

wwPDB EM Validation Summary Report (i)

Jun 25, 2023 – 12:08 AM JST

PDB ID	:	8HPO
EMDB ID	:	EMD-34935
Title	:	Cryo-EM structure of a SIN3/HDAC complex from budding yeast
Authors	:	Guo, Z.; Zhan, X.; Wang, C.
Deposited on	:	2022-12-12
Resolution	:	2.60 Å(reported)

This is a wwPDB EM Validation Summary 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 (i)) were used in the production of this report:

EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 Å.

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



Metric	(# Entries)	(#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%

Mol	Chain	Length	Qı	uality of chain		
1	K	460		86%		• 10%
2	D	327	28% 16%	6%	50%	
3	F	433	66%		21%	•• 9%
4	G	433	63%		22% •	11%
5	Ι	201	38%	23% ••	35%	
6	А	1536	26% 14%		59%	
6	В	1536	22% 16% ·		60%	
7	Н	405	36%	18% •	42%	
8	С	330	27% 13%		58%	



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Mol	Chain	Length	Quality of chain					
9	Е	430	40%	16% •	41%			
10	J	294	47%	22%	• 29%			

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SEP	F	265	-	-	Х	-
3	TPO	F	365	-	-	Х	-
9	TPO	Е	167	-	-	Х	-



2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 27951 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 Transcriptional regulatory protein UME1.

Mol	Chain	Residues		Ator	AltConf	Trace		
1	K	413	Total 2038	C 1212	N 413	0 413	0	0

• Molecule 2 is a protein called Transcriptional regulatory protein SDS3.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	165	Total 1385	C 863	N 248	0 271	Р 1	${ m S} { m 2}$	0	0

• Molecule 3 is a protein called Histone deacetylase RPD3.

Mol	Chain	Residues		A	AltConf	Trace				
3	F	392	Total 3132	C 1982	N 524	O 596	Р 5	${ m S}\ 25$	0	0

• Molecule 4 is a protein called Histone deacetylase RPD3.

Mol	Chain	Residues		At	AltConf	Trace			
4	G	385	Total 3057	C 1948	N 513	0 571	$\begin{array}{c} \mathrm{S} \\ \mathrm{25} \end{array}$	0	0

• Molecule 5 is a protein called Transcriptional regulatory protein SAP30.

Mol	Chain	Residues		I	AltConf	Trace				
5	Ι	130	Total 1104	C 696	N 203	O 201	Р 1	${ m S} { m 3}$	0	0

• Molecule 6 is a protein called Transcriptional regulatory protein SIN3.

Mol	Chain	Residues		At	AltConf	Trace			
6	А	637	Total 5283	C 3392	N 887	0 987	S 17	0	0



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Mol	Chain	Residues		At	AltConf	Trace			
6	В	613	Total 5129	C 3295	N 862	O 955	S 17	0	0

• Molecule 7 is a protein called Transcriptional regulatory protein DEP1.

Mol	Chain	Residues		At	AltConf	Trace			
7	Н	233	Total 1936	C 1218	N 340	O 368	S 10	0	0

• Molecule 8 is a protein called Transcriptional regulatory protein PHO23.

Mol	Chain	Residues		At	oms	AltConf	Trace		
8	С	138	Total 1116	C 703	N 195	0 211	${ m S} 7$	0	0

• Molecule 9 is a protein called Transcriptional regulatory protein RXT2.

Mol	Chain	Residues		A	AltConf	Trace				
9	Е	255	Total 2077	C 1306	N 375	0 391	Р 2	$\frac{S}{3}$	0	0

• Molecule 10 is a protein called Transcriptional regulatory protein RXT3.

Mol	Chain	Residues		Ate	AltConf	Trace			
10	J	209	Total 1676	C 1069	N 284	0 321	${ m S} { m 2}$	0	0

• Molecule 11 is PHOSPHOTHREONINE (three-letter code: TPO) (formula: $C_4H_{10}NO_6P$).





Mol	Chain	Residues		Atoms									
11	F	1	Total 12	$\begin{array}{c} \mathrm{C} \\ 4 \end{array}$	N 1	0 6	Р 1	0					

• Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
12	F	1	Total Zn 1 1	0
12	G	1	Total Zn 1 1	0

• Molecule 13 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
13	F	2	Total K 2 2	0
13	G	2	Total K 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. 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. 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 K: 86% 10% ASP 3LY SER SER ARG 3LU VAL VAL VAL ALA ALA ALA ALA ALA SER • Molecule 2: Transcriptional regulatory protein SDS3 Chain D: 28% 50% 16% 6% MET MEA SLNE SLN SLN SER SER SER SER TYR ALA MET ASN SER ARG PRO GLN GLN GLN CYS LYS LYS ASN ASN ARG • Molecule 3: Histone deacetylase RPD3 Chain F: 9% 66% 21% . .
- Molecule 1: Transcriptional regulatory protein UME1





Chain G:	63%		22% •	11%
MET V2 V2 K14 F15 B16 B16 R19 R19 R20 F24 F24 F24	V29 K41 I46 I46 S50 S50 N54 N54 Y64	K67 K71 G72 G75 G75 G75 G75 F77 H78 H78	D84 F85 L86 S87 R88 R88 V89 F91 D92	E95 M96 F97 K98 R99 R99 V102 K103 F104
N105 N105 D114 D114 C115 C115 C115 C124 C124 C124 C124 C124	E129 E129 D140 V141 V141 C139 C139 C139 C146 C148 C148 C148 C153 K153 K153	8156 8156 8157 8157 8159 8159 8159 1166 1166 1171	L174 1185 D196 D191 T199	1205 H209 E213 E213 (219 (219 E220
L221 R222 N231 N235 L238 L238 L238 L238 L238 L238 D244 D244	1246 2249 V250 V250 1258 W261 V261 0271 0271 0272 0272	8277 8280 8280 8292 8293 8293 7295 7295 7295 7295 7302	M305 G311 L328 L328 N341	Y346 D350 R356 N359 M360
P366 P366 E367 F368 F368 F368 F370 F370 F370 F371 F374 F374 F374 F375 F374 F376 F376 F376 F376 F376 F376 F376 F376	A386 PRO VAL VAL GLN GLN CGLN CGLN ASN PRO ASP ALA ALA ALA CGLA	ASP GLY GLY ASP ASP CLU GLU GLU SER ALA ALA	LYS ASP THR LYS GLY GLY SER GLN ALA	ARG ASP ASP LEU HIS CLU ASP ASP
GLU TYR				
• Molecule 5: Trans	scriptional regulator	y protein SAP30		
Chain I:	38%	23% • •	35%	_
MET ALA ARG PRC PRC PRC ARG GLU GLU SER SER SER	GLY THR PRO GLY GLY GLY ASN ASN ASN	SER CYS ASN ASN ASN GLY SER ASN ASN ASN	ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN	ASN ASN SER ASN ASN ASN GLY PRO
THR SER SER SER SER ARG ARG ARG GLY CT2 TT2 A74 A74	978 779 1990 1990 1992 1993 1993 1993 1993 1900 1900 1900	E105 E106 F107 7107 7108 0109 A110 A111 A111 A111 F113 F119	Q120 L121 V122 V123 V126 L127 L128 L128 Q130	C131 Y132 L133 S136 N148 N148 T149
R156 1157 1158 8159 8159 8159 1161 1171 1171 1173 8173 8173 8173	K176 Ex77 T178 0179 C380 C380 C380 C380 C380 C380 F198 K190 K192 K192 K192	F 195 K196 G201		
• Molecule 6: Trans	scriptional regulator	y protein SIN3		
Chain A: 26%	5 14% •	5	9%	
MET SER GLN VAL TRP HIS ASN SER SER SER SER SER SER SER	VAL VAL THR SER ASP ASP ASP ASP CLY SER ASS ASS ASS ASS	LYS CUU PRO PRO CLU SER CLU CUN CLU ASN LYS CUY CUY PHE	VAL GLN GLN GLN GLN ARG THR THR THR FRO	SER LEU SER ALA LEU SER THR LYS GLU
GLU ASP ARG ARG ARG ARG ARG ARG ARG CLN GLN GLN CLN CLN CLN SER SER	HIS ALA ALA ALA HIS TIE LEU CLY GLY PRO PRO PRO PRO PRO ASN	MET MET SER SER ILE ASP ASP ASP ALA LEU LYS GLN	PRO HIS GLU TYR HIS PRO PRO LYS SER	SER SER SER SER PRO SER ILE ASN ALA
SER LEU MET MET ALA ALA ALA PRO PRO PRO PRO CLY CAL	ALA ALA SER SER SER EEU SER ARG ARG ARG ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP	LYS ALA PRO VAL HIS THR GLU CLU PRO CLU SER SER	ASN GLY LLEU GLU GLU GLU CLU ALA ALA THR	GLN ARG PRO GLN ASP CYS CYS CYS CYS VAL
PRO ALA ALA CLY VAL CLN VAL ALA ALA ALA ALA ASP PRO ASP PRO SER SER	ASN HIS ALA ASP ASP ASN ASP ASN ASN ASN ASN ASN ASN ASN ASN ASN	HIS ASP GLU ASP ASP ASP ASP ASP PRO PRO LEU ASN VAL	LYS ASP ALA LEU SER TYR LEU GLU GLU VAL	LYS PHE GLN PHE SER SER ARG PRO ASP









• Molecule 6: Transcriptional regulatory protein SIN3

Chai	in	B			2	22%	6					10	5%			·			_							6	50%	Ď							_	_				
MET SER GLN	VAL TRP	SIH	SER	SER	GLN	ASN	ASP VAL	ALA	THR	ASN	ASP	ALA	GLY	SER	ASN	GLU ARG	ASN	GLU	LYS	PRO	SER	CI.N	GLY	ASN	LYS PRO	GLY	PHE	GLN	GLN	GLN	ARG	THR	LEU	PRO	LEU	SER	ALA LEU	SER	THR	GLU
GLU ASP ARG	ARG	SER	GLY	GLN	ALA I.FII	THR	SER HIS	ALA	ALA	HIS	TEU	GLY	PRO	PRO	PRO	SER	ASN	ALA	MET	SER	ILE	ALA THR	ASP	SER	ALA LEU	TAS	GLN	HIS	GLU	SIH	PRO	PRO	LYS	SER	SER	SER	SER PRO	SER	ASN	ALA
SER LEU MET	ASN	GLY	ALA	LEU	THR	VAL	GLY ALA	ALA	SER	PHE SFR	TEU	SER	PHE	ASP	ASN	PRU LEU	PRO	ILE	LYS	PRO	VAL	THR	GLU	CLU	PR0 LYS	SER	TYR	GLY	CT N	GLU	GLU	LYS	ALA	THR.	ARG	PRO	GLN ASP	CYS	GLU	VAL
PRO ALA GLY	GLN	PRO	ALA	PR0	PRD	SER	SER	HIS	ALA	ASP	ASN	ASP	ASN	ASN	ASN	ASN GLU	ASN	SER	ASP	GLU	ASP	ALA	TYR	ARG	PR.0 L.E.U	ASN	VAL	ASP	ALA	SER	TYR	GLU	GLN	VAL	PHE	GLN	PHE SER	SER	ARG PRO	ASP
ILE TYR ASN	DHE	LEU	ILE	TAS	ASP PHF	TAS	GLN	ALA	ILE	ASP THR	PRO	GLY	VAL ILE	GLU	ARG	VAL SFR	THR	LEU	PHE	GLY	TYR	PRO TLE	LEU	ILE	GLN	PHE	ASN	PHE	LEU	GLN	GLY	ARG	ILE	GLU	SER	SER	ASN PRO	ASP	ASP PRO	ILE
ARG VAL THR	THR PRO	MET	THR	THE	V AL A SN	ASN	ASN ILE	SER	PRO	SER	ARG	GLY	THR	ASP	ALA	GLU	LEU	GLY	SER	PRO	GLU	SER ASP	GLY	ASN	GLY VAL	GLN	GLN	SER	ASN	PRO	MET	PRO	SER	SER VAL	TYR	GLN	GLU	GLN	GLN	ASP
GLN GLN GLN	LEU	PRO		THR	SER	GLY	LEU PRO	SER	ILE	GLN	PRO	GLU	PRO	ALA	SIH	GI.N	ILE	PRO	GLN SFR	GLN	SER	LEU VAL	PRO	CLN	GLU ASP	ALA	LYS	ASN	VAL	VAL	GLU	SER	GLN	ALA TLE	SER	TYR	VAL ASN	LYS	ILE	THR
ARG PHE ALA	GLN	PRO	ILE	TYS	HTS DHF	LEU	GLU	TEU	GLN	THR	GLN	ARG	GLN	LYS	PRO TT T	ASN	CLU	VAL	TYR AT A	GLN	VAL	THR	TEU	PHE	GLN	ALA	PRO ACD	LEU	LEU	ASP	PHE	LYS	PHE	LEU PRO	ASP	SER	SER	SER	ALA ASN	GLN
GLN VAL GLN	ALA	GLN	SIH	GLN	GL.N	SIH	GLU ALA	GLN	MET	ALA	GLN	ALA	GLN	GLN	ALA	GLN AT.A	GLN	ALA	GLN VAL	GLU	GLN	GLN	GLN	GLN	GLN GLN	PHE	LEU	PRO	ALA	GLY	TYR TVP	GLY	HIS	PROSER	ASN	ARG	GLY	PRO	GLN	ASN
LEU PRO PRO	GLY	SER	SER	PRO	ASN	GLY	SER THR	VAL	HIS	GLU	TYR	GLN	GLN	GLN	HIS	UET.	PRO	PRO	HIS	MET	PRO	LEU PRO	SER	ILE	VAL GLN	SIH	GLY	ASN	MET VAI	SIH	GLN	ILE	ALA	ASN GLII	ASN	PRO	PRO LEU	SER	ASP LEU	ARG
THR SER LEU	GLU	GLN	ALA	SER	SER TLE	GLN	SIH	GLN	GLN	PRO	GLN	SER	SER	PRO	ILE	ALA ASN	THR	GLN	TYR CI V	ASP	ILE	PRO VAL	ARG	PRO	GLU TI.E	ASP	LEU	P643	V648		E651 D657	T653	E654	F657		L662	N663 E664		F669 E670	K671
N678 K679	H680	E684	L686	V00/	N690 1.691		D695 1696	L697		D700	L702			-	4709	K714		K721	V706		K7 29	T730 K731	C732	I733	E734 N735	1736	V737	E739	K740 H741	R742	L743		C748	K760		M7 65	S768	G769	R770	W775
V787 W788	A789 S790			7101	D818 F819	Y820	R826		C830	L831	1838 1838		1 84.2 E843	N844	E845	F849	K850	L851	T REP	G856	H857	T858 3859	M860		Y863 K864		1867 1867	K869	V870 V871	D872	K873 E874	E014 R875		1880 D881	A882	L883	H884 E885	H886	V889	T890
A891	L895 K896	R897		D902	R906		R910	N913	-	W916 R917	E918	L919	ES 20	V9 <mark>23</mark>	F924	2002	L928	D929	K036	0937 0937	A938	1.942	L943	•	K946 0947	L948	1949 5050	E951	1952 4953	S954	1955 Voef	V957	D958	0959 Т960	N961	K962	K963	P971	K972 S973	Q974
D978 F979	P980 D981	t COL	1984 F985	D987	1 988 1.989	C990	L991 A992	D993	T994	F995 T996	1997	H998	1 399	N1004	P1005	N1006 K1007	E1008	R1009	L1010	D1012	L1013	L1014 K1015	Y1016	F1017	I1018 S1019	L1020	F1021	S1025	F1026	I1029	E1030 E1031	E1031 S1032	L1033	Y1034 S1035	H1036	K1037	Q1038 N1039	V1040	<mark>S1041</mark> GLU	SER
SER GLY SER	ASP ASP	GLY	SER	ALA	ARG	LYS	ARG PRO	TYR	GLN	GLN	M1063	S1064	L1066	D1067	I1068	L1069 H1070	ARG	SER	ARG TVR	GLN	LYS	LEU	ARG	SER	ASN	GLU	ASP	LYS	VAL	GLN	LEU	GLU	PRO	PRO GLII	GLU	GLU	ASN	THR	GLU	GLU











4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	665105	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	50	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	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: SEP, K, ZN, TPO

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	nd lengths	B	ond angles
WIOI	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	Κ	0.24	0/2033	0.44	0/2822
2	D	0.50	1/1393~(0.1%)	0.69	1/1866~(0.1%)
3	F	0.55	3/3156~(0.1%)	0.63	6/4262~(0.1%)
4	G	0.35	0/3137	0.48	0/4246
5	Ι	0.38	0/1119	0.61	1/1500~(0.1%)
6	А	0.32	0/5400	0.48	0/7289
6	В	0.30	0/5245	0.51	1/7077~(0.0%)
7	Н	0.34	0/1976	0.50	0/2674
8	С	0.30	0/1134	0.50	0/1529
9	Е	0.42	0/2082	0.58	1/2799~(0.0%)
10	J	0.38	1/1718~(0.1%)	0.54	0/2335
All	All	0.37	5/28393~(0.0%)	0.53	10/38399~(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
3	F	0	1
5	Ι	0	1
6	А	0	1
6	В	0	2
7	Н	0	4
9	Е	0	2
All	All	0	11

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	10	PRO	N-CA	13.06	1.69	1.47



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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	
2	D	294	PRO	C-N	8.63	1.50	1.34	
3	F	14	LYS	C-N	8.37	1.50	1.34	
10	J	123	PRO	C-N	7.87	1.49	1.34	
3	F	9	ASP	C-N	6.27	1.46	1.34	

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The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	D	307	ASP	CB-CA-C	-11.25	87.91	110.40
3	F	9	ASP	CB-CA-C	-7.49	95.42	110.40
3	F	266	ALA	N-CA-CB	7.36	120.40	110.10
3	F	10	PRO	CA-N-CD	-6.63	102.21	111.50
6	В	1033	LEU	CA-CB-CG	6.06	129.25	115.30

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	А	891	ALA	Peptide
3	F	265	SEP	Mainchain
7	Н	314	LYS	Peptide
7	Н	342	GLU	Peptide
5	Ι	174	SEP	Mainchain

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	K	2038	0	890	9	0
2	D	1385	0	1388	84	0
3	F	3132	0	2978	85	0
4	G	3057	0	2932	69	0
5	Ι	1104	0	1087	46	0
6	А	5283	0	5216	166	0
6	В	5129	0	5096	193	0
7	H	1936	0	1896	65	0
8	С	1116	0	1133	38	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	Ε	2077	0	2136	75	0
10	J	1676	0	1637	44	0
11	F	12	0	5	3	0
12	F	1	0	0	0	0
12	G	1	0	0	0	0
13	F	2	0	0	0	0
13	G	2	0	0	0	0
All	All	27951	0	26394	767	0

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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 14.

The worst 5 of 767 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)
3:F:10:PRO:N	3:F:10:PRO:CA	1.69	1.36
3:F:6:TPO:CG2	3:F:7:PRO:HD2	1.68	1.23
9:E:176:ILE:CD1	9:E:374:LEU:HD12	1.77	1.15
9:E:167:TPO:CG2	9:E:168:PRO:HD2	1.81	1.10
5:I:177:GLU:O	5:I:179:ASP:N	1.82	1.09

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	K	403/460~(88%)	396~(98%)	7 (2%)	0	100	100
2	D	160/327~(49%)	157 (98%)	3 (2%)	0	100	100
3	F	385/433~(89%)	356 (92%)	26 (7%)	3 (1%)	19	39
4	G	383/433~(88%)	360 (94%)	23~(6%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
5	Ι	127/201~(63%)	110 (87%)	14 (11%)	3~(2%)	6	10
6	А	627/1536~(41%)	593~(95%)	32~(5%)	2~(0%)	41	64
6	В	605/1536~(39%)	551 (91%)	54 (9%)	0	100	100
7	Н	231/405~(57%)	208 (90%)	20 (9%)	3~(1%)	12	24
8	С	134/330~(41%)	128 (96%)	3~(2%)	3~(2%)	6	12
9	Е	245/430~(57%)	217 (89%)	24 (10%)	4 (2%)	9	19
10	J	205/294~(70%)	188 (92%)	17 (8%)	0	100	100
All	All	3505/6385~(55%)	3264 (93%)	223 (6%)	18 (0%)	32	52

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5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	Ι	177	GLU
5	Ι	178	THR
7	Н	344	ILE
9	Е	42	GLN
9	Е	71	ARG

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
2	D	153/289~(53%)	124 (81%)	29~(19%)	1 2
3	F	328/362~(91%)	301~(92%)	27~(8%)	11 22
4	G	326/367~(89%)	292~(90%)	34 (10%)	7 13
5	Ι	119/178~(67%)	105~(88%)	14~(12%)	5 9
6	А	585/1391~(42%)	524 (90%)	61 (10%)	7 13
6	В	574/1391~(41%)	513~(89%)	61 (11%)	6 12
7	Н	213/371~(57%)	190 (89%)	23~(11%)	6 12
8	С	129/290~(44%)	123 (95%)	6(5%)	26 50
9	Е	234/391~(60%)	210 (90%)	24 (10%)	7 13



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Mol	Chain	Analysed	Rotameric	Outliers	Percenti	les
10	J	190/269~(71%)	167~(88%)	23~(12%)	5 9	
All	All	2851/5299~(54%)	2549~(89%)	302 (11%)	10 12	

5 of 302 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	В	765	MET
10	J	109	ASP
6	В	881	ASP
6	В	1152	THR
10	J	273	LYS

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such side chains are listed below:

Mol	Chain	Res	Type
6	В	1233	ASN
6	В	1296	ASN
6	А	848	ASN
6	А	836	ASN
10	J	120	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

9 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol Type Ch	Chain	Dog	Link	Bond lengths			Bond angles			
	туре	Ullalli	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	SEP	Е	171	9	8,9,10	0.69	0	8,12,14	1.52	1 (12%)



Mal	Turne	Chain	Dec	Tink	B	ond leng	gths	Bond angles			
1VIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2	
5	SEP	Ι	174	5	8,9,10	0.96	0	8,12,14	0.82	0	
3	SEP	F	388	3	8,9,10	0.73	0	8,12,14	1.08	1 (12%)	
3	TPO	F	365	3	8,10,11	0.86	0	10,14,16	1.19	2 (20%)	
2	SEP	D	309	2	8,9,10	0.94	0	8,12,14	0.94	0	
9	TPO	Е	167	9	8,10,11	2.98	1 (12%)	10,14,16	1.56	2 (20%)	
3	SEP	F	265	3	8,9,10	1.97	1 (12%)	8,12,14	2.22	3 (37%)	
3	TPO	F	6	3	8,10,11	0.99	0	10,14,16	1.33	1 (10%)	
3	TPO	F	12	3	8,10,11	0.81	0	10,14,16	1.12	1 (10%)	

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SEP	Е	171	9	-	2/5/8/10	-
5	SEP	Ι	174	5	-	1/5/8/10	-
3	SEP	F	388	3	-	3/5/8/10	-
3	TPO	F	365	3	-	7/9/11/13	-
2	SEP	D	309	2	-	2/5/8/10	-
9	TPO	Е	167	9	-	6/9/11/13	-
3	SEP	F	265	3	-	4/5/8/10	-
3	TPO	F	6	3	-	0/9/11/13	-
3	TPO	F	12	3	-	1/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Е	167	TPO	P-OG1	-7.95	1.44	1.59
3	F	265	SEP	O-C	-4.57	1.01	1.19

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	F	265	SEP	O2P-P-OG	-4.51	94.74	106.73
9	Е	167	TPO	P-OG1-CB	-3.55	112.48	123.21
9	Е	171	SEP	O3P-P-OG	-2.75	99.41	106.73
3	F	265	SEP	OG-P-O1P	2.72	114.11	106.47
3	F	388	SEP	OG-CB-CA	2.70	110.78	108.14



There are no chirality outliers.

Mol	Chain	Res	Type	Atoms
3	F	12	TPO	O-C-CA-CB
3	F	265	SEP	N-CA-CB-OG
3	F	265	SEP	CB-OG-P-O2P
3	F	265	SEP	CB-OG-P-O3P
3	F	365	TPO	N-CA-CB-CG2

5 of 26 torsion outliers are listed below:

There are no ring outliers.

5 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	388	SEP	1	0
3	F	365	TPO	8	0
9	Е	167	TPO	8	0
3	F	265	SEP	6	0
3	F	6	TPO	5	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 for Mogul analysis.

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

Mol Type	Turne	Chain	Dec	es Link	Bond lengths			Bond angles		
	туре		nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	TPO	F	501	3	9,11,11	0.83	0	13,16,16	1.79	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.



'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	TPO	F	501	3	-	5/13/13/13	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
11	F	501	TPO	CB-CA-C	5.25	122.46	110.32

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	F	501	TPO	O-C-CA-N
11	F	501	TPO	OXT-C-CA-N
11	F	501	TPO	O-C-CA-CB
11	F	501	TPO	OXT-C-CA-CB
11	F	501	TPO	CG2-CB-OG1-P

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	F	501	TPO	3	0

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.

