47:GLU:HG3	8:F:64:PHE:HE1	1.01	1.11
4:A:920:VAL:CG2	4:A:921:PRO:HD3	1.80	1.09
4:A:854:ILE:HG23	4:A:917:SER:HB3	1.15	1.09
4:A:920:VAL:CG2	4:A:921:PRO:CD	2.30	1.07
4:A:854:ILE:CG2	4:A:917:SER:CB	2.31	1.07
5:B:24:LEU:HG	5:B:232:ASN:HD21	1.17	1.06
4:A:920:VAL:HG13	4:A:921:PRO:HD2	1.37	1.06
8:F:123:ARG:HB2	8:F:124:PRO:HD3	1.08	1.04
8:F:123:ARG:CB	8:F:124:PRO:CD	2.33	1.04
4:A:888:THR:O	4:A:890:LYS:CD	2.04	1.04
4:A:857:VAL:CG1	4:A:919:ARG:NH2	2.19	1.04
4:A:880:GLY:CA	4:A:921:PRO:O	2.07	1.03
4:A:857:VAL:HG13	4:A:919:ARG:HH21	1.23	1.02
3:7:32:U:H5'	4:A:1259:LEU:HD21	1.40	1.02
4:A:895:LEU:CD2	5:B:69:GLU:OE2	2.07	1.01
4:A:854:ILE:HG21	4:A:917:SER:CB	1.88	1.01
4:A:920:VAL:CG1	4:A:921:PRO:HD2	1.89	1.00
8:F:123:ARG:HD3	8:F:124:PRO:HD2	1.36	1.00
4:A:549:ASP:OD2	5:B:750:PRO:HB3	1.60	0.99
4:A:920:VAL:HG22	4:A:921:PRO:HD3	1.00	0.99
4:A:1268:GLN:NE2	5:B:352:ARG:HD2	1.79	0.97
8:F:47:GLU:CG	8:F:64:PHE:HE1	1.76	0.97
3:7:32:U:OP1	4:A:1250:SER:OG	1.83	0.96
5:B:111:THR:HG23	5:B:300:GLN:CD	1.86	0.96
1:5:94:DG:O6	2:6:30:DC:N4	1.99	0.95
2:6:15:DC:N4	2:6:16:DC:N4	2.15	0.94
4:A:914:LYS:NZ	4:A:916:SER:OG	2.00	0.94
5:B:68:TYR:O	5:B:75:TYR:CE2	2.20	0.94
4:A:855:PRO:HG3	4:A:915:ASP:CG	1.88	0.94
4:A:879:GLY:O	4:A:922:ASN:HB3	1.68	0.94
4:A:857:VAL:HG13	4:A:919:ARG:NH2	1.80	0.93
4:A:641:GLU:OE2	5:B:749:LYS:NZ	2.00	0.93
4:A:854:ILE:HG21	4:A:917:SER:HB3	1.46	0.92
4:A:920:VAL:HG22	4:A:921:PRO:HD2	1.50	0.91
4:A:920:VAL:CG2	4:A:921:PRO:HD2	1.97	0.91
8:F:114:ARG:HB2	8:F:119:GLY:HA2	1.49	0.91
8:F:123:ARG:HB2	8:F:124:PRO:HD2	1.49	0.91
4:A:845:LEU:HD11	4:A:909:LYS:NZ	1.85	0.91



	jue pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
5:B:136:GLU:OE1	5:B:312:ARG:NH1	2.04	0.90
4:A:920:VAL:CB	4:A:921:PRO:HD2	2.03	0.89
4:A:845:LEU:CD1	4:A:909:LYS:HZ3	1.86	0.89
5:B:24:LEU:HB2	5:B:232:ASN:OD1	1.72	0.89
5:B:202:ARG:HG2	5:B:202:ARG:HH11	1.35	0.88
4:A:857:VAL:HG12	4:A:919:ARG:NH2	1.82	0.87
1:5:114:DC:H5"	5:B:1148:ARG:NH2	1.87	0.87
5:B:24:LEU:HG	5:B:232:ASN:ND2	1.90	0.87
5:B:290:ILE:CG2	8:F:93:ILE:HG22	2.03	0.87
4:A:879:GLY:C	4:A:922:ASN:HB3	1.96	0.86
5:B:68:TYR:O	5:B:75:TYR:HE2	1.58	0.85
5:B:425:ARG:NH1	5:B:458:ASN:O	2.08	0.85
4:A:808:ASN:H	5:B:633:ALA:HB2	1.41	0.85
4:A:920:VAL:CB	4:A:921:PRO:CD	2.56	0.84
5:B:68:TYR:HB3	5:B:75:TYR:OH	1.76	0.84
5:B:68:TYR:C	5:B:75:TYR:HE2	1.80	0.84
4:A:888:THR:H	4:A:889:PRO:HD2	1.42	0.83
5:B:26:SER:HB2	5:B:236:TRP:CZ2	2.12	0.83
8:F:130:PRO:HG3	8:F:151:VAL:HG22	1.59	0.83
4:A:845:LEU:HD21	4:A:912:ASP:OD1	1.79	0.83
1:5:95:DA:H8	1:5:95:DA:H5"	1.43	0.82
4:A:898:GLU:HB2	4:A:901:LEU:HB2	1.61	0.82
2:6:21:DA:N1	3:7:36:G:N2	2.26	0.82
5:B:111:THR:HG23	5:B:300:GLN:OE1	1.81	0.81
8:F:129:GLU:CB	8:F:130:PRO:CD	2.36	0.81
8:F:123:ARG:CD	8:F:124:PRO:HD2	2.10	0.81
2:6:21:DA:N1	3:7:36:G:C2	2.49	0.81
4:A:888:THR:H	4:A:889:PRO:CD	1.92	0.81
1:5:89:DG:C2	2:6:36:DG:C2	2.69	0.81
5:B:141:PHE:CE2	5:B:296:LYS:HB2	2.15	0.81
5:B:87:LYS:HA	5:B:87:LYS:HE3	1.63	0.80
5:B:1169:THR:OG1	5:B:1192:LYS:NZ	2.13	0.80
4:A:618:GLN:HG3	5:B:770:LEU:HD13	1.61	0.80
5:B:141:PHE:HE2	5:B:296:LYS:HB2	1.45	0.80
2:6:18:DC:H42	3:7:38:G:H1	1.27	0.80
5:B:37:GLU:O	5:B:61:ILE:HD11	1.81	0.79
5:B:144:TYR:HE1	5:B:162:GLU:OE2	1.64	0.79
8:F:116:GLN:HA	8:F:116:GLN:NE2	1.98	0.79
4:A:845:LEU:CD2	4:A:912:ASP:OD1	2.31	0.78
1:5:96:DT:H1'	1:5:97:DC:H5'	1.66	0.78
4:A:903:ARG:NE	4:A:903:ARG:H	1.82	0.78



	h a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
5:B:90:VAL:O	5:B:90:VAL:HG13	1.81	0.78
5:B:186:GLN:HG3	5:B:238:ILE:HG13	1.65	0.78
2:6:30:DC:OP2	2:6:30:DC:H6	1.67	0.77
5:B:123:ARG:HG3	5:B:1337:VAL:HG11	1.67	0.77
5:B:1075:ARG:NH2	5:B:1168:GLU:OE2	2.17	0.77
2:6:15:DC:C4	2:6:16:DC:N4	2.53	0.76
5:B:110:PRO:HG2	5:B:183:GLU:HG3	1.68	0.75
8:F:129:GLU:HB3	8:F:130:PRO:HD3	0.77	0.75
5:B:202:ARG:HG2	5:B:202:ARG:NH1	2.00	0.74
2:6:18:DC:N3	3:7:38:G:N2	2.31	0.74
8:F:123:ARG:CD	8:F:123:ARG:H	1.99	0.74
8:F:129:GLU:OE2	8:F:148:VAL:HG11	1.86	0.74
5:B:44:ILE:HD12	5:B:252:LEU:CD2	2.18	0.74
1:5:115:DA:OP1	5:B:1148:ARG:NE	2.21	0.73
5:B:210:SER:HB3	5:B:213:LYS:HB2	1.70	0.73
3:7:35:U:H4'	5:B:322:ARG:CD	2.18	0.72
5:B:44:ILE:HD12	5:B:252:LEU:HD21	1.71	0.72
5:B:120:LEU:O	5:B:1330:ARG:NH1	2.21	0.72
5:B:142:GLU:HG3	5:B:142:GLU:O	1.89	0.72
5:B:157:GLN:HA	5:B:157:GLN:OE1	1.89	0.72
5:B:107:LEU:HD11	5:B:242:LEU:HB2	1.70	0.72
5:B:220:ARG:HG2	5:B:220:ARG:HH11	1.55	0.72
2:6:21:DA:C6	3:7:36:G:N2	2.57	0.72
5:B:211:GLU:HG2	5:B:215:LYS:HE3	1.70	0.72
5:B:105:ILE:HD12	5:B:242:LEU:HD22	1.71	0.71
8:F:130:PRO:HG3	8:F:151:VAL:CG2	2.21	0.71
3:7:32:U:C5'	4:A:1259:LEU:HD21	2.21	0.71
5:B:1143:ASP:OD1	5:B:1148:ARG:NH1	2.21	0.70
4:A:1268:GLN:HE22	5:B:352:ARG:HD2	1.55	0.70
4:A:65:ASN:HB3	4:A:105:TYR:HB2	1.73	0.70
2:6:27:DG:OP1	8:F:18:PHE:CE1	2.45	0.69
3:7:35:U:H4'	5:B:322:ARG:HD2	1.73	0.69
4:A:1332:SER:O	5:B:243:PRO:HG2	1.93	0.69
8:F:159:LYS:HA	8:F:172:GLU:HA	1.75	0.69
6:D:48:LEU:HB2	6:D:183:ILE:HD11	1.75	0.68
8:F:123:ARG:CB	8:F:124:PRO:HD3	2.04	0.68
5:B:39:LYS:O	5:B:273:ILE:CG2	2.41	0.68
5:B:54:ASP:OD1	5:B:54:ASP:N	2.24	0.68
2:6:8:DC:C6	2:6:9:DT:H72	2.28	0.68
4:A:879:GLY:C	4:A:922:ASN:CB	2.62	0.68
5:B:128:LEU:HD11	5:B:189:LEU:HG	1.73	0.68



	had page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
5:B:141:PHE:CD2	5:B:293:ARG:O	2.47	0.68
5:B:117:LEU:O	5:B:117:LEU:HD12	1.94	0.68
8:F:132:GLU:OE2	8:F:134:VAL:HG12	1.94	0.68
5:B:161:THR:HG22	5:B:164:GLN:HB2	1.76	0.68
4:A:887:VAL:HG12	4:A:917:SER:HA	1.75	0.67
2:6:16:DC:H1'	5:B:426:ALA:HB1	1.77	0.67
8:F:115:LEU:HD12	8:F:123:ARG:HH21	1.59	0.67
2:6:21:DA:C2	3:7:36:G:N2	2.61	0.67
2:6:27:DG:OP1	8:F:18:PHE:HE1	1.78	0.67
4:A:895:LEU:HD22	4:A:895:LEU:H	1.59	0.67
5:B:94:GLN:HB2	5:B:97:VAL:HG23	1.75	0.67
5:B:1355:ARG:NH1	5:B:1369:ARG:HH12	1.93	0.67
8:F:114:ARG:HG3	8:F:114:ARG:O	1.94	0.67
5:B:68:TYR:HB3	5:B:75:TYR:HH	1.59	0.67
5:B:108:ALA:HB3	5:B:279:LEU:HD22	1.77	0.67
5:B:984:LEU:HB3	5:B:993:GLU:HB2	1.76	0.67
3:7:41:G:OP1	4:A:1073:LYS:NZ	2.25	0.66
5:B:1037:PHE:HB3	5:B:1040:MET:HB2	1.78	0.66
8:F:115:LEU:O	8:F:115:LEU:HG	1.93	0.66
4:A:920:VAL:HG13	4:A:921:PRO:CD	2.19	0.66
4:A:845:LEU:CD1	4:A:909:LYS:NZ	2.53	0.66
5:B:84:ILE:HG13	5:B:84:ILE:O	1.96	0.66
5:B:108:ALA:CB	5:B:279:LEU:HD22	2.25	0.66
5:B:290:ILE:HG22	8:F:93:ILE:HG22	1.78	0.66
5:B:193:ASP:HB3	5:B:196:GLN:HB2	1.78	0.66
5:B:978:ARG:HG2	5:B:1197:ASN:HD21	1.60	0.65
5:B:68:TYR:C	5:B:75:TYR:CE2	2.65	0.65
4:A:888:THR:N	4:A:889:PRO:CD	2.59	0.65
3:7:29:A:H5"	3:7:29:A:N3	2.11	0.64
4:A:813:GLU:HB2	5:B:461:PHE:HD2	1.61	0.64
5:B:975:ILE:HG22	5:B:977:SER:H	1.62	0.64
3:7:29:A:N3	3:7:29:A:H3'	2.13	0.64
4:A:848:GLU:HG2	4:A:888:THR:HG21	1.80	0.64
5:B:141:PHE:HD2	5:B:293:ARG:O	1.80	0.64
5:B:832:LYS:C	5:B:1242:ARG:HH12	2.01	0.64
4:A:528:ARG:NH2	4:A:576:SER:O	2.30	0.64
5:B:68:TYR:HB3	5:B:75:TYR:CE2	2.32	0.64
4:A:314:ASN:HD21	4:A:348:SER:HA	1.62	0.64
4:A:1280:ALA:HB1	5:B:918:ILE:HG22	1.79	0.64
5:B:162:GLU:HA	5:B:162:GLU:OE1	1.97	0.63
5:B:395:LYS:HZ2	5:B:399:LYS:CD	2.10	0.63



	h a c	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:6:27:DG:H2"	2:6:28:DA:OP2	1.97	0.63
5:B:67:ASP:OD1	5:B:95:THR:OG1	2.15	0.63
5:B:245:LEU:HG	5:B:246:PRO:HD2	1.80	0.63
8:F:129:GLU:HG3	8:F:151:VAL:HG13	1.79	0.63
8:F:130:PRO:HA	8:F:148:VAL:HG12	1.81	0.63
1:5:101:DT:OP2	5:B:275:ARG:NH2	2.31	0.63
4:A:879:GLY:O	4:A:922:ASN:CB	2.45	0.63
4:A:1282:GLY:HA3	7:E:17:PHE:HE1	1.63	0.63
5:B:44:ILE:CD1	5:B:252:LEU:HD21	2.29	0.63
1:5:98:DA:C2'	1:5:99:DT:H72	2.28	0.62
1:5:100:DA:H4'	8:F:16:SER:OG	1.98	0.62
1:5:92:DA:C2	2:6:33:DG:C2	2.87	0.62
2:6:15:DC:N4	2:6:16:DC:H41	1.96	0.62
5:B:92:VAL:HG12	5:B:92:VAL:O	1.99	0.62
1:5:95:DA:H2"	1:5:96:DT:H5'	1.81	0.62
3:7:32:U:OP1	4:A:1250:SER:CB	2.48	0.62
5:B:68:TYR:HD2	5:B:75:TYR:HH	1.47	0.62
8:F:123:ARG:CB	8:F:124:PRO:HD2	2.13	0.62
4:A:55:SER:OG	4:A:465:ARG:NH1	2.33	0.62
4:A:1287:LEU:HD13	5:B:1357:ILE:HD11	1.81	0.62
5:B:201:LEU:HB2	5:B:221:ILE:HD13	1.80	0.62
6:D:211:ILE:HG12	6:D:219:ARG:HH12	1.65	0.62
4:A:618:GLN:CG	5:B:770:LEU:HD13	2.30	0.62
4:A:880:GLY:N	4:A:921:PRO:O	2.32	0.61
4:A:1328:LYS:HE2	5:B:100:GLU:HA	1.82	0.61
5:B:1355:ARG:NH1	5:B:1369:ARG:NH1	2.47	0.61
5:B:68:TYR:HB3	5:B:75:TYR:CZ	2.35	0.61
5:B:111:THR:CG2	5:B:300:GLN:NE2	2.63	0.61
2:6:15:DC:C4	2:6:16:DC:C4	2.89	0.61
5:B:90:VAL:O	5:B:90:VAL:CG1	2.48	0.61
5:B:223:LEU:O	5:B:223:LEU:HG	2.00	0.61
4:A:120:GLN:NE2	4:A:490:GLN:OE1	2.32	0.61
8:F:123:ARG:H	8:F:123:ARG:HD2	1.65	0.61
1:5:110:DA:N7	4:A:183:TRP:CH2	2.69	0.60
5:B:154:LEU:HD21	5:B:160:LEU:HD21	1.83	0.60
4:A:806:PRO:O	5:B:633:ALA:HA	2.01	0.60
4:A:1072:ASN:ND2	4:A:1111:GLN:OE1	2.34	0.60
1:5:94:DG:C2	1:5:95:DA:C2	2.89	0.60
5:B:395:LYS:NZ	5:B:399:LYS:HD3	2.15	0.60
5:B:951:GLN:NE2	5:B:1014:GLY:O	2.35	0.60
6:D:112:ALA:HB3	6:D:126:PRO:HA	1.83	0.60



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:A:895:LEU:HD21	5:B:69:GLU:CD	2.18	0.60
5:B:67:ASP:OD1	5:B:67:ASP:N	2.34	0.60
5:B:370:LYS:HG2	5:B:441:LEU:HD23	1.84	0.60
5:B:412:LEU:HD22	5:B:441:LEU:HD21	1.84	0.60
5:B:1161:GLY:HA3	5:B:1179:PRO:HA	1.83	0.60
8:F:134:VAL:N	8:F:146:GLY:O	2.33	0.60
8:F:106:LYS:HD2	8:F:106:LYS:O	2.01	0.60
1:5:95:DA:H5"	1:5:95:DA:C8	2.31	0.59
5:B:24:LEU:CG	5:B:232:ASN:ND2	2.63	0.59
5:B:926:PRO:HG2	5:B:1248:ILE:HD11	1.84	0.59
8:F:126:THR:HG22	8:F:130:PRO:HG2	1.84	0.59
4:A:69:GLN:HE21	4:A:101:ARG:HD2	1.67	0.59
5:B:416:ILE:HG13	5:B:441:LEU:HD11	1.83	0.59
6:C:45:ARG:HD3	6:D:38:THR:HB	1.83	0.59
4:A:1101:LEU:HD23	5:B:725:MET:SD	2.42	0.59
3:7:32:U:H5'	4:A:1259:LEU:CD2	2.24	0.59
5:B:342:LEU:HD23	5:B:1352:ILE:HG23	1.83	0.59
5:B:395:LYS:HZ2	5:B:399:LYS:HD3	1.66	0.59
5:B:99:ARG:NH1	5:B:99:ARG:HG3	2.18	0.59
5:B:118:LYS:HD2	5:B:312:ARG:NH2	2.17	0.59
4:A:901:LEU:HD21	4:A:904:ALA:HB2	1.83	0.59
5:B:144:TYR:CE1	5:B:162:GLU:OE2	2.51	0.59
1:5:99:DT:H2"	1:5:100:DA:H5"	1.85	0.59
5:B:638:SER:OG	5:B:639:VAL:N	2.36	0.59
4:A:1284:ALA:HB3	5:B:1361:THR:HB	1.85	0.58
4:A:707:ALA:O	4:A:711:ASP:HB2	2.03	0.58
5:B:111:THR:CG2	5:B:300:GLN:CD	2.66	0.58
5:B:201:LEU:HD11	5:B:220:ARG:HH11	1.67	0.58
8:F:47:GLU:CG	8:F:64:PHE:CE1	2.64	0.58
4:A:918:LEU:HD23	4:A:918:LEU:O	2.02	0.58
5:B:161:THR:HG23	5:B:164:GLN:H	1.68	0.58
5:B:136:GLU:CD	5:B:312:ARG:HH22	2.06	0.58
5:B:37:GLU:O	5:B:61:ILE:CD1	2.52	0.58
5:B:514:THR:HG21	5:B:596:LEU:HD12	1.84	0.58
5:B:615:LYS:HG2	7:E:5:THR:HG21	1.85	0.58
8:F:106:LYS:HD2	8:F:106:LYS:C	2.24	0.58
2:6:18:DC:N4	3:7:38:G:H1	1.99	0.58
5:B:491:LEU:HB2	5:B:904:ALA:HA	1.86	0.58
8:F:112:MET:HA	8:F:115:LEU:HB3	1.86	0.58
1:5:88:DC:O2	2:6:37:DG:N2	2.37	0.58
5:B:510:LEU:HD22	5:B:601:ILE:HD12	1.86	0.57



	h h	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
5:B:97:VAL:HG11	5:B:101:ARG:NH2	2.18	0.57
5:B:275:ARG:NH1	5:B:278:ARG:NH1	2.51	0.57
4:A:1142:ARG:NH1	4:A:1161:LEU:O	2.36	0.57
5:B:124:ILE:O	5:B:124:ILE:HG22	2.04	0.57
5:B:241:VAL:HG12	5:B:241:VAL:O	2.04	0.57
1:5:115:DA:OP2	5:B:1148:ARG:HG3	2.04	0.57
4:A:1122:LYS:NZ	4:A:1126:ASP:OD1	2.38	0.57
5:B:741:ALA:O	5:B:762:ASN:ND2	2.38	0.57
4:A:516:ASP:OD1	4:A:516:ASP:O	2.23	0.57
4:A:1268:GLN:HE21	5:B:352:ARG:HD2	1.68	0.57
3:7:38:G:OP2	4:A:540:ARG:NH1	2.37	0.57
5:B:903:LEU:HD21	5:B:1249:ASN:HD22	1.70	0.57
5:B:1046:ILE:HD12	5:B:1059:LEU:HB3	1.86	0.57
6:C:82:LEU:HD11	6:C:171:LEU:HD23	1.86	0.57
4:A:1142:ARG:NH2	4:A:1166:ASP:OD1	2.38	0.56
5:B:99:ARG:CG	5:B:99:ARG:HH11	2.18	0.56
5:B:198:CYS:HA	5:B:221:ILE:HD11	1.86	0.56
2:6:21:DA:N6	3:7:36:G:H1	2.04	0.56
5:B:74:LYS:HD2	5:B:85:CYS:SG	2.45	0.56
5:B:160:LEU:HD22	5:B:164:GLN:HB3	1.86	0.56
5:B:39:LYS:O	5:B:273:ILE:HG21	2.06	0.56
4:A:839:VAL:HG12	4:A:1049:ILE:HG12	1.87	0.56
4:A:985:GLU:HB3	4:A:988:LYS:HB2	1.88	0.56
5:B:343:LEU:HD11	5:B:1324:SER:HB3	1.87	0.56
3:7:27:U:O2	3:7:27:U:H5'	2.05	0.55
5:B:102:MET:HG2	5:B:246:PRO:HG3	1.87	0.55
5:B:247:PRO:HA	5:B:250:ARG:HG3	1.87	0.55
6:C:28:LEU:HD22	6:C:201:LEU:HD23	1.88	0.55
4:A:818:VAL:HG22	4:A:1096:ILE:HG12	1.87	0.55
4:A:1101:LEU:HD21	5:B:508:LEU:HD22	1.88	0.55
5:B:171:GLU:HA	5:B:171:GLU:OE1	2.05	0.55
4:A:633:LEU:HD13	4:A:644:LEU:HD23	1.89	0.55
4:A:855:PRO:HG3	4:A:915:ASP:OD1	2.06	0.55
1:5:89:DG:N2	2:6:36:DG:C2	2.75	0.55
5:B:1175:LEU:HD22	5:B:1190:ILE:HD11	1.88	0.55
8:F:116:GLN:HA	8:F:116:GLN:HE21	1.69	0.55
3:7:32:U:P	4:A:1250:SER:HG	2.26	0.55
5:B:136:GLU:OE1	5:B:312:ARG:CZ	2.55	0.55
3:7:41:G:O2'	5:B:425:ARG:NH2	2.40	0.54
4:A:103:VAL:HB	4:A:114:VAL:HG11	1.89	0.54
4:A:143:ARG:NH2	4:A:512:SER:O	2.40	0.54



	h a c	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:A:29:SER:O	4:A:33:ASP:HB2	2.07	0.54
4:A:360:LEU:HD13	4:A:378:ARG:HH11	1.72	0.54
5:B:833:GLU:HB2	5:B:1242:ARG:NH1	2.22	0.54
5:B:1166:GLY:HA3	5:B:1174:ARG:HB2	1.88	0.54
3:7:26:U:H2'	3:7:27:U:H5"	1.89	0.54
5:B:26:SER:HB2	5:B:236:TRP:CE2	2.42	0.54
5:B:1155:ILE:HG13	5:B:1210:ILE:HB	1.89	0.54
5:B:58:CYS:SG	5:B:59:ALA:N	2.80	0.54
7:E:3:ARG:NH1	7:E:55:GLU:OE2	2.40	0.54
3:7:36:G:H2'	3:7:37:A:C8	2.43	0.54
4:A:143:ARG:NH1	4:A:507:GLY:O	2.32	0.54
4:A:549:ASP:OD2	5:B:750:PRO:CB	2.45	0.54
5:B:30:ILE:HG21	5:B:241:VAL:O	2.08	0.54
2:6:30:DC:OP2	2:6:30:DC:C6	2.56	0.54
5:B:746:LEU:HG	5:B:758:PRO:HG3	1.90	0.54
2:6:2:DC:H2"	2:6:3:DC:C5	2.43	0.54
2:6:22:DC:H4'	4:A:508:SER:OG	2.07	0.54
4:A:684:ASN:OD1	4:A:687:ARG:NH2	2.41	0.54
5:B:124:ILE:HG23	5:B:128:LEU:HD12	1.89	0.54
5:B:145:VAL:HG23	5:B:159:ILE:HG22	1.89	0.53
5:B:56:LEU:CD1	5:B:273:ILE:HD12	2.39	0.53
5:B:290:ILE:HG23	8:F:93:ILE:HG22	1.85	0.53
5:B:759:ILE:HG23	5:B:771:GLN:HB3	1.89	0.53
6:C:100:LEU:HD23	6:C:115:ILE:HG21	1.89	0.53
4:A:895:LEU:HD23	5:B:69:GLU:OE2	2.02	0.53
6:D:28:LEU:HD12	6:D:201:LEU:HD23	1.91	0.53
4:A:628:HIS:HB3	4:A:647:ARG:HH21	1.74	0.53
4:A:890:LYS:HA	4:A:914:LYS:HG3	1.90	0.53
5:B:814:CYS:SG	5:B:883:ARG:NH2	2.81	0.53
5:B:975:ILE:HD11	5:B:1003:LEU:HD11	1.91	0.53
1:5:110:DA:N7	4:A:183:TRP:HH2	2.06	0.53
4:A:917:SER:O	4:A:919:ARG:HG3	2.07	0.53
5:B:111:THR:HG22	5:B:300:GLN:NE2	2.23	0.53
5:B:785:ASP:O	5:B:789:LYS:HB2	2.08	0.53
1:5:97:DC:H2"	1:5:98:DA:C8	2.43	0.53
5:B:832:LYS:HB3	5:B:1242:ARG:NH1	2.24	0.53
4:A:618:GLN:HG3	5:B:770:LEU:CD1	2.37	0.53
5:B:39:LYS:O	5:B:273:ILE:HG23	2.08	0.53
4:A:886:LYS:HB3	4:A:918:LEU:HD22	1.89	0.53
6:D:16:ILE:HG23	6:D:26:VAL:HG22	1.91	0.53
4:A:786:GLY:N	4:A:789:THR:OG1	2.41	0.53



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
8:F:147:VAL:HG13	8:F:161:SER:HB3	1.91	0.53
4:A:811:ASN:HA	4:A:815:SER:HB2	1.90	0.52
5:B:205:LEU:HG	5:B:217:LEU:HB3	1.90	0.52
4:A:524:ILE:HG21	4:A:708:VAL:HG13	1.91	0.52
4:A:1117:LEU:HD12	4:A:1195:ILE:HG12	1.90	0.52
5:B:78:LEU:HD13	5:B:78:LEU:O	2.08	0.52
4:A:246:LEU:HB3	4:A:269:ILE:HD13	1.91	0.52
4:A:243:PRO:HB2	4:A:274:ILE:HG23	1.90	0.52
4:A:714:VAL:HB	4:A:787:PRO:HD2	1.92	0.52
4:A:1070:HIS:NE2	4:A:1114:GLU:OE1	2.36	0.52
4:A:1278:LEU:HD21	5:B:484:MET:HE1	1.91	0.52
5:B:112:ALA:HA	5:B:238:ILE:HA	1.92	0.52
5:B:802:ASP:OD1	5:B:1348:LYS:NZ	2.31	0.52
5:B:804:ALA:O	5:B:806:ASP:N	2.41	0.52
6:C:43:LEU:HD13	6:C:217:ILE:HD11	1.90	0.52
3:7:38:G:H2'	3:7:39:A:C8	2.44	0.52
5:B:68:TYR:CA	5:B:75:TYR:HE2	2.22	0.52
5:B:209:ASN:HA	5:B:214:ARG:HH21	1.74	0.52
5:B:290:ILE:HG21	8:F:93:ILE:O	2.09	0.52
6:D:100:LEU:HD21	6:D:121:VAL:HG11	1.91	0.52
4:A:125:GLY:HA2	4:A:499:SER:HB2	1.92	0.52
1:5:96:DT:OP2	5:B:47:ARG:NH1	2.43	0.52
4:A:255:ILE:HB	4:A:263:VAL:HB	1.92	0.52
4:A:903:ARG:N	4:A:903:ARG:CD	2.73	0.52
5:B:99:ARG:HG3	5:B:99:ARG:HH11	1.74	0.52
3:7:36:G:H2'	3:7:37:A:H8	1.75	0.51
4:A:808:ASN:N	5:B:633:ALA:HB2	2.19	0.51
4:A:93:SER:HA	4:A:128:PRO:HA	1.92	0.51
5:B:390:LEU:N	5:B:390:LEU:CD1	2.73	0.51
1:5:89:DG:C2	2:6:36:DG:N2	2.78	0.51
5:B:88:CYS:HB3	5:B:90:VAL:HG12	1.92	0.51
5:B:215:LYS:HA	5:B:218:THR:HG22	1.91	0.51
5:B:1321:SER:OG	5:B:1349:GLU:OE2	2.21	0.51
3:7:29:A:N3	3:7:29:A:C5'	2.73	0.51
3:7:37:A:H2'	3:7:38:G:C8	2.45	0.51
4:A:974:ARG:HD2	4:A:1014:LEU:HD21	1.92	0.51
5:B:201:LEU:HD12	5:B:224:LEU:HD12	1.91	0.51
1:5:101:DT:H72	5:B:271:ARG:CZ	2.41	0.51
5:B:99:ARG:HA	5:B:248:ASP:HB2	1.92	0.51
4:A:855:PRO:HD2	4:A:887:VAL:HG11	1.92	0.51
5:B:749:LYS:HB3	5:B:755:ILE:HD11	1.93	0.51



	h h	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
5:B:850:LYS:HB2	5:B:857:LEU:HB2	1.91	0.51
5:B:395:LYS:NZ	5:B:399:LYS:CD	2.74	0.51
5:B:683:ILE:HD12	5:B:754:ILE:HG21	1.93	0.51
4:A:1245:ALA:O	5:B:375:GLU:HG2	2.10	0.50
5:B:144:TYR:HE1	5:B:162:GLU:CD	2.14	0.50
8:F:130:PRO:HA	8:F:148:VAL:CG1	2.40	0.50
4:A:374:GLU:HB2	8:F:80:TRP:HH2	1.76	0.50
4:A:812:PHE:HA	5:B:505:ASP:OD2	2.11	0.50
5:B:972:LYS:HD2	5:B:1004:ALA:HA	1.93	0.50
4:A:400:VAL:HG11	4:A:452:ARG:HD2	1.94	0.50
5:B:290:ILE:HG22	8:F:93:ILE:CG2	2.40	0.50
5:B:275:ARG:HH12	5:B:278:ARG:NH1	2.09	0.50
5:B:421:VAL:O	5:B:436:ALA:HA	2.11	0.50
1:5:98:DA:N9	1:5:99:DT:H72	2.27	0.50
4:A:738:GLU:HA	4:A:741:MET:HE2	1.94	0.50
4:A:18:ARG:HE	4:A:620:ASN:HA	1.77	0.50
5:B:437:PHE:HZ	5:B:453:VAL:HG11	1.76	0.50
5:B:799:ARG:HG2	5:B:1325:PHE:HZ	1.77	0.50
4:A:232:ILE:HG12	4:A:237:LEU:HG	1.93	0.49
4:A:9:LYS:HG2	4:A:1171:ARG:HH12	1.77	0.49
5:B:1371:ARG:HE	5:B:1372:ARG:NH1	2.10	0.49
4:A:146:VAL:HG21	4:A:513:GLN:HE21	1.77	0.49
4:A:400:VAL:HG21	4:A:452:ARG:HE	1.76	0.49
4:A:857:VAL:HG12	4:A:919:ARG:CZ	2.42	0.49
5:B:800:LEU:HB3	5:B:920:ALA:HB1	1.95	0.49
4:A:903:ARG:H	4:A:903:ARG:CD	2.24	0.49
8:F:115:LEU:HB2	8:F:123:ARG:HE	1.78	0.49
1:5:108:DT:H73	4:A:199:ASP:HB3	1.95	0.49
4:A:554:HIS:HD2	4:A:558:VAL:HB	1.77	0.49
5:B:46:TYR:CD1	5:B:46:TYR:C	2.86	0.49
5:B:152:THR:HB	5:B:172:PHE:CZ	2.48	0.49
5:B:550:VAL:O	5:B:569:LEU:HA	2.13	0.49
5:B:1027:VAL:HB	5:B:1121:LEU:HB2	1.95	0.49
4:A:854:ILE:HG21	4:A:917:SER:HB2	1.89	0.48
5:B:809:VAL:HG21	5:B:909:ILE:HG12	1.95	0.48
8:F:71:VAL:HG12	8:F:73:MET:HB2	1.93	0.48
5:B:53:ARG:HA	5:B:54:ASP:HA	1.55	0.48
5:B:115:TRP:O	5:B:1333:THR:HG21	2.13	0.48
5:B:220:ARG:HG2	5:B:220:ARG:NH1	2.26	0.48
8:F:150:GLU:HG3	8:F:159:LYS:HB3	1.95	0.48
4:A:529:ARG:HH11	4:A:572:ILE:HG22	1.77	0.48



	juo puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:A:836:LEU:HD13	:A:836:LEU:HD13 4:A:1054:LEU:HD13		0.48
5:B:111:THR:HG23	5:B:300:GLN:NE2	2.24	0.48
5:B:117:LEU:HG	5:B:118:LYS:HG3	1.95	0.48
5:B:833:GLU:N	5:B:1242:ARG:HH12	2.12	0.48
5:B:968:ASN:HA	5:B:1117:SER:HB2	1.96	0.48
8:F:133:MET:HA	8:F:147:VAL:HA	1.94	0.48
2:6:37:DG:H2"	2:6:38:DT:OP2	2.14	0.48
4:A:318:SER:OG	4:A:320:ASP:OD1	2.31	0.48
5:B:114:ILE:HG12	5:B:311:ARG:HD2	1.95	0.48
1:5:95:DA:C8	1:5:95:DA:C5'	2.96	0.48
8:F:116:GLN:NE2	8:F:116:GLN:CA	2.73	0.48
5:B:102:MET:HG2	5:B:246:PRO:HD3	1.94	0.48
2:6:21:DA:N6	3:7:36:G:N1	2.61	0.48
4:A:411:ARG:NH2	4:A:427:ASP:OD2	2.44	0.48
5:B:141:PHE:CE2	5:B:296:LYS:CB	2.94	0.48
5:B:201:LEU:HD11	5:B:220:ARG:HG2	1.95	0.48
5:B:1036:ARG:HE	5:B:1081:VAL:HG11	1.79	0.48
5:B:1167:LYS:HZ2	5:B:1170:LYS:HB2	1.78	0.48
4:A:400:VAL:HG22	4:A:584:TYR:HB3	1.96	0.48
5:B:47:ARG:HB2	5:B:47:ARG:CZ	2.44	0.48
4:A:1314:GLN:HB2	7:E:28:ARG:HH12	1.78	0.48
5:B:513:MET:HE1	5:B:579:LEU:HD13	1.96	0.48
6:D:100:LEU:HB2	6:D:144:ILE:HG23	1.94	0.48
4:A:1311:GLY:O	7:E:31:GLN:NE2	2.48	0.47
5:B:1261:LEU:HD12	5:B:1304:ARG:HH21	1.79	0.47
5:B:145:VAL:HG12	5:B:184:ALA:HB1	1.94	0.47
5:B:395:LYS:NZ	5:B:399:LYS:CE	2.77	0.47
4:A:565:GLU:HA	4:A:569:ILE:HG12	1.95	0.47
4:A:732:ILE:HD11	4:A:769:PRO:HB3	1.95	0.47
5:B:1060:VAL:HG13	5:B:1106:ILE:HG12	1.96	0.47
5:B:1221:LEU:HD22	5:B:1306:LEU:HB2	1.97	0.47
1:5:95:DA:H8	1:5:95:DA:C5'	2.20	0.47
4:A:1245:ALA:HB3	5:B:375:GLU:HB3	1.97	0.47
6:C:64:VAL:HG11	6:C:78:ILE:HG21	1.97	0.47
3:7:29:A:N3	3:7:29:A:C3'	2.77	0.47
3:7:37:A:H2'	3:7:38:G:H8	1.80	0.47
4:A:363:LEU:HB3	4:A:381:ALA:HB1	1.96	0.47
4:A:855:PRO:CG	4:A:915:ASP:CG	2.73	0.47
4:A:689:ALA:HB2	4:A:1233:LEU:HD23	1.97	0.47
4:A:1279:GLU:HG2	5:B:1357:ILE:HD13	1.97	0.47
4:A:1336:ASN:ND2	5:B:29:MET:HG2	2.29	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
5:B:891:ASP:OD2	5:B:1290:ARG:NH2	2.47	0.47
6:D:182:ARG:O	6:D:205:MET:HA	2.14	0.47
3:7:38:G:H2'	3:7:39:A:H8	1.80	0.47
4:A:894:GLN:HA	4:A:894:GLN:NE2	2.27	0.47
4:A:902:LEU:HB2	4:A:903:ARG:NH1	2.30	0.47
4:A:1268:GLN:NE2	5:B:352:ARG:HB2	2.30	0.47
5:B:144:TYR:CE1	5:B:162:GLU:CD	2.88	0.47
6:C:102:LEU:HD12	6:C:115:ILE:HG12	1.96	0.47
4:A:103:VAL:HG12	4:A:117:ILE:HG22	1.97	0.47
5:B:1146:GLU:OE2	5:B:1310:THR:HG22	2.14	0.47
5:B:1167:LYS:NZ	5:B:1170:LYS:HB2	2.30	0.47
5:B:1219:ASP:O	5:B:1223:LEU:HB2	2.15	0.47
6:D:35:PHE:HA	6:D:38:THR:HG22	1.97	0.46
5:B:103:GLY:H	5:B:244:VAL:HG22	1.79	0.46
5:B:902:ASP:OD2	5:B:905:ARG:HB2	2.15	0.46
6:D:15:ASP:OD1	6:D:27:THR:OG1	2.30	0.46
6:D:59:VAL:HG22	6:D:144:ILE:HA	1.97	0.46
4:A:207:THR:OG1	4:A:354:ASP:OD2	2.32	0.46
5:B:1347:LEU:HG	5:B:1357:ILE:HG23	1.96	0.46
3:7:30:U:H5"	3:7:30:U:H6	1.80	0.46
6:D:212:ASP:OD1	6:D:212:ASP:N	2.48	0.46
5:B:105:ILE:HD12	5:B:242:LEU:CD2	2.44	0.46
8:F:129:GLU:OE2	8:F:148:VAL:CG1	2.61	0.46
4:A:735:LYS:HA	4:A:748:ILE:HG22	1.98	0.46
1:5:116:DG:OP1	5:B:1311:LYS:NZ	2.46	0.46
4:A:1286:THR:O	4:A:1290:MET:HB2	2.14	0.46
4:A:1314:GLN:HA	7:E:28:ARG:HH22	1.80	0.46
3:7:26:U:H3'	3:7:26:U:H6	1.81	0.46
7:E:25:ARG:NH1	7:E:61:ASN:OD1	2.49	0.46
8:F:116:GLN:HB3	8:F:117:GLN:NE2	2.31	0.46
1:5:94:DG:N1	1:5:95:DA:C2	2.84	0.46
5:B:198:CYS:HA	5:B:221:ILE:CD1	2.45	0.46
5:B:420:PRO:HA	5:B:437:PHE:O	2.15	0.46
5:B:1150:PRO:HG3	5:B:1214:PRO:HB2	1.96	0.46
4:A:28:LEU:HD21	4:A:524:ILE:HG13	1.98	0.46
5:B:24:LEU:CB	5:B:232:ASN:OD1	2.54	0.46
5:B:128:LEU:HD21	5:B:188:LEU:HB3	1.97	0.46
3:7:32:U:P	4:A:1250:SER:OG	2.74	0.45
4:A:561:ILE:HG21	5:B:772:TYR:HE2	1.80	0.45
5:B:115:TRP:HB3	5:B:1333:THR:CG2	2.47	0.45
6:D:185:TYR:HA	6:D:202:VAL:O	2.16	0.45



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
4:A:855:PRO:CG	4:A:915:ASP:HB3	2.46	0.45	
5:B:842:ARG:HH22	5:B:1250:ASP:HB2	1.80	0.45	
1:5:108:DT:O4	4:A:199:ASP:OD2	2.34	0.45	
5:B:43:THR:HG22	5:B:57:PHE:HE1	1.80	0.45	
5:B:319:SER:HA	5:B:320:ASN:HA	1.64	0.45	
5:B:506:VAL:HG23	5:B:628:GLY:HA3	1.98	0.45	
6:C:218:ARG:NH1	6:D:231:PHE:O	2.50	0.45	
2:6:15:DC:N3	2:6:16:DC:C4	2.84	0.45	
5:B:24:LEU:CG	5:B:232:ASN:HD21	2.05	0.45	
5:B:109:SER:HB2	5:B:296:LYS:HG2	1.98	0.45	
5:B:478:LEU:HD21	7:E:47:THR:HG23	1.99	0.45	
4:A:1334:GLY:O	5:B:25:ALA:HB3	2.16	0.45	
1:5:110:DA:N1	4:A:536:GLY:O	2.50	0.45	
4:A:892:GLU:OE2	4:A:892:GLU:HA	2.17	0.45	
4:A:1246:ARG:HH11	4:A:1266:GLY:HA2	1.82	0.45	
4:A:1336:ASN:OD1	5:B:33:TRP:HZ2	2.00	0.45	
5:B:515:ARG:NH2	5:B:718:SER:O	2.48	0.45	
5:B:526:VAL:HG12	5:B:549:LYS:HB2	1.96	0.45	
3:7:35:U:H2'	3:7:36:G:C8	2.51	0.45	
4:A:230:PHE:HB2	4:A:333:ILE:HB	1.97	0.45	
4:A:998:LEU:HG	4:A:1011:LEU:HB3	1.99	0.45	
5:B:211:GLU:CG	5:B:215:LYS:HE3	2.44	0.45	
5:B:1227:HIS:HA	5:B:1230:THR:HG22	1.99	0.45	
2:6:15:DC:C4	2:6:16:DC:C5	3.05	0.45	
4:A:674:ASP:OD2	4:A:1070:HIS:ND1	2.50	0.45	
4:A:712:SER:OG	4:A:713:GLY:N	2.49	0.45	
4:A:746:ALA:O	4:A:974:ARG:NH2	2.45	0.45	
5:B:201:LEU:CD1	5:B:224:LEU:HD12	2.46	0.45	
5:B:209:ASN:HA	5:B:214:ARG:NH2	2.31	0.45	
5:B:395:LYS:NZ	5:B:399:LYS:HE2	2.32	0.45	
4:A:557:ARG:NH2	4:A:607:SER:O	2.49	0.45	
4:A:1002:LEU:HD21	4:A:1007:LYS:HB2	1.98	0.45	
4:A:1247:SER:HB3	5:B:375:GLU:O	2.16	0.45	
1:5:115:DA:P	5:B:1148:ARG:HG3	2.58	0.44	
8:F:123:ARG:CG	8:F:124:PRO:HD2	2.47	0.44	
4:A:176:ILE:HD11	4:A:428:VAL:HG21	1.98	0.44	
4:A:694:ARG:HH22	6:C:80:GLU:HG3	1.82	0.44	
4:A:1105:SER:HB2	5:B:731:ARG:HB3	2.00	0.44	
4:A:1278:LEU:HD21	5:B:484:MET:CE	2.47	0.44	
5:B:1158:GLU:HA	5:B:1223:LEU:HD21	1.99	0.44	
2:6:21:DA:C6	3:7:36:G:C2	3.03	0.44	



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
5:B:76:LYS:NZ	5:B:76:LYS:HB3	2.32	0.44	
5:B:111:THR:HG21	5:B:303:VAL:HB	2.00	0.44	
5:B:385:LEU:HD23	5:B:390:LEU:HB2	1.98	0.44	
6:D:29:GLU:HB3	6:D:200:LYS:HG3	1.99	0.44	
7:E:72:GLN:O	7:E:76:GLU:HG2	2.17	0.44	
8:F:130:PRO:CG	8:F:151:VAL:CG2	2.94	0.44	
1:5:89:DG:N1	2:6:36:DG:N1	2.65	0.44	
3:7:31:U:H5"	3:7:31:U:H6	1.82	0.44	
5:B:201:LEU:CB	5:B:221:ILE:HD13	2.47	0.44	
5:B:245:LEU:CG	5:B:246:PRO:HD2	2.48	0.44	
5:B:926:PRO:HB2	5:B:1241:TYR:HE1	1.82	0.44	
5:B:75:TYR:O	5:B:75:TYR:CD2	2.70	0.44	
5:B:123:ARG:HA	5:B:123:ARG:HD3	1.49	0.44	
5:B:201:LEU:HD11	5:B:220:ARG:NH1	2.31	0.44	
5:B:1024:THR:HG23	5:B:1123:ARG:HA	2.00	0.44	
1:5:116:DG:C6	1:5:117:DA:C6	3.06	0.44	
4:A:148:GLN:NE2	4:A:535:PRO:O	2.40	0.44	
4:A:444:ASP:OD1	4:A:444:ASP:N	2.51	0.44	
4:A:886:LYS:HE3	4:A:918:LEU:HD13	1.99	0.44	
4:A:888:THR:O	4:A:890:LYS:CE	2.64	0.44	
5:B:388:ARG:NH1	5:B:388:ARG:HG2	2.32	0.44	
5:B:1108:GLN:HG3	5:B:1109:LEU:HD12	1.99	0.44	
5:B:1106:ILE:O	5:B:1123:ARG:N	2.45	0.44	
6:D:192:VAL:HG12	6:D:193:GLU:H	1.83	0.44	
4:A:1294:LYS:HG2	5:B:472:LEU:CD1	2.47	0.44	
5:B:108:ALA:HB1	5:B:279:LEU:HD22	1.96	0.44	
5:B:294:ASN:ND2	8:F:68:TYR:OH	2.51	0.44	
5:B:26:SER:CB	5:B:236:TRP:CZ2	2.95	0.43	
5:B:515:ARG:HH12	5:B:724:MET:HG2	1.83	0.43	
5:B:1026:PRO:HB2	5:B:1028:ILE:HG23	2.00	0.43	
8:F:122:PRO:CB	8:F:123:ARG:HD2	2.47	0.43	
4:A:811:ASN:ND2	4:A:1098:LEU:O	2.51	0.43	
4:A:1275:VAL:HG13	4:A:1287:LEU:HD11	2.01	0.43	
5:B:107:LEU:HA	5:B:276:ASN:ND2	2.33	0.43	
5:B:213:LYS:HE3	5:B:213:LYS:CA	2.47	0.43	
5:B:213:LYS:HE3	5:B:213:LYS:HA	1.99	0.43	
8:F:7:LYS:HG2	8:F:74:VAL:HG13	2.01	0.43	
8:F:126:THR:HA	8:F:130:PRO:HD2	1.99	0.43	
4:A:857:VAL:HG12	4:A:919:ARG:HE	1.83	0.43	
6:D:78:ILE:HA	6:D:81:ILE:HG22	2.00	0.43	
8:F:130:PRO:CG	8:F:151:VAL:HG22	2.39	0.43	



	hi a	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
4:A:11:ILE:HG22	4:A:1172:LEU:HD11	1.99	0.43	
5:B:128:LEU:CD2	5:B:188:LEU:HB3	2.47	0.43	
5:B:190:LYS:HB2	5:B:190:LYS:HE3	1.41	0.43	
5:B:847:ASP:N	5:B:847:ASP:OD1	2.49	0.43	
5:B:1357:ILE:HG22	5:B:1359:ALA:H	1.83	0.43	
7:E:58:LEU:HD12	7:E:59:ILE:HG12	2.00	0.43	
8:F:115:LEU:HA	8:F:123:ARG:NH2	2.33	0.43	
2:6:31:DA:C2'	2:6:32:DT:H72	2.48	0.43	
4:A:557:ARG:HB3	4:A:587:LEU:HD13	2.00	0.43	
5:B:62:PHE:CD1	5:B:62:PHE:N	2.86	0.43	
5:B:824:PRO:HD3	5:B:835:LEU:HD12	2.00	0.43	
6:D:68:TYR:HE1	6:D:79:LEU:HD13	1.82	0.43	
4:A:300:ASP:OD1	4:A:313:ALA:N	2.51	0.43	
5:B:111:THR:CG2	5:B:300:GLN:HA	2.48	0.43	
5:B:978:ARG:HD3	5:B:999:TYR:H	1.82	0.43	
8:F:106:LYS:C	8:F:106:LYS:CD	2.86	0.43	
1:5:94:DG:C2	1:5:95:DA:N3	2.85	0.43	
4:A:1274:GLU:HG3	5:B:434:ILE:HD11	2.00	0.43	
4:A:1298:VAL:HG11	5:B:96:LYS:NZ	2.34	0.43	
5:B:141:PHE:HE2	5:B:296:LYS:CB	2.22	0.43	
5:B:894:VAL:HG22	5:B:1258:ARG:HH11	1.83	0.43	
2:6:12:DC:H6	2:6:12:DC:O5'	2.01	0.43	
4:A:857:VAL:CG1	4:A:919:ARG:CZ	2.95	0.43	
4:A:1274:GLU:CG	5:B:434:ILE:HD11	2.49	0.43	
5:B:58:CYS:SG	5:B:60:ARG:HG2	2.59	0.43	
5:B:161:THR:H	5:B:164:GLN:HB2	1.82	0.43	
5:B:850:LYS:HB3	5:B:855:ASP:HB2	2.00	0.43	
6:D:31:LEU:HD21	6:D:39:LEU:HD12	2.00	0.43	
4:A:1245:ALA:CB	5:B:375:GLU:HB3	2.48	0.43	
5:B:220:ARG:NH1	5:B:220:ARG:CG	2.82	0.43	
5:B:1033:GLY:HA3	5:B:1081:VAL:O	2.18	0.43	
4:A:861:ALA:HB1	4:A:882:ILE:HD13	2.01	0.43	
5:B:126:LEU:HD12	5:B:223:LEU:HD22	1.99	0.43	
8:F:157:ARG:O	8:F:158:LEU:HD12	2.18	0.43	
1:5:90:DT:C2	1:5:91:DC:C4	3.07	0.42	
4:A:22:LEU:HB3	4:A:655:VAL:HG11	2.01	0.42	
4:A:27:LEU:O	4:A:528:ARG:NH1	2.43	0.42	
4:A:590:PRO:HB2	4:A:655:VAL:HG21	2.01	0.42	
4:A:829:THR:HG23	4:A:1059:ARG:HG2	2.00	0.42	
5:B:26:SER:HB2	5:B:236:TRP:CH2	2.51	0.42	
5:B:388:ARG:HG2	5:B:388:ARG:HH11	1.84	0.42	



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
5:B:513:MET:HG3	5:B:544:LEU:HD11	2.01	0.42	
5:B:647:PRO:HG3	5:B:697:MET:HB3	2.01	0.42	
5:B:1079:LYS:HD3	5:B:1098:GLN:HB3	2.00	0.42	
5:B:1350:ASN:HA	5:B:1353:VAL:HG12	2.01	0.42	
3:7:26:U:C6	3:7:26:U:C3'	3.03	0.42	
4:A:1157:GLN:HG3	4:A:1159:VAL:HG13	2.00	0.42	
5:B:141:PHE:CD2	5:B:297:ARG:HB2	2.54	0.42	
5:B:568:SER:HB3	5:B:570:LYS:NZ	2.34	0.42	
6:D:76:GLU:HB3	6:D:80:GLU:HB3	2.01	0.42	
1:5:94:DG:C6	1:5:95:DA:C2	3.08	0.42	
4:A:616:ILE:HG13	4:A:652:TYR:HB2	2.01	0.42	
4:A:646:SER:OG	4:A:647:ARG:N	2.52	0.42	
4:A:699:LEU:HG	4:A:799:ASN:HD22	1.85	0.42	
4:A:908:GLU:H	4:A:908:GLU:HG3	1.56	0.42	
5:B:24:LEU:CD1	5:B:232:ASN:ND2	2.82	0.42	
5:B:68:TYR:O	5:B:75:TYR:CD2	2.70	0.42	
5:B:390:LEU:N	5:B:390:LEU:HD13	2.35	0.42	
5:B:395:LYS:HB3	5:B:395:LYS:HE3	1.45	0.42	
5:B:797:THR:HG22	5:B:924:GLY:HA3	2.01	0.42	
4:A:1313:HIS:CD2	7:E:31:GLN:HE22	2.37	0.42	
5:B:102:MET:HG2	5:B:246:PRO:CG	2.49	0.42	
5:B:559:ALA:HB3	5:B:562:GLU:HB3	2.01	0.42	
5:B:609:TYR:HD2	5:B:610:ARG:NH1	2.17	0.42	
4:A:478:ARG:HD2	4:A:492:MET:HA	2.02	0.42	
5:B:1289:ASN:O	5:B:1293:GLU:HB2	2.20	0.42	
1:5:89:DG:N2	2:6:36:DG:N3	2.67	0.42	
1:5:114:DC:H5"	5:B:1148:ARG:CZ	2.46	0.42	
3:7:34:G:H8	3:7:34:G:H5"	1.84	0.42	
4:A:125:GLY:H	4:A:495:ALA:HB1	1.84	0.42	
4:A:845:LEU:HD23	4:A:912:ASP:OD1	2.18	0.42	
5:B:394:ILE:O	5:B:394:ILE:HG13	2.18	0.42	
5:B:1046:ILE:HG22	5:B:1061:VAL:HA	2.00	0.42	
4:A:469:VAL:HA	4:A:472:GLU:HG2	2.02	0.42	
5:B:137:ARG:HA	5:B:142:GLU:HG2	2.02	0.42	
3:7:34:G:H8	3:7:34:G:C5'	2.33	0.42	
5:B:586:GLY:HA3	5:B:612:LEU:HD11	2.01	0.42	
5:B:596:LEU:HD23	5:B:596:LEU:HA	1.91	0.42	
4:A:1282:GLY:O	5:B:1361:THR:OG1	2.28	0.42	
5:B:47:ARG:HA	5:B:47:ARG:NE	2.35	0.42	
5:B:385:LEU:CD2	5:B:390:LEU:HB2	2.50	0.42	
5:B:1272:SER:OG	5:B:1273:ASP:N	2.53	0.42	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:A:1069:ARG:NH2	4:A:1114:GLU:OE2	2.44	0.41
5:B:144:TYR:CE1	5:B:162:GLU:OE1	2.73	0.41
5:B:244:VAL:HA	5:B:269:TYR:OH	2.19	0.41
5:B:616:PRO:HA	5:B:619:ILE:HG22	2.02	0.41
5:B:839:VAL:HG12	5:B:864:LEU:HD12	2.02	0.41
8:F:169:THR:HA	8:F:170:PRO:HD3	1.88	0.41
4:A:741:MET:SD	4:A:974:ARG:NH2	2.93	0.41
5:B:923:ILE:O	5:B:1241:TYR:OH	2.31	0.41
5:B:950:ILE:HB	5:B:1018:ALA:HB3	2.01	0.41
5:B:1002:VAL:N	5:B:1019:ASN:O	2.46	0.41
4:A:144:VAL:HG23	4:A:515:MET:HB2	2.02	0.41
4:A:856:ASN:O	4:A:919:ARG:NH2	2.53	0.41
4:A:903:ARG:NE	4:A:903:ARG:N	2.60	0.41
5:B:68:TYR:HB3	5:B:75:TYR:HE2	1.81	0.41
5:B:136:GLU:OE1	5:B:312:ARG:NH2	2.53	0.41
5:B:279:LEU:HD13	5:B:299:LEU:HD13	2.02	0.41
8:F:103:ILE:HG13	8:F:104:SER:H	1.85	0.41
1:5:95:DA:C2'	1:5:96:DT:H5'	2.50	0.41
4:A:22:LEU:HD22	4:A:603:ILE:HG21	2.02	0.41
5:B:450:HIS:HA	5:B:451:PRO:HD3	1.90	0.41
5:B:1050:THR:HG23	5:B:1057:SER:HB3	2.03	0.41
3:7:25:U:O2	3:7:25:U:H2'	2.20	0.41
4:A:559:CYS:HA	4:A:560:PRO:HD3	1.90	0.41
4:A:1294:LYS:HG2	5:B:472:LEU:HD11	2.03	0.41
5:B:126:LEU:CD1	5:B:223:LEU:HD22	2.49	0.41
5:B:139:LEU:HD23	5:B:139:LEU:HA	1.90	0.41
5:B:515:ARG:HG2	5:B:516:ASP:H	1.85	0.41
7:E:26:ARG:HA	7:E:26:ARG:HD2	1.92	0.41
5:B:239:LEU:N	5:B:239:LEU:HD23	2.36	0.41
5:B:576:ARG:HD3	5:B:593:ASN:HA	2.03	0.41
4:A:936:ARG:HB2	4:A:1042:LEU:HD12	2.03	0.41
5:B:109:SER:CB	5:B:296:LYS:HG2	2.51	0.41
5:B:144:TYR:OH	5:B:162:GLU:OE1	2.34	0.41
5:B:271:ARG:HE	5:B:271:ARG:HB2	1.58	0.41
8:F:117:GLN:N	8:F:117:GLN:CD	2.73	0.41
4:A:524:ILE:HD12	4:A:712:SER:HB2	2.02	0.41
4:A:800:MET:HE3	4:A:800:MET:HB2	1.86	0.41
4:A:998:LEU:HD21	4:A:1015:ALA:HB2	2.02	0.41
8:F:153:TYR:HD1	8:F:153:TYR:HA	1.75	0.41
3:7:27:U:O2	3:7:27:U:H3'	2.20	0.41
3:7:39:A:O3'	4:A:688:GLN:NE2	2.54	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:A:657:THR:HG21	4:A:1188:ASP:HB2	2.03	0.41
4:A:879:GLY:CA	4:A:922:ASN:HA	2.50	0.41
4:A:899:GLU:OE1	4:A:899:GLU:HA	2.18	0.41
5:B:47:ARG:NE	5:B:47:ARG:CA	2.84	0.41
5:B:144:TYR:N	5:B:144:TYR:CD1	2.88	0.41
5:B:805:GLN:HG3	5:B:1348:LYS:HD3	2.03	0.41
6:D:46:ILE:HD11	6:D:224:LEU:HD13	2.02	0.41
5:B:848:VAL:HB	5:B:858:VAL:HG22	2.02	0.41
5:B:1263:LYS:NZ	5:B:1315:ALA:O	2.49	0.41
6:C:228:LEU:HD21	6:D:224:LEU:HD23	2.03	0.41
4:A:213:LEU:HD13	4:A:422:LYS:HG2	2.03	0.40
5:B:506:VAL:H	5:B:506:VAL:HG12	1.59	0.40
4:A:618:GLN:CD	5:B:770:LEU:HD13	2.42	0.40
5:B:351:GLY:O	5:B:467:ALA:HA	2.22	0.40
5:B:930:LEU:HA	5:B:1244:GLN:HG3	2.02	0.40
1:5:98:DA:C2'	1:5:99:DT:C7	2.96	0.40
4:A:310:ILE:HG21	4:A:325:LEU:HB3	2.03	0.40
5:B:244:VAL:HA	5:B:269:TYR:CZ	2.57	0.40
1:5:98:DA:H2'	1:5:99:DT:H72	2.01	0.40
4:A:979:LEU:HD11	4:A:1011:LEU:HD11	2.03	0.40
5:B:390:LEU:HD13	5:B:390:LEU:H	1.85	0.40
5:B:1064:SER:OG	5:B:1168:GLU:OE1	2.31	0.40
3:7:26:U:C6	3:7:26:U:O5'	2.75	0.40
4:A:899:GLU:HG3	4:A:900:LYS:HE3	2.04	0.40
5:B:117:LEU:HD22	5:B:139:LEU:CD1	2.52	0.40
5:B:820:ILE:HG12	5:B:884:SER:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
4	А	1338/1342~(100%)	1207 (90%)	125~(9%)	6 (0%)	34	72
5	В	1329/1407~(94%)	1199 (90%)	121 (9%)	9 (1%)	22	62
6	С	217/329~(66%)	203~(94%)	12 (6%)	2 (1%)	17	56
6	D	214/329~(65%)	198~(92%)	16 (8%)	0	100	100
7	Ε	73/91~(80%)	70~(96%)	3 (4%)	0	100	100
8	F	157/181~(87%)	136 (87%)	15 (10%)	6 (4%)	3	27
All	All	3328/3679~(90%)	3013 (90%)	292 (9%)	23 (1%)	26	62

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	А	888	THR
8	F	122	PRO
8	F	123	ARG
8	F	129	GLU
4	А	918	LEU
5	В	175	GLU
8	F	118	VAL
4	А	899	GLU
5	В	51	PRO
5	В	805	GLN
8	F	127	LEU
4	А	921	PRO
5	В	174	ASP
5	В	193	ASP
6	С	193	GLU
4	А	905	ILE
5	В	91	GLU
8	F	126	THR
5	В	49	PHE
5	В	73	GLY
5	В	904	ALA
6	С	192	VAL
4	А	1317	PRO

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.



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
4	А	1155/1157~(100%)	1136 (98%)	19~(2%)	62	79
5	В	1120/1168~(96%)	1051 (94%)	69~(6%)	18	45
6	С	186/286~(65%)	186 (100%)	0	100	100
6	D	185/286~(65%)	185 (100%)	0	100	100
7	Ε	65/75~(87%)	64~(98%)	1 (2%)	65	80
8	F	138/158~(87%)	115~(83%)	23~(17%)	2	14
All	All	2849/3130~(91%)	2737 (96%)	112 (4%)	36	57

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

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	А	888	THR
4	А	890	LYS
4	А	893	THR
4	А	894	GLN
4	А	895	LEU
4	А	896	THR
4	А	898	GLU
4	А	899	GLU
4	А	900	LYS
4	А	901	LEU
4	А	903	ARG
4	А	905	ILE
4	А	908	GLU
4	А	909	LYS
4	А	913	VAL
4	А	914	LYS
4	А	915	ASP
4	А	918	LEU
4	А	920	VAL
5	В	40	LYS
5	В	42	GLU
5	В	44	ILE
5	В	46	TYR
5	В	47	ARG
5	В	49	PHE
5	В	50	LYS
5	В	52	GLU



Mol	Chain	Res Type	
5	В	53	ARG
5	В	54	ASP
5	В	60	ARG
5	В	67	ASP
5	В	70	CYS
5	В	72	CYS
5	В	74	LYS
5	В	76	LYS
5	В	77	ARG
5	В	78	LEU
5	В	81	ARG
5	В	87	LYS
5	В	88	CYS
5	В	91	GLU
5	В	94	GLN
5	В	95	THR
5	В	99	ARG
5	В	100	GLU
5	В	117	LEU
5	В	119	SER
5	В	123	ARG
5	В	132	LEU
5	В	135	ILE
5	В	142	GLU
5	В	144	TYR
5	В	145	VAL
5	В	147	ILE
5	В	152	THR
5	В	154	LEU
5	В	157	GLN
5	В	159	ILE
5	В	175	GLU
5	B	180	MET
5	B	190	LYS
5	B	193	ASP
5	B	196	GLN
5	B	210	SER
5	B	215	LYS
5	B	216	LYS
5	B	222	LYS
5	B	223	LEU
5	В	227	PHE



Mol	Chain	Res Type	
5	В	232	ASN
5	В	233	LYS
5	В	237	MET
5	В	238	ILE
5	В	239	LEU
5	В	240	THR
5	В	244	VAL
5	В	271	ARG
5	В	385	LEU
5	В	386	GLU
5	В	390	LEU
5	В	393	THR
5	В	394	ILE
5	В	395	LYS
5	В	514	THR
5	В	709	ARG
5	В	836	ARG
5	В	1172	LYS
5	В	1373	ARG
7	Е	76	GLU
8	F	21	ARG
8	F	104	SER
8	F	105	ASP
8	F	106	LYS
8	F	114	ARG
8	F	116	GLN
8	F	117	GLN
8	F	123	ARG
8	F	125	LYS
8	F	127	LEU
8	F	129	GLU
8	F	132	GLU
8	F	143	ASP
8	F	147	VAL
8	F	152	ASP
8	F	153	TYR
8	F	155	LYS
8	F	158	LEU
8	F	162	VAL
8	F	164	ILE
8	F	169	THR
8	F	175	PHE



 $Continued \ from \ previous \ page...$

Mol	Chain	Res	Type
8	F	176	SER

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

Mol	Chain	Res	Type	
4	А	69 GLN		
4	А	150	HIS	
4	А	314	ASN	
4	А	513	GLN	
4	А	554	HIS	
4	А	580	GLN	
4	А	604	HIS	
4	А	688	GLN	
4	А	894	GLN	
4	А	1268	GLN	
4	А	1313	HIS	
5	В	294	ASN	
6	С	147	GLN	
6	D	66	HIS	
6	D	117 HIS		
6	D	227	GLN	
7	Е	31	GLN	
8	F	116	GLN	

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	7	16/41~(39%)	8 (50%)	0

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	7	26	U
3	7	27	U
3	7	28	G
3	7	29	А
3	7	31	U
3	7	32	U
3	7	33	G
3	7	34	G



There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-27916. 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: 192



Y Index: 192



Z Index: 192

6.2.2 Raw 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: 209



Y Index: 228



Z Index: 186

6.3.2 Raw map



X Index: 209

Y Index: 231



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 0.0041. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

6.5 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 747 $\rm nm^3;$ this corresponds to an approximate mass of 675 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 0.227 ${\rm \AA^{-1}}$



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 0.227 ${\rm \AA^{-1}}$



8.2 Resolution estimates (i)

$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	Estimation criterion (FSC cut-off)		
Resolution estimate (A)	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.91	8.92	7.23

*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 6.91 differs from the reported value 4.4 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-27916 and PDB model 8E5O. 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 0.0041 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 (0.0041).



9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 95% 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 (0.0041) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score	1.0
All	0.9480	0.1510	
5	0.9246	0.1390	
6	0.9706	0.2090	
7	0.9918	0.2660	
А	0.9574	0.1700	
В	0.9463	0.1390	
С	0.9543	0.1440	
D	0.9215	0.1250	
E	0.9110	0.1280	0.0 0 .0
F	0.9031	0.0730	

