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PDB ID	:	6MZM
EMDB ID	:	EMD-9306
Title	:	Human TFIID bound to promoter DNA and TFIIA
Authors	:	Patel, A.B.; Louder, R.K.; Greber, B.J.; Grunberg, S.; Luo, J.; Fang, J.; Liu,
		Y.; Ranish, J.; Hahn, S.; Nogales, E.
Deposited on	:	2018-11-05
Resolution	:	7.50 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

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

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

EMDB validation analysis	:	0.0.1. dev 70
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 7.50 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.



Motria	Whole archive	EM structures
wietric	$(\# {\rm Entries})$	$(\# {\rm Entries})$
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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 <=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			Qu	ality of	chain			
1	А	496	22%		79%				10%	10%
2	В	1199	9%		64%			16%	19%	
3	D	1025	• 12% •			8	8%			
4	G	800	14%	48%		11%		41	%	
5	Н	677	319	%	7%		629	%		
6	Ι	677	6%	43%		6%		50%		_
7	J	349	10%	6	5%		65%			
8	К	310	12%	56	%		9%		35%	



Mol	Chain	Length			Qual	ity of ch	ain		
9	L	264	—	37%	•		61%		
10	Ο	218	30	%	8%		62%		
11	R	161	11%	40%	6%		54%		
12	Т	339	23%	46%		7%	47	%	
13	U	80	15%			94%			6%
14	V	80	15%			94%			6%
15	W	90		40%	91	۱%			9%
16	Х	97		51%	9	2%			7% •
17	Z	238	25%			98%			



2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 32243 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 initiation factor TFIID subunit 1, TAF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	А	445	Total 3610	C 2300	N 642	0 645	S 23	0	0

• Molecule 2 is a protein called Transcription initiation factor TFIID subunit 2, TAF2.

Mol	Chain	Residues		Α	AltConf	Trace			
2	В	968	Total 7832	C 5031	N 1322	0 1421	S 58	0	0

• Molecule 3 is a protein called Transcription initiation factor TFIID subunit 4, TAF4.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
3	D	128	Total 816	C 501	N 156	O 159	0	0

• Molecule 4 is a protein called Transcription initiation factor TFIID subunit 5, TAF5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	473	Total 3646	C 2314	N 638	0 679	S 15	0	0

• Molecule 5 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Н	257	Total 1943	C 1230	N 347	0 355	S 11	0	0

• Molecule 6 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Ι	339	Total 2520	C 1585	N 445	0 474	S 16	0	0



• Molecule 7 is a protein called Transcription initiation factor TFIID subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	123	Total 998	C 638	N 184	0 172	${S \atop 4}$	0	0

• Molecule 8 is a protein called Transcription initiation factor TFIID subunit 8, TAF8.

Mol	Chain	Residues		At	AltConf	Trace			
8	K	202	Total 1449	C 906	N 260	0 278	${ m S}{ m 5}$	0	0

• Molecule 9 is a protein called Transcription initiation factor TFIID subunit 9, TAF9.

Mol	Chain	Residues		At	AltConf	Trace			
9	L	104	Total 732	C 456	N 129	0 142	${f S}{5}$	0	0

• Molecule 10 is a protein called Transcription initiation factor TFIID subunit 10.

Mol	Chain	Residues		At	AltConf	Trace			
10	Ο	82	Total 645	C 413	N 102	0 126	$\frac{S}{4}$	0	0

• Molecule 11 is a protein called Transcription initiation factor TFIID subunit 12.

Mol	Chain	Residues		At	oms			AltConf	Trace
11	R	74	Total 611	C 381	N 107	O 120	${ m S} { m 3}$	0	0

• Molecule 12 is a protein called TATA-box-binding protein.

Mol	Chain	Residues		At	AltConf	Trace			
12	Т	180	Total 1429	C 927	N 252	0 243	${f S}7$	0	0

• Molecule 13 is a DNA chain called SCP DNA (80-MER).

Mol	Chain	Residues		At	AltConf	Trace			
13	U	80	Total 1626	C 770	N 292	0 484	Р 80	0	0

• Molecule 14 is a DNA chain called SCP DNA (80-MER).



Mol	Chain	Residues		\mathbf{A}	AltConf	Trace			
14	V	80	Total 1654	C 778	N 320	O 476	Р 80	0	0

• Molecule 15 is a protein called Transcription initiation factor IIA subunit 1.

Mol	Chain	Residues		At	AltConf	Trace			
15	W	90	Total 749	C 478	N 126	0 141	$\frac{S}{4}$	0	0

• Molecule 16 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues		At	AltConf	Trace			
16	Х	97	Total 793	C 502	N 140	0 149	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 17 is a protein called Unk.

Mol	Chain	Residues		Ato	ms		AltConf	Trace
17	Z	238	Total 1190	C 714	N 238	O 238	0	0



3 Residue-property plots (i)

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



• Molecule 1: Transcription initiation factor TFIID subunit 1, TAF1

N328	5332 1335	E338	L041 T342 R343 R344	0348	S349	1353 1353	1359 8360 R361	M362	D366 E367	K371	M382	G387 V388	N389 E390 V391	K396	1402	K408	H4 <mark>15</mark> P416	I417 F418	G419 G420	G421 K422	E423 K424	D425	H432	-
W443	Y446	H454 L455	R458 M467	R463	u4/1 S485 ♦	F488	H491	M492	V498 S499	D514	V528	K530	N538 R539	K540 R541	N542 E545	L546 E547	1548 K549 0550	D551 Y552	K559	L564 K565		H577	1579 1580	•
E583	K587	P591 C592 UE03	R597	R598	K602	NGO8	G609 E610	E611 V612	M619	D620 A621	1630	M634	R638 K639	L653	R657	U658 V659 V660	0663	1666	L669 E670	R678	T682	F6 <mark>91</mark> Y692 R693	V694	S711
T714	M719 B725	C728	C729 K730 S731	1735 V736	K737	A756	D762 V763	H764	R785	L802	V805 T807 P808	A809	V810 S811	V812 N813	N814 E815	V816 R817	T818 L819	D820 N821 1822	1829	R835	roso L837 N838	M839 E840 K841	L842 L843 P844	R847 H848 H848
T849 1850	T851 R856 ♦	P871	F874 K875	D885 1886 R887	1888 L891	V894	T898 K899	L907	D917	R923	1926	м929 1930 т931	K932	P935	N939	N946	K955 L956	<mark>M957</mark> N958 S959	G960 T961	R966	F976	F979 G980 L981	P984	
S985 C986	L987 PRO LEU	PRO GLU LEU	GLY LEU VAL	LEU LEU	LYS GLU	LYS ALA VAL	LEU ASN	THR TLE	ILE PRO	GLU SER VAT	VAL ALA GLY	ASN GLN	GLU ALA	ALA ASN ASN	PR0 SER	SER HIS	GLN	VAL GLY DHE	GLN	PRO PHE SFR	SER	GLN GLU	GLU	
GLU	ASP MET ASP	THR VAL HIS	SER GLN	PHE ILE SFR	SIH SIH	ASN MET	LEU GLU ARG	PRO SER	THR PRO	LEU SER	LYS TYR	ARG PRO	ALA SER SEP	ARG	ALA LEU	PRO GLN	HIS SER	ALA GLY CYS	ASP SER TUD	PRO THR	THR LYS	PRU GLN TRP SFD	NEC	
GLU GLU	LEU ALA ARG	LYS GLY THR	CL N CL N CL N	ALA PRO	GLU MET	MET HIS	PRO ALA ALA	SER	PRO LEU SEB	VAL PHE	THR LYS	GLU SER	THR ALA SEP	SIH	SER ASP	SIH SIH	HIS	HIS GLU	HIS LYS	LYS	LYS	STH STH	FIS	
SIH	HIS LYS HIS	LYS HIS ASP	LYS GLU AS	ASP	PRO PHE	PHE SER	SER PRO ALA	SER GLY	ARG SER	ARG SER	PRO SER	LEU SER	ASP											
• 1	Mole	cule	3: T	rans	crip	tion	ı ini	tiat	ion	fa	cto	r T	FII	D s	ubı	ınit	4,	TA	F4					
Ch	ain 1	D: 📕	12%	•	-	-	-	-	-	-	-	8	8%	-	-	-	-	-	-	-				
HIS VAL	VAL SER GLY	SER PRO ALA	ALA ALA ALA	ALA GLY PRO	ALA ALA	ALA GLU	GLY ALA PRO	GLY ALA	ALA PRO	PRO PRO	PRO ALA	GLY ARG	ALA ARG PPO	GLY GLY	GLY GLY	GLN ARG	PRO GLY	PRO PRO SER	PRO ARG	PRO LEU	VAL PRO	ALA GLY PRO	WTW	
PRO PRO	ALA ALA LYS	LEU ARG PRO	PRO GLU GLU	SER ALA GLY	SER	ALA PRO VAL	PRO ALA ALA	ALA ALA	VAL ALA	GLY PRO	GLU PRO	ALA PRO	ALA GLY DDO	ALA LYS	PRO ALA	GLY PRO ALA	ALA LEU	ALA ALA ARG	ALA GLY DDO	GLY PRO	GLY PRO	GLY PRO GLY PPO	rw	
GLY PRO	GLY PRO GLY	PRO GLY LYS	ALA GLY PRD	GLY ALA ALA	GLN THR	ASN GLY	SER ALA ALA	LEU	ASN SER UTS	ALA	ALA ALA	PRO ALA	VAL SER LEII	VAL	ASN GLY	PRU ALA ALA	LEU	PRO LEU PRO	LYS PRO AT A	ALA PRO	GL Y THR	VAL ILE GLN THD	UUT	
PRO PRO	PHE VAL GLY	ALA ALA ALA	PRO ALA PRO	ALA ALA PRO	SER PRO	PKU ALA ALA	PRO ALA PRO	ALA ALA	PRO ALA ATA	ALA ALA PRO	PRO PRO	PRO PRO	PRO ALA PPO	ALA THR	LEU ALA	ARG PRO PRO	GLY GLY	PRO ALA GLY	PRO PRO TUD	ALA ALA	PRO ALA	VAL PRO PRO	LIN	
ALA ALA	ALA GLN ASN	GLY GLY SER	ALA GLY ALA ATA	PRO ALA PRO	ALA PRO	ALA ALA GLY	GLY PRO ALA	GLY VAL	SER GLY CIN	PRO GLY	PRO GLY	ALA ALA	ALA ALA ATA	PRO ALA	PRO GLY	VAL LYS ALA	GLU SER	PR0 LYS ARG	VAL VAL CTN	ALA ALA	PRO PRO	ALA GLN THP	VIIIT	
LEU ALA	ALA SER GLY	PRO ALA SER	ALA ALA ALA SFR	MET VAL TIF	GLY PRO	MET GLN	GLY ALA LEU	PRO SER	PRO ALA	ALA VAL PRO	PRO PRO	ALA PRO	GLY THR PBO	THR	LEU PRO	LYS GLY ALA	ALA GLY	ALA VAL THR	GLN SER 1 EII	SER	THR PRO	THR ALA THR	WHIT	
SER GLY	ILE ARG ALA	THR LEU THR	THR VAL	ALA PRO	LEU PRO	GLN PRO PRO	GLN ASN PRO	THR	GLN	PHE GLN	LEU PRO	PRO GLY	MET VAL 1 EU	VAL	SER GLU	GLY GLN	LEU	MET ILE PRO	GLN GLN	LEU ALA	GLN	GLN GLN AT A	ALA	



























4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	25180	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT $(4k \ge 4k)$	Depositor
Maximum map value	0.119	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	380.16, 380.16, 380.16	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor



5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol Chain		Bond lengths		Bond angles	
	Ullaili	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.27	0/3694	0.51	1/4967~(0.0%)
2	В	0.30	0/8029	0.60	1/10882~(0.0%)
3	D	0.25	0/821	0.44	0/1124
4	G	0.28	0/3537	0.59	0/4802
5	Н	0.30	0/1978	0.58	1/2693~(0.0%)
6	Ι	0.26	0/2506	0.50	0/3402
7	J	0.26	0/1017	0.53	0/1370
8	Κ	0.26	0/1212	0.50	1/1640~(0.1%)
9	L	0.25	0/705	0.49	0/955
10	0	0.26	0/657	0.46	0/891
11	R	0.26	0/618	0.50	0/835
12	Т	0.28	0/1455	0.52	0/1958
13	U	0.69	0/1819	0.99	6/2802~(0.2%)
14	V	0.67	0/1859	0.93	1/2870~(0.0%)
15	W	0.29	0/762	0.56	0/1026
16	Х	0.29	0/803	0.63	1/1088~(0.1%)
All	All	0.35	0/31472	0.62	12/43305~(0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	А	0	1
2	В	0	8
4	G	0	3
5	Н	0	4
6	Ι	0	1
8	Κ	0	3
15	W	0	1
16	Х	0	1
17	Ζ	0	1



Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	23

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
13	U	151	DT	O4'-C1'-N1	7.93	113.55	108.00
13	U	149	DT	O4'-C1'-N1	7.02	112.92	108.00
16	Х	76	LEU	CA-CB-CG	6.36	129.94	115.30
8	Κ	227	LEU	CA-CB-CG	5.75	128.53	115.30
1	А	1020	LEU	CA-CB-CG	5.74	128.51	115.30
13	U	149	DT	O4'-C4'-C3'	-5.71	102.22	104.50
13	U	151	DT	C1'-O4'-C4'	-5.62	104.48	110.10
14	V	1	DA	O4'-C4'-C3'	-5.54	102.28	104.50
13	U	149	DT	C1'-O4'-C4'	-5.38	104.72	110.10
13	U	94	DT	O4'-C1'-N1	5.20	111.64	108.00
2	B	159	LEU	CA-CB-CG	5.13	127.11	115.30
5	Н	426	LEU	CA-CB-CG	5.05	126.93	115.30

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	949	GLU	Peptide
2	В	193	VAL	Peptide
2	В	259	ASP	Peptide
2	В	316	VAL	Peptide
2	В	415	HIS	Peptide
2	В	737	LYS	Peptide
2	В	821	ASN	Peptide
2	В	822	LEU	Peptide
2	В	843	LEU	Peptide
4	G	668	HIS	Peptide
4	G	721	ARG	Peptide
4	G	783	LEU	Peptide
5	Н	313	VAL	Peptide
5	Н	314	SER	Peptide
5	Н	348	THR	Peptide
5	Н	441	PRO	Peptide
6	Ι	256	LEU	Peptide
8	K	113	ARG	Peptide



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Mol	Chain	\mathbf{Res}	Type	Group	
8	Κ	144	UNK	Peptide	
8	Κ	217	ARG	Peptide	
15	W	345	SER	Peptide	
16	Х	85	THR	Peptide	
17	Ζ	364	UNK	Peptide	

Continued from previous page...

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	3610	0	3640	31	0
2	В	7832	0	7789	121	0
3	D	816	0	632	5	0
4	G	3646	0	3312	51	0
5	Н	1943	0	1922	23	0
6	Ι	2520	0	2422	26	0
7	J	998	0	1055	13	0
8	K	1449	0	1281	20	0
9	L	732	0	624	5	0
10	0	645	0	640	14	0
11	R	611	0	610	9	0
12	Т	1429	0	1521	15	0
13	U	1626	0	897	1	0
14	V	1654	0	893	6	0
15	W	749	0	740	4	0
16	Х	793	0	801	4	0
17	Z	1190	0	276	4	0
All	All	32243	0	29055	313	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 5.

All (313) 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)
2:B:31:GLN:HA	2:B:50:GLU:O	1.41	1.17



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:835:ARG:HH21	8:K:188:ARG:HD2	1.58	0.68
2:B:564:LEU:H	2:B:580:GLN:HB2	1.59	0.68
4:G:718:ARG:HG2	4:G:771:GLY:H	1.59	0.67
4:G:321:LEU:HD22	4:G:327:ASN:HD21	1.60	0.66
2:B:230:ARG:HG3	2:B:231:LYS:HG3	1.77	0.66
1:A:854:ARG:HH12	14:V:68:DG:H21	1.43	0.65
1:A:666:ARG:HG3	1:A:667:THR:HG23	1.77	0.65
6:I:392:ILE:HA	6:I:395:ARG:HB2	1.79	0.65
4:G:586:TYR:HB3	4:G:605:HIS:HB3	1.77	0.65
2:B:206:PHE:O	2:B:233:THR:HA	1.96	0.64
2:B:443:TRP:HE1	2:B:966:ARG:HB2	1.63	0.64
2:B:214:ALA:HB1	2:B:249:LEU:HD11	1.80	0.64
2:B:92:GLU:HG2	2:B:958:ASN:HB3	1.78	0.63
2:B:31:GLN:CA	2:B:50:GLU:O	2.33	0.63
2:B:314:VAL:HG12	2:B:316:VAL:H	1.63	0.63
10:O:130:ILE:HG13	10:O:160:GLN:HE21	1.64	0.62
12:T:257:ASN:ND2	14:V:12:DA:N3	2.43	0.62
4:G:733:ASN:HB3	4:G:761:LEU:HB2	1.81	0.62
4:G:286:THR:HG22	4:G:287:LYS:HG3	1.82	0.62
4:G:472:GLY:HA3	4:G:783:LEU:HD13	1.82	0.62
5:H:324:ASP:HA	5:H:327:TRP:HD1	1.65	0.62
4:G:468:ASN:HA	4:G:786:THR:HG23	1.82	0.61
4:G:546:VAL:HA	4:G:562:SER:HA	1.82	0.61
2:B:678:ARG:NH1	2:B:682:THR:OG1	2.33	0.61
2:B:159:LEU:HD23	2:B:179:SER:HB3	1.82	0.61
4:G:726:LEU:HB2	4:G:738:TRP:HB2	1.83	0.61
10:O:170:ALA:O	10:O:174:CYS:HB2	2.01	0.61
2:B:538:ASN:HD22	2:B:547:GLU:HB2	1.66	0.60
4:G:229:LEU:HB2	4:G:232:HIS:HD2	1.67	0.60
2:B:344:ARG:NH1	2:B:382:MET:SD	2.74	0.60
2:B:838:ASN:HD22	8:K:191:THR:HG23	1.66	0.60
2:B:75:VAL:HG13	2:B:148:ILE:HG12	1.84	0.60
2:B:396:LYS:HD2	2:B:660:VAL:HA	1.83	0.59
2:B:538:ASN:HA	2:B:542:ASN:HD22	1.68	0.59
12:T:187:ALA:HB2	12:T:244:LEU:HD11	1.85	0.58
8:K:73:GLY:HA3	10:O:142:ALA:HB1	1.84	0.58
1:A:635:SER:HB3	7:J:40:LYS:HB2	1.84	0.58
2:B:48:PHE:HA	2:B:148:ILE:O	2.04	0.58
6:I:338:ALA:HB2	6:I:382:GLU:HB3	1.86	0.57
2:B:530:LYS:HG2	2:B:639:LYS:HB3	1.85	0.57
2:B:549:LYS:HG2	2:B:587:LYS:HG2	1.86	0.57



	t i a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
8:K:65:LEU:HD11	10:O:159:ALA:HB1	1.86	0.57
12:T:303:LEU:HB2	12:T:311:VAL:HB	1.86	0.57
2:B:549:LYS:HE2	2:B:587:LYS:HE2	1.87	0.57
1:A:927:VAL:O	1:A:933:ASN:ND2	2.35	0.56
8:K:191:THR:O	8:K:195:ALA:HB2	2.05	0.56
2:B:32:VAL:HB	2:B:50:GLU:HB2	1.87	0.56
2:B:187:ARG:NH2	2:B:194:ASP:OD1	2.35	0.56
2:B:539:ARG:HG3	2:B:545:GLU:HA	1.88	0.56
12:T:171:THR:HG22	12:T:220:VAL:HG22	1.87	0.56
2:B:371:LYS:NZ	2:B:446:TYR:OH	2.39	0.56
4:G:692:ARG:NH2	4:G:706:GLU:OE1	2.39	0.56
8:K:195:ALA:HB1	8:K:212:PRO:HG2	1.87	0.56
4:G:237:SER:HA	4:G:240:PHE:HD2	1.71	0.56
6:I:215:UNK:O	6:I:254:GLN:NE2	2.38	0.56
2:B:946:ASN:ND2	2:B:986:CYS:SG	2.76	0.56
4:G:240:PHE:HB3	4:G:271:GLN:HE22	1.71	0.56
2:B:530:LYS:HE2	2:B:639:LYS:HD3	1.87	0.55
6:I:323:VAL:HA	6:I:326:HIS:HD2	1.70	0.55
1:A:961:GLU:OE1	7:J:147:ARG:NH1	2.40	0.55
4:G:475:ALA:HB3	4:G:781:VAL:HG11	1.88	0.55
16:X:87:LEU:HD21	16:X:89:LYS:HE3	1.87	0.55
5:H:381:ALA:HA	5:H:388:ILE:HD11	1.87	0.55
9:L:49:THR:OG1	9:L:78:ARG:NH1	2.40	0.55
11:R:106:ARG:HH22	11:R:112:GLU:HB2	1.70	0.55
1:A:996:ARG:HA	1:A:1026:ILE:HD13	1.87	0.55
2:B:550:GLN:HE22	2:B:580:GLN:HG2	1.72	0.55
6:I:260:SER:HB2	6:I:304:LEU:HD21	1.88	0.55
8:K:108:PRO:O	8:K:111:ALA:HB3	2.07	0.55
12:T:169:VAL:HB	12:T:257:ASN:HB3	1.88	0.55
1:A:670:ASP:O	7:J:78:LYS:NZ	2.37	0.54
2:B:26:TYR:HB2	2:B:53:ILE:HD11	1.89	0.54
2:B:32:VAL:HG22	2:B:203:LYS:HB3	1.89	0.54
1:A:903:TYR:HE2	1:A:926:GLU:HB3	1.72	0.54
1:A:999:SER:O	1:A:1001:LYS:N	2.41	0.54
2:B:630:ILE:O	2:B:638:ARG:NH1	2.40	0.54
4:G:298:LEU:O	4:G:302:THR:OG1	2.25	0.54
9:L:57:TYR:OH	11:R:122:ARG:NH2	2.37	0.54
2:B:85:ILE:HD11	2:B:129:LYS:HE3	1.89	0.53
2:B:183:GLN:OE1	2:B:361:ARG:NH2	2.41	0.53
2:B:396:LYS:HZ3	2:B:663:GLN:HB2	1.72	0.53
4:G:609:ALA:HB3	4:G:623:PHE:HB2	1.89	0.53



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:G:684:LEU:HB2	4:G:696:TRP:HB2	1.90	0.53
2:B:208:VAL:HG11	2:B:214:ALA:HB2	1.91	0.53
2:B:24:ARG:NH1	2:B:120:ASP:OD1	2.42	0.52
12:T:168:ILE:HG12	12:T:258:MET:HG2	1.90	0.52
2:B:359:ILE:HG23	2:B:498:VAL:HB	1.90	0.52
4:G:671:PRO:O	4:G:689:THR:OG1	2.27	0.52
6:I:410:PRO:O	6:I:417:ARG:NH2	2.40	0.52
1:A:702:ASN:HB2	1:A:722:THR:HA	1.92	0.52
1:A:680:LEU:HD11	7:J:91:ILE:HD12	1.91	0.52
1:A:753:TYR:OH	1:A:1074:ASN:OD1	2.27	0.52
3:D:892:THR:H	11:R:109:SER:HB2	1.75	0.52
8:K:31:LEU:HD11	8:K:34:ARG:HH21	1.74	0.52
2:B:338:GLU:HG2	2:B:341:LEU:HD12	1.91	0.52
2:B:32:VAL:HA	2:B:203:LYS:O	2.09	0.52
2:B:307:VAL:HB	2:B:324:ILE:HG12	1.92	0.51
2:B:431:LEU:HD13	2:B:976:PHE:HB2	1.92	0.51
11:R:120:LEU:O	11:R:124:TRP:N	2.40	0.51
4:G:470:TYR:HD2	6:I:63:ARG:HH22	1.59	0.51
4:G:476:VAL:HG22	4:G:768:LEU:HD22	1.91	0.51
4:G:564:ASP:HB2	4:G:566:THR:HG22	1.92	0.51
2:B:691:PHE:HD2	2:B:694:VAL:H	1.58	0.51
8:K:51:GLU:OE1	10:O:192:LYS:N	2.43	0.51
4:G:730:SER:OG	4:G:732:ASP:OD1	2.29	0.51
3:D:873:LEU:HD23	11:R:58:LEU:HD13	1.92	0.51
6:I:314:SER:OG	17:Z:200:UNK:O	2.29	0.51
2:B:313:TYR:O	2:B:966:ARG:NH1	2.44	0.51
1:A:784:GLN:H	1:A:1073:GLN:HE22	1.58	0.51
2:B:268:PHE:HB2	2:B:307:VAL:HG22	1.91	0.51
2:B:451:CYS:HA	2:B:454:HIS:HD2	1.76	0.51
2:B:539:ARG:HD3	2:B:546:LEU:HG	1.93	0.51
2:B:38:ILE:HD11	2:B:177:VAL:HG11	1.93	0.50
5:H:233:GLY:O	5:H:239:ARG:NH1	2.44	0.50
2:B:219:ASP:O	2:B:236:TYR:HA	2.10	0.50
3:D:912:ASN:HB2	11:R:124:TRP:HH2	1.76	0.50
4:G:332:ILE:HA	4:G:336:HIS:HD2	1.75	0.50
4:G:783:LEU:HD21	4:G:787:ARG:HG3	1.94	0.50
6:I:57:PHE:O	6:I:61:GLY:N	2.41	0.50
12:T:188:ARG:HH11	16:X:64:THR:HG21	1.77	0.50
8:K:172:TYR:OH	8:K:176:ARG:NH1	2.44	0.50
6:I:55:LEU:HD13	9:L:28:ILE:HD12	1.92	0.50
2:B:663:GLN:HA	2:B:666:ILE:HB	1.94	0.50



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:752:ILE:HG22	1:A:782:VAL:HG22	1.92	0.49
2:B:118:ASP:O	2:B:123:ASN:ND2	2.44	0.49
4:G:277:ASP:OD1	4:G:649:ARG:NH2	2.45	0.49
4:G:695:LEU:HB3	4:G:705:GLY:H	1.77	0.49
5:H:404:ARG:NH2	5:H:452:PHE:O	2.45	0.49
2:B:599:ASN:HA	2:B:602:LYS:HB2	1.94	0.49
3:D:934:TYR:O	10:O:150:ARG:NH2	2.44	0.49
8:K:112:LYS:HA	8:K:116:ARG:HD2	1.94	0.49
2:B:891:LEU:HA	2:B:894:VAL:HG12	1.95	0.49
12:T:174:LEU:HD12	12:T:178:LEU:HD11	1.94	0.49
2:B:929:MET:HA	2:B:932:LYS:HB2	1.95	0.49
4:G:479:THR:O	4:G:555:ARG:NH2	2.44	0.49
2:B:402:ILE:HD12	2:B:455:LEU:HD12	1.94	0.49
2:B:328:ASN:O	2:B:847:ARG:NH2	2.33	0.48
2:B:597:ARG:NH1	2:B:621:ALA:O	2.44	0.48
1:A:1026:ILE:HA	1:A:1029:VAL:HG12	1.95	0.48
5:H:389:LYS:HG3	5:H:438:LEU:HD11	1.95	0.48
2:B:566:VAL:O	2:B:577:HIS:HA	2.13	0.48
5:H:410:PRO:O	5:H:417:ARG:NH2	2.47	0.48
1:A:996:ARG:HG2	1:A:1026:ILE:HG21	1.95	0.48
2:B:299:TYR:OH	2:B:353:GLN:NE2	2.47	0.48
2:B:539:ARG:NH1	2:B:593:HIS:O	2.37	0.48
5:H:306:PRO:HB3	17:Z:406:UNK:HA	1.95	0.48
2:B:917:ASP:OD1	2:B:923:ARG:NE	2.34	0.47
9:L:57:TYR:HH	11:R:122:ARG:HH21	1.59	0.47
1:A:1014:GLU:O	1:A:1018:LYS:HB2	2.13	0.47
2:B:565:LYS:HA	2:B:578:THR:O	2.14	0.47
4:G:653:LEU:HD12	4:G:663:ARG:HB2	1.95	0.47
12:T:268:ILE:HD13	12:T:332:LEU:HD22	1.96	0.47
2:B:338:GLU:OE2	2:B:847:ARG:NH2	2.48	0.47
2:B:917:ASP:H	2:B:923:ARG:HH21	1.62	0.47
4:G:558:LEU:HB3	4:G:570:TRP:HB2	1.96	0.47
1:A:926:GLU:OE1	7:J:149:ARG:NH1	2.39	0.47
5:H:418:ILE:O	5:H:422:HIS:ND1	2.45	0.47
6:I:258:ARG:HD3	17:Z:422:UNK:HA	1.97	0.47
12:T:300:ILE:HD11	12:T:320:GLU:HB3	1.95	0.47
2:B:565:LYS:HE3	2:B:577:HIS:HB3	1.97	0.47
2:B:669:LEU:HB3	2:B:678:ARG:HE	1.80	0.47
5:H:387:VAL:HG13	5:H:391:LEU:HD12	1.96	0.47
5:H:411:VAL:HA	5:H:417:ARG:HH21	1.79	0.47
1:A:661:GLU:OE1	2:B:471:GLN:NE2	2.47	0.47



	h i o	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:765:ILE:HB	1:A:772:TYR:HB2	1.96	0.47
2:B:366:ASP:HB3	2:B:499:SER:HB2	1.97	0.47
2:B:692:TYR:HE1	2:B:745:GLN:HG2	1.81	0.46
5:H:370:TRP:HZ2	5:H:406:VAL:HG21	1.80	0.46
2:B:259:ASP:HB3	2:B:263:HIS:HA	1.97	0.46
2:B:389:ASN:HB3	2:B:659:VAL:HG21	1.97	0.46
6:I:258:ARG:NH1	17:Z:421:UNK:O	2.48	0.46
7:J:21:PRO:HB2	7:J:24:TYR:HD2	1.80	0.46
2:B:463:ARG:NH1	2:B:514:ASP:O	2.48	0.46
2:B:570:GLU:OE1	2:B:593:HIS:ND1	2.48	0.46
2:B:898:THR:HG21	2:B:907:LEU:HD13	1.98	0.46
1:A:673:GLY:O	1:A:774:ARG:NH1	2.49	0.46
1:A:929:THR:HG22	1:A:954:ALA:HA	1.97	0.46
8:K:109:ALA:O	8:K:112:LYS:HB2	2.15	0.46
8:K:202:SER:HB2	8:K:207:ASP:HB2	1.98	0.46
2:B:51:LEU:HB2	2:B:146:ILE:HB	1.97	0.46
2:B:387:GLY:O	2:B:391:TYR:N	2.46	0.46
4:G:768:LEU:HB3	4:G:769:LEU:H	1.66	0.46
15:W:333:ASN:HA	15:W:359:ASN:O	2.16	0.46
15:W:335:VAL:HB	16:X:95:ILE:HG12	1.97	0.46
2:B:529:VAL:HG22	2:B:559:LYS:HB3	1.97	0.46
2:B:608:ASN:O	2:B:657:ARG:NH2	2.49	0.46
2:B:806:VAL:HG12	2:B:808:PRO:HD3	1.98	0.46
6:I:320:ARG:HD3	6:I:415:ILE:HD13	1.98	0.45
4:G:241:TYR:HD1	4:G:271:GLN:HG3	1.82	0.45
5:H:217:SER:OG	5:H:218:VAL:N	2.46	0.45
6:I:263:ILE:HG23	6:I:282:LEU:HD22	1.98	0.45
12:T:295:MET:O	12:T:299:ARG:HA	2.17	0.45
16:X:62:LEU:HA	16:X:76:LEU:HD13	1.99	0.45
5:H:370:TRP:O	5:H:374:TYR:HB2	2.17	0.45
1:A:854:ARG:NH2	14:V:69:DA:N3	2.65	0.45
12:T:292:ILE:HG21	14:V:11:DT:H5"	1.98	0.45
2:B:361:ARG:HD2	2:B:367:GLU:HG3	1.98	0.45
6:I:311:CYS:O	6:I:316:GLN:NE2	2.49	0.45
2:B:332:SER:H	2:B:335:ILE:HD12	1.81	0.45
2:B:840:GLU:HG3	2:B:850:ILE:HB	1.99	0.45
4:G:558:LEU:HD23	4:G:572:LEU:HD21	1.98	0.45
5:H:380:LEU:HD23	5:H:383:LEU:HD12	1.98	0.45
10:O:119:PHE:HA	10:O:122:GLN:HG2	1.98	0.45
2:B:835:ARG:HH22	8:K:184:ARG:HE	1.63	0.45
10:O:139:LEU:HB3	10:O:144:PHE:HB3	1.99	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
10:O:149:PRO:HG2	10:O:153:ARG:HH12	1.81	0.45
2:B:206:PHE:HB2	2:B:234:PHE:HB2	1.99	0.44
5:H:403:ILE:HG23	5:H:420:ALA:HB1	1.98	0.44
8:K:120:THR:HA	10:O:129:THR:HG23	1.99	0.44
2:B:956:LEU:O	2:B:961:THR:OG1	2.24	0.44
4:G:730:SER:OG	4:G:734:THR:OG1	2.32	0.44
2:B:26:TYR:HA	2:B:55:PRO:HA	1.99	0.44
2:B:76:ARG:HD2	2:B:79:ASP:HA	1.99	0.44
2:B:259:ASP:O	2:B:261:TYR:N	2.51	0.44
8:K:75:SER:O	8:K:79:TYR:HB2	2.16	0.44
15:W:22:ILE:HG23	15:W:39:LEU:HD11	2.00	0.44
1:A:1083:LEU:O	7:J:141:LYS:NZ	2.49	0.44
2:B:50:GLU:HA	2:B:146:ILE:O	2.18	0.44
6:I:276:LEU:HB3	6:I:326:HIS:CE1	2.53	0.44
12:T:167:ASN:HB3	12:T:259:VAL:HB	1.99	0.44
2:B:432:HIS:HB2	2:B:440:THR:HG22	2.00	0.44
5:H:308:VAL:O	5:H:311:CYS:HB2	2.18	0.44
8:K:191:THR:O	8:K:195:ALA:CB	2.65	0.44
4:G:491:ASP:HA	4:G:540:TYR:HB3	1.99	0.44
6:I:380:LEU:HD13	6:I:391:LEU:HD13	1.98	0.44
8:K:115:GLN:HE22	10:O:126:TYR:HB3	1.82	0.44
4:G:651:VAL:HB	4:G:665:PHE:HB2	2.00	0.43
10:O:139:LEU:HA	10:O:142:ALA:HB3	2.00	0.43
2:B:458:ARG:O	2:B:462:ASN:ND2	2.51	0.43
6:I:257:PRO:O	6:I:261:THR:N	2.51	0.43
7:J:77:LEU:HG	7:J:87:LYS:HA	2.01	0.43
2:B:820:ASP:HB2	2:B:822:LEU:HD23	2.01	0.43
4:G:461:ILE:HG12	4:G:792:LEU:HB3	2.00	0.43
4:G:735:VAL:HG22	4:G:766:GLN:HE22	1.83	0.43
2:B:76:ARG:HH11	2:B:79:ASP:H	1.66	0.43
2:B:871:PRO:O	2:B:875:LYS:N	2.41	0.43
6:I:216:UNK:HA	6:I:220:GLN:HE21	1.84	0.43
1:A:874:GLU:HA	1:A:877:ARG:HD2	2.01	0.43
2:B:899:LYS:HA	2:B:935:PRO:HB3	2.01	0.43
6:I:263:ILE:O	6:I:267:VAL:N	2.49	0.43
6:I:309:MET:HA	6:I:312:ILE:HD12	2.01	0.43
2:B:39:ASN:HB3	2:B:44:SER:H	1.83	0.43
2:B:64:LYS:HD3	2:B:119:PRO:HB3	1.99	0.43
4:G:608:VAL:HG12	4:G:624:ALA:HB2	2.00	0.43
7:J:65:SER:HA	7:J:96:VAL:O	2.18	0.43
10:O:123:LEU:HA	10:O:126:TYR:HD2	1.83	0.43



	Jus puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:G:552:SER:HB3	4:G:557:TYR:HB2	1.99	0.43
4:G:605:HIS:ND1	4:G:629:ASP:OD1	2.52	0.43
2:B:842:LEU:HD23	2:B:842:LEU:HA	1.88	0.42
5:H:305:ILE:HD11	5:H:340:ILE:HG21	2.01	0.42
1:A:650:ARG:HH11	7:J:80:ILE:HD11	1.84	0.42
2:B:926:ILE:O	2:B:930:LEU:HB2	2.19	0.42
15:W:353:LEU:HB2	15:W:370:ALA:HB3	2.00	0.42
2:B:815:GLU:HA	2:B:819:LEU:HD12	2.01	0.42
6:I:274:ASN:HD21	6:I:317:LEU:H	1.67	0.42
2:B:66:ASN:N	2:B:192:CYS:O	2.45	0.42
2:B:83:ALA:HB3	2:B:129:LYS:HB2	2.01	0.42
2:B:530:LYS:HB2	2:B:552:TYR:HE1	1.84	0.42
7:J:39:LEU:HA	7:J:42:ARG:HB2	2.00	0.42
1:A:680:LEU:HD23	1:A:776:LEU:HD22	2.01	0.42
2:B:305:LYS:O	2:B:322:MET:HA	2.20	0.42
2:B:885:ASP:HA	2:B:888:ILE:HG22	2.02	0.42
1:A:749:ARG:HB3	1:A:786:CYS:HB2	2.02	0.42
2:B:49:VAL:HG12	2:B:148:ILE:HB	2.00	0.42
8:K:75:SER:O	8:K:79:TYR:CB	2.68	0.42
1:A:1007:LEU:HD22	1:A:1012:VAL:HG21	2.01	0.42
2:B:802:LEU:HD22	2:B:829:ILE:HG12	2.02	0.42
10:O:126:TYR:O	10:O:153:ARG:NE	2.53	0.42
5:H:324:ASP:HA	5:H:327:TRP:CD1	2.50	0.42
6:I:337:VAL:HA	6:I:340:ILE:HD12	2.01	0.42
1:A:623:TYR:HE2	1:A:766:ARG:HE	1.66	0.41
2:B:220:LEU:HD23	2:B:236:TYR:HE1	1.85	0.41
2:B:256:ILE:HD12	2:B:277:LEU:HD12	2.02	0.41
4:G:636:HIS:HA	4:G:677:PHE:HD2	1.85	0.41
4:G:678:SER:HG	4:G:682:ARG:H	1.65	0.41
11:R:68:ARG:NH1	11:R:72:PRO:O	2.52	0.41
1:A:692:MET:O	7:J:87:LYS:NZ	2.42	0.41
2:B:258:VAL:HG11	2:B:281:THR:HB	2.02	0.41
2:B:891:LEU:HD13	2:B:926:ILE:HD11	2.03	0.41
2:B:719:MET:HE1	2:B:756:ALA:HB3	2.02	0.41
6:I:23:ALA:HB1	6:I:28:ILE:HD12	2.02	0.41
6:I:270:ASN:HA	6:I:273:GLN:HB2	2.03	0.41
2:B:318:ALA:HB2	2:B:349:SER:HA	2.01	0.41
2:B:710:VAL:HG22	2:B:762:ASP:HA	2.02	0.41
2:B:955:LYS:O	2:B:959:SER:N	2.47	0.41
2:B:735:ILE:HD12	8:K:173:GLN:HE21	1.85	0.41
4:G:716:SER:HB2	4:G:769:LEU:HB2	2.03	0.41



	Clash		
Atom-1	Atom-2	distance $\begin{pmatrix} \lambda \end{pmatrix}$	$\operatorname{Clash}_{\operatorname{overlap}}(\lambda)$
4.C.766.CI N.HE91	4.C.799.IUC.CE1	D 20	0.41
4:G:700:GLN:HE21	4:G:782:HIS:CE1	2.39	0.41
6:1:374:1YR:HD1	6:1:423:VAL:HG13	1.80	0.41
2:B:68:LYS:HD3	2:B:188:PHE:HE1	1.86	0.41
5:H:386:ASP:HA	5:H:389:LYS:HB3	2.02	0.41
13:U:129:DA:H2"	13:U:130:DA:C8	2.55	0.41
2:B:848:HIS:CD2	2:B:886:ILE:HD11	2.56	0.41
4:G:249:LEU:HD22	4:G:301:ARG:HG2	2.03	0.41
5:H:366:GLU:HG2	5:H:367:LYS:H	1.86	0.41
7:J:17:ILE:O	7:J:94:MET:HA	2.20	0.41
12:T:301:VAL:HG11	14:V:11:DT:H4'	2.02	0.41
2:B:848:HIS:HB3	2:B:851:THR:HB	2.02	0.41
2:B:946:ASN:ND2	2:B:984:PRO:O	2.35	0.41
5:H:419:GLY:HA2	5:H:422:HIS:CE1	2.56	0.41
4:G:485:ILE:HG21	4:G:787:ARG:HG2	2.03	0.40
4:G:779:PRO:HA	4:G:791:VAL:HA	2.03	0.40
4:G:251:LEU:HD13	4:G:260:ALA:HA	2.04	0.40
9:L:77:CYS:SG	11:R:122:ARG:NH2	2.94	0.40
4:G:594:SER:HB2	4:G:597:GLY:H	1.86	0.40
5:H:278:LEU:HD23	5:H:281:TYR:HD2	1.87	0.40
3:D:910:LEU:HD23	3:D:913:LEU:HD12	2.04	0.40
4:G:486:ALA:HA	4:G:492:SER:HA	2.03	0.40
4:G:783:LEU:HD23	4:G:783:LEU:HA	1.80	0.40
5:H:257:PRO:HG3	5:H:300:TYR:CZ	2.56	0.40
12:T:292:ILE:HG12	14:V:11:DT:H5"	2.03	0.40
2:B:62:ARG:HG2	2:B:129:LYS:HG2	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
1	А	437/496~(88%)	431 (99%)	4 (1%)	2(0%)	29	69



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
2	В	966/1199~(81%)	823~(85%)	143~(15%)	0	100	100
3	D	124/1025~(12%)	118 (95%)	6 (5%)	0	100	100
4	G	429/800 (54%)	382 (89%)	47 (11%)	0	100	100
5	Н	255/677~(38%)	237~(93%)	17 (7%)	1 (0%)	34	72
6	Ι	326/677~(48%)	303 (93%)	21 (6%)	2 (1%)	25	66
7	J	119/349~(34%)	117 (98%)	2 (2%)	0	100	100
8	К	149/310 (48%)	140 (94%)	9 (6%)	0	100	100
9	L	96/264~(36%)	93~(97%)	3 (3%)	0	100	100
10	Ο	78/218~(36%)	74 (95%)	4 (5%)	0	100	100
11	R	72/161~(45%)	70 (97%)	2 (3%)	0	100	100
12	Т	178/339~(52%)	175 (98%)	3 (2%)	0	100	100
15	W	86/90~(96%)	85 (99%)	1 (1%)	0	100	100
16	X	95/97~(98%)	91 (96%)	3 (3%)	1 (1%)	14	52
All	All	3410/6702~(51%)	3139 (92%)	265 (8%)	6 (0%)	50	81

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	1000	LEU
1	А	950	VAL
16	Х	86	GLU
6	Ι	256	LEU
6	Ι	257	PRO
5	Н	321	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.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	393/437~(90%)	389~(99%)	4 (1%)	76 86
2	В	879/1083~(81%)	876 (100%)	3~(0%)	92 95



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	D	52/771~(7%)	52~(100%)	0	100 100
4	G	367/619~(59%)	365 (100%)	2 (0%)	88 93
5	Н	200/574~(35%)	200 (100%)	0	100 100
6	Ι	252/564~(45%)	252 (100%)	0	100 100
7	J	113/322~(35%)	113 (100%)	0	100 100
8	Κ	132/223~(59%)	132 (100%)	0	100 100
9	L	61/229~(27%)	60~(98%)	1 (2%)	62 79
10	Ο	71/154~(46%)	71 (100%)	0	100 100
11	R	70/141~(50%)	69~(99%)	1 (1%)	67 80
12	Т	155/293~(53%)	154 (99%)	1 (1%)	86 92
15	W	84/84 (100%)	84 (100%)	0	100 100
16	Х	89/89~(100%)	89 (100%)	0	100 100
All	All	2918/5583~(52%)	2906 (100%)	12 (0%)	91 94

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	766	ARG
1	А	798	ARG
1	А	922	LYS
1	А	1022	ARG
2	В	74	ARG
2	В	343	ARG
2	В	361	ARG
4	G	558	LEU
4	G	607	ARG
9	L	73	LEU
11	R	125	ASN
12	Т	193	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	1073	GLN
1	А	1074	ASN
2	В	184	ASN
2	В	353	GLN



Mol	Chain	Res	Type
2	В	454	HIS
2	В	462	ASN
2	В	538	ASN
2	В	542	ASN
2	В	550	GLN
2	В	644	GLN
2	В	740	ASN
2	В	838	ASN
2	В	848	HIS
2	В	924	HIS
2	В	946	ASN
3	D	895	HIS
4	G	232	HIS
4	G	271	GLN
4	G	327	ASN
4	G	336	HIS
4	G	626	HIS
4	G	710	HIS
4	G	766	GLN
6	Ι	220	GLN
6	Ι	244	GLN
6	Ι	302	HIS
6	Ι	326	HIS
6	Ι	385	HIS
7	J	48	HIS
8	K	173	GLN
10	0	160	GLN
11	R	125	ASN
12	Т	193	ASN
15	W	343	HIS
15	W	352	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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



5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
17	Ζ	8
15	W	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Ζ	95:UNK	С	119:UNK	Ν	129.92
1	Ζ	52:UNK	С	81:UNK	Ν	114.22
1	Ζ	143:UNK	С	195:UNK	Ν	96.41
1	Ζ	223:UNK	С	309:UNK	Ν	55.85
1	Ζ	386:UNK	С	401:UNK	Ν	34.49
1	Ζ	328:UNK	С	358:UNK	Ν	34.04
1	Ζ	428:UNK	С	551:UNK	Ν	25.25
1	W	51:MET	С	330:ASP	Ν	15.43
1	Ζ	571:UNK	С	573:UNK	Ν	4.33



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-9306. 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: 144



Y Index: 144



Z Index: 144

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: 153



Y Index: 122



Z Index: 158

6.3.2 Raw map



X Index: 245

Y Index: 172



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



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

6.4.1 Primary map







6.4.2 Raw map



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



6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. 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 384 nm^3 ; this corresponds to an approximate mass of 347 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 0.133 ${\rm \AA^{-1}}$



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 0.133 ${\rm \AA^{-1}}$



8.2 Resolution estimates (i)

$\mathbf{B}_{\mathrm{assolution ostimato}}(\mathbf{\hat{\lambda}})$	Estimation criterion (FSC cut-off)			
Resolution estimate (A)	0.143	0.5	Half-bit	
Reported by author	7.50	-	-	
Author-provided FSC curve	-	-	-	
Unmasked-calculated*	9.22	18.05	9.35	

*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 9.22 differs from the reported value 7.5 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-9306 and PDB model 6MZM. 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 0.03 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 (0.03).



9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 65% of all non-hydrogen atoms, are inside the map.



1.0

0.0 <0.0

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6540	0.1350
А	0.5890	0.1280
В	0.6840	0.1460
D	0.7430	0.1970
G	0.6550	0.1160
Н	0.7130	0.1520
Ι	0.7050	0.1420
J	0.5950	0.1050
К	0.6580	0.1590
L	0.7170	0.1700
О	0.6510	0.1420
R	0.5760	0.1460
Т	0.4820	0.0480
U	0.7070	0.1370
V	0.7070	0.1340
W	0.5140	0.0710
Х	0.4370	0.0390
Ζ	0.7250	0.2280

