



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 08:55 PM GMT

PDB ID : 4XSZ
Title : Crystal structure of CBR 9393 bound to Escherichia coli RNA polymerase holoenzyme
Authors : Bae, B.; Darst, S.A.
Deposited on : 2015-01-22
Resolution : 3.68 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

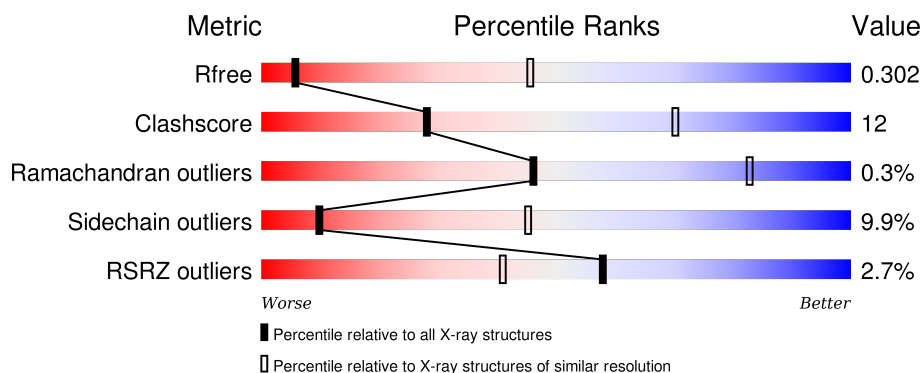
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.68 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}	91344	1033 (3.86-3.50)
Clashscore	102246	1148 (3.86-3.50)
Ramachandran outliers	100387	1100 (3.86-3.50)
Sidechain outliers	100360	1098 (3.86-3.50)
RSRZ outliers	91569	1040 (3.86-3.50)

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 on the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	239	<div> <div>2%</div> <div>64%</div> <div>26%</div> <div>6%</div> </div>
1	B	239	<div> <div>3%</div> <div>63%</div> <div>26%</div> <div>8%</div> </div>
1	G	239	<div> <div>3%</div> <div>67%</div> <div>24%</div> <div>5%</div> </div>
1	H	239	<div> <div>7%</div> <div>61%</div> <div>27%</div> <div>9%</div> </div>
2	C	1342	<div> <div>0%</div> <div>66%</div> <div>30%</div> <div>0%</div> </div>

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Mol	Chain	Length	Quality of chain
2	I	1342	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>67%</div><div>30%</div><div></div></div><div></div></div>
3	D	1407	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>55%</div><div>24%</div><div></div><div>17%</div></div><div></div></div>
3	J	1407	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>58%</div><div>26%</div><div></div><div>12%</div></div><div></div></div>
4	E	91	<div><div><div></div><div></div><div></div></div><div><div></div><div>74%</div><div>21%</div><div></div></div><div></div></div>
4	K	91	<div><div><div></div><div></div><div></div></div><div><div></div><div>65%</div><div>18%</div><div></div><div>13%</div></div><div></div></div>
5	F	522	<div><div><div></div><div></div><div></div></div><div><div>5%</div><div>62%</div><div>24%</div><div></div><div>10%</div></div><div></div></div>
5	L	522	<div><div><div></div><div></div><div></div></div><div><div>5%</div><div>63%</div><div>23%</div><div></div><div>10%</div></div><div></div></div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 55744 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 subunit alpha,DNA-directed RNA polymerase subunit alpha,DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1730	1076	308	340	6			
1	B	220	Total	C	N	O	S	0	0	0
			1687	1053	298	330	6			
1	G	228	Total	C	N	O	S	0	0	0
			1750	1088	312	344	6			
1	H	217	Total	C	N	O	S	0	0	0
			1667	1041	293	327	6			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	235	GLU	-	linker	UNP A7ZSI4
A	236	VAL	-	linker	UNP A7ZSI4
A	237	LEU	-	linker	UNP A7ZSI4
A	238	PHE	-	linker	UNP A7ZSI4
A	239	GLN	-	linker	UNP A7ZSI4
B	235	GLU	-	linker	UNP A7ZSI4
B	236	VAL	-	linker	UNP A7ZSI4
B	237	LEU	-	linker	UNP A7ZSI4
B	238	PHE	-	linker	UNP A7ZSI4
B	239	GLN	-	linker	UNP A7ZSI4
G	235	GLU	-	linker	UNP A7ZSI4
G	236	VAL	-	linker	UNP A7ZSI4
G	237	LEU	-	linker	UNP A7ZSI4
G	238	PHE	-	linker	UNP A7ZSI4
G	239	GLN	-	linker	UNP A7ZSI4
H	235	GLU	-	linker	UNP A7ZSI4
H	236	VAL	-	linker	UNP A7ZSI4
H	237	LEU	-	linker	UNP A7ZSI4
H	238	PHE	-	linker	UNP A7ZSI4
H	239	GLN	-	linker	UNP A7ZSI4

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0	0
			10570	6631	1841	2055	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10566	6629	1840	2054	43			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1166	Total	C	N	O	S	0	0	0
			9107	5723	1634	1704	46			
3	J	1236	Total	C	N	O	S	0	0	0
			9638	6058	1726	1807	47			

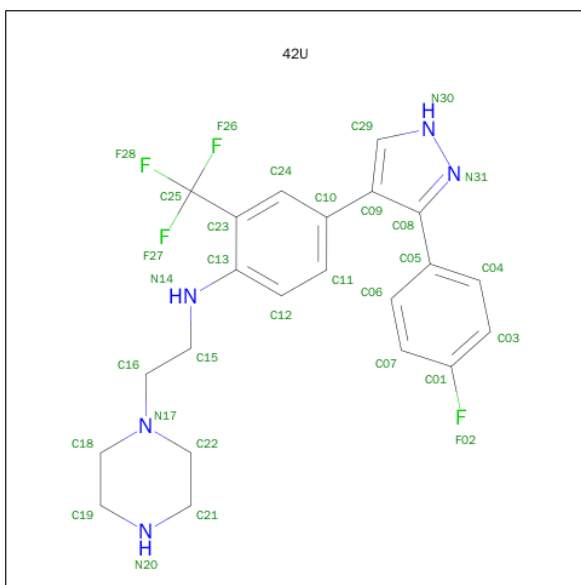
- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	89	Total	C	N	O	S	0	0	0
			691	421	129	140	1			
4	K	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	470	Total	C	N	O	S	0	0	0
			3822	2394	680	725	23			
5	L	469	Total	C	N	O	S	0	0	0
			3821	2393	679	726	23			

- Molecule 6 is 4-[3-(4-fluorophenyl)-1H-pyrazol-4-yl]-N-[2-(piperazin-1-yl)ethyl]-2-(trifluoromethyl)aniline (three-letter code: 42U) (formula: C₂₂H₂₃F₄N₅).



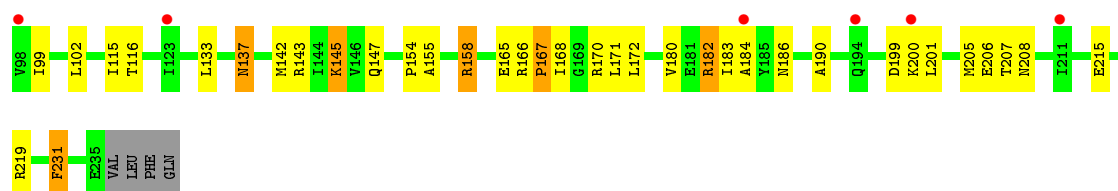
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	F	N	0	0
			31	22	4	5		
6	I	1	Total	C	F	N	0	0
			31	22	4	5		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

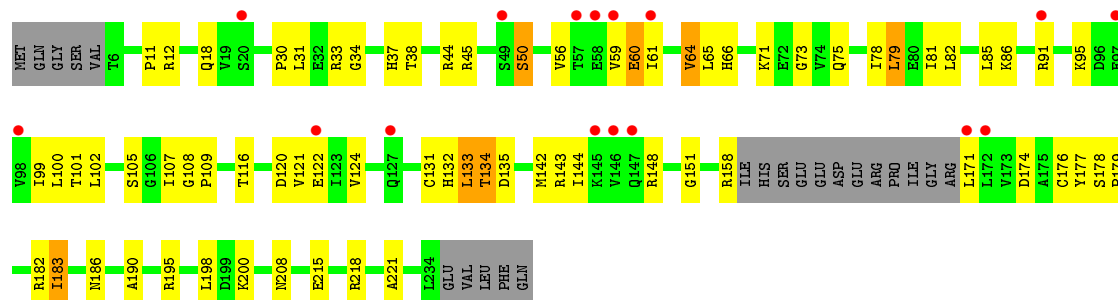
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	J	1	Total	Mg	0	0
			1	1		
7	D	1	Total	Mg	0	0
			1	1		

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

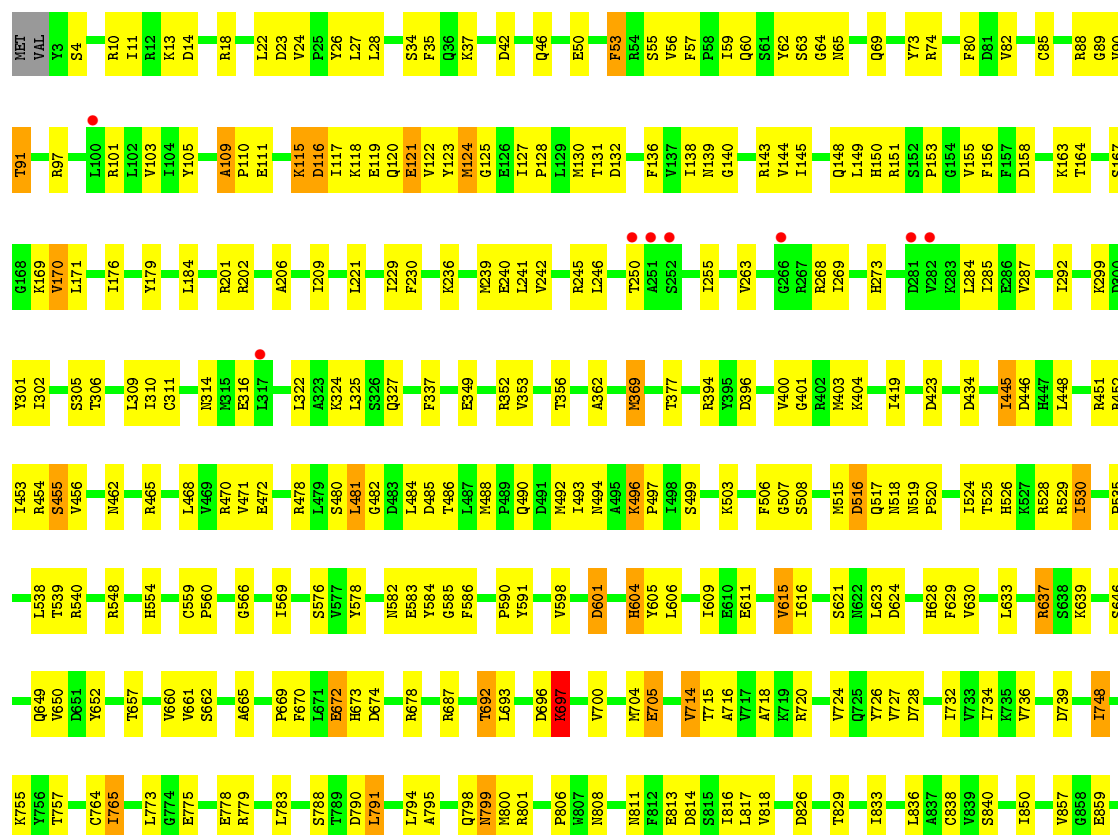
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	J	2	Total	Zn	0	0
			2	2		
8	D	2	Total	Zn	0	0
			2	2		

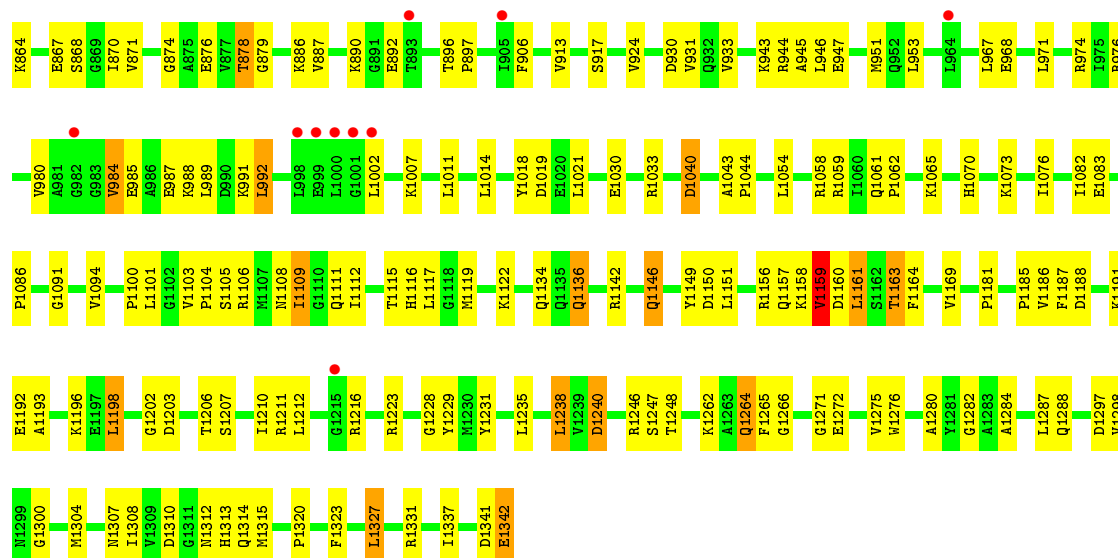


- Molecule 1: DNA-directed RNA polymerase subunit alpha,DNA-directed RNA polymerase subunit alpha,DNA-directed RNA polymerase subunit alpha

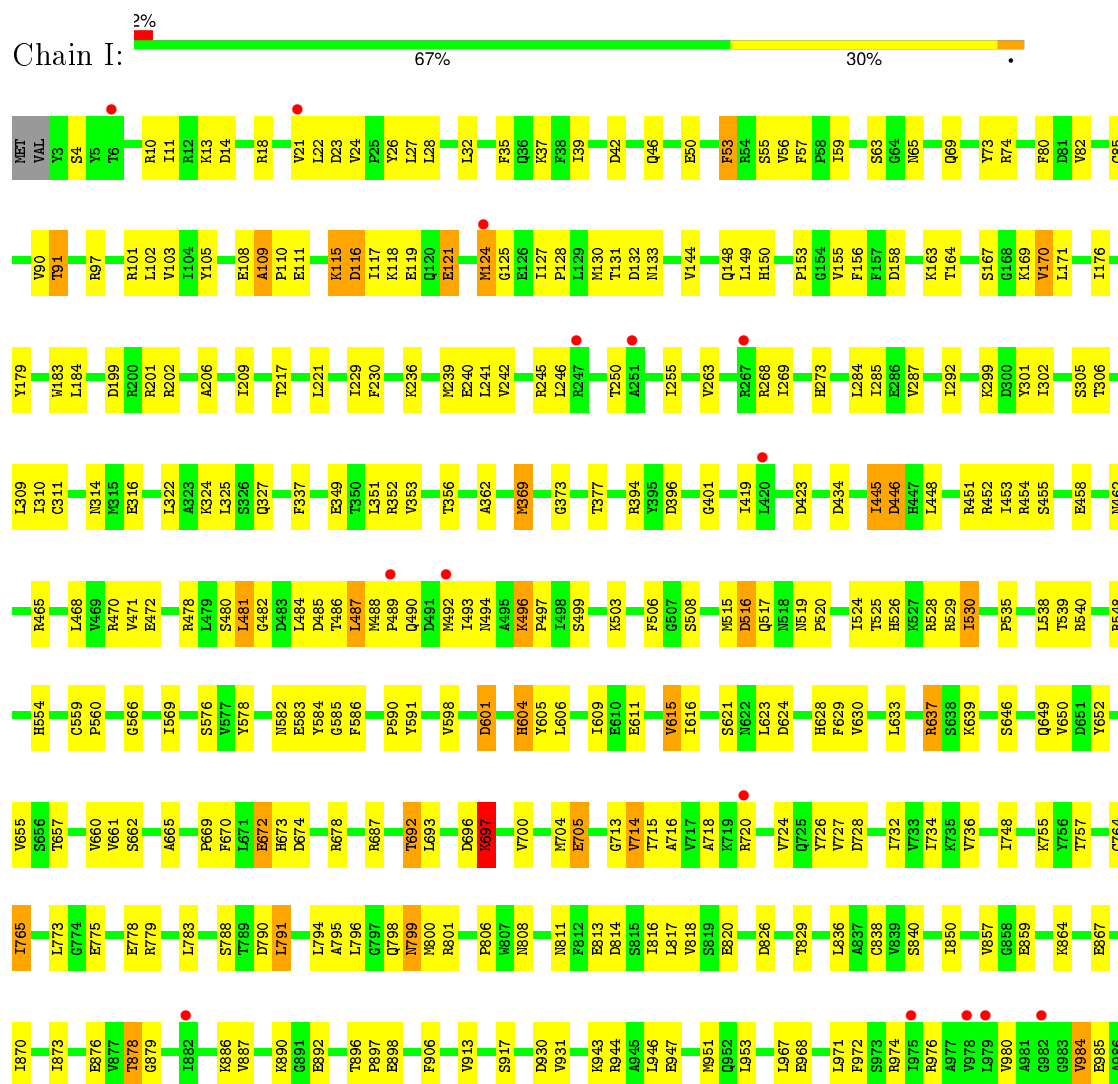


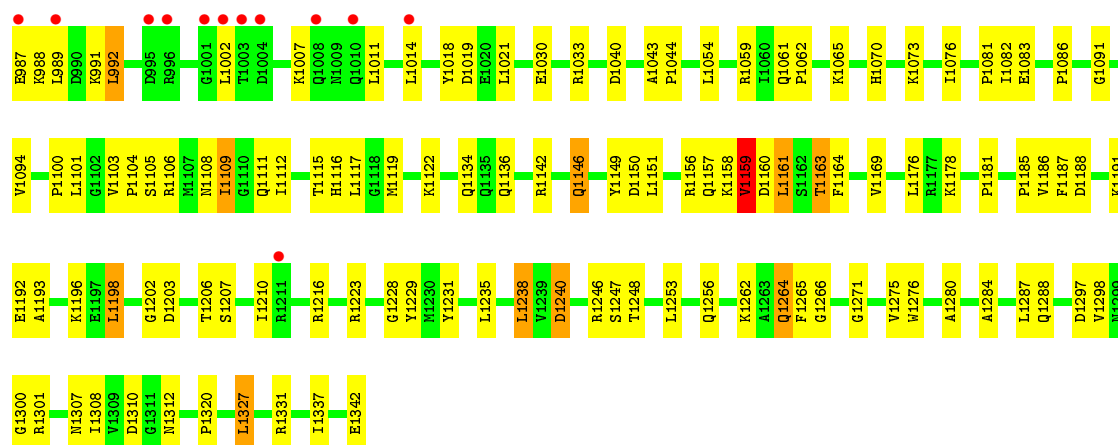
- Molecule 2: DNA-directed RNA polymerase subunit beta



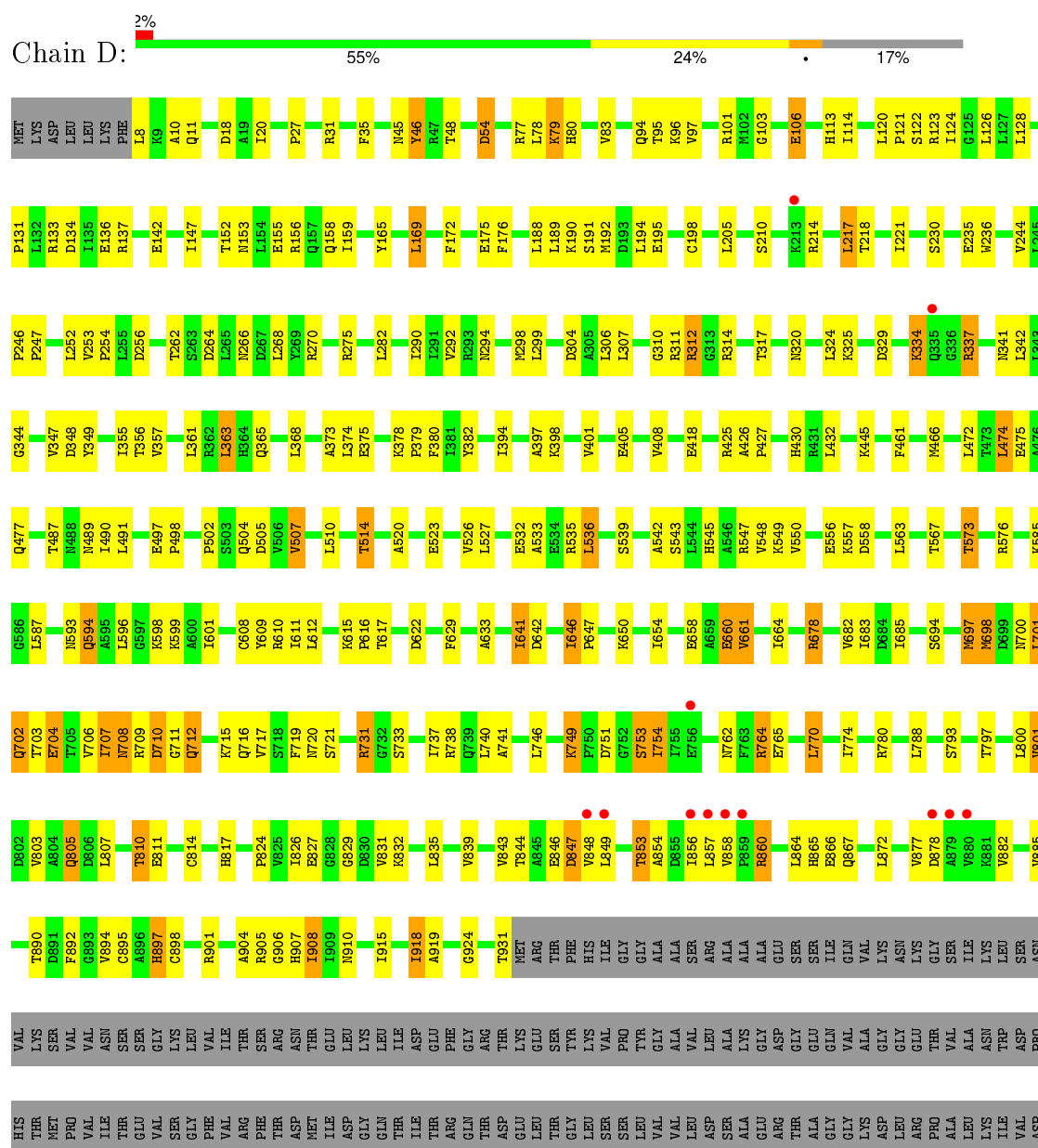


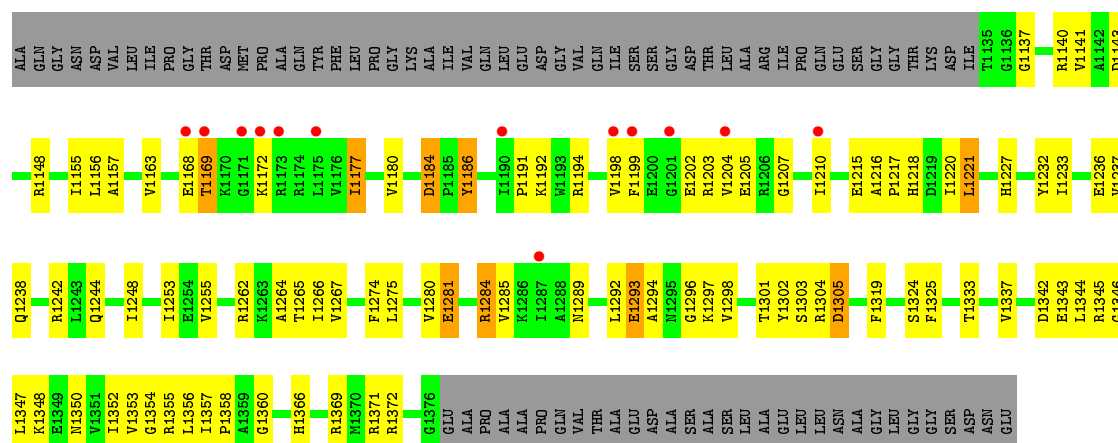
• Molecule 2: DNA-directed RNA polymerase subunit beta



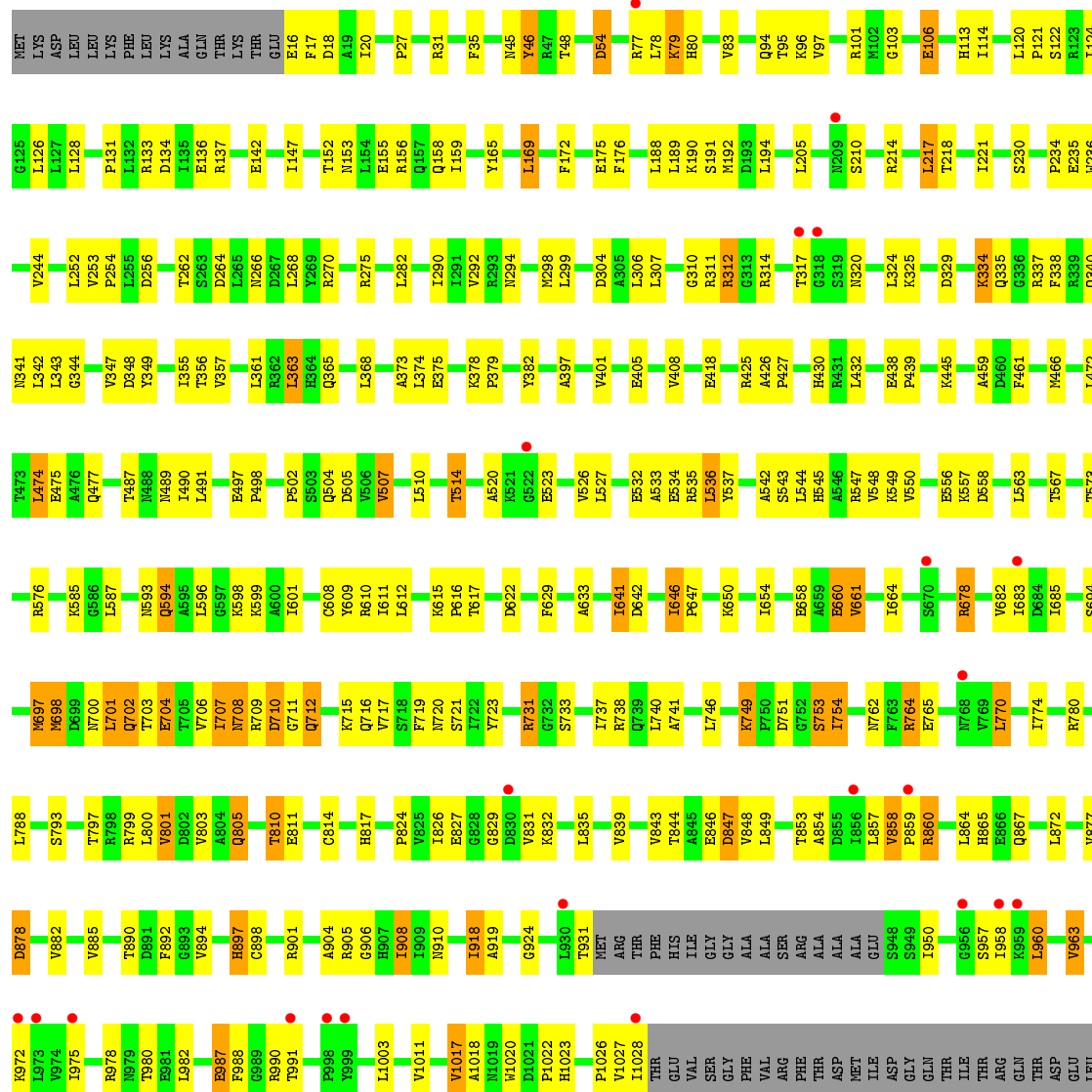


• Molecule 3: DNA-directed RNA polymerase subunit beta'





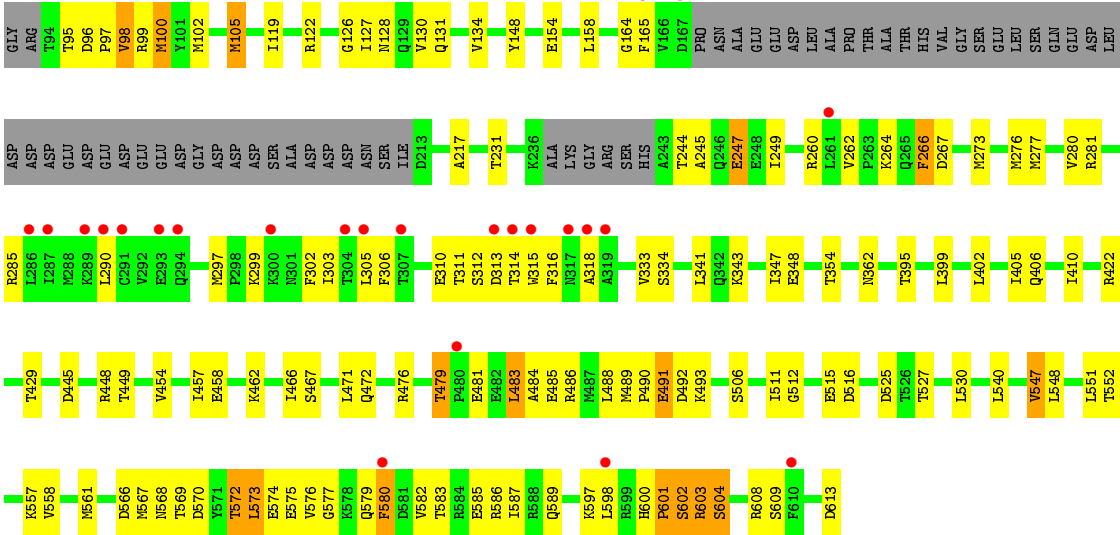
• Molecule 3: DNA-directed RNA polymerase subunit beta'







● Molecule 5: RNA polymerase sigma factor RpoD



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	184.44Å 206.33Å 309.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.93 – 3.68 39.93 – 3.68	Depositor EDS
% Data completeness (in resolution range)	88.5 (39.93-3.68) 88.5 (39.93-3.68)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.66Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.240 , 0.286 0.263 , 0.302	Depositor DCC
R_{free} test set	5687 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	139.9	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 46.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 113219 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	55744	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 42U, 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 > 5$	RMSZ	# $ Z > 5$
1	A	0.25	0/1751	0.54	0/2373
1	B	0.27	0/1707	0.53	0/2314
1	G	0.26	0/1771	0.56	0/2401
1	H	0.27	0/1686	0.51	0/2285
2	C	0.27	0/10739	0.52	0/14489
2	I	0.27	0/10735	0.51	0/14484
3	D	0.26	0/9246	0.51	0/12478
3	J	0.26	0/9785	0.51	0/13206
4	E	0.27	0/693	0.52	0/935
4	K	0.28	0/629	0.51	0/847
5	F	0.29	0/3873	0.51	1/5206 (0.0%)
5	L	0.29	0/3872	0.51	1/5205 (0.0%)
All	All	0.27	0/56487	0.52	2/76223 (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
2	C	0	3
2	I	0	3
3	D	0	3
3	J	0	3
5	F	0	1
5	L	0	1
All	All	0	14

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	602	SER	N-CA-C	-6.49	93.48	111.00
5	L	602	SER	N-CA-C	-6.47	93.53	111.00

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	109	ALA	Peptide
2	C	1161	LEU	Peptide
2	C	236	LYS	Peptide
3	D	1168	GLU	Peptide
3	D	1184	ASP	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.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1730	0	1756	49	0
1	B	1687	0	1700	47	0
1	G	1750	0	1764	45	0
1	H	1667	0	1689	55	0
2	C	10570	0	10582	277	0
2	I	10566	0	10576	256	0
3	D	9107	0	9309	251	0
3	J	9638	0	9853	261	0
4	E	691	0	695	19	0
4	K	627	0	634	10	0
5	F	3822	0	3885	91	0
5	L	3821	0	3884	81	0
6	C	31	0	23	0	0
6	I	31	0	23	0	0
7	D	1	0	0	0	0
7	J	1	0	0	0	0
8	D	2	0	0	0	0
8	J	2	0	0	0	0
All	All	55744	0	56373	1308	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 12.

The worst 5 of 1308 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:D:660:GLU:HB3	3:D:685:ILE:HD12	1.50	0.94
3:J:660:GLU:HB3	3:J:685:ILE:HD12	1.51	0.93
1:G:45:ARG:NH1	1:H:34:GLY:O	2.11	0.83
3:D:1372:ARG:HH21	3:J:854:ALA:HB3	1.42	0.83
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.62	0.81

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	222/239 (93%)	194 (87%)	26 (12%)	2 (1%)	21	68
1	B	216/239 (90%)	192 (89%)	24 (11%)	0	100	100
1	G	226/239 (95%)	196 (87%)	28 (12%)	2 (1%)	21	68
1	H	213/239 (89%)	190 (89%)	23 (11%)	0	100	100
2	C	1338/1342 (100%)	1231 (92%)	102 (8%)	5 (0%)	39	80
2	I	1338/1342 (100%)	1230 (92%)	103 (8%)	5 (0%)	39	80
3	D	1162/1407 (83%)	1077 (93%)	81 (7%)	4 (0%)	46	83
3	J	1230/1407 (87%)	1145 (93%)	81 (7%)	4 (0%)	46	83
4	E	87/91 (96%)	82 (94%)	5 (6%)	0	100	100
4	K	77/91 (85%)	74 (96%)	3 (4%)	0	100	100
5	F	464/522 (89%)	429 (92%)	35 (8%)	0	100	100
5	L	463/522 (89%)	427 (92%)	36 (8%)	0	100	100
All	All	7036/7680 (92%)	6467 (92%)	547 (8%)	22 (0%)	46	83

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	1159	VAL
2	I	1159	VAL
2	C	170	VAL
2	I	170	VAL
3	J	340	GLN

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 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	191/206 (93%)	174 (91%)	17 (9%)	12	51
1	B	184/206 (89%)	165 (90%)	19 (10%)	9	43
1	G	191/206 (93%)	174 (91%)	17 (9%)	12	51
1	H	183/206 (89%)	165 (90%)	18 (10%)	10	46
2	C	1155/1157 (100%)	1043 (90%)	112 (10%)	10	46
2	I	1154/1157 (100%)	1040 (90%)	114 (10%)	10	45
3	D	975/1168 (84%)	874 (90%)	101 (10%)	9	43
3	J	1036/1168 (89%)	929 (90%)	107 (10%)	9	43
4	E	72/75 (96%)	66 (92%)	6 (8%)	14	54
4	K	67/75 (89%)	60 (90%)	7 (10%)	9	43
5	F	417/462 (90%)	377 (90%)	40 (10%)	10	47
5	L	418/462 (90%)	376 (90%)	42 (10%)	9	44
All	All	6043/6548 (92%)	5443 (90%)	600 (10%)	10	45

5 of 600 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	448	ARG
2	I	82	VAL
4	K	28	ARG
5	F	489	MET

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Mol	Chain	Res	Type
1	G	145	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	518	HIS
2	I	628	HIS
5	L	362	ASN
5	F	600	HIS
2	I	69	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	42U	C	1401	-	33,34,34	1.66	7 (21%)	40,48,48	3.10	17 (42%)
6	42U	I	1401	-	33,34,34	1.67	6 (18%)	40,48,48	3.14	18 (45%)

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
6	42U	C	1401	-	-	0/20/28/28	1/4/4/4
6	42U	I	1401	-	-	0/20/28/28	1/4/4/4

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1401	42U	C16-N17	2.02	1.52	1.47
6	C	1401	42U	C09-C10	2.02	1.52	1.49
6	C	1401	42U	C16-C15	2.04	1.57	1.51
6	C	1401	42U	C12-C13	2.10	1.43	1.39
6	I	1401	42U	C16-C15	2.12	1.58	1.51

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	1401	42U	C12-C13-C23	-8.95	110.85	119.91
6	C	1401	42U	C12-C13-C23	-8.72	111.08	119.91
6	I	1401	42U	C05-C08-N31	-6.70	111.37	120.58
6	C	1401	42U	C05-C08-N31	-6.65	111.44	120.58
6	I	1401	42U	C11-C10-C24	-5.89	110.71	118.17

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1401	42U	C18-C19-C21-C22-N17-N20
6	I	1401	42U	C18-C19-C21-C22-N17-N20

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	224/239 (93%)	-0.18	4 (1%) 71 55	54, 87, 128, 162	0
1	B	220/239 (92%)	0.06	8 (3%) 46 30	71, 115, 149, 168	0
1	G	228/239 (95%)	-0.03	7 (3%) 52 35	74, 113, 149, 176	0
1	H	217/239 (90%)	0.23	16 (7%) 17 10	73, 129, 157, 174	0
2	C	1340/1342 (99%)	-0.20	18 (1%) 79 64	29, 79, 134, 171	0
2	I	1340/1342 (99%)	-0.11	27 (2%) 68 52	32, 96, 144, 171	0
3	D	1166/1407 (82%)	-0.13	25 (2%) 67 50	24, 78, 144, 177	0
3	J	1236/1407 (87%)	-0.04	34 (2%) 56 39	33, 95, 148, 172	0
4	E	89/91 (97%)	-0.37	0 100 100	40, 86, 123, 133	0
4	K	79/91 (86%)	-0.27	0 100 100	60, 92, 142, 160	0
5	F	470/522 (90%)	-0.02	27 (5%) 27 16	45, 121, 158, 182	0
5	L	469/522 (89%)	-0.13	24 (5%) 32 19	49, 117, 159, 180	0
All	All	7078/7680 (92%)	-0.10	190 (2%) 58 41	24, 96, 149, 182	0

The worst 5 of 190 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	160	HIS	6.5
3	D	1204	VAL	6.2
1	H	146	VAL	6.0
3	D	1198	VAL	5.4
5	F	167	ASP	5.3

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	42U	C	1401	31/31	0.89	0.33	1.62	31,71,93,105	0
6	42U	I	1401	31/31	0.92	0.33	1.58	48,83,117,134	0
8	ZN	J	1503	1/1	0.98	0.27	0.76	126,126,126,126	0
8	ZN	D	1503	1/1	0.94	0.25	0.30	76,76,76,76	0
8	ZN	J	1502	1/1	0.93	0.16	-0.39	160,160,160,160	0
8	ZN	D	1502	1/1	0.96	0.17	-0.56	176,176,176,176	0
7	MG	J	1501	1/1	0.84	0.61	-	75,75,75,75	0
7	MG	D	1501	1/1	0.93	0.35	-	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.