wwPDB X-ray Structure Validation Summary Report (i)

Jun 23, 2024 – 05:43 PM EDT

PDB ID	:	5C44
Title	:	Crystal structure of a transcribing RNA Polymerase II complex reveals a complete transcription bubble
Authors	:	Barnes, C.O.; Calero, M.; Malik, I.; Spahr, H.; Zhang, Q.; Pullara, F.; Kaplan, C.D.; Calero, G.
Deposited on	:	2015-06-17
Resolution	:	3.95 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp
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:

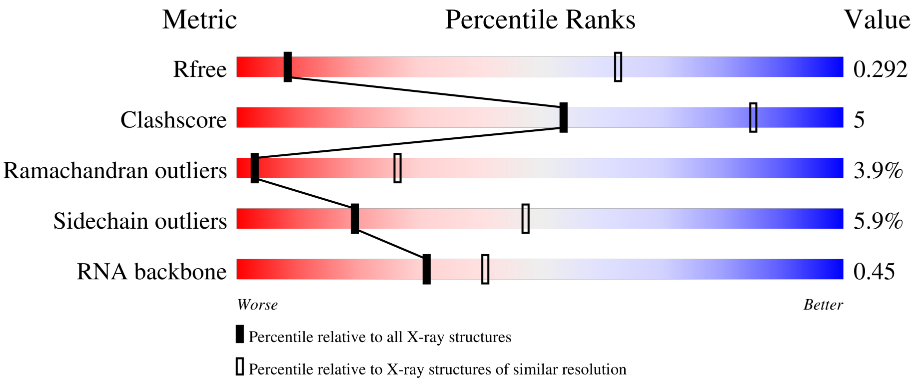
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.95 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1025 (4.22-3.70)
Clashscore	141614	1085 (4.22-3.70)
Ramachandran outliers	138981	1047 (4.22-3.70)
Sidechain outliers	138945	1039 (4.22-3.70)
RNA backbone	3102	1041 (4.84-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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	Quality of chain
1	A	1733	66% 15% • 17%
2	B	1224	73% 20% • 5%
3	C	318	66% 15% • 17%
4	D	221	67% 13% • 19%
5	E	215	86% 13% •
6	F	155	43% 14% 44%

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Mol	Chain	Length	Quality of chain
7	G	179	79% 16% • •
8	H	146	79% 14% 8%
9	I	120	86% 8% • 5%
10	J	70	71% 20% • 7%
11	K	120	78% 17% • •
12	L	70	43% 19% • 37%
13	R	9	56% 22% 22%
14	S	53	6% 17% • 75%
15	U	53	13% 19% 17% • 49%

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 32540 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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					ZeroOcc	AltConf	Trace
1	A	1434	Total 11249	C 7083	N 1967	O 2137	S 62	0	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1158	Total 9175	C 5795	N 1603	O 1721	S 56	0	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	265	Total 2086	C 1312	N 347	O 414	S 13	0	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	178	Total 1417	C 875	N 254	O 286	S 2	0	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	214	Total 1752	C 1111	N 309	O 321	S 11	0	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	87	Total 705	C 451	N 119	O 132	S 3	0	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	171	1339	861	222	248	8	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	172	LEU	-	expression tag	UNP P34087
G	173	GLU	-	expression tag	UNP P34087
G	174	HIS	-	expression tag	UNP P34087
G	175	HIS	-	expression tag	UNP P34087
G	176	HIS	-	expression tag	UNP P34087
G	177	HIS	-	expression tag	UNP P34087
G	178	HIS	-	expression tag	UNP P34087
G	179	HIS	-	expression tag	UNP P34087

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	135	1080	679	182	214	5	0	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	114	921	568	165	178	10	0	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	115	924	593	157	172	2	0	0	0

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	44	346	214	67	61	4	0	0	0

- Molecule 13 is a RNA chain called Synthetic RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
13	R	9	197	88	40	60	9	0	0	0

- Molecule 14 is a DNA chain called Synthetic DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
14	S	13	268	128	46	81	13	0	0	0

- Molecule 15 is a DNA chain called Synthetic DNA.

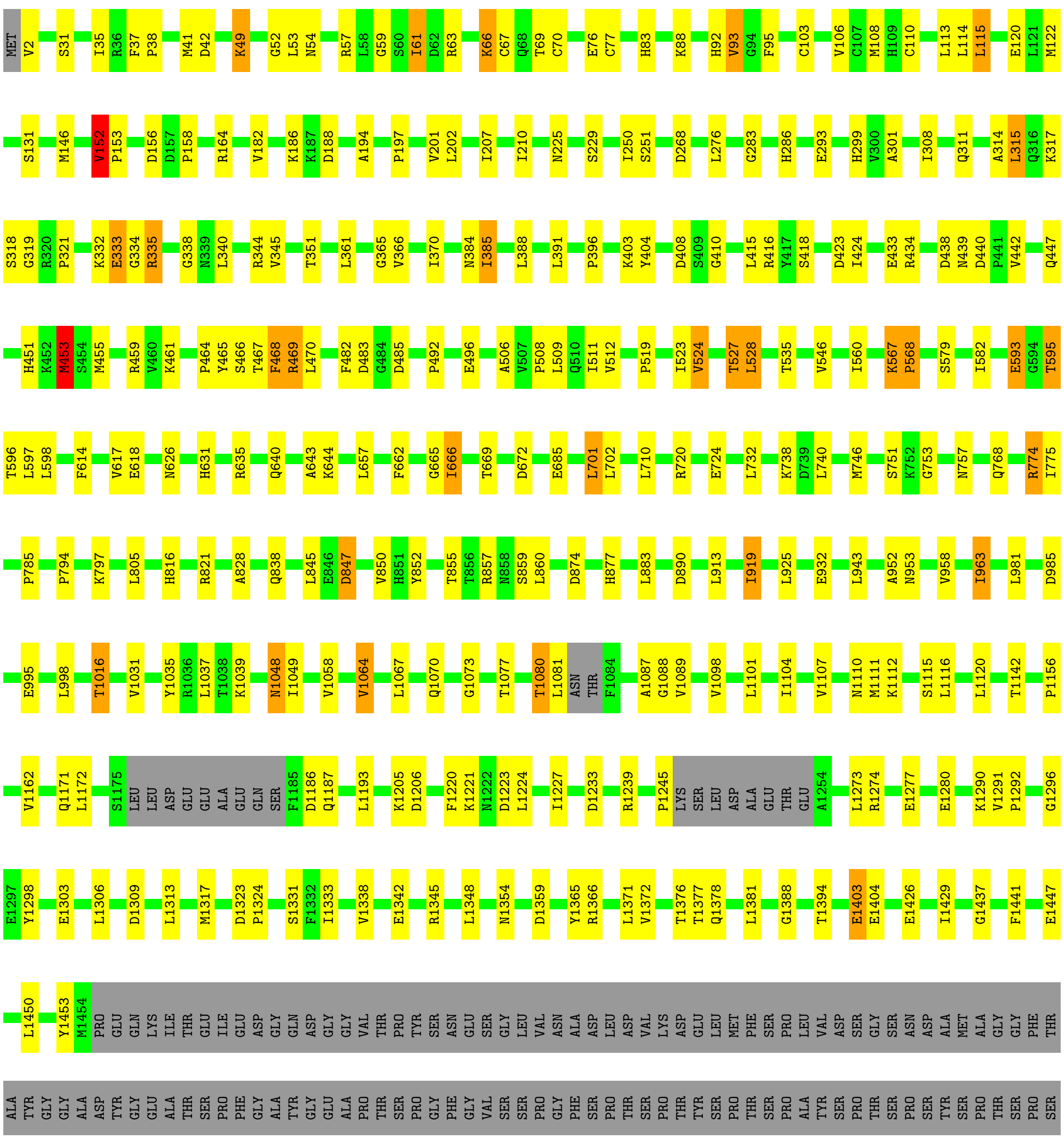
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
15	U	27	549	261	102	159	27	0	0	0

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. 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.

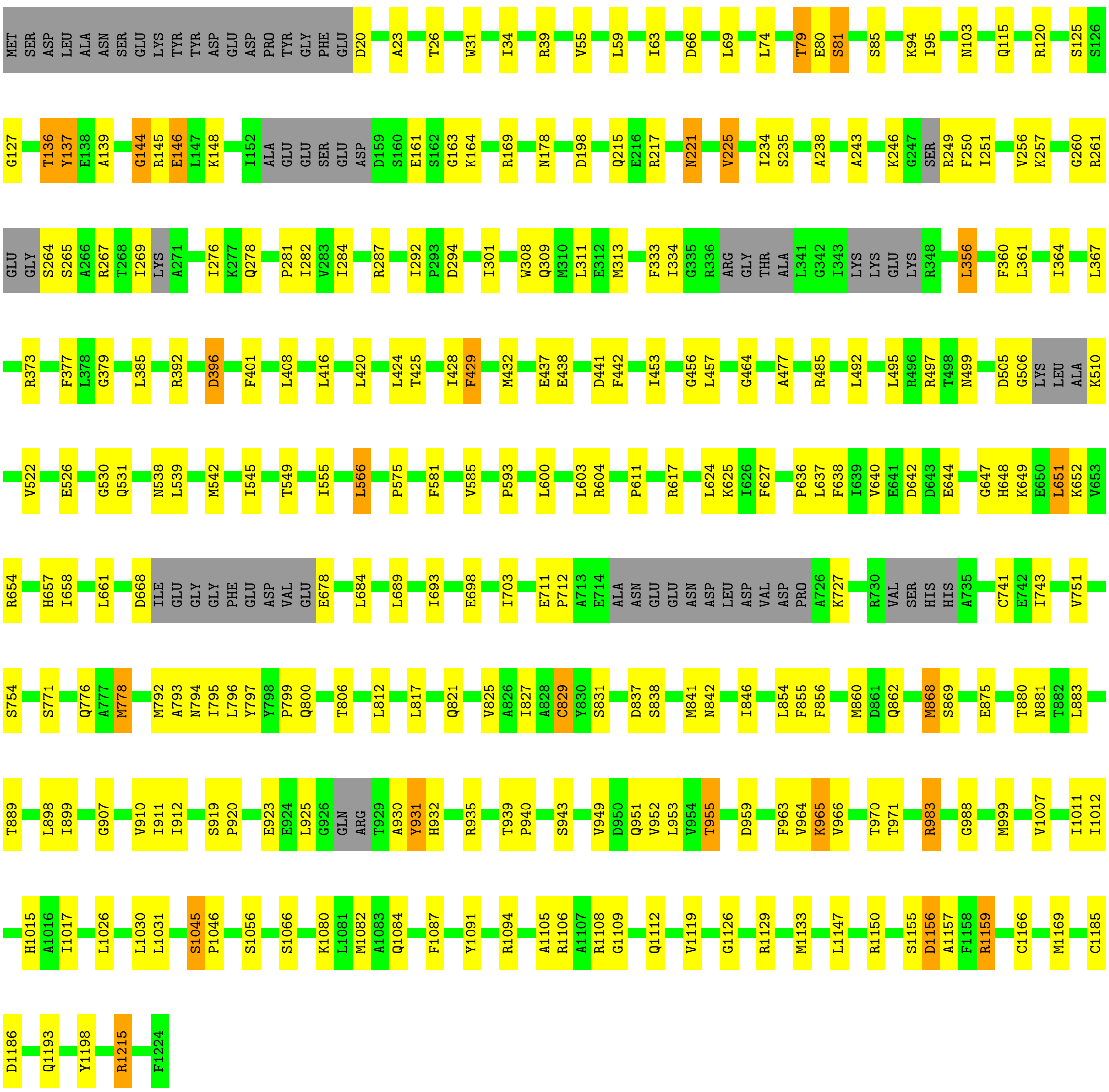
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1

Chain A:



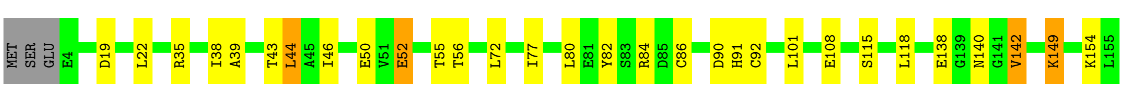
- Molecule 2: DNA-directed RNA polymerase II subunit RPB2

Chain B:



- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:



T156 A159 K160 K161 A164 P172 A173 A174 A175 I176 L186 K187 H188 T189 D190 Y191 Q203 E215 A223 V232 V235 D241 Q242 V243 V244 V245 I248 I258 L259 L262 Q267 D268 LYS VAL ASN PHE ALA SER GLY ASP ASN ASN THR ALA SER ASN

MET LEU GLY SER ASN GLU ASP VAL MET MET THR GLY ALA GLU GLN ASP PRO TYR SER ASN ALA SER GLN MET GLY ASN THR GLY SER GLY GLY TYR ASP ASN ALA TRP

• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

Chain D: 67% 13% • 19%

MET ASN VAL S4 T5 S6 T7 F8 R11 R12 L15 K16 K17 V18 E19 E20 N23 L35 I38 L50 R56 L57 V58 I59 K71 Q74 K75 K76 HIS LYS LYS LYS HIS LEU LYS HIS GLU ASN ALA ASN ASP GLU THR THR ALA VAL GLU ASP GLU ASP ASP

ASP LEU ASP GLU ASP ASP VAL ASN ALA ASP ASP ASP ASP PHE MET HIS SER E117 T149 K168 S169 V177 T187 L198 N199 I202 L207 E208 L211 L214 E218 Y221

• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 86% 13% •

MET D2 Q3 R14 V23 Y28 L37 P38 L39 E40 D41 P64 L78 G89 T92 I100 N104 F105 N115 I116 T117 V124 I132 V142 N143 I144 D159 E160 K161 L165 E172 L175 L190 I198 C214 M215

• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 43% 14% 44%

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

HIS GLU GLN ILE ARG ARG LYS THR L69 K72 A73 I74 Q78 T81 Y84 M85 T86 E89 R97 A98 L99 Q100 P117 I120 K129 I130 P131 L132 E144 V148 L151 I152 L155

• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G: 79% 16% • •

M1 L13 H14 P15 S16 F17 T39 F42 L46 L49 R60 P63 T64 V77 F82 E85 S93 E100 V108 T120 E134 I137 S141 R142 I143 I147 Q153 V154 A159 E165 D166 Y167 L168 I171 LEU GLU HIS HIS

HIS HIS HIS HIS

• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 79% 14% 8%

M1 S2 F6 V15 D16 P17 I26 K37 D53 N64 LEU GLU ASP THR PRO ALA ASN ASP SER SER A75 S78 Q83 V96 A101 S108 F118 L121 L122 E126 Y129 R130 L135 LYS Q137 E138 R146

• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I: 86% 8% • 5%

MET T2 N11 N12 P16 L25 P41 I52 E82 C103 L104 S105 C106 K115 ASN LYS ARG THR GLN

• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 71% 20% • 7%

M1 I2 V3 R6 C7 F8 S9 C10 V14 G15 D16 K17 R43 Y44 C45 C46 M49 N64 P65 LEU GLU LYS ARG ASP

• Molecule 11: DNA-directed RNA polymerase II subunit RPB11

Chain K: 78% 17% • •

M1 P4 F7 L11 L12 L19 K20 T34 F35 T41 R47 A48 E49 F58 Y61 R70 L73 R74 I75 L87 C91 I94 W109 A115 ALA ASP ASP ALA PHE

• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L: 43% 19% • 37%

MET SER ARG GLU GLY PHE GLN ILE PRO THR ASN LEU ASP ALA ALA ALA ALA GLY THR SER GLN ALA ARG THR ALA THR L27 I30 E33 K37 L38 S39 L40 T43 D44 A45 C48 I55 L56 L57 K58 A59 L64 R70

• Molecule 13: Synthetic RNA

Chain R: 56% 22% 22%

U2 C3 G6 G9 A10

• Molecule 14: Synthetic DNA

Chain S: 6% 17% • 75%

DC DG DC DT DT DG DT DA DT DA DT DA DA DA DG DA DG DT DC DC DG DT DG DG DA DA DG DC DT DC DT DC DC DT DA DG DC DA DG T27 G28 C29 T30 T31 A32 T33 C34 G35 G36 T37 A38 G39 DG

• Molecule 15: Synthetic DNA

Chain U: 13% 19% 17% • 49%

DC C2 T3 A4 C5 C6 G7 A8 T9 A10 A11 G12 C13 A14 G15 A16 C17 G18 A19 T20 C21 G27 A28 DA DC DC DA DC DG DG DA DC DT DC DT DT DT DA DT DA DT DA DC DA DA DG DC DG

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	220.22Å 391.84Å 282.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.00 – 3.95 90.88 – 3.95	Depositor EDS
% Data completeness (in resolution range)	94.3 (79.00-3.95) 94.6 (90.88-3.95)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	0.23	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 4.01Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.215 , 0.236 0.271 , 0.292	Depositor DCC
R_{free} test set	3013 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å^2)	114.2	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 214.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.32$, $< L^2 > = 0.15$	Xtriage
Estimated twinning fraction	0.178 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.186 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	32540	wwPDB-VP
Average B, all atoms (Å^2)	197.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.41	0/11452	0.64	0/15492
2	B	0.41	1/9347 (0.0%)	0.63	6/12601 (0.0%)
3	C	0.40	0/2124	0.60	0/2879
4	D	0.40	0/1427	0.59	0/1911
5	E	0.38	0/1788	0.57	0/2406
6	F	0.40	0/717	0.63	0/967
7	G	0.39	0/1367	0.62	0/1844
8	H	0.37	0/1097	0.57	0/1484
9	I	0.38	0/939	0.59	0/1266
10	J	0.38	0/541	0.58	0/727
11	K	0.37	0/942	0.56	0/1272
12	L	0.40	0/348	0.64	0/461
13	R	0.82	0/221	0.90	1/343 (0.3%)
14	S	3.47	54/299 (18.1%)	1.36	1/460 (0.2%)
15	U	2.78	61/615 (9.9%)	1.12	0/945
All	All	0.64	116/33224 (0.3%)	0.65	8/45058 (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
14	S	0	1
15	U	0	1
All	All	0	2

The worst 5 of 116 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	U	4	DA	N3-C4	12.86	1.42	1.34
15	U	14	DA	N3-C4	12.21	1.42	1.34
15	U	11	DA	N3-C4	11.55	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	S	27	DT	P-O5'	11.27	1.71	1.59
15	U	11	DA	N9-C4	11.21	1.44	1.37

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	260	GLY	O-C-N	-8.44	109.19	122.70
2	B	260	GLY	CA-C-N	5.98	130.37	117.20
13	R	2	U	P-O3'-C3'	-5.93	112.58	119.70
2	B	79	THR	C-N-CA	5.90	136.46	121.70
14	S	27	DT	O4'-C1'-N1	5.64	111.95	108.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	S	32	DA	Sidechain
15	U	8	DA	Sidechain

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	A	11249	0	11277	114	0
2	B	9175	0	9138	123	0
3	C	2086	0	2049	25	0
4	D	1417	0	1428	9	0
5	E	1752	0	1776	11	0
6	F	705	0	731	13	0
7	G	1339	0	1357	12	0
8	H	1080	0	1049	9	0
9	I	921	0	877	9	0
10	J	532	0	546	5	0
11	K	924	0	934	11	0
12	L	346	0	367	3	0
13	R	197	0	97	4	0
14	S	268	0	149	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	U	549	0	303	33	0
All	All	32540	0	32078	342	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.

The worst 5 of 342 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)
14:S:38:DA:N6	15:U:2:DC:N4	2.15	0.93
14:S:38:DA:N6	15:U:2:DC:C4	2.43	0.86
1:A:567:LYS:HB3	1:A:568:PRO:CD	2.07	0.85
1:A:67:CYS:HG	1:A:77:CYS:HG	1.12	0.85
14:S:38:DA:H62	15:U:2:DC:N4	1.74	0.83

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 X-ray entries followed by that with respect to entries of similar resolution.

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	1426/1733 (82%)	1227 (86%)	135 (10%)	64 (4%)	2	24
2	B	1134/1224 (93%)	967 (85%)	121 (11%)	46 (4%)	3	25
3	C	263/318 (83%)	228 (87%)	26 (10%)	9 (3%)	3	30
4	D	174/221 (79%)	152 (87%)	12 (7%)	10 (6%)	1	19
5	E	212/215 (99%)	198 (93%)	10 (5%)	4 (2%)	8	40
6	F	85/155 (55%)	79 (93%)	3 (4%)	3 (4%)	3	29
7	G	169/179 (94%)	143 (85%)	21 (12%)	5 (3%)	4	32
8	H	129/146 (88%)	111 (86%)	14 (11%)	4 (3%)	4	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	112/120 (93%)	98 (88%)	13 (12%)	1 (1%)	17	54
10	J	63/70 (90%)	56 (89%)	3 (5%)	4 (6%)	1	18
11	K	113/120 (94%)	110 (97%)	3 (3%)	0	100	100
12	L	42/70 (60%)	31 (74%)	8 (19%)	3 (7%)	1	16
All	All	3922/4571 (86%)	3400 (87%)	369 (9%)	153 (4%)	3	26

5 of 153 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	LYS
1	A	66	LYS
1	A	319	GLY
1	A	385	ILE
1	A	567	LYS

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	1244/1520 (82%)	1156 (93%)	88 (7%)	14	42
2	B	996/1061 (94%)	938 (94%)	58 (6%)	20	48
3	C	233/274 (85%)	219 (94%)	14 (6%)	19	47
4	D	156/200 (78%)	147 (94%)	9 (6%)	20	48
5	E	196/197 (100%)	186 (95%)	10 (5%)	24	51
6	F	77/137 (56%)	77 (100%)	0	100	100
7	G	152/160 (95%)	145 (95%)	7 (5%)	27	54
8	H	118/128 (92%)	117 (99%)	1 (1%)	81	88
9	I	107/114 (94%)	105 (98%)	2 (2%)	57	75
10	J	60/65 (92%)	57 (95%)	3 (5%)	24	52
11	K	99/102 (97%)	93 (94%)	6 (6%)	18	47
12	L	38/57 (67%)	32 (84%)	6 (16%)	2	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3476/4015 (87%)	3272 (94%)	204 (6%)	19	47

5 of 204 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	624	LEU
2	B	1159	ARG
12	L	33	GLU
2	B	698	GLU
2	B	931	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	9	GLN
9	I	11	ASN
9	I	89	GLN
9	I	46	HIS
1	A	1171	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	R	7/9 (77%)	2 (28%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	R	3	C
13	R	6	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.