

#### Apr 18, 2024 - 01:58 pm BST

PDB ID	:	8PFJ
EMDB ID	:	EMD-17647
Title	:	fully recruited RfaH bound to E. coli transcription complex paused at ops site
		(not fully complementary scaffold; alternative state of RfaH)
Authors	:	Zuber, P.K.; Said, N.; Hilal, T.; Loll, B.; Wahl, M.C.; Knauer, S.H.
Deposited on	:	2023-06-16
Resolution	:	3.40  Å(reported)
This is	a F	ull 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.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 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	Quality of c	hain
1	Р	164	46% 15%	• 38%
2	Ι	1342	• 76%	21% •••
3	J	1416	<b>•</b> 72%	21% · 5%
4	Κ	91	64%	24% • 8%
5	R	17	35% 24% 65'	% 12%
6	А	40	55%	40% 5%
7	В	40	42%	52% 5%



Mol	Chain	Length	Quality	of chain			
8	G	329	<b>•</b> 50%	18%	•	29%	_
8	Н	329	<b>•</b> 51%	17%	•	30%	_



# 2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 27856 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 Transcription antitermination protein RfaH.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Р	101	Total 811	C 523	N 144	0 140	${S \atop 4}$	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Р	-1	GLY	-	expression tag	UNP P0AFW0
Р	0	HIS	-	expression tag	UNP P0AFW0

• Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues		A	toms			AltConf	Trace
9	т	1201	Total	С	Ν	Ο	$\mathbf{S}$	0	0
		1521	10423	6539	1816	2024	44	U	U

• Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	1343	Total 10449	$\begin{array}{c} \mathrm{C} \\ 6565 \end{array}$	N 1862	O 1972	S 50	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1	VAL	-	expression tag	UNP P0A8T7
J	1408	LEU	-	expression tag	UNP P0A8T7
J	1409	GLU	-	expression tag	UNP P0A8T7
J	1410	VAL	-	expression tag	UNP P0A8T7
J	1411	HIS	-	expression tag	UNP P0A8T7
J	1412	HIS	-	expression tag	UNP P0A8T7
J	1413	HIS	-	expression tag	UNP P0A8T7
J	1414	HIS	-	expression tag	UNP P0A8T7
J	1415	HIS	-	expression tag	UNP P0A8T7



Chain	Residue	Modelled	Actual	Comment	Reference
J	1416	HIS	-	expression tag	UNP P0A8T7

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	84	Total 663	C 404	N 124	0 133	${S \over 2}$	0	0

• Molecule 5 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms			AltConf	Trace		
5	R	17	Total 355	C 160	N 58	0 121	Р 16	0	0

• Molecule 6 is a DNA chain called non-template DNA.

Mol	Chain	Residues	Atoms			AltConf	Trace		
6	А	38	Total 771	C 367	N 131	0 235	Р 38	0	0

• Molecule 7 is a DNA chain called template DNA.

Mol	Chain	Residues	Atoms				AltConf	Trace	
7	В	38	Total 786	C 371	N 160	0 218	Р 37	0	0

• Molecule 8 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms			AltConf	Trace			
8	G	933	Total	С	Ν	0	S	1	0	
0		200	1811	1127	323	355	6			
8	Н	Н	221	Total	С	Ν	0	$\mathbf{S}$	0	0
8			201	1784	1110	315	353	6		U

• Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
9	J	2	Total Zn 2 2	0

• Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).



Mol	Chain	Residues	Atoms	AltConf
10	J	1	Total Mg 1 1	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Transcription antitermination protein RfaH



# W1276 K1140 K1141 L1014 F1291 T1141 L1014 M1201 T1143 L1014 M1201 T1149 L1014 M1301 T1149 L1014 M1301 T1151 M1015 M1301 W1169 D1019 M1301 W1169 D1014 M170 M117 L1044 M1305 M1177 L1044 M1305 M1183 P10019 M1305 M1184 P1004 M1183 M1184 P1064 M1190 M1190 M1072 M1190 M1190 M1072 M1190 M1190 M1072 M1190 M1190 M1072 M1190 M1202 M1092 M1206 M1208 M1072 M1208 M1208 M1072 M1209 M1208 M1072 M1208 M1208 M108 M1208 M1208 M108

• Molecule 3: DNA-directed RNA polymerase subunit beta'





#### R1258 R1273 E1278 E1278 E1278 E1278 E1278 E1278 E1326 E1326 E1326 E1326 E1346 E

#### ASN ASN GLY GLY CLL ULEU GLY ASN ASP CLU CLU CLU CLU VAL CLU VAL HISS HISS HISS HISS

• Molecule 4: DNA-directed RNA polymerase subunit omega





#### 

• Molecule 8: DNA-directed RNA polymerase subunit alpha





# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	51791	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 $(e^-/\text{\AA}^2)$	42	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.522	Depositor
Minimum map value	0.000	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	319.488, 319.488, 319.488	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles $(^{\circ})$	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	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	Bond	lengths	Bo	ond angles
1VIOI		RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	Р	0.28	0/832	0.60	0/1131
2	Ι	0.25	0/10589	0.50	2/14286~(0.0%)
3	J	0.24	0/10607	0.51	0/14321
4	K	0.26	0/665	0.58	0/896
5	R	0.20	0/395	0.80	0/613
6	А	0.51	0/860	0.97	0/1324
7	В	0.49	0/886	0.84	0/1367
8	G	0.25	0/1836	0.57	1/2487~(0.0%)
8	H	0.25	0/1806	0.53	0/2448
All	All	0.27	0/28476	0.56	3/38873~(0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	Ι	102	LEU	CA-CB-CG	5.28	127.43	115.30
2	Ι	484	LEU	CA-CB-CG	5.18	127.20	115.30
8	G	193	GLU	CB-CA-C	5.00	120.40	110.40

There are no chirality outliers.

There are no planarity outliers.

#### 5.2 Too-close contacts (i)

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Р	811	0	826	15	0
2	Ι	10423	0	10436	172	0
3	J	10449	0	10666	192	0
4	Κ	663	0	675	18	0
5	R	355	0	182	7	0
6	А	771	0	430	15	0
7	В	786	0	424	19	0
8	G	1811	0	1843	54	0
8	Н	1784	0	1806	34	0
9	J	2	0	0	0	0
10	J	1	0	0	0	0
All	All	27856	0	27288	484	0

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

All (484) 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)
3:J:275:ARG:HH22	3:J:278:ARG:HE	1.27	0.78
2:I:633:LEU:HB3	2:I:644:LEU:HD12	1.69	0.75
3:J:443:GLU:OE2	3:J:443:GLU:N	2.23	0.71
8:H:192:VAL:HG13	8:H:193:GLU:HG3	1.73	0.70
2:I:104:ILE:HG12	2:I:484:LEU:HD11	1.74	0.70
2:I:808:ASN:H	3:J:633:ALA:HB2	1.56	0.69
1:P:10:LYS:NZ	6:A:16:DG:N7	2.41	0.69
3:J:255:LEU:HD21	3:J:261:ALA:HB2	1.76	0.68
2:I:729:ALA:O	2:I:755:LYS:NZ	2.28	0.67
3:J:584:PRO:HG2	3:J:587:LEU:HD23	1.75	0.67
3:J:1326:GLN:HG3	3:J:1327:GLU:HG3	1.75	0.67
3:J:24:LEU:HD11	3:J:232:ASN:HB3	1.76	0.67
2:I:812:PHE:O	2:I:1099:ASN:ND2	2.28	0.67
2:I:1101:LEU:HD13	3:J:725:MET:HE3	1.76	0.66
7:B:36:DT:H2"	7:B:37:DG:C8	2.31	0.65
8:G:45:ARG:HD3	8:H:38:THR:HG22	1.78	0.65
2:I:44:GLU:HB2	2:I:46:GLN:HE22	1.60	0.65
2:I:255:ILE:HD11	2:I:263:VAL:H	1.62	0.65
2:I:975:ILE:HG22	2:I:1014:LEU:HD13	1.79	0.65
3:J:502:PRO:HB3	3:J:506:VAL:HB	1.78	0.65
2:I:254:ASP:HB2	2:I:265:LYS:HG2	1.80	0.64
3:J:648:GLU:OE2	3:J:648:GLU:N	2.31	0.64
8:G:188:GLU:OE2	8:G:200:LYS:NZ	2.29	0.64



	A + 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:I:1084:ASP:OD1	8:G:45:ARG:NH2	2.30	0.64
7:B:21:DC:H2'	7:B:22:DG:H8	1.63	0.64
2:I:371:ARG:NH1	6:A:20:DG:OP2	2.31	0.64
4:K:13:ILE:HG13	4:K:19:LEU:HD23	1.80	0.64
8:G:72:GLU:N	8:G:72:GLU:OE2	2.27	0.64
2:I:1245:ALA:HB2	3:J:372:MET:HG2	1.80	0.63
2:I:44:GLU:O	2:I:46:GLN:NE2	2.31	0.63
2:I:213:LEU:HD22	2:I:422:LYS:HG2	1.80	0.63
8:H:98:VAL:HG13	8:H:146:VAL:HG13	1.81	0.62
2:I:539:THR:HB	2:I:542:ARG:HB2	1.81	0.62
8:H:183:ILE:HD13	8:H:205:MET:HG2	1.82	0.62
8:G:193:GLU:CD	8:G:194:GLN:H	2.04	0.61
8:G:194:GLN:N	8:G:194:GLN:OE1	2.32	0.61
8:G:102:LEU:HD12	8:G:115:ILE:HG12	1.81	0.61
2:I:1185:PRO:HD2	2:I:1189:GLY:HA2	1.82	0.61
3:J:72:CYS:HB3	3:J:88:CYS:SG	2.41	0.61
3:J:399:LYS:HB3	3:J:403:ARG:HH21	1.65	0.61
3:J:930:LEU:HA	3:J:1244:GLN:HG3	1.81	0.60
3:J:318:GLY:N	3:J:322:ARG:O	2.34	0.60
2:I:1244:HIS:NE2	2:I:1266:GLY:O	2.33	0.60
2:I:1269:ARG:NH1	7:B:20:DA:OP1	2.34	0.60
3:J:527:LEU:HB2	3:J:550:VAL:HG12	1.83	0.60
3:J:363:LEU:HD23	3:J:618:VAL:HG12	1.84	0.60
8:G:155:ALA:HA	8:G:158:ARG:HH12	1.67	0.60
2:I:244:GLU:HG3	2:I:247:ARG:HH22	1.65	0.59
2:I:1132:LEU:HD13	2:I:1177:ARG:HH21	1.67	0.59
3:J:1173:ARG:NH1	3:J:1192:LYS:O	2.35	0.59
4:K:42:GLU:O	4:K:43:ASN:ND2	2.35	0.59
6:A:8:DA:H2"	6:A:9:DC:H5'	1.83	0.59
2:I:563:THR:O	2:I:684:ASN:ND2	2.30	0.59
3:J:215:LYS:O	3:J:219:LYS:HG2	2.03	0.59
3:J:1051:ASP:HB2	3:J:1055:GLY:H	1.68	0.59
8:G:5:VAL:O	8:H:150:ARG:NH1	2.36	0.59
2:I:444:ASP:HB3	2:I:447:HIS:HB2	1.85	0.58
3:J:321:LYS:N	3:J:321:LYS:HE2	2.18	0.58
8:G:67:GLU:HB3	8:G:171:LEU:HG	1.85	0.58
3:J:1368:ASP:HA	3:J:1371:ARG:HD3	1.84	0.58
8:H:158:ARG:NH2	8:H:173:VAL:O	2.35	0.58
2:I:1273:MET:HB3	3:J:428:THR:HB	1.85	0.58
3:J:151:MET:H	3:J:151:MET:CE	2.16	0.58
3:J:179:LYS:HB3	3:J:184:ALA:HB2	1.84	0.58



	tus page	Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
7:B:21:DC:H2'	7:B:22:DG:C8	2.39	0.58	
3:J:552:ILE:HD11	3:J:570:LYS:HG3	1.86	0.58	
3:J:968:ASN:OD1	3:J:972:LYS:N	2.37	0.57	
2:I:288:PRO:HG2	2:I:291:TYR:HB2	1.86	0.57	
3:J:460:ASP:OD1	3:J:460:ASP:N	2.37	0.57	
8:G:157:THR:O	8:G:160:HIS:ND1	2.37	0.57	
2:I:197:ARG:HD3	2:I:200:ARG:HA	1.87	0.57	
2:I:233:ARG:HG3	2:I:238:GLN:HB2	1.86	0.57	
8:G:111:THR:HG22	8:G:129:VAL:HA	1.87	0.57	
3:J:808:VAL:HG12	3:J:914:ALA:HA	1.87	0.57	
8:H:99:ILE:HD11	8:H:145:LYS:HE2	1.86	0.57	
2:I:646:SER:HB3	2:I:649:GLN:HG3	1.86	0.57	
5:R:8:G:N2	7:B:28:DC:O2	2.38	0.56	
2:I:315:MET:HA	2:I:352:ARG:HE	1.70	0.56	
8:H:95:LYS:NZ	8:H:120:ASP:OD2	2.36	0.56	
2:I:391:SER:OG	2:I:393:ASP:OD1	2.23	0.56	
4:K:8:ASP:OD2	4:K:8:ASP:N	2.35	0.56	
3:J:978:ARG:HH22	3:J:1198:VAL:HA	1.70	0.56	
8:G:56:VAL:HG22	8:G:146:VAL:HG12	1.86	0.56	
8:H:102:LEU:HB2	8:H:115:ILE:HD13	1.88	0.56	
2:I:563:THR:HG22	2:I:680:LEU:HD11	1.87	0.56	
2:I:386:GLU:OE1	2:I:387:ASN:ND2	2.40	0.55	
3:J:492:SER:HB2	3:J:499:ILE:HD13	1.87	0.55	
3:J:1157:ALA:HB3	3:J:1208:ASP:H	1.71	0.55	
7:B:3:DA:H2"	7:B:4:DA:C8	2.41	0.55	
3:J:587:LEU:HD21	3:J:608:CYS:HA	1.87	0.55	
3:J:1183:SER:OG	3:J:1184:ASP:N	2.39	0.55	
8:G:33:ARG:HG3	8:G:33:ARG:HH11	1.72	0.55	
3:J:197:GLU:OE2	3:J:220:ARG:NH2	2.40	0.55	
3:J:824:PRO:HD3	3:J:835:LEU:HB2	1.87	0.55	
4:K:1:MET:SD	4:K:3:ARG:NH1	2.80	0.55	
1:P:13:GLN:HB3	1:P:16:ARG:HD3	1.88	0.55	
2:I:411:ARG:NH2	2:I:427:ASP:OD2	2.40	0.55	
8:G:67:GLU:HG2	8:G:68:TYR:HD1	1.72	0.55	
2:I:979:LEU:HD22	2:I:989:LEU:HD11	1.89	0.55	
2:I:1269:ARG:HA	3:J:346:ARG:HA	1.89	0.55	
2:I:648:ASP:N	2:I:648:ASP:OD1	2.38	0.55	
3:J:370:LYS:HG2	3:J:441:LEU:HD12	1.89	0.55	
2:I:422:LYS:O	2:I:426:ILE:HD12	2.06	0.55	
2:I:925:SER:OG	2:I:926:GLY:N	2.40	0.55	
1:P:73:ARG:NH1	2:I:477:GLU:OE1	2.40	0.54	



	e us page	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:I:196:VAL:N	2:I:204:LEU:O	2.37	0.54	
2:I:516:ASP:OD1	2:I:516:ASP:N	2.33	0.54	
3:J:981:GLU:OE1	3:J:983:LYS:NZ	2.37	0.54	
2:I:972:PHE:HD2	2:I:994:ARG:HD2	1.71	0.54	
8:G:57:THR:HG22	8:G:58:GLU:HG3	1.89	0.54	
3:J:615:LYS:HG2	4:K:5:THR:HG21	1.89	0.54	
2:I:257:ALA:HB3	2:I:262:TYR:HE2	1.71	0.54	
3:J:709:ARG:HH11	3:J:712:GLN:HG2	1.71	0.54	
6:A:16:DG:H1'	6:A:19:DA:H61	1.72	0.54	
2:I:1073:LYS:NZ	5:R:16:G:OP1	2.34	0.54	
2:I:339:ASN:HB3	2:I:343:HIS:H	1.73	0.54	
8:G:207:THR:OG1	8:G:208:ASN:N	2.40	0.54	
2:I:406:ASN:ND2	2:I:413:GLU:O	2.41	0.54	
3:J:431:ARG:HD3	3:J:493:PRO:HG3	1.90	0.53	
3:J:67:ASP:OD1	3:J:67:ASP:N	2.40	0.53	
2:I:263:VAL:HA	2:I:267:ARG:HH21	1.73	0.53	
3:J:1174:ARG:HD3	3:J:1187:GLU:HB3	1.89	0.53	
8:G:191:ARG:HH22	8:G:194:GLN:HA	1.74	0.53	
8:H:74:VAL:HG21	8:H:81:ILE:HD11	1.89	0.53	
2:I:489:PRO:HA	2:I:492:MET:HB2	1.89	0.53	
2:I:102:LEU:HD11	2:I:118:LYS:HD2	1.91	0.53	
3:J:1048:ARG:HE	3:J:1059:LEU:HB3	1.74	0.53	
5:R:8:G:H2'	5:R:9:U:C6	2.43	0.53	
8:G:185:TYR:HB2	8:G:201:LEU:HD11	1.91	0.53	
8:H:65:LEU:HD12	8:H:168:ILE:HG13	1.90	0.53	
2:I:842:ASP:HA	2:I:847:PRO:HA	1.91	0.53	
8:G:190:ALA:HB2	8:G:200:LYS:HB3	1.89	0.52	
3:J:572:THR:HG21	3:J:589:TYR:HE2	1.74	0.52	
2:I:33:ASP:N	2:I:33:ASP:OD1	2.41	0.52	
2:I:1290:MET:HA	2:I:1294:LYS:HD3	1.91	0.52	
3:J:381:ILE:HD11	3:J:412:LEU:HD13	1.91	0.52	
2:I:444:ASP:O	2:I:450:ASN:ND2	2.42	0.52	
3:J:393:THR:HG23	3:J:396:ALA:H	1.75	0.52	
2:I:705:GLU:HB3	2:I:794:LEU:H	1.74	0.52	
2:I:1301:ARG:NE	5:R:1:U:O5'	2.42	0.52	
3:J:656:GLU:OE2	3:J:692:ARG:NH1	2.43	0.52	
4:K:9:ALA:HB2	4:K:55:GLU:HG2	1.92	0.52	
6:A:33:DG:H2"	6:A:34:DA:C8	2.44	0.52	
2:I:1291:LEU:HD21	3:J:1351:VAL:HG13	1.90	0.52	
2:I:516:ASP:O	2:I:522:SER:OG	2.28	0.51	
2:I:1223:ARG:NH2	3:J:721:SER:OG	2.43	0.51	



	<b>A t</b> and <b>D</b>	Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
3:J:174:ASP:OD1	3:J:174:ASP:N	2.37	0.51	
2:I:937:ASP:N	2:I:937:ASP:OD1	2.43	0.51	
3:J:322:ARG:HB3	3:J:322:ARG:NH1	2.26	0.51	
2:I:160:ASP:N	2:I:160:ASP:OD1	2.43	0.51	
3:J:404:GLU:OE1	3:J:404:GLU:N	2.43	0.51	
8:G:183:ILE:HD13	8:G:205:MET:HG2	1.93	0.51	
1:P:52:PRO:HG2	3:J:278:ARG:HH12	1.75	0.51	
3:J:1164:SER:HB2	3:J:1176:VAL:HG13	1.92	0.51	
8:G:33:ARG:HH22	8:G:197:ASP:HB2	1.74	0.51	
2:I:998:LEU:HD23	2:I:998:LEU:H	1.74	0.51	
2:I:148:GLN:OE1	2:I:454:ARG:NH2	2.44	0.51	
3:J:1140:ARG:NH2	3:J:1236:GLU:OE1	2.44	0.51	
2:I:1332:SER:HA	3:J:243:PRO:HB2	1.93	0.51	
3:J:153:ASN:OD1	3:J:153:ASN:N	2.44	0.50	
2:I:233:ARG:H	2:I:237:LEU:HA	1.76	0.50	
2:I:533:LEU:HD21	2:I:571:LEU:HD13	1.94	0.50	
3:J:321:LYS:HE2	3:J:321:LYS:H	1.75	0.50	
3:J:1230:THR:HG23	3:J:1257:VAL:HG11	1.93	0.50	
2:I:1253:LEU:H	2:I:1253:LEU:HD12	1.76	0.50	
8:G:154:PRO:HG2	8:G:157:THR:HG23	1.94	0.50	
3:J:473:THR:HG23	3:J:476:ALA:H	1.74	0.50	
3:J:1087:ASP:OD1	3:J:1087:ASP:N	2.43	0.50	
4:K:3:ARG:CZ	4:K:3:ARG:HA	2.41	0.50	
7:B:6:DA:H2"	7:B:7:DT:H71	1.94	0.50	
2:I:222:ASP:HA	2:I:227:LYS:HE3	1.93	0.50	
2:I:961:SER:OG	2:I:965:GLN:OE1	2.29	0.50	
2:I:1041:ASP:OD1	2:I:1041:ASP:N	2.38	0.50	
2:I:1100:PRO:HB3	3:J:639:VAL:HG22	1.93	0.50	
1:P:70:ASN:O	6:A:17:DG:N2	2.44	0.50	
2:I:996:ARG:HH21	2:I:999:GLU:HB3	1.76	0.49	
3:J:789:LYS:NZ	3:J:928:THR:O	2.38	0.49	
3:J:984:LEU:HB3	3:J:993:GLU:HB2	1.93	0.49	
3:J:1344:LEU:H	3:J:1344:LEU:HD22	1.77	0.49	
8:G:155:ALA:HA	8:G:158:ARG:NH1	2.26	0.49	
1:P:60:ASP:OD1	1:P:63:VAL:HG13	2.13	0.49	
8:G:17:GLU:HB3	8:G:25:LYS:HB2	1.94	0.49	
2:I:132:ASP:OD1	2:I:132:ASP:N	2.41	0.49	
3:J:846:GLU:HG2	3:J:881:LYS:HD3	1.95	0.49	
8:G:127:GLN:OE1	8:G:127:GLN:N	2.37	0.49	
3:J:848:VAL:HB	3:J:858:VAL:HG22	1.94	0.49	
2:I:724:VAL:HA	2:I:734:ILE:HG12	1.95	0.49	



	the case of the ca	Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
8:H:175:ALA:HB1	8:H:177:TYR:CD1	2.47	0.49	
2:I:12:ARG:HG3	2:I:1181:PRO:HB2	1.94	0.49	
2:I:593:LYS:O	2:I:600:THR:OG1	2.29	0.49	
2:I:106:GLU:HA	2:I:115:LYS:HE2	1.93	0.49	
3:J:443:GLU:OE1	8:H:196:THR:OG1	2.19	0.49	
3:J:520:ALA:HB1	3:J:543:SER:HB3	1.93	0.49	
3:J:1109:LEU:HD11	3:J:1113:VAL:HG11	1.93	0.49	
2:I:17:LYS:NZ	2:I:1194:GLU:OE2	2.43	0.49	
2:I:813:GLU:OE1	3:J:460:ASP:HA	2.13	0.49	
3:J:355:ILE:HG21	3:J:466:MET:SD	2.53	0.49	
8:G:91:ARG:NH1	8:G:122:GLU:OE2	2.41	0.49	
2:I:235:ASN:O	2:I:236:LYS:HG2	2.13	0.49	
3:J:984:LEU:HD23	3:J:992:LYS:HB3	1.95	0.49	
3:J:827:GLU:OE1	3:J:832:LYS:NZ	2.41	0.48	
8:G:158:ARG:NH1	8:G:158:ARG:HB3	2.28	0.48	
1:P:35:LEU:HD12	1:P:37:LYS:HD2	1.94	0.48	
3:J:1189:MET:HA	3:J:1189:MET:HE2	1.95	0.48	
4:K:12:LYS:NZ	4:K:55:GLU:O	2.46	0.48	
7:B:24:DT:H2'	7:B:25:DG:C8	2.48	0.48	
2:I:242:VAL:HB	2:I:245:ARG:HG3	1.95	0.48	
2:I:1142:ARG:HG3	2:I:1169:VAL:HG11	1.95	0.48	
3:J:1167:LYS:HE3	3:J:1167:LYS:HB3	1.67	0.48	
8:G:58:GLU:HG2	8:G:172:LEU:HD23	1.95	0.48	
3:J:511:TYR:OH	3:J:515:ARG:NH1	2.47	0.48	
2:I:602:GLU:OE2	2:I:604:HIS:NE2	2.47	0.48	
3:J:201:LEU:HB2	3:J:221:ILE:HD11	1.95	0.48	
2:I:45:GLY:HA3	2:I:54:ARG:HD2	1.95	0.48	
3:J:816:THR:HG22	3:J:818:GLU:H	1.79	0.48	
8:H:23:HIS:HE1	8:H:204:GLU:HG3	1.78	0.48	
3:J:208:THR:HG23	3:J:214:ARG:HG2	1.94	0.48	
3:J:807:LEU:HD11	3:J:1258:ARG:HE	1.79	0.48	
3:J:821:MET:HE1	3:J:879:ALA:HB1	1.96	0.48	
7:B:5:DG:H4'	7:B:6:DA:OP1	2.14	0.48	
7:B:31:DC:H2"	7:B:32:DG:N7	2.29	0.48	
8:G:235:ARG:NH2	8:H:14:VAL:O	2.47	0.48	
3:J:978:ARG:NH2	3:J:1198:VAL:HA	2.29	0.47	
2:I:727:VAL:HG12	2:I:773:LEU:HG	1.96	0.47	
2:I:878:THR:OG1	2:I:879:GLY:N	2.46	0.47	
2:I:972:PHE:O	2:I:975:ILE:HG13	2.15	0.47	
7:B:27:DC:H2"	7:B:28:DC:C6	2.49	0.47	
2:I:225:PHE:HZ	2:I:345:PRO:HA	1.79	0.47	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:I:1062:PRO:HA	2:I:1076:ILE:HB	1.97	0.47	
3:J:952:VAL:O	3:J:1014:GLY:N	2.36	0.47	
3:J:965:SER:HB2	3:J:973:LEU:HG	1.96	0.47	
3:J:1159:ILE:HD12	3:J:1179:PRO:HG3	1.96	0.47	
3:J:113:HIS:HB3	3:J:116:PHE:HD2	1.79	0.47	
3:J:532:GLU:OE2	8:H:152:TYR:OH 2.26		0.47	
3:J:821:MET:HE3	3:J:822:MET:H	1.79	0.47	
8:G:91:ARG:NH2	8:G:209:GLY:O	2.46	0.47	
3:J:117:LEU:HD12	3:J:124:ILE:HD13	1.96	0.47	
3:J:1188:GLU:OE1	3:J:1188:GLU:N	2.48	0.47	
1:P:62:GLU:OE2	1:P:62:GLU:N	2.39	0.47	
2:I:165:HIS:NE2	2:I:167:SER:HB2	2.30	0.47	
2:I:642:SER:HB2	3:J:770:LEU:HD21	1.97	0.47	
2:I:1080:ASN:OD1	2:I:1084:ASP:HB2	2.14	0.47	
2:I:1276:TRP:CE2	3:J:801:VAL:HG11	2.49	0.47	
7:B:23:DC:H2'	7:B:24:DT:C6	2.49	0.47	
8:G:33:ARG:NH2	8:G:197:ASP:HB2	2.30	0.47	
8:G:67:GLU:HG2	8:G:68:TYR:CD1	2.48	0.47	
8:H:104:LYS:HG2	8:H:110:VAL:HG22	1.96	0.47	
2:I:689:ALA:HB2	2:I:1233:LEU:HD23	1.97	0.47	
4:K:78:ALA:HA	4:K:81:GLN:HE21	1.80	0.47	
8:G:191:ARG:NH2	8:G:193:GLU:O	2.48	0.47	
6:A:32:DC:H2"	6:A:33:DG:C8	2.50	0.47	
8:H:187:VAL:HG13	8:H:199:ASP:HB3	1.97	0.47	
2:I:102:LEU:HG	2:I:118:LYS:HB2	1.96	0.47	
2:I:1103:VAL:HG21	3:J:639:VAL:HG21	1.96	0.47	
3:J:903:LEU:HD12	3:J:903:LEU:HA	1.82	0.47	
3:J:481:ARG:NH1	4:K:2:ALA:O	2.48	0.46	
2:I:196:VAL:HG21	2:I:209:ILE:HG13	1.96	0.46	
2:I:1121:ALA:HB2	2:I:1182:ILE:HD12	1.97	0.46	
3:J:1360:GLY:O	3:J:1363:TYR:HB3	2.16	0.46	
8:G:46:ILE:HD11	8:G:224:LEU:HD13	1.97	0.46	
2:I:236:LYS:O	2:I:237:LEU:HD12	2.15	0.46	
3:J:773:PHE:O	3:J:776:THR:OG1	2.33	0.46	
8:G:125:LYS:HD2	8:G:127:GLN:NE2	2.31	0.46	
2:I:275:ARG:O 2:I:279:LYS:HG2		2.15	0.46	
3:J:478:LEU:HB3	4:K:20:VAL:HG13	1.97	0.46	
2:I:562:GLU:HG2	2:I:574:SER:HB2	1.96	0.46	
3:J:342:LEU:HD13	3:J:1352:ILE:HG23	1.98	0.46	
3:J:591:ILE:O	3:J:594:GLN:NE2	2.47	0.46	
3:J:964:LYS:HB2	3:J:964:LYS:HE2	1.72	0.46	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:J:1160:SER:OG	3:J:1203:ARG:NH1	2.22	0.46
3:J:721:SER:O	3:J:725:MET:HG3	2.15	0.46
3:J:275:ARG:HH12	3:J:278:ARG:HD3	1.81	0.46
7:B:19:DC:H2'	7:B:20:DA:C8	2.51	0.46
8:H:226:GLU:O	8:H:229:GLU:HG3	2.15	0.46
2:I:255:ILE:HB	2:I:285:ILE:HD11	1.97	0.46
2:I:269:ILE:HG23	2:I:273:HIS:HB2	1.98	0.46
3:J:16:GLU:OE2	3:J:1355:ARG:NH2	2.44	0.46
6:A:16:DG:H1'	6:A:19:DA:N6	2.30	0.46
3:J:349:TYR:HE1	3:J:379:PRO:HG2	1.80	0.46
2:I:678:ARG:CZ	2:I:1106:ARG:HG2	2.46	0.46
3:J:450:HIS:HE1	3:J:452:LEU:HD12	1.81	0.46
3:J:653:ILE:O	3:J:656:GLU:HG3	2.15	0.46
3:J:215:LYS:O	3:J:218:THR:HG22	2.16	0.45
3:J:953:LYS:NZ	3:J:954:ASN:OD1	2.49	0.45
8:H:97:GLU:HG3	8:H:147:GLN:HE21	1.82	0.45
2:I:802:VAL:HG12	2:I:1096:ILE:HB	1.97	0.45
3:J:613:GLY:O	3:J:617:THR:OG1	2.26	0.45
8:H:11:PRO:O	8:H:12:ARG:NH1	2.49	0.45
2:I:104:ILE:HB	2:I:116:ASP:HB2	1.97	0.45
2:I:877:VAL:HG13	2:I:881:ASP:HB2 1.99		0.45
3:J:505:ASP:HB2	3:J:629:PHE:HE1	1.81	0.45
4:K:78:ALA:O	4:K:81:GLN:NE2	2.50	0.45
2:I:1216:ARG:HA	8:G:45:ARG:HE	1.81	0.45
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.99	0.45
3:J:555:TYR:CE2	3:J:565:ALA:HB2	2.51	0.45
8:G:77:ASP:OD1	8:G:77:ASP:N	2.50	0.45
2:I:944:ARG:HD2	2:I:944:ARG:HA	1.73	0.45
2:I:1059:ARG:NH1	8:G:152:TYR:OH	2.49	0.45
3:J:93:THR:OG1	3:J:94:GLN:N	2.50	0.45
8:G:133:LEU:HD11	8:G:140:ILE:HG22	1.99	0.45
2:I:1216:ARG:HA	8:G:45:ARG:HH21	1.81	0.45
3:J:1205:GLU:N	3:J:1208:ASP:OD2	2.49	0.45
7:B:19:DC:H2'	7:B:20:DA:H8	1.81	0.45
2:I:15:PHE:CG	2:I:1190:ALA:HB2	2.52	0.45
2:I:992:LEU:HD21	2:I:1000:LEU:HD11	1.98	0.45
2:I:14:ASP:HA	2:I:1183:ALA:HB3	1.99	0.45
2:I:1336:ASN:HA	3:J:33:TRP:HH2	1.81	0.45
2:I:915:ASP:OD1	2:I:915:ASP:N	2.50	0.44
3:J:1167:LYS:HB3	3:J:1174:ARG:HH21	1.82	0.44
2:I:1122:LYS:HG2	2:I:1229:TYR:CE1	2.52	0.44



	A + 2	Interatomic	Clash	
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)	
3:J:832:LYS:HE2	3:J:832:LYS:HB2	1.81	0.44	
3:J:1078:LEU:HD12	3:J:1121:LEU:HD13	2.00	0.44	
2:I:59:ILE:HD11	2:I:476:LYS:HD3	1.99	0.44	
2:I:129:LEU:HD23	2:I:129:LEU:HA	1.84	0.44	
2:I:1108:ASN:OD1	2:I:1108:ASN:N	2.50	0.44	
2:I:1140:LYS:O	2:I:1143:GLU:HG3	2.18	0.44	
3:J:1156:LEU:HD23	3:J:1223:LEU:HD12	1.98	0.44	
8:G:224:LEU:HD23	8:H:228:LEU:HD11	1.98	0.44	
3:J:591:ILE:HG13	3:J:592:VAL:HG13	2.00	0.44	
3:J:1021:ASP:OD1	3:J:1023:HIS:ND1	2.50	0.44	
6:A:19:DA:H1'	6:A:20:DG:O4'	2.16	0.44	
8:G:61:ILE:HB	8:G:64:VAL:HB	1.98	0.44	
3:J:1173:ARG:HG3	3:J:1190:ILE:HG23	1.99	0.44	
8:G:100:LEU:HD21	8:G:121:VAL:HG11	1.99	0.44	
2:I:540:ARG:HH22	5:R:12:G:P	2.41	0.44	
3:J:694:SER:HB2	3:J:738:ARG:HH11	1.83	0.44	
2:I:104:ILE:HD12	2:I:116:ASP:HB2	1.99	0.44	
3:J:151:MET:H	3:J:151:MET:HE3	1.83	0.44	
3:J:572:THR:HG21	3:J:589:TYR:CE2	2.52	0.44	
3:J:655:SER:O	3:J:658:GLU:HG2	2.17	0.44	
3:J:803:VAL:HG21	3:J:1309:ILE:HG23	2.00	0.44	
3:J:1082:ASP:OD1	3:J:1082:ASP:N	2.49	0.44	
4:K:8:ASP:O	4:K:11:GLU:HG3	2.18	0.44	
8:G:10:LYS:HA	8:G:10:LYS:HD2	1.75	0.44	
1:P:10:LYS:HG3	1:P:76:SER:HB2	1.99	0.43	
2:I:1016:GLU:HA	2:I:1019:ASP:OD2	2.18	0.43	
2:I:1082:ILE:HD11	2:I:1093:PRO:HG2	2.00	0.43	
2:I:657:THR:HB	2:I:1187:PHE:HB2	2.00	0.43	
2:I:914:LYS:NZ	2:I:915:ASP:O	2.46	0.43	
3:J:1193:TRP:HE3	3:J:1193:TRP:H	1.67	0.43	
2:I:402:ARG:HA	2:I:402:ARG:HD3	1.73	0.43	
2:I:576:SER:HB2	2:I:579:ALA:HB2	2.00	0.43	
2:I:1129:ASN:OD1	2:I:1177:ARG:NH1	2.51	0.43	
3:J:515:ARG:NH2	3:J:718:SER:O	2.50	0.43	
3:J:663:GLU:O	3:J:666:GLU:HG3	2.17	0.43	
3:J:678:ARG:HG3	3:J:679:TYR:N	2.33	0.43	
8:G:61:ILE:HG12	8:G:142:MET:HG2	2.00	0.43	
8:H:23:HIS:CE1	8:H:204:GLU:HG3	2.53	0.43	
8:H:102:LEU:HB3	8:H:142:MET:SD	2.58	0.43	
3:J:35:PHE:CG	3:J:101:ARG:HD3	2.53	0.43	
3:J:55:GLY:H	3:J:58:CYS:HB2	1.83	0.43	



Atom-1	Atom-2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
3:J:91:GLU:OE1	3:J:101:ARG:NH2	2.45	0.43	
4:K:38:LEU:HB3	4:K:58:LEU:HD23	2.01	0.43	
7:B:24:DT:H2'	7:B:25:DG:H8	1.83	0.43	
2:I:1047:LEU:HD12	2:I:1048:LYS:HB2	2.00	0.43	
3:J:331:ILE:HD13	3:J:331:ILE:HA	1.87	0.43	
1:P:27:ASN:HB2	1:P:58:GLU:HB3	2.01	0.43	
3:J:215:LYS:HD3	3:J:215:LYS:HA	1.68	0.43	
8:G:23:HIS:CE1	8:G:204:GLU:HG3	2.54	0.43	
3:J:102:MET:HG2	3:J:246:PRO:HD3	2.01	0.43	
8:H:224:LEU:HD12	8:H:224:LEU:HA	1.83	0.43	
2:I:233:ARG:HE	2:I:233:ARG:HB3	1.62	0.43	
2:I:351:LEU:HD23	2:I:351:LEU:HA	1.91	0.43	
2:I:519:ASN:OD1	2:I:522:SER:HB3	2.19	0.43	
2:I:1151:LEU:HD22	2:I:1198:LEU:HD13	2.01	0.43	
3:J:819:GLY:HA3	3:J:882:VAL:O	2.18	0.43	
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.54	0.42	
2:I:1262:LYS:N	7:B:22:DG:OP1	2.52	0.42	
2:I:678:ARG:HA	2:I:678:ARG:HD2	1.71	0.42	
2:I:791:LEU:HD23	2:I:791:LEU:HA 1.84		0.42	
3:J:272:VAL:HG21	3:J:306:LEU:HD22	2.00	0.42	
3:J:425:ARG:HD2	3:J:459:ALA:HB2	1.99	0.42	
1:P:94:HIS:HD1	1:P:94:HIS:C	2.23	0.42	
5:R:8:G:O2'	5:R:9:U:O4'	2.34	0.42	
6:A:33:DG:H2"	6:A:34:DA:H8	1.85	0.42	
7:B:35:DG:H2"	7:B:36:DT:OP2	2.19	0.42	
8:G:92:VAL:HG22	8:G:121:VAL:HB	2.00	0.42	
3:J:886:VAL:HA	3:J:1258:ARG:HB2	2.01	0.42	
3:J:1248:ILE:HD13	3:J:1248:ILE:HA	1.92	0.42	
8:G:44:ARG:O	8:G:48:LEU:HD23	2.19	0.42	
1:P:21:LEU:HD22	1:P:72:THR:HG21	2.01	0.42	
2:I:312:ALA:HB3	2:I:315:MET:HE2	2.01	0.42	
2:I:388:LEU:HD12	2:I:388:LEU:HA	1.87	0.42	
2:I:545:PHE:CD1	2:I:545:PHE:C	2.92	0.42	
2:I:996:ARG:NH2	2:I:999:GLU:HB3	2.35	0.42	
3:J:1346:GLY:O	3:J:1350:ASN:ND2	2.35	0.42	
8:H:64:VAL:HG13	8:H:69:SER:HB2	2.01	0.42	
2:I:661:VAL:HG21 2:I:1186:VAL:HG21		2.00	0.42	
6:A:27:DT:H2'	6:A:28:DT:H71	2.02	0.42	
8:H:76:GLU:OE1	8:H:132:HIS:N	2.48	0.42	
2:I:143:ARG:NH1	2:I:512:SER:OG	2.52	0.42	
2:I:487:LEU:HD23	2:I:487:LEU:H	1.84	0.42	



	the case of the ca	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
3:J:919:ALA:O	3:J:923:ILE:HG12	2.20	0.42	
3:J:415:VAL:HG23	3:J:416:ILE:HG23	2.01	0.42	
3:J:1156:LEU:HD12	3:J:1209:VAL:HA	2.02	0.42	
8:G:104:LYS:HD2	8:G:104:LYS:HA	1.89	0.42	
2:I:3:TYR:HB2	2:I:8:LYS:HG3	2.02	0.42	
2:I:347:ILE:HD13	2:I:347:ILE:HA	1.96	0.42	
2:I:1178:LYS:HE2	2:I:1178:LYS:HB2	1.88	0.42	
2:I:1336:ASN:N	3:J:23:ALA:O	2.51	0.42	
3:J:804:ALA:O	3:J:916:GLY:HA3	2.20	0.42	
3:J:870:ASP:O	3:J:873:GLU:HG3	2.20	0.42	
3:J:1306:LEU:HD22	3:J:1306:LEU:HA	1.87	0.42	
3:J:644:MET:H	3:J:644:MET:HG2	1.55	0.41	
3:J:980:THR:HB	3:J:997:VAL:HG22	2.01	0.41	
3:J:1063:ASP:N	3:J:1063:ASP:OD1	2.43	0.41	
2:I:819:SER:HB2	2:I:1085:MET:HG3	2.02	0.41	
6:A:28:DT:H2'	6:A:29:DT:H71	2.02	0.41	
1:P:21:LEU:HD12	1:P:26:VAL:HG21	2.02	0.41	
1:P:54:TYR:CE2	3:J:291:ILE:HD11	2.55	0.41	
3:J:403:ARG:HB3	3:J:405:GLU:OE1 2.20		0.41	
3:J:1077:ALA:HB1	3:J:1098:GLN:OE1	2.21	0.41	
8:H:151:GLY:O	8:H:177:TYR:HB2	2.20	0.41	
2:I:714:VAL:O	2:I:767:GLN:NE2	2.53	0.41	
2:I:842:ASP:OD1	2:I:842:ASP:N	2.44	0.41	
5:R:2:C:N4	5:R:6:A:N7	2.69	0.41	
2:I:1072:ASN:OD1	2:I:1072:ASN:N	2.48	0.41	
3:J:960:LEU:HB3	3:J:963:VAL:HG11	2.03	0.41	
3:J:1273:ASP:OD1	3:J:1273:ASP:N	2.36	0.41	
4:K:70:GLN:O	4:K:73:GLN:HG3	2.21	0.41	
6:A:5:DA:H2"	6:A:6:DC:C5	2.56	0.41	
6:A:11:DC:H2"	6:A:12:DG:N7	2.35	0.41	
7:B:20:DA:H2'	7:B:21:DC:C6	2.55	0.41	
8:G:195:ARG:HB3	8:G:197:ASP:OD1	2.20	0.41	
1:P:100:LYS:HA	1:P:100:LYS:HD3	1.86	0.41	
3:J:836:ARG:NH1	3:J:870:ASP:OD1	2.53	0.41	
4:K:72:GLN:HG2	4:K:75:GLN:HE21	1.85	0.41	
7:B:12:DA:H2"	7:B:13:DA:H8	1.86	0.41	
8:H:154:PRO:HG2	8:H:157:THR:HG23	2.03	0.41	
2:I:960:LEU:HD23	2:I:960:LEU:HA	1.92	0.41	
3:J:84:ILE:HG13	3:J:91:GLU:HG3	2.03	0.41	
3:J:222:LYS:HE3	3:J:1278:GLU:HG3	2.02	0.41	
3:J:731:ARG:HA	3:J:731:ARG:HD2	1.74	1.74 0.41	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:I:230:PHE:CE1	2:I:239:MET:HG2	2.55	0.41	
2:I:302:ILE:HG13	2:I:308:GLU:O	2.21	0.41	
2:I:446:ASP:OD2	2:I:446:ASP:N	2.53	0.41	
3:J:197:GLU:O	3:J:201:LEU:HG	2.21	0.41	
3:J:221:ILE:HD13	3:J:221:ILE:HA	1.86	0.41	
3:J:265:LEU:HD23	3:J:265:LEU:HA	1.89	0.41	
3:J:357:VAL:HG23	3:J:451:PRO:HG3	2.03	0.41	
3:J:709:ARG:NH1	3:J:710:ASP:O	2.53	0.41	
3:J:715:LYS:HE2	3:J:715:LYS:HB3	1.92	0.41	
8:G:16:ILE:HD13	8:G:16:ILE:HA	1.89	0.41	
8:H:137:ASN:OD1	8:H:137:ASN:N	2.49	0.41	
2:I:11:ILE:O	2:I:1149:TYR:OH	2.32	0.41	
2:I:23:ASP:OD1	2:I:23:ASP:N	2.53	0.41	
2:I:195:PHE:CG	2:I:203:LYS:HE2	2.55	0.41	
2:I:317:LEU:HD23	2:I:317:LEU:HA	1.87	0.41	
2:I:371:ARG:HD3	2:I:371:ARG:HA	1.79	0.41	
3:J:46:TYR:OH	6:A:8:DA:H3'	2.20	0.41	
3:J:114:ILE:HD12	3:J:114:ILE:HA	1.91	0.41	
3:J:179:LYS:HG3	3:J:180:MET:H 1.85		0.41	
3:J:845:ALA:HB3	3:J:881:LYS:HG2	2.03	0.41	
3:J:872:LEU:HD21	3:J:880:VAL:HG21	2.03	0.41	
4:K:64:LEU:HD23	4:K:64:LEU:HA	1.87	0.41	
8:H:109:PRO:HB3	8:H:132:HIS:NE2	2.36	0.41	
2:I:1088:ASP:OD1	2:I:1088:ASP:N	2.51	0.41	
2:I:1120:ALA:HB2	2:I:1199:LEU:HG	2.03	0.41	
3:J:245:LEU:O	3:J:250:ARG:NH2	2.54	0.41	
3:J:614:LEU:HD23	4:K:7:GLN:HB2	2.02	0.41	
3:J:933:ARG:HH11	3:J:933:ARG:HA	1.86	0.41	
3:J:1028:ILE:H	3:J:1028:ILE:HG13	1.80	0.41	
3:J:1169:THR:HG23	3:J:1171:GLY:H	1.86	0.40	
8:G:64:VAL:HG11	8:G:78:ILE:HG21	2.03	0.40	
8:H:188:GLU:OE1	8:H:200:LYS:NZ	2.52	0.40	
2:I:478:ARG:HH21	2:I:492:MET:HE3	1.86	0.40	
2:I:1117:LEU:HD12	2:I:1117:LEU:HA	1.91	0.40	
3:J:287:ALA:HB1	3:J:291:ILE:HG21	2.03	0.40	
3:J:411:ILE:HD13	3:J:411:ILE:HA	1.88	0.40	
3:J:640:GLY:N	3:J:643:ASP:OD2	2.52	0.40	
3:J:844:THR:HG23	3:J:864:LEU:HD11	2.03	0.40	
3:J:1250:ASP:OD1	3:J:1250:ASP:N	2.54	0.40	
8:G:193:GLU:CD	8:G:194:GLN:N	2.73	0.40	
2:I:1005:GLU:HG3	2:I:1007:LYS:H	1.86 0.40		



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1116:HIS:HE1	2:I:1226:THR:HG23	1.87	0.40
3:J:220:ARG:HG3	3:J:224:LEU:HD23	2.02	0.40
3:J:292:VAL:HG22 3:J:296:LYS:H		2.02	0.40
3:J:424:ASN:HB2 3:J:434:ILE:HI		2.04	0.40
2:I:631:GLU:OE1 2:I:631:GLU:N		2.54	0.40
2:I:1022:LYS:HE3	2:I:1022:LYS:HB2	1.94	0.40
2:I:204:LEU:HD23	2:I:204:LEU:HA	1.98	0.40
2:I:967:LEU:HD13 2:I:1021:LEU:HD11		2.03	0.40
8:H:47:LEU:HB3	8:H:180:VAL:HG11	2.04	0.40
8:H:79:LEU:H	8:H:79:LEU:HD23	1.86	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
1	Р	99/164~(60%)	96~(97%)	3~(3%)	0	100	100
2	Ι	1317/1342~(98%)	1291 (98%)	26~(2%)	0	100	100
3	J	1337/1416~(94%)	1301 (97%)	36 (3%)	0	100	100
4	Κ	82/91~(90%)	80 (98%)	2(2%)	0	100	100
8	G	232/329~(70%)	228 (98%)	4 (2%)	0	100	100
8	Η	229/329 $(70%)$	222 (97%)	6 (3%)	1 (0%)	34	67
All	All	3296/3671~(90%)	3218 (98%)	77 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	Н	193	GLU



#### 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	Percentiles
1	Р	89/143~(62%)	83~(93%)	6~(7%)	16 46
2	Ι	1140/1157~(98%)	1062 (93%)	78 (7%)	16 45
3	J	1126/1177~(96%)	1066~(95%)	60~(5%)	22 52
4	Κ	71/75~(95%)	65~(92%)	6 (8%)	10 35
8	G	201/286~(70%)	190 (94%)	11 (6%)	21 51
8	Н	198/286~(69%)	179 (90%)	19 (10%)	8 29
All	All	2825/3124~(90%)	2645~(94%)	180 (6%)	21 47

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Р	28	CYS
1	Р	36	GLU
1	Р	37	LYS
1	Р	84	SER
1	Р	95	GLN
1	Р	99	TYR
2	Ι	1	MET
2	Ι	21	VAL
2	Ι	30	ILE
2	Ι	55	SER
2	Ι	70	TYR
2	Ι	113	THR
2	Ι	147	SER
2	Ι	158	ASP
2	Ι	159	SER
2	Ι	163	LYS
2	Ι	165	HIS
2	Ι	188	PHE
2	Ι	189	ASP
2	Ι	234	ASP
2	Ι	237	LEU
2	Ι	239	MET



Mol	Chain	Res	Type
2	Ι	245	ARG
2	Ι	252	SER
2	Ι	264	GLU
2	Ι	280	ASP
2	Ι	287	VAL
2	Ι	300	ASP
2	Ι	315	MET
2	Ι	318	SER
2	Ι	341	LEU
2	Ι	348	SER
2	Ι	369	MET
2	Ι	370	MET
2	Ι	378	ARG
2	Ι	387	ASN
2	Ι	391	SER
2	Ι	393	ASP
2	Ι	421	SER
2	Ι	423	ASP
2	Ι	441	GLU
2	Ι	452	ARG
2	Ι	472	GLU
2	Ι	478	ARG
2	Ι	481	LEU
2	Ι	488	MET
2	Ι	503	LYS
2	Ι	509	SER
2	Ι	512	SER
2	Ι	514	PHE
2	Ι	516	ASP
2	Ι	522	SER
2	Ι	529	ARG
2	Ι	541	GLU
2	Ι	545	PHE
2	Ι	554	HIS
2	Ι	563	THR
2	Ι	565	GLU
2	Ι	584	TYR
2	Ι	643	SER
2	Ι	697	LYS
2	Ι	741	MET
2	Ι	758	ARG
2	Ι	770	CYS



Mol	Chain	Res	Type
2	Ι	773	LEU
2	Ι	805	MET
2	Ι	811	ASN
2	Ι	819	SER
2	Ι	913	VAL
2	Ι	925	SER
2	Ι	998	LEU
2	Ι	1046	VAL
2	Ι	1059	ARG
2	Ι	1131	MET
2	Ι	1170	MET
2	Ι	1178	LYS
2	Ι	1225	VAL
2	Ι	1227	VAL
2	Ι	1243	MET
2	Ι	1270	PHE
2	Ι	1289	GLU
2	Ι	1315	MET
2	Ι	1319	MET
2	Ι	1339	LEU
3	J	24	LEU
3	J	29	MET
3	J	46	TYR
3	J	74	LYS
3	J	88	CYS
3	J	117	LEU
3	J	133	ARG
3	J	151	MET
3	J	172	PHE
3	J	174	ASP
3	J	179	LYS
3	J	227	PHE
3	J	232	ASN
3	J	259	ARG
3	J	281	ARG
3	J	290	ILE
3	J	312	ARG
3	J	357	VAL
3	J	472	LEU
3	J	485	MET
3	J	553	THR
3	J	599	LYS



Mol	Chain	Res	Type
3	J	644	MET
3	J	649	LYS
3	J	651	HIS
3	J	670	SER
3	J	673	VAL
3	J	678	ARG
3	J	743	MET
3	J	747	MET
3	J	763	PHE
3	J	814	CYS
3	J	821	MET
3	J	857	LEU
3	J	891	ASP
3	J	895	CYS
3	J	910	ASN
3	J	922	SER
3	J	964	LYS
3	J	990	ARG
3	J	999	TYR
3	J	1023	HIS
3	J	1025	MET
3	J	1036	ARG
3	J	1040	MET
3	J	1059	LEU
3	J	1169	THR
3	J	1173	ARG
3	J	1186	TYR
3	J	1193	TRP
3	J	1199	PHE
3	J	1224	ARG
3	J	1239	ASP
3	J	1250	ASP
3	J	1273	ASP
3	J	1306	LEU
3	J	1321	SER
3	J	$1\overline{365}$	TYR
3	J	1366	HIS
3	J	1373	ARG
4	K	1	MET
4	К	3	ARG
4	Κ	43	ASN
4	K	66	VAL



Mol	Chain	Res	Type
4	K	69	ARG
4	K	70	GLN
8	G	4	SER
8	G	18	GLN
8	G	77	ASP
8	G	80	GLU
8	G	117	HIS
8	G	121	VAL
8	G	129	VAL
8	G	152	TYR
8	G	171	LEU
8	G	185	TYR
8	G	207	THR
8	Н	20	SER
8	Н	23	HIS
8	Н	38	THR
8	Н	68	TYR
8	Н	74	VAL
8	Н	77	ASP
8	Н	98	VAL
8	Н	117	HIS
8	Н	133	LEU
8	Н	137	ASN
8	Н	142	MET
8	Н	160	HIS
8	Н	176	CYS
8	Н	182	ARG
8	Н	192	VAL
8	Н	193	GLU
8	Н	207	THR
8	Н	229	GLU
8	Н	231	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	Ι	46	GLN
2	Ι	1116	HIS
4	Κ	81	GLN
8	G	23	HIS
8	Н	147	GLN



#### 5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	R	16/17~(94%)	8~(50%)	0

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	R	2	С
5	R	3	U
5	R	4	А
5	R	5	U
5	R	6	А
5	R	7	U
5	R	13	С
5	R	17	U

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-17647. 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





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: 189





Z Index: 161

#### 6.3.2 Raw map



X Index: 189

Y Index: 195



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



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

#### 6.4.1 Primary map



6.4.2 Raw map



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



#### 6.5 Orthogonal surface views (i)

#### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

#### 6.5.2 Raw map



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

#### 6.6 Mask visualisation (i)

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



# 7 Map analysis (i)

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

### 7.1 Map-value distribution (i)



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



#### 7.2 Volume estimate (i)



The volume at the recommended contour level is  $251 \text{ nm}^3$ ; this corresponds to an approximate mass of 227 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 0.294  $\rm \AA^{-1}$ 



# 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 0.294  $\mathrm{\AA^{-1}}$ 



#### 8.2 Resolution estimates (i)

$\begin{bmatrix} Bosolution ostimato (Å) \end{bmatrix}$	Estimation criterion (FSC cut-off)		
resolution estimate (A)	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.27	3.69	3.30
Unmasked-calculated*	3.84	6.93	3.91

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.84 differs from the reported value 3.4 by more than 10 %



# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-17647 and PDB model 8PFJ. Per-residue inclusion information can be found in section 3 on page 7.

## 9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.25 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 (0.25).



#### 9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 86% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score	1.0
All	0.8630	0.4340	
А	0.8560	0.3100	
В	0.8930	0.3110	
G	0.8820	0.4720	
Н	0.8670	0.4350	
I	0.8770	0.4570	
J	0.8540	0.4290	
K	0.8020	0.4310	
Р	0.8740	0.4280	0.0 <0.0
R	0.6230	0.3020	

