



wwPDB EM Map/Model Validation Report ⓘ

May 26, 2016 – 01:37 PM EDT

PDB ID : 5FYW
EMDB ID: : 3378
Title : Transcription initiation complex structures elucidate DNA opening (OC)
Authors : Plaschka, C.; Hantsche, M.; Dienemann, C.; Burzinski, C.; Plitzko, J.; Cramer, P.
Deposited on : 2016-03-10
Resolution : 4.35 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027674

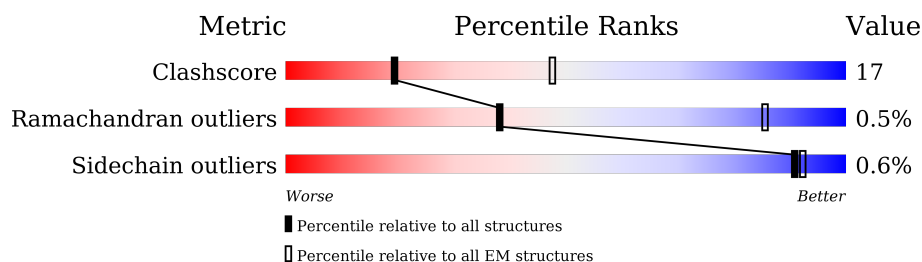
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.35 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	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	1733	58% 23% 19%
2	B	1224	62% 32% 5%
3	C	318	52% 31% 18%
4	D	221	45% 26% 29%
5	E	215	75% 24% .
6	F	155	42% 12% 46%
7	G	171	51% 48% .
8	H	146	52% 39% .. 7%
9	I	122	61% 34% 5%

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Mol	Chain	Length	Quality of chain
10	J	70	
11	K	120	
12	L	70	
13	M	345	
14	N	72	
15	O	240	
16	Q	735	
17	R	400	
18	T	72	
19	U	286	
20	V	122	
21	W	482	
22	X	328	

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 41710 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-DIRECTED RNA POLYMERASE II SUBUNIT RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1398	Total	C	N	O	S	0	0
			10997	6931	1927	2078	61		

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1157	Total	C	N	O	S	0	0
			9203	5822	1613	1713	55		

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	262	Total	C	N	O	S	0	0
			2061	1299	343	406	13		

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	157	Total	C	N	O	S	0	0
			1253	779	220	252	2		

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	213	Total	C	N	O	S	0	0
			1744	1107	308	318	11		

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	83	Total	C	N	O	S	0	0
			670	428	114	125	3		

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	136	Total	C	N	O	S	0	0
			1089	686	184	215	4		

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	116	Total	C	N	O	S	0	0
			944	581	172	181	10		

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	65	Total	C	N	O	S	0	0
			532	339	93	94	6		

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	112	Total	C	N	O	S	0	0
			904	580	154	168	2		

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			358	221	71	62	4		

- Molecule 13 is a protein called TRANSCRIPTION INITIATION FACTOR IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	231	Total	C	N	O	S	0	0
			1785	1145	299	326	15		

- Molecule 14 is a DNA chain called NONTEMPLATE DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	47	Total	C	N	O	P	0	0
			919	461	178	234	46		

- Molecule 15 is a protein called TATA-BOX-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	180	Total	C	N	O	S	0	0
			1416	921	242	247	6		

- Molecule 16 is a protein called TRANSCRIPTION INITIATION FACTOR IIF SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	148	Total	C	N	O	S	0	0
			1144	733	195	212	4		

- Molecule 17 is a protein called TRANSCRIPTION INITIATION FACTOR IIF SUBUNIT BETA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	199	Total	C	N	O	S	0	0
			1347	838	247	255	7		

- Molecule 18 is a DNA chain called NONTEMPLATE DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	47	Total	C	N	O	P	0	0
			909	458	172	233	46		

- Molecule 19 is a protein called TRANSCRIPTION INITIATION FACTOR IIA LARGE SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	92	Total	C	N	O	S	0	0
			757	474	130	150	3		

- Molecule 20 is a protein called TRANSCRIPTION INITIATION FACTOR IIA SUBUNIT

2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	100	Total	C	N	O	S	0	0
			782	492	130	156	4		

- Molecule 21 is a protein called TRANSCRIPTION INITIATION FACTOR IIE SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	168	Total	C	N	O		0	0
			835	499	168	168			

- Molecule 22 is a protein called TRANSCRIPTION INITIATION FACTOR IIE SUBUNIT BETA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	143	Total	C	N	O		0	0
			710	424	143	143			

- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
23	J	1	Total	Zn	0
			1	1	
23	B	1	Total	Zn	0
			1	1	
23	I	2	Total	Zn	0
			2	2	
23	C	1	Total	Zn	0
			1	1	
23	W	1	Total	Zn	0
			1	1	
23	A	2	Total	Zn	0
			2	2	
23	L	1	Total	Zn	0
			1	1	
23	M	1	Total	Zn	0
			1	1	

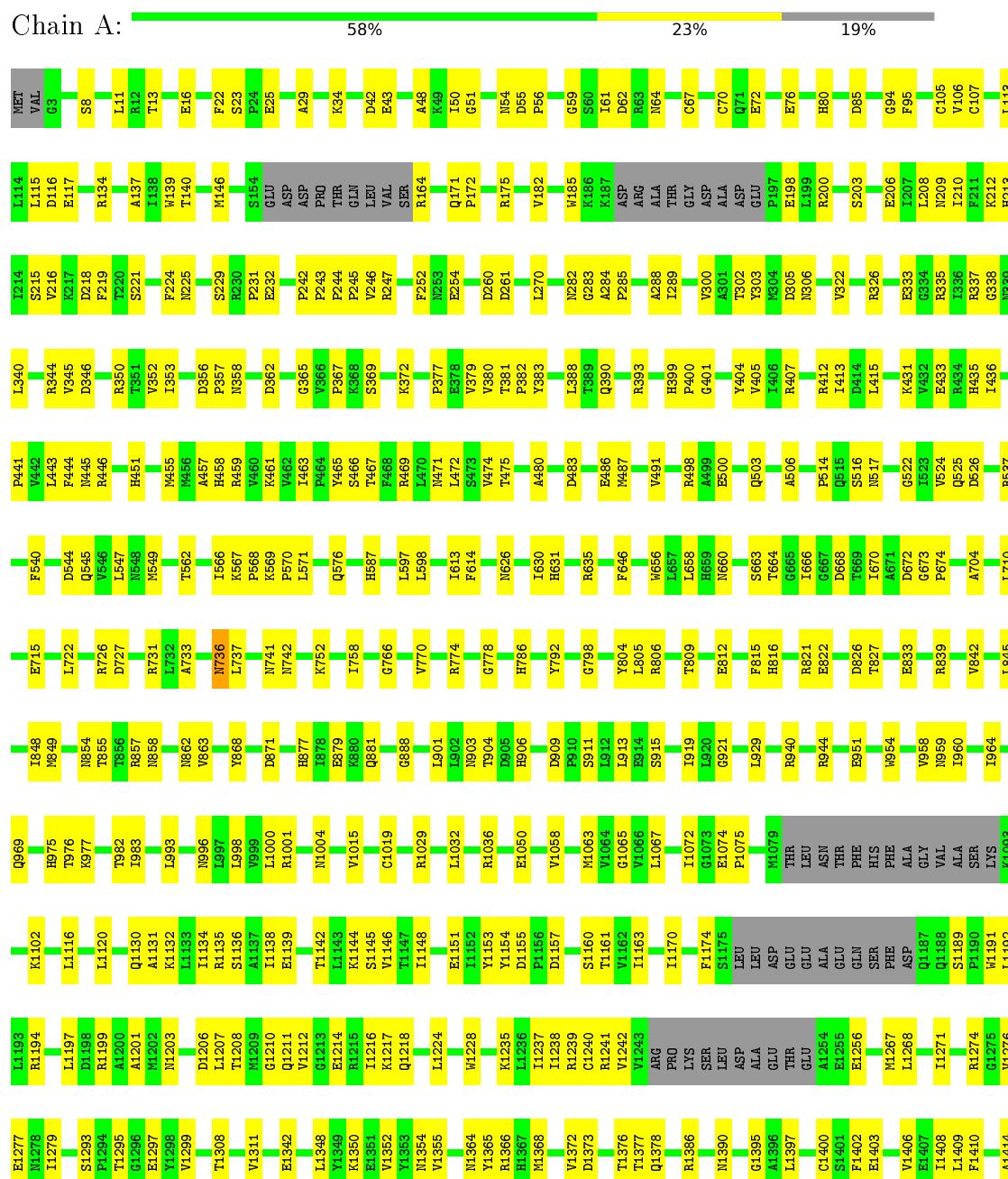
- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
24	A	1	Total	Mg	0
			1	1	

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

- Molecule 1: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1



MET SER ASP TYR GLU ALA PHE ASN ASP GLU ASN ASP PHE ASP VAL HIS PHE SER ASP GLU GLU THR TYR GLU GLU LYS PRO GLN PHE LYS ASP GLY THR THR THR GLY GLY ASP PHE GLN

HIS GLU GLN ILE ARG ARG LYS THR LEU LYS K72 T82 P83 Y84 R90 A91 A92 I93 L94 L99 S102 A105 V133 I134 R135 R136 Y137 D140 F143 S147 E150 D154 LEU

• Molecule 7: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

Chain G:  51% 48%

M1 F2 F3 I4 K5 K6 L7 M10 H14 P15 S16 F17 F18 R21 M22 K23 Q24 Y25 L26 V34 F35 G36 K41 F42 G43 Y44 I45 L46 C47 D50 N53 Q57 R58 G59 R60 I61 L62 P63 F70 Y74 V77 F78 F79 R80 P81 F82 R83 G84 E85

V86 S93 C94 S95 S96 H97 G98 F99 E100 V101 V108 F109 V110 T111 K112 H113 L114 M115 L119 T120 F121 R122 A123 P127 Y130 Q131 S132 S133 I137 T138 I139 R140 S141 R142 I143 R144 V145 K146 T147 E148 G149 C150 I151 I157 H158 A159 I160 G161 S162 Y167 A170

I171

• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3

Chain H:  52% 39% 7%

MET S2 R3 T4 K5 L6 D7 I9 F10 S13 R22 V23 C24 R25 I26 E27 S30 Q35 C36 D41 I42 M43 V44 L46 T56 A60 S61 N64 L65 GLU ASP THR PRO ALA ASN ASP SER SER A75 L89 A90 D91 D92 Y93 D94 Y95 Y96 T100

A101 Y102 K103 F104 E105 E106 V107 S108 K109 D110 L111 L112 Y115 Y116 S117 C120 G120 I121 L122 M123 R124 L125 E126 Y129 R130 M131 L132 N133 K136 Q137 E138 N139 L143 I144 R145 R146

• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9

Chain I:  61% 34% 5%

MET T2 C7 R8 D9 L14 D19 I23 F27 E28 T31 V35 L42 V43 Y44 L48 I49 T50 E54 T55 A56 G57 V58 V59 D60 D61 R70 S71 E74 C78 R81 E82 R83 V84 D87 S88 Q89 R90 R91 S96 F100 F101 V102

G103 L104 S105 I109 S112 K117 ARG THR GLN PHE SER

• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5

Chain J:  64% 27% 7%

M1 I2 R6 C7 F8 V13 D16 K17 M18 Y21 L25 L30 T34 R38 L41 K42 R43 C45 C46 R47 R48 T52 E58 N64 P65 LEU GLU LYS ARG ASP

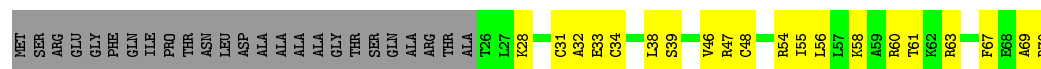
• Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11

Chain K:  71% 23% 7%

M1 N2 F7 E8 L9 F10 L11 K18 L19 K20 I33 T34 F35 E38 T41 L42 L45 I46 R47 A48 E49 F58 A59 V63 E64 R65 R70 F71 R74 I94 L101 M104 F105 Q112 THR LEU ALA ASP ASP ALA PHE

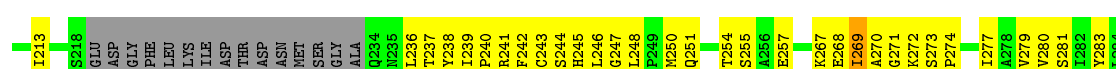
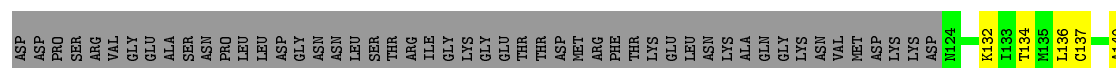
- Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4

Chain L: 




- Molecule 13: TRANSCRIPTION INITIATION FACTOR IIB

Chain M: 



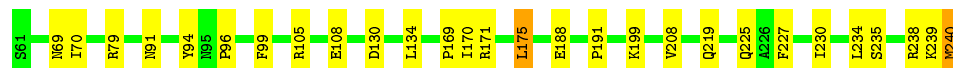
- Molecule 14: NONTEMPLATE DNA

Chain N: 



- Molecule 15: TATA-BOX-BINDING PROTEIN

Chain O: 



- Molecule 16: TRANSCRIPTION INITIATION FACTOR IIF SUBUNIT ALPHA

Chain Q: 



THR	GLU	ASP	ALA	VAL	ASN	ALA	THR	THR	ALA	ALA	SER	GLY	PRO	SER	ALA	ALA	ASN	ALA	LYS	PRO	ASN	ASP	GLY	ASP	ASP	ASP	ASP	ASP	ASP	ASP	GLU	MET	ILE	ASP	GLU	PHE	GLU	ASP	VAL
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

Chain X: 41% • 56%

GLU VAL LYS LYS LYS ARG GLN ARG LYS LYS LYS THR ASN THR HIS MET THR GLY ILE LEU LYS ASP TYR SER HIS ARG VAL

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	33	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	4200	Depositor
Magnification	37000	Depositor
Image detector	GATAN K2 SUMMIT (4K X 4K)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.46	0/11192	0.55	1/15128 (0.0%)
10	J	0.53	0/541	0.56	0/727
11	K	0.43	0/922	0.53	0/1244
12	L	0.40	0/360	0.60	0/478
13	M	0.40	0/1809	0.60	0/2435
14	N	1.07	12/1036 (1.2%)	1.30	5/1530 (0.3%)
15	O	0.59	0/1443	0.78	1/1942 (0.1%)
16	Q	0.53	0/1168	0.68	1/1579 (0.1%)
17	R	0.43	0/1354	0.68	1/1832 (0.1%)
18	T	1.24	16/1023 (1.6%)	1.44	13/1507 (0.9%)
19	U	0.39	0/766	0.61	0/1032
2	B	0.51	0/9381	0.59	1/12650 (0.0%)
20	V	0.38	0/789	0.62	1/1066 (0.1%)
21	W	0.33	1/832 (0.1%)	0.47	0/1157
22	X	0.26	0/706	0.47	0/979
3	C	0.52	0/2099	0.57	0/2845
4	D	0.25	0/1262	0.44	0/1693
5	E	0.40	0/1780	0.49	0/2395
6	F	0.47	0/682	0.52	0/922
7	G	0.31	0/1368	0.50	0/1844
8	H	0.61	1/1107 (0.1%)	0.97	6/1499 (0.4%)
9	I	0.40	0/962	0.50	0/1295
All	All	0.52	30/42582 (0.1%)	0.65	30/57779 (0.1%)

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
10	J	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	M	0	1
2	B	0	1
8	H	0	2
All	All	0	5

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	131	ASN	C-N	-13.08	1.03	1.34
18	T	53	DA	P-O5'	-11.50	1.48	1.59
18	T	47	DA	C1'-N9	-10.28	1.32	1.47
18	T	56	DG	C1'-N9	-6.75	1.37	1.47
18	T	64	DC	C1'-N1	6.24	1.57	1.49

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	131	ASN	N-CA-C	16.18	154.67	111.00
8	H	131	ASN	O-C-N	-15.85	97.34	122.70
8	H	131	ASN	C-N-CA	15.68	160.91	121.70
18	T	46	DT	O4'-C4'-C3'	-11.75	98.95	106.00
17	R	336	VAL	CB-CA-C	-10.95	90.60	111.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1175	LEU	Peptide
8	H	131	ASN	Mainchain,Peptide
10	J	2	ILE	Peptide
13	M	292	PRO	Peptide

5.2 Too-close contacts ⓘ

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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10997	0	11082	291	0
2	B	9203	0	9203	371	0
3	C	2061	0	2029	72	0
4	D	1253	0	1273	62	0
5	E	1744	0	1772	32	0
6	F	670	0	690	15	0
7	G	1340	0	1356	95	0
8	H	1089	0	1061	40	0
9	I	944	0	899	30	0
10	J	532	0	543	22	0
11	K	904	0	911	20	0
12	L	358	0	380	24	0
13	M	1785	0	1891	170	0
14	N	919	0	533	33	0
15	O	1416	0	1493	69	0
16	Q	1144	0	1034	100	0
17	R	1347	0	1130	92	0
18	T	909	0	533	65	0
19	U	757	0	747	21	0
20	V	782	0	790	16	0
21	W	835	0	349	12	0
22	X	710	0	287	4	0
23	A	2	0	0	0	0
23	B	1	0	0	0	0
23	C	1	0	0	0	0
23	I	2	0	0	0	0
23	J	1	0	0	0	0
23	L	1	0	0	0	0
23	M	1	0	0	0	0
23	W	1	0	0	0	0
24	A	1	0	0	0	0
All	All	41710	0	39986	1351	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 17.

The worst 5 of 1351 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:865:LYS:CE	13:M:145:ILE:HD11	1.46	1.44
2:B:405:ARG:NH1	2:B:632:ARG:HG2	1.23	1.40
2:B:868:MET:HB2	13:M:149:CYS:SG	1.64	1.35
13:M:267:LYS:HE3	15:O:208:VAL:CG1	1.59	1.31
13:M:272:LYS:HB3	18:T:53:DA:P	1.71	1.29

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	Percentiles	
1	A	1386/1733 (80%)	1306 (94%)	77 (6%)	3 (0%)	52	86
2	B	1139/1224 (93%)	1086 (95%)	48 (4%)	5 (0%)	39	80
3	C	260/318 (82%)	246 (95%)	14 (5%)	0	100	100
4	D	153/221 (69%)	145 (95%)	8 (5%)	0	100	100
5	E	211/215 (98%)	209 (99%)	2 (1%)	0	100	100
6	F	81/155 (52%)	76 (94%)	5 (6%)	0	100	100
7	G	169/171 (99%)	160 (95%)	8 (5%)	1 (1%)	30	74
8	H	132/146 (90%)	114 (86%)	14 (11%)	4 (3%)	5	44
9	I	114/122 (93%)	105 (92%)	9 (8%)	0	100	100
10	J	63/70 (90%)	57 (90%)	5 (8%)	1 (2%)	12	57
11	K	110/120 (92%)	107 (97%)	3 (3%)	0	100	100
12	L	43/70 (61%)	37 (86%)	6 (14%)	0	100	100
13	M	225/345 (65%)	202 (90%)	20 (9%)	3 (1%)	15	60
15	O	178/240 (74%)	174 (98%)	4 (2%)	0	100	100
16	Q	140/735 (19%)	124 (89%)	13 (9%)	3 (2%)	9	52
17	R	181/400 (45%)	171 (94%)	9 (5%)	1 (1%)	30	74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	U	88/286 (31%)	82 (93%)	3 (3%)	3 (3%)	5	42
20	V	96/122 (79%)	87 (91%)	8 (8%)	1 (1%)	19	65
21	W	162/482 (34%)	154 (95%)	7 (4%)	1 (1%)	30	74
22	X	135/328 (41%)	125 (93%)	9 (7%)	1 (1%)	26	71
All	All	5066/7503 (68%)	4767 (94%)	272 (5%)	27 (0%)	38	77

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	343	ILE
2	B	476	ARG
8	H	132	LEU
13	M	269	ILE
17	R	259	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain 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	A	1221/1520 (80%)	1219 (100%)	2 (0%)	95	97
2	B	1000/1061 (94%)	999 (100%)	1 (0%)	95	97
3	C	230/274 (84%)	230 (100%)	0	100	100
4	D	139/200 (70%)	139 (100%)	0	100	100
5	E	195/197 (99%)	195 (100%)	0	100	100
6	F	73/137 (53%)	73 (100%)	0	100	100
7	G	152/152 (100%)	152 (100%)	0	100	100
8	H	119/128 (93%)	119 (100%)	0	100	100
9	I	110/116 (95%)	110 (100%)	0	100	100
10	J	60/65 (92%)	60 (100%)	0	100	100
11	K	97/102 (95%)	97 (100%)	0	100	100
12	L	40/57 (70%)	40 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	201/299 (67%)	200 (100%)	1 (0%)	92	96
15	O	152/205 (74%)	141 (93%)	11 (7%)	18	57
16	Q	109/641 (17%)	109 (100%)	0	100	100
17	R	107/363 (30%)	107 (100%)	0	100	100
19	U	84/260 (32%)	79 (94%)	5 (6%)	24	63
20	V	90/108 (83%)	85 (94%)	5 (6%)	26	65
All	All	4179/5885 (71%)	4154 (99%)	25 (1%)	91	95

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	O	219	GLN
15	O	235	SER
20	V	57	GLN
15	O	225	GLN
15	O	240	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
15	O	95	ASN
15	O	158	GLN
19	U	280	GLN
4	D	173	HIS
16	Q	122	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.