

wwPDB EM Validation Summary Report (i)

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PDB ID	:	7PMN
EMDB ID	:	EMD-13539
Title	:	S. cerevisiae replisome-SCF(Dia2) complex bound to double-stranded DNA
		(conformation II)
Authors	:	Jenkyn-Bedford, M.; Yeeles, J.T.P.; Deegan, T.D.
Deposited on	:	2021-09-02
Resolution	:	3.20 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 following versions of software and data (see references (i)) were used in the production of this report:

EMDB validation analysis	:	0.0.0.dev 97
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.24

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 3.20 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.



Motric	Whole archive	EM structures		
IVIEUTIC	$(\# {\rm Entries})$	$(\# { m Entries})$		
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	Quality of chai	n
1	2	868	5%	• 24%
2	3	1009	60% ·	39%
3	4	933	63%	36%
4	5	775	83%	• 15%
5	6	1017	62%	37%
6	7	845	28%	• 25%
7	А	208	92%	• 5%
8	В	213	89%	• 10%



Mol	Chain	Length	(Quality of chain				
9	С	194	•	88%	12%			
10	D	294	–	82%	• 17%			
11	Е	657	85% • 14%					
12	F	962	44%	56%				
12	G	962	44%	56%				
12	Н	962	44%	56%				
13	Ι	115	27% •	70%				
14	J	122	24%	73%				
15	K	194	9%	•	29%			
16	L	735	• 64%		35%			
17	Q	2222	34% •	66%				
18	R	689	9%	8%	• 20%			
19	Х	1238	52%	• 469	%			
20	Y	319	31%	69%				

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2 Entry composition (i)

There are 23 unique types of molecules in this entry. The entry contains 74640 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 DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	656	Total 5183	C 3261	N 933	0 971	S 18	0	0

• Molecule 2 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	615	Total 4834	$\begin{array}{c} \mathrm{C} \\ \mathrm{3055} \end{array}$	N 859	O 907	S 13	0	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	-37	MET	-	initiating methionine	UNP P24279
3	-36	LYS	-	expression tag	UNP P24279
3	-35	ARG	-	expression tag	UNP P24279
3	-34	ARG	-	expression tag	UNP P24279
3	-33	TRP	-	expression tag	UNP P24279
3	-32	LYS	-	expression tag	UNP P24279
3	-31	LYS	-	expression tag	UNP P24279
3	-30	ASN	-	expression tag	UNP P24279
3	-29	PHE	-	expression tag	UNP P24279
3	-28	ILE	-	expression tag	UNP P24279
3	-27	ALA	-	expression tag	UNP P24279
3	-26	VAL	-	expression tag	UNP P24279
3	-25	SER	-	expression tag	UNP P24279
3	-24	ALA	-	expression tag	UNP P24279
3	-23	ALA	-	expression tag	UNP P24279
3	-22	ASN	-	expression tag	UNP P24279
3	-21	ARG	-	expression tag	UNP P24279
3	-20	PHE	-	expression tag	UNP P24279
3	-19	LYS	-	expression tag	UNP P24279
3	-18	LYS	-	expression tag	UNP P24279
3	-17	ILE	-	expression tag	UNP P24279



Chain	Residue	Modelled	Actual	Comment	Reference
3	-16	SER	-	expression tag	UNP P24279
3	-15	SER	-	expression tag	UNP P24279
3	-14	SER	-	expression tag	UNP P24279
3	-13	GLY	-	expression tag	UNP P24279
3	-12	ALA	-	expression tag	UNP P24279
3	-11	LEU	-	expression tag	UNP P24279
3	-10	GLU	-	expression tag	UNP P24279
3	-9	ASN	-	expression tag	UNP P24279
3	-8	LEU	-	expression tag	UNP P24279
3	-7	TYR	-	expression tag	UNP P24279
3	-6	PHE	-	expression tag	UNP P24279
3	-5	GLN	-	expression tag	UNP P24279
3	-4	GLY	-	expression tag	UNP P24279
3	-3	GLU	-	expression tag	UNP P24279
3	-2	ALA	-	expression tag	UNP P24279
3	-1	PRO	-	expression tag	UNP P24279
3	0	VAL	-	expression tag	UNP P24279

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• Molecule 3 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	595	Total 4731	C 2986	N 813	0 904	S 28	0	0

• Molecule 4 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	660	Total 5231	C 3289	N 912	O 1007	S 23	0	0

• Molecule 5 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	641	Total 5042	C 3177	N 886	0 954	${ m S}\ 25$	0	0

• Molecule 6 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	633	Total 4936	C 3121	N 857	O 932	S 26	0	0



• Molecule 7 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	А	197	Total 1611	C 1012	N 277	0 313	S 9	0	0

• Molecule 8 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
8	В	192	Total 1609	C 1034	N 285	O 286	$\frac{S}{4}$	0	0

• Molecule 9 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms				AltConf	Trace	
9	С	171	Total 1381	C 900	N 223	0 252	S 6	0	0

• Molecule 10 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues		At	\mathbf{oms}			AltConf	Trace
10	D	243	Total 2004	C 1276	N 327	O 389	S 12	0	0

• Molecule 11 is a protein called Cell division control protein 45,Cell division control protein 45.

Mol	Chain	Residues		At	oms			AltConf	Trace
11	Е	564	Total 4569	C 2916	N 772	O 867	S 14	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	167F	ASP	-	expression tag	UNP Q08032
E	167G	TYR	-	expression tag	UNP Q08032
Е	167H	LYS	-	expression tag	UNP Q08032
E	167I	ASP	-	expression tag	UNP Q08032
Е	167J	ASP	-	expression tag	UNP Q08032
E	167K	ASP	-	expression tag	UNP Q08032
Е	167L	GLY	-	expression tag	UNP Q08032
Е	167M	ASP	-	expression tag	UNP Q08032
E	167N	TYR	-	expression tag	UNP Q08032
E	167O	LYS	-	expression tag	UNP Q08032



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Chain	Residue	Modelled	Actual	Comment	Reference
E	167P	ASP	-	expression tag	UNP Q08032
Е	167Q	ASP	-	expression tag	UNP Q08032

• Molecule 12 is a protein called DNA polymerase alpha-binding protein.

Mol	Chain	Residues		Atoms					Trace
19	F	494	Total	С	Ν	0	S	0	0
12	Ľ	424	3404	2188	564	637	15	0	0
10	С	499	Total	С	Ν	0	S	0	0
12	G	422	3380	2172	557	636	15	0	0
10	ц	425	Total	С	Ν	0	S	0	0
12 H		420	3411	2193	565	638	15		0

There are 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-34	MET	-	initiating methionine	UNP Q01454
F	-33	LYS	-	expression tag	UNP Q01454
F	-32	ARG	-	expression tag	UNP Q01454
F	-31	ARG	-	expression tag	UNP Q01454
F	-30	TRP	-	expression tag	UNP Q01454
F	-29	LYS	-	expression tag	UNP Q01454
F	-28	LYS	-	expression tag	UNP Q01454
F	-27	ASN	-	expression tag	UNP Q01454
F	-26	PHE	-	expression tag	UNP Q01454
F	-25	ILE	-	expression tag	UNP Q01454
F	-24	ALA	-	expression tag	UNP Q01454
F	-23	VAL	-	expression tag	UNP Q01454
F	-22	SER	-	expression tag	UNP Q01454
F	-21	ALA	-	expression tag	UNP Q01454
F	-20	ALA	-	expression tag	UNP Q01454
F	-19	ASN	-	expression tag	UNP Q01454
F	-18	ARG	-	expression tag	UNP Q01454
F	-17	PHE	-	expression tag	UNP Q01454
F	-16	LYS	-	expression tag	UNP Q01454
F	-15	LYS	-	expression tag	UNP Q01454
F	-14	ILE	-	expression tag	UNP Q01454
F	-13	SER	-	expression tag	UNP Q01454
F	-12	SER	-	expression tag	UNP Q01454
F	-11	SER	-	expression tag	UNP Q01454
F	-10	GLY	-	expression tag	UNP Q01454
F	-9	ALA	-	expression tag	UNP Q01454



Chain	Residue	Modelled	Actual	Comment	Reference
F	-8	LEU	-	expression tag	UNP Q01454
F	-7	GLU	-	expression tag	UNP Q01454
F	-6	ASN	_	expression tag	UNP Q01454
F	-5	LEU	-	expression tag	UNP Q01454
F	-4	TYR	-	expression tag	UNP Q01454
F	-3	PHE	-	expression tag	UNP Q01454
F	-2	GLN	-	expression tag	UNP Q01454
F	-1	GLY	-	expression tag	UNP Q01454
F	0	GLU	-	expression tag	UNP Q01454
G	-34	MET	-	initiating methionine	UNP Q01454
G	-33	LYS	-	expression tag	UNP Q01454
G	-32	ARG	-	expression tag	UNP Q01454
G	-31	ARG	-	expression tag	UNP Q01454
G	-30	TRP	-	expression tag	UNP Q01454
G	-29	LYS	-	expression tag	UNP Q01454
G	-28	LYS	-	expression tag	UNP Q01454
G	-27	ASN	-	expression tag	UNP Q01454
G	-26	PHE	-	expression tag	UNP Q01454
G	-25	ILE	-	expression tag	UNP Q01454
G	-24	ALA	_	expression tag	UNP Q01454
G	-23	VAL	-	expression tag	UNP Q01454
G	-22	SER	-	expression tag	UNP Q01454
G	-21	ALA	-	expression tag	UNP Q01454
G	-20	ALA	-	expression tag	UNP Q01454
G	-19	ASN	-	expression tag	UNP Q01454
G	-18	ARG	-	expression tag	UNP Q01454
G	-17	PHE	-	expression tag	UNP Q01454
G	-16	LYS	-	expression tag	UNP Q01454
G	-15	LYS	-	expression tag	UNP Q01454
G	-14	ILE	-	expression tag	UNP Q01454
G	-13	SER	-	expression tag	UNP Q01454
G	-12	SER	-	expression tag	UNP Q01454
G	-11	SER	-	expression tag	UNP Q01454
G	-10	GLY	-	expression tag	UNP Q01454
G	-9	ALA	-	expression tag	UNP Q01454
G	-8	LEU	-	expression tag	UNP Q01454
G	-7	GLU	-	expression tag	UNP Q01454
G	-6	ASN	-	expression tag	UNP Q01454
G	-5	LEU	-	expression tag	UNP Q01454
G	-4	TYR	-	expression tag	UNP Q01454
G	-3	PHE	-	expression tag	UNP Q01454
G	-2	GLN	-	expression tag	UNP Q01454

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0 0		regener			
Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	GLY	-	expression tag	UNP Q01454
G	0	GLU	-	expression tag	UNP Q01454
Н	-34	MET	-	initiating methionine	UNP Q01454
Н	-33	LYS	-	expression tag	UNP Q01454
Н	-32	ARG	-	expression tag	UNP Q01454
Н	-31	ARG	-	expression tag	UNP Q01454
Н	-30	TRP	-	expression tag	UNP Q01454
Н	-29	LYS	-	expression tag	UNP Q01454
H	-28	LYS	-	expression tag	UNP Q01454
Н	-27	ASN	-	expression tag	UNP Q01454
H	-26	PHE	-	expression tag	UNP Q01454
Н	-25	ILE	-	expression tag	UNP Q01454
Н	-24	ALA	-	expression tag	UNP Q01454
Н	-23	VAL	-	expression tag	UNP Q01454
H	-22	SER	-	expression tag	UNP Q01454
H	-21	ALA	-	expression tag	UNP Q01454
Н	-20	ALA	-	expression tag	UNP Q01454
H	-19	ASN	-	expression tag	UNP Q01454
H	-18	ARG	-	expression tag	UNP Q01454
H	-17	PHE	-	expression tag	UNP Q01454
H	-16	LYS	-	expression tag	UNP Q01454
H	-15	LYS	-	expression tag	UNP Q01454
H	-14	ILE	-	expression tag	UNP Q01454
H	-13	SER	-	expression tag	UNP Q01454
H	-12	SER	-	expression tag	UNP Q01454
H	-11	SER	-	expression tag	UNP Q01454
H	-10	GLY	-	expression tag	UNP Q01454
H	-9	ALA	-	expression tag	UNP Q01454
H	-8	LEU	-	expression tag	UNP Q01454
<u>H</u>	-7	GLU	-	expression tag	UNP Q01454
H	-6	ASN	-	expression tag	UNP Q01454
H	-5	LEU	-	expression tag	UNP Q01454
H	-4	TYR	-	expression tag	UNP Q01454
H	-3	PHE	-	expression tag	UNP Q01454
H	-2	GLN	-	expression tag	UNP Q01454
H	-1	GLY	-	expression tag	UNP Q01454
H	0	GLU	-	expression tag	UNP Q01454

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• Molecule 13 is a DNA chain called Leading strand template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Ι	34	Total 742	C 340	N 161	O 207	Р 34	0	0



• Molecule 14 is a DNA chain called Lagging strand template DNA.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	AltConf	Trace			
14	J	33	Total 629	C 298	N 101	0 197	Р 33	0	0

• Molecule 15 is a protein called Suppressor of kinetochore protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Κ	137	Total 1120	C 709	N 195	0 212	${S \over 4}$	0	0

• Molecule 16 is a protein called Protein DIA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	475	Total 3921	C 2533	N 654	0 710	S 24	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	-2	GLY	-	expression tag	UNP Q08496
L	-1	ALA	-	expression tag	UNP Q08496
L	0	GLY	-	expression tag	UNP Q08496

• Molecule 17 is a protein called DNA polymerase epsilon catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	0	766	Total	С	Ν	Ο	S	0	0
11	Q	700	6203	4028	1015	1124	36	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	290	ALA	ASP	variant	UNP P21951
Q	292	ALA	GLU	variant	UNP P21951

• Molecule 18 is a protein called DNA polymerase epsilon subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	552	Total 4427	C 2843	N 759	O 807	S 18	0	0



• Molecule 19 is a protein called Topoisomerase 1-associated factor 1.

Mol	Chain	Residues		At	AltConf	Trace			
19	Х	665	Total 5410	$ m C \ 3505$	N 912	0 974	S 19	0	0

• Molecule 20 is a protein called Chromosome segregation in meiosis protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Y	98	Total 791	C 511	N 138	0 138	$\frac{S}{4}$	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-1	GLY	-	expression tag	UNP Q04659
Y	0	GLU	-	expression tag	UNP Q04659

• Molecule 21 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (threeletter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
21	2	1	Total	С	Ν	Ο	Р	0
21	2	L	31	10	6	12	3	0
21	F	1	Total	С	Ν	0	Р	0
21	5	T	31	10	6	12	3	0

• Molecule 22 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Lig-



and of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
22	2	1	Total Mg 1 1	0
22	5	1	Total Mg 1 1	0

• Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
23	2	1	Total Zn 1 1	0
23	4	1	Total Zn 1 1	0
23	5	1	Total Zn 1 1	0
23	6	1	Total Zn 1 1	0
23	7	1	Total Zn 1 1	0
23	Q	2	Total Zn 2 2	0



3 Residue-property plots (i)

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

• Molecule 1: DNA replication licensing factor MCM2 Chain 2: 75% 24% ASN THR ALA ALA ASN 3LY 3LY 3LU 3LU 3LU • Molecule 2: DNA replication licensing factor MCM3 12% Chain 3: 60% 39% PRO PRO PRO ASN ASN ALA ALA VAL VAL SER SER











• Molecule 7: DNA replication complex GINS protein PSF1



Chain A:	92%		• 5%
M V2 V2 822 833 825 926 163 163 164	C78 C78 L107 ASP ASP ASP ASP ASP ASP C10 C10 C10 C10 C10 C10 C10 C12 C12 C12 C12 C12 C12 C12 C12 C12 C12	1137 11208	
• Molecule 8: DNA	replication complex GINS	protein PSF2	
Chain B:	89%		• 10%
MET 82 82 82 85 85 85 85 71 11 85 85 85 85 85 85 85 85 85 85 85 85 85	WSO DE6 S113 S113 A1A A13 A13 A13 A13 A13 A13 A13 A13	111	
• Molecule 9: DNA	replication complex GINS	protein PSF3	
Chain C:	88%		12%
MET 62 63 658 658 614 614 711 711 711 711 711 711 711 711 711 7	1144 ASP ASP ASP ASN ASP ASS SER THR ALA ALA ALA ALA ASN SSR ASS ASS ASS ASS ASS ASS ASS ASS ASS		
• Molecule 10: DNA	A replication complex GIN	S protein SLD5	
Chain D:	82%		17%
MET D2 13 613 613 613 718 718 718 718 718 718 718 718 718 718	THR LYS THR GLN GLN GLN GLN GLN GLN GLN ASR ASR ASR ASR ASR ASR ASR ASR ASR ASR	SER SER SER LEU ASP ASN ASN ASN ASN CIU CIU CIU CIU CIU CIU CIU	L106 D107 MET GLN GLN GLN ASN ASN ASN ASN PRO PRO
MET PR0 1126 1126 K181 T185 T185			
• Molecule 11: Cell	division control protein 45	,Cell division control	protein 45
Chain E:	85%		14%
M V2 D108 D108 C10 C112 D166 C112 C112 C112 C112 C112 C112 C112 C	ASP ASP GLU GLU CLU LEU CLU SER ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP	ASP ALLA ASP GLU VAL THR THR ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP	TYR LYS ASP ASP ASP ASP CLU CLU SER ASN LYS
ARG GLY ASN SER ASN SER ILE CLL ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN	R307 N308 N308 N357 N357 N357 N357 N357 A58 A58 A58 A58 L175 A58 L175 A58 L175 A58 L175 A58 A58 A58 A58 A58 A58 A58 A58 A58 A5	ASN ASN ASP ASN ASP ASP ASP ASP CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	A463 A463 Q464 D563 THR THR THR THS THS THS K598
D617 A618 A619 L650			
• Molecule 12: DNA	A polymerase alpha-binding	g protein	
Chain F:	44%	56%	

WORLDWIDE PROTEIN DATA BANK









• Molecule 12: DNA polymerase alpha-binding protein







ASP	ILE	GLU	TYR	VAL	PRO TVD	SIH	VAL	VAL	SER	ILE ASP	LYS	ASP	ARG	VAL	GLY	TRP	TYR	LYS	VAL THR	GLN	GLN	GLY	TLE	GLU	ASP	ARG	LYS	ALA	PHE	ALA ASP	PRO	VAL VAL	MET	ALA PHF.	ALA	ILE ALA	THR	THR L.YS	PRO	PRO LEU	LYS PHE
PRO	ASP	ALA	VAL	GLN	ILE	MET	ILE SFR	TYR	MET	ASP	GLY	CLU	GLY PHF	LEU	ILE	ASN	ARG	GLU	TLE	SER	GLU	ASP	GLU	ASP	PHE	TYR	THR	PRO	PRO	GLU TYR	PRO	GLY	PHE	THR TLF	PHE	ASN	ASN	ASP GLU	VAL	ALA LEU	GLN
ARG	PHE	CLU	HIS	ARG	ASP	ARG	PR.O THR	VAL	ILE	SER THR	PHE	ASN	GLY	PHE	PHE	TRP	PRO	PHE	ILE HTS	ASN	ARG	SER	LYS	HIS	GLY	ASP	MET	PHE	GLU	GLY	PHE	PRO	ASP	ALA GLU	GLY	GLU TVR	LYS	SER	TYR	CYS SER	HIS MET
ASP	CYS	ARG	TRP	LYS	ARG	SER	TYR LEH	PRO	GLN	GLY SER	GLN	CLY	LEU LYS	ALA	VAL	GI.N	SER	LYS	CLLV CLLV	TYR	ASN	PRO TI D	GLU	LEU	ASP	GLU	LEU	THR	PRO	TYR ALA	PHE	GLU	PRO	GLN	TEU	SER	TYR	SER VAL	SER	ASP ALA	VAL ALA
THR	TYR	LEU	TYR	LYS	TYR	SIH	PRO PHF	ILE	PHE	SER LEU	CYS	THR	TLE	PRO	LEU	PRD	ASP	GLU	THR	ARG	LYS	GLY	GLY	THR	LEU	GLU	MET	LEU	MET	VAL GLN	ALA	GLN	SIH	ASN TLF.	LEU	LEU PRO	ASN	LYS HTS	THR	ASP PRO	GLU
ARG	PHE	ASP	GLY	LEU	LEU	SER	GLU THR	TYR	VAL	GLY GLY	SIH	VAL	GLU	LEU	GLU	ALA GLY	VAL	PHE	ARG	ASP	LEU	LYS	GLU	PHE	LYS	ASP	PRO	SER	ILE	ASP GLU	LEU	GLN	GLU	LEU PRO	GLU	ALA LEII	LYS	PHE SER	VAL	GLU VAL	GLU ASN
LYS	SER	VAL	ASP	VAL	THR	PHE	GLU	ILE	LYS	ASN GLN	ILE	THR	GLN LYS	LEU	LEU	GLU LEU	LYS	GLU	ASN	ILE	ARG	ASN	GLU	PRO	LEU	TYR	SIH	VAL ASP	VAL	ALA SER	MET	PRO	ASN	ILE MET	THR	THR	ARG	CEU GL.N	PRO	ASP SER	ILE LYS
ALA	GLU	ASP	CYS AT A	SER	CYS	PHE	ASN	PRO	GLY	LYS THR	CYS	ALA	ARG LYS	TEU	LYS	AL.A	TRP	ARG	GL Y GL II	PHE	PHE	PRO	LYS	MET	ASP	TYR	ASN	TLE	LYS	ARG ALA	LEU	ASN	CLU	THR PHF.	PRO	ASN	ASN	LYS PHF	SER	LYS LYS	LYS VAL
LEU	THR	ASP	GLU	SER	TYR	ASP	GLN	ILE	SIH	ILE	LYS	ARG	THR	GLU	TYR	ARG	LYS	VAL	TYR HTS	ARG	VAL	LYS	VAL SER	GLU	TLE	GLU	ARG	GLU ALA	ILE	VAL CYS	GLN	GLU	ASN	PRO PHF.	TYR	VAL	THR	VAL LYS	SER	PHE ARG	ASP ARG
ARG	TYR	PHE	LYS	LEU	ALA	THR	TRP	GLY	ASN	LEU SER	LYS	ILE	ASP PRO	SER	ASP	LIS	ALA	ARG	ASP GLII	ALA	LYS	LYS	TLE	VAL	LEU	ASP	SER	GLN	LEU	ALA HIS	LYS	VAL ILE	LEU	ASN SER	PHE	TYR GLV	TYR	VAL MET	ARG	GLY	SER ARG
TRP	TYR	MET	GLU	ALA	GLY GLY	THR	CYS	THR	GLY	ALA THR	ILE	ILE	GLN	ALA	ARG	ALA LEU	VAL	GLU	ARG VAL.	GLY	ARG	PR.O	0TU CLU	LEU	ASP	ASP	GL Y	TRP	CYS	ILEU	PRO	LYS SER	PHE	GI.II	THR	TYR	PHE	THR	GLU	ASN GLY	LYS
LEU	TYR	SER	TYR	CYS	SER	TEU	ASN TVR	ARG	VAL	GLN	LYS	PHE	THR	HIS	GLN	GI.N	GLU	LEU	LYS	PRO	LEU	ASN	ITR	TYR	GLU	SIH	SER	GLU	THR	TLE PHE	PHE	VAL	ASP	GLY PRO	TYR	LYS	MET	ILEU	PRO	SER SER	CLU GLU
GLU	CLY GLY	GLY	ILE	LYS	ARG	ALA	VAL	ASN	GLU	ASP GLY	SER	LEU	GLU	TEU	LYS	GLY PHF.	GLU	LEU	LYS Arg	ARG	GLY	GLU	GLN	LEU	ILE	ASN	PHE	GLN SER	ASP	TLE PHE	LYS	VAL PHE	LEU	GLU	ASP	THR	GLU	GLY CYS	TYR	SER ALA	VAL ALA
SER	VAL	ASN	ARG	LEU	ASP	LEU	ASP SFR	HIS	GLY	LEU MET	LEU	GLU	GLU	ASP	LEU	V AL SFR	LEU	ILE	CYS	ASN	ARG	SER	NET	LYS	THR	LYS	GLU	TYR GLU	GLY	GLN	SER	SER	ILE	THR	ALA	ARG	LEU	GLY ASP	PHE	GLY	GLU ASP
MET	VAL	ASP	LYS	LEU	GLN	LYS	TYR	ILE	SER	SER LYS	PRO	PHE	ASN AL.A	PRO	VAL	GI.U	ARG	ALA	TLE	VAL	ALA	ILE	PHE	ALA	ASP	PRO	ILE	LYS ARG	SER	PHE LEU	ARG	TRP	THR	ASP	PRO	SER	GLU	ASP LEU	ASP	ILE ARG	THR ILE
ILE	ASP	GLY	TYR	ARG	GLU	TEU	GLY SFR	ALA	ILE	GLN	ILE	ILE	THR	PRO	ALA	ALA LEU	GLN	GLY	VAL SER	ASN	PRO	VAL	ARG	VAL	GLU	PRO	ASP	TRP LEU	LYS	ARG LYS	ILE	THR	LYS	GLU ASP	LYS	PHE	GLN	THR SER	LEU	THR	PHE
SER	LYS	TYS	ASN	PRO	THR	GLY	LYS	TAS	ASP	GLU	ASP	LEU	PHE GLU	PRO	THR	GLU	GLU	ASP	ASN AL.A	LYS	ILE	LYS	ALA	ARG	THR	THR	LYS	ALA	VAL	SER LYS	ARG	ARG	ASN	G L.N L.F.U	THR	ASN	GLU	ASP PRO	LEU	VAL LEU	PRO SER
GLU	ILE	SER	MET	GLU	ASP	VAL	GLY TRP	LEU	ASN	TYR GLN	LYS	ILE	LYS TRP	LYS	ILE	AL.A	ARG	ASP	ARG	ARG	ARG	ASP	GLN	PHE	GLY	THR	ASN	SER	ARG	GLU ARG	SER	ALA LEU	GLY	NET	ILE	ARG	GLN	ALA GLU	SER	TYR ALA	ASN SER
T1321	1 200	CTN CTT	LYS	LYS	ASN	L1375	N1 385	ASN	PRO	LYS THR	SER	ASN	AI.A	GLY	GLY	41390	T1430		V1445 THR	PHE	ARG	SER	ALA	MET	GLY	LEU	GLY	GLY	ILE	GLN	G1462	M1470	ALA	GLU	GLU	ARG TVR	TEU	SER G1479		P1491 THR	SER ILE
GLY	TYR E1407	10110	V1513 TETT	LYS	PRO	ASN	GLN	GLN	GLU	I1523	D1551	ILE	GLU	ASP	I1556	F1563	THR	ASP	ILE SER	K1568		M1610	S1616	LEU	ASN	VAL	LEU	LEU PRO	GLN	LEU ASN	TRP	PRO	T1630	R1664		N1690	Q1702	N1729		A1748 LEU	ILE ASN

WORLDWIDE PROTEIN DATA BANK





• Molecule 18: DNA polymerase epsilon subunit B





GLU GLN GLN GLY GLY GLV GLV GLV GLV GLY ASP ASP ASP ASP TYR	ASN ASP PRO TTR TTR TTR TCE PRO ASP CLM TLE CLM TLE SER SER SER ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP	ALA PHE PHE LYS ASP LEU ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP	LYS GLY TILE ARG SER LYS LYS LYS LYS LYS ASP
LYS ARG LYS LYS ARG ARG CLY GLY GLY GLY THR THR ALA LEU	PRIO MET PHE GLY GLY ASP GLU ASP GLU CHN CHL CHN CHU CHN CHN CHN CHN CHN CHN CHN CHN CHN CHN	H13 GLY VAL PHE PHE F13 PHE L13 PHE T11 PHE C13 V ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN	PRIO TILE PHE CLU ASN CLU TTRR TTRR TTRR
ARG TRP LEU LEU LEU ASP ASN ASN ASN ASN ASN ASN ASN CLY CLU	ASP ARG TYR TILE CLN CLN CLN CLN ALA ALA ALA ALA ALA ALA ALA ALA ALA A	0LY VAL THR THR GLY GLY GLY ASP ASP ASP CLY CLEU CLY CLY CLY CLY CLY SER SER SER SER SER	ILE ARG ALA THR GLU SER SER SER PHE ALA
PRO ASP LYS SER SER LEU LEU LEU LEU ALA SER HIS VAL	SER GLU MET MET MET MET PHE ASP ASN ASN ASN ASN ASN ASN ASN ASN ASN SER SER SER	ASP ASP VAL VAL VAL SER SER ASN SER ASN CLV CLV CLV CLN SER SER SER SER SER	GLN ASN MET PHE GLN SER CLU VAL TYR SER SER
ARG LYS GLU SER THR LYS SER ARG SER LEU CLU ALA SER ALA	ALA ASP GLU GLU ASP GLU GLU ASP GLU CLU CLU CLU CLU CLU CLU CLU CLU CLU C	ASER VAL VAL LEU SER GLN ASP ASP ASP ASP	
• Molecule 20: Cl	nromosome segregation	in meiosis protein 3	
		-	
Chain Y:	31%	69%	
Chain Y:	PHE ASN ASP ASP ASP ASP SER VAL LYS ASP PRO THR THR THR THR THR CLY CLY CLY CLY LEU	ASP GLY SER VAL VAL ASP PRO ALA ALA ALA A42 A45 A45 A45 A45 A45 A45 A45 A45 A45 A45	R48 R48 SER SER PHE ASP ASP CLY THR ARG CLY GLU
Chain Y:	GLU PHE HIS ASN VAL ASN SER ASN SER ASN ALA SER GLU 0.1N ALA SER PRO 0.1N ALA DAL ASN ASN PRO 1.1YS PRO 0.1N ALA VAL TAR ALA VAL ASN PRO 6.1V ALA VAL LEU VAL	GLM ASP GLY LYS KAR LYS SER ASN VAL VAL ASN VAL ASN THR ASN THR ASP PRO ASP AIA ASP PRO ASP PRO ASP 143 ASP 144 ASP 14	HIS MAC LEU PAS SER TYR H139 ARG SER ASN PHE ARG VAL GLY GLY ARG THR ARG CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU
Chain Y: ATD ATD ATD ATD ATD ATD ATD ATD ATD ATD	ASN GLU PHE VAL HLS ASN PRO SER ASN PRO SER ASN ASP DLU CLU SER ASN ASP DLU CLU ASP DLU CLU ASP PRO CLU CLN ASP PRO ASN ALA SER ASN ALA VAL THR LEU VAL THR ALA VAL LEU AAA ARG ASN ALA LEU LEU	VAL GLM ASP GUN ASP CUN ASP PRO VAL ASN UNL CUN ASN VAL GUN ASN VAL ASN VAL ASN VAL ASN VAL ASN ASP CUU ASP CU	ALA HIS A4 ARG LEU M48 ARG SRR LYS TYR M139 MET ARG SRR GLU ASN PRE GLY ARG VAL SER GLY GLY MET ARG THR MET ARG THR AGG GLY GLY MET GLY GLY GLY



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	369254	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 $(e^-/\text{\AA}^2)$	38.8	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	63.838	Depositor
Minimum map value	-32.137	Depositor
Average map value	0.038	Depositor
Map value standard deviation	1.533	Depositor
Recommended contour level	6.82	Depositor
Map size (Å)	398.55997, 398.55997, 398.55997	wwPDB
Map dimensions	376, 376, 376	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: ANP, MG, ZN

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	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5
1	2	0.35	0/5272	0.69	0/7122
2	3	0.31	0/4918	0.65	0/6668
3	4	0.32	0/4801	0.66	1/6488~(0.0%)
4	5	0.34	0/5303	0.67	0/7155
5	6	0.33	0/5125	0.68	0/6916
6	7	0.32	0/5010	0.65	1/6779~(0.0%)
7	А	0.32	0/1631	0.63	0/2194
8	В	0.29	0/1642	0.63	0/2221
9	С	0.31	0/1414	0.55	0/1911
10	D	0.33	0/2040	0.59	0/2755
11	Е	0.31	0/4653	0.64	0/6297
12	F	0.31	0/3489	0.62	0/4724
12	G	0.32	0/3465	0.63	0/4696
12	Н	0.32	0/3496	0.63	0/4735
13	Ι	0.76	1/839~(0.1%)	1.14	2/1303~(0.2%)
14	J	1.18	1/694~(0.1%)	1.39	3/1053~(0.3%)
15	Κ	0.33	0/1139	0.68	0/1539
16	L	0.37	0/3996	0.66	0/5395
17	Q	0.33	0/6332	0.61	0/8548
18	R	0.34	0/4526	0.66	0/6125
19	Х	0.32	0/5512	0.61	0/7426
20	Y	0.35	0/807	0.60	0/1084
All	All	0.35	2/76104~(0.0%)	0.66	7/103134~(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	2	0	1



Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
18	R	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	J	104	DC	C1'-N1	7.40	1.58	1.49
13	Ι	105	DT	C1'-N1	5.42	1.56	1.49

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
13	Ι	103	DT	OP1-P-OP2	-7.29	108.66	119.60
14	J	1	DC	OP1-P-OP2	-6.81	109.39	119.60
13	Ι	1	DG	OP1-P-OP2	-6.68	109.58	119.60
14	J	101	DC	OP1-P-OP2	-6.50	109.85	119.60
3	4	710	ASP	CB-CG-OD1	6.25	123.93	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	678	ASP	Peptide
18	R	489	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	5183	0	5225	2	0
2	3	4834	0	4903	2	0
3	4	4731	0	4796	2	0
4	5	5231	0	5303	6	0
5	6	5042	0	5045	3	0
6	7	4936	0	4970	3	0
7	А	1611	0	1615	3	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	В	1609	0	1662	1	0
9	С	1381	0	1394	0	0
10	D	2004	0	2001	2	0
11	Е	4569	0	4556	0	0
12	F	3404	0	3352	2	0
12	G	3380	0	3310	0	0
12	Н	3411	0	3355	1	0
13	Ι	742	0	379	0	0
14	J	629	0	365	0	0
15	Κ	1120	0	1111	1	0
16	L	3921	0	4025	1	0
17	Q	6203	0	6270	4	0
18	R	4427	0	4480	10	0
19	Х	5410	0	5573	4	0
20	Y	791	0	811	0	0
21	2	31	0	13	1	0
21	5	31	0	13	2	0
22	2	1	0	0	0	0
22	5	1	0	0	0	0
23	2	1	0	0	0	0
23	4	1	0	0	0	0
23	5	1	0	0	0	0
23	6	1	0	0	0	0
23	7	1	0	0	0	0
23	Q	2	0	0	0	0
All	All	74640	0	74527	45	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 0.

The worst 5 of 45 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom_1	Atom_2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
12:F:584:THR:OG1	12:F:622:ASN:O	2.08	0.70
19:X:566:SER:O	19:X:569:ARG:NH1	2.25	0.69
18:R:543:ARG:NH1	18:R:545:ASP:OD1	2.28	0.67
18:R:413:ILE:HD13	18:R:665:ILE:HD12	1.85	0.56
1:2:546:GLY:H	21:2:1500:ANP:HNB1	1.54	0.55

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	n Analysed Favoured Allowed Outli		Outliers	Percentiles		
1	2	650/868~(75%)	630~(97%)	20 (3%)	0	100	100
2	3	603/1009~(60%)	585~(97%)	18 (3%)	0	100	100
3	4	583/933~(62%)	565~(97%)	18 (3%)	0	100	100
4	5	644/775~(83%)	626~(97%)	18 (3%)	0	100	100
5	6	631/1017~(62%)	608~(96%)	23~(4%)	0	100	100
6	7	617/845~(73%)	594 (96%)	23~(4%)	0	100	100
7	А	193/208~(93%)	186 (96%)	7 (4%)	0	100	100
8	В	188/213~(88%)	184 (98%)	4 (2%)	0	100	100
9	С	165/194~(85%)	164 (99%)	1 (1%)	0	100	100
10	D	237/294~(81%)	234~(99%)	3 (1%)	0	100	100
11	Ε	554/657~(84%)	539~(97%)	15 (3%)	0	100	100
12	F	418/962~(44%)	409 (98%)	9 (2%)	0	100	100
12	G	416/962~(43%)	404 (97%)	12 (3%)	0	100	100
12	Н	419/962~(44%)	408 (97%)	11 (3%)	0	100	100
15	Κ	131/194~(68%)	124 (95%)	7 (5%)	0	100	100
16	L	469/735~(64%)	450 (96%)	19 (4%)	0	100	100
17	Q	740/2222~(33%)	721 (97%)	19 (3%)	0	100	100
18	R	544/689~(79%)	525~(96%)	19 (4%)	0	100	100
19	X	$6\overline{49/1238}~(52\%)$	637~(98%)	12 (2%)	0	100	100
20	Y	96/319~(30%)	95~(99%)	1 (1%)	0	100	100
All	All	8947/15296 (58%)	8688 (97%)	259 (3%)	0	100	100

There are no Ramachandran outliers to report.



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 Ou		Outliers	Perce	ntiles
1	2	569/770~(74%)	564~(99%)	5 (1%)	78	91
2	3	532/866~(61%)	528~(99%)	4 (1%)	81	93
3	4	537/848~(63%)	537 (100%)	0	100	100
4	5	591/688~(86%)	584 (99%)	7 (1%)	71	88
5	6	553/886~(62%)	545~(99%)	8 (1%)	67	86
6	7	545/753~(72%)	536~(98%)	9 (2%)	60	83
7	А	182/193~(94%)	179~(98%)	3(2%)	62	84
8	В	182/198~(92%)	181 (100%)	1 (0%)	88	95
9	С	154/173~(89%)	154 (100%)	0	100	100
10	D	234/279~(84%)	233 (100%)	1 (0%)	91	95
11	Ε	507/592~(86%)	503~(99%)	4 (1%)	81	93
12	F	375/854~(44%)	374 (100%)	1 (0%)	92	96
12	G	372/854~(44%)	370~(100%)	2~(0%)	88	95
12	Н	375/854~(44%)	372~(99%)	3 (1%)	81	93
15	Κ	124/179~(69%)	122~(98%)	2(2%)	62	84
16	L	456/686~(66%)	450~(99%)	6 (1%)	69	87
17	Q	701/2012~(35%)	697~(99%)	4 (1%)	86	94
18	R	$\overline{498/629}~(79\%)$	495 (99%)	3 (1%)	86	94
19	Х	607/1125~(54%)	598~(98%)	9 (2%)	65	85
20	Y	85/286~(30%)	85 (100%)	0	100	100
All	All	8179/13725 (60%)	8107 (99%)	72 (1%)	79	91

 $5~{\rm of}~72$ residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
17	Q	1664	ARG
19	Х	687	ASP
17	Q	1729	ASN



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

Mol	Chain	Res	Type
19	Х	280	ASP
6	7	82	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
19	Х	433	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)

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 11 ligands modelled in this entry, 9 are monoatomic - leaving 2 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	Typo	Chain	Dec	Link	Bo	ond leng	$_{\rm ths}$	Bond angles			
IVIOI	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
21	ANP	5	1500	22	29,33,33	1.11	4 (13%)	31,52,52	1.08	2 (6%)	
21	ANP	2	1500	22	29,33,33	1.12	4 (13%)	31,52,52	1.05	2 (6%)	

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 tl	ne '	Torsion	and	Rings	columns	5.
'-' means	no outliers o	of that kind	were ide	ntified.									

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	ANP	5	1500	22	-	6/14/38/38	0/3/3/3
21	ANP	2	1500	22	-	4/14/38/38	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
21	2	1500	ANP	PB-O3A	-3.22	1.55	1.59
21	5	1500	ANP	PB-O3A	-3.01	1.55	1.59
21	5	1500	ANP	PG-01G	2.40	1.50	1.46
21	2	1500	ANP	PG-01G	2.35	1.49	1.46
21	2	1500	ANP	PG-N3B	2.29	1.69	1.63

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
21	5	1500	ANP	PB-O3A-PA	-3.92	118.83	132.62
21	2	1500	ANP	PB-O3A-PA	-3.55	120.12	132.62
21	2	1500	ANP	C5-C6-N6	2.32	123.88	120.35
21	5	1500	ANP	C5-C6-N6	2.29	123.84	120.35

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms
21	2	1500	ANP	PB-N3B-PG-O1G
21	2	1500	ANP	C5'-O5'-PA-O2A
21	5	1500	ANP	PB-N3B-PG-O1G
21	5	1500	ANP	PA-O3A-PB-O1B
21	5	1500	ANP	PA-O3A-PB-O2B

There are no ring outliers.

2 monomers are involved in 3 short contacts:

	Mol	Chain	Res	Type	Clashes	Symm-Clashes
ſ	21	5	1500	ANP	2	0
	21	2	1500	ANP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In



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







5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-13539. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections (i)

6.1.1 Primary map



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

6.2 Central slices (i)

6.2.1 Primary map



X Index: 188



Y Index: 188



Z Index: 188

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: 178

Y Index: 155

Z Index: 167

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 6.82. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



6.5 Mask visualisation (i)

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



7 Map analysis (i)

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

7.1 Map-value distribution (i)



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



7.2 Volume estimate (i)



The volume at the recommended contour level is 634 $\rm nm^3;$ this corresponds to an approximate mass of 572 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 0.312 ${\rm \AA^{-1}}$



8 Fourier-Shell correlation (i)

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



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-13539 and PDB model 7PMN. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 6.82 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 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

