



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 01:54 pm BST

PDB ID : 4ZH2
Title : Crystal structure of Escherichia coli RNA polymerase in complex with CBR703
Authors : Feng, Y.; Ebright, R.H.
Deposited on : 2015-04-24
Resolution : 4.20 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
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) : 2.11

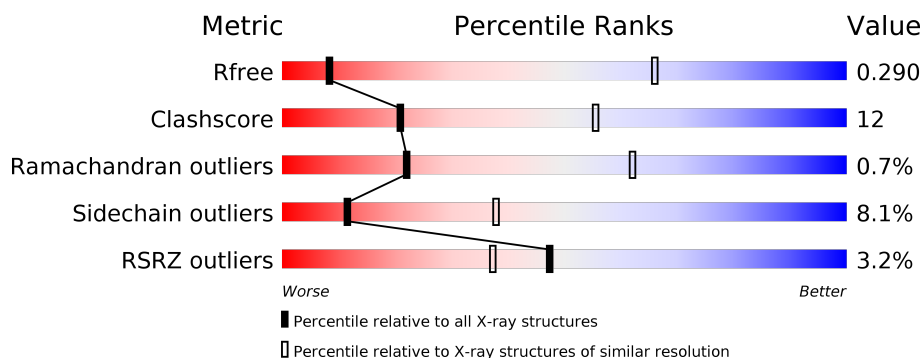
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1005 (4.62-3.78)
Clashscore	141614	1044 (4.60-3.80)
Ramachandran outliers	138981	1000 (4.60-3.80)
Sidechain outliers	138945	1007 (4.62-3.78)
RSRZ outliers	127900	1063 (4.70-3.70)

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 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 $\leq 5\%$. 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	335	<div> <div>2%</div> <div> <div></div> <div>62%</div> <div>25%</div> <div>•</div> <div>10%</div> </div> </div>
1	B	335	<div> <div>2%</div> <div> <div></div> <div>39%</div> <div>24%</div> <div>•</div> <div>36%</div> </div> </div>
1	G	335	<div> <div>0%</div> <div> <div></div> <div>41%</div> <div>24%</div> <div>•</div> <div>33%</div> </div> </div>
1	H	335	<div> <div>2%</div> <div> <div></div> <div>42%</div> <div>20%</div> <div>••</div> <div>36%</div> </div> </div>
2	C	1342	<div> <div>2%</div> <div> <div></div> <div>68%</div> <div>30%</div> <div>•</div> </div> </div>
2	I	1342	<div> <div>4%</div> <div> <div></div> <div>68%</div> <div>30%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	D	1407	
3	J	1407	
4	E	91	
4	K	91	
5	F	613	
5	L	613	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	4OB	C	2001	-	-	X	-
6	4OB	I	2001	-	-	X	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 57763 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	0	0
			2328	1456	413	451	8			
1	B	216	Total	C	N	O	S	0	0	0
			1667	1041	294	326	6			
1	G	224	Total	C	N	O	S	0	0	0
			1730	1076	308	340	6			
1	H	216	Total	C	N	O	S	0	0	0
			1662	1038	292	326	6			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	expression tag	UNP P0A7Z4
A	-4	HIS	-	expression tag	UNP P0A7Z4
A	-3	HIS	-	expression tag	UNP P0A7Z4
A	-2	HIS	-	expression tag	UNP P0A7Z4
A	-1	HIS	-	expression tag	UNP P0A7Z4
A	0	HIS	-	expression tag	UNP P0A7Z4
A	1	HIS	-	expression tag	UNP P0A7Z4
B	-5	MET	-	expression tag	UNP P0A7Z4
B	-4	HIS	-	expression tag	UNP P0A7Z4
B	-3	HIS	-	expression tag	UNP P0A7Z4
B	-2	HIS	-	expression tag	UNP P0A7Z4
B	-1	HIS	-	expression tag	UNP P0A7Z4
B	0	HIS	-	expression tag	UNP P0A7Z4
B	1	HIS	-	expression tag	UNP P0A7Z4
G	-5	MET	-	expression tag	UNP P0A7Z4
G	-4	HIS	-	expression tag	UNP P0A7Z4
G	-3	HIS	-	expression tag	UNP P0A7Z4
G	-2	HIS	-	expression tag	UNP P0A7Z4
G	-1	HIS	-	expression tag	UNP P0A7Z4
G	0	HIS	-	expression tag	UNP P0A7Z4
G	1	HIS	-	expression tag	UNP P0A7Z4

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-5	MET	-	expression tag	UNP P0A7Z4
H	-4	HIS	-	expression tag	UNP P0A7Z4
H	-3	HIS	-	expression tag	UNP P0A7Z4
H	-2	HIS	-	expression tag	UNP P0A7Z4
H	-1	HIS	-	expression tag	UNP P0A7Z4
H	0	HIS	-	expression tag	UNP P0A7Z4
H	1	HIS	-	expression tag	UNP P0A7Z4

- 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	1334	Total	C	N	O	S	0	0	0
			10369	6513	1850	1957	49			

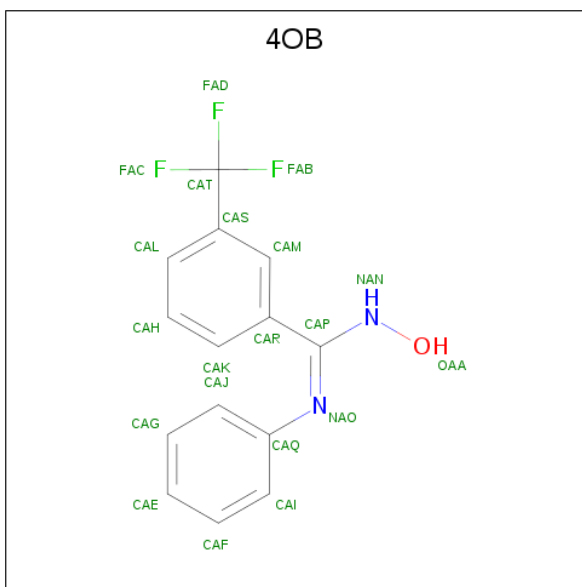
- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

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	542	Total	C	N	O	S	0	0	0
			4204	2625	752	801	26			
5	L	539	Total	C	N	O	S	0	0	0
			4196	2619	749	802	26			

- Molecule 6 is N-hydroxy-N'-phenyl-3-(trifluoromethyl)benzenecarboximidamide (three-letter code: 4OB) (formula: C₁₄H₁₁F₃N₂O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	F	N	O	0	0
			20	14	3	2	1		
6	I	1	Total	C	F	N	O	0	0
			20	14	3	2	1		

- 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		

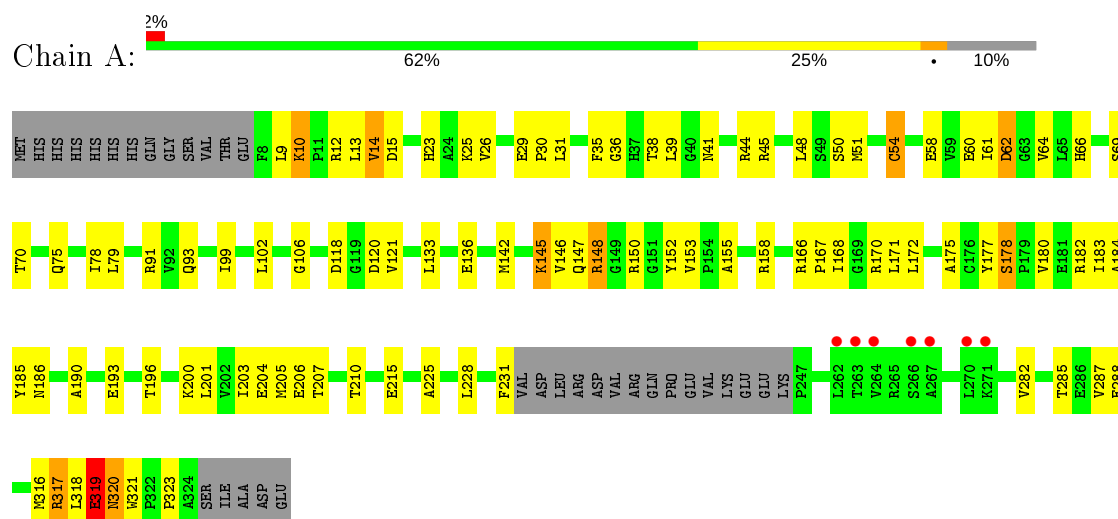
- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

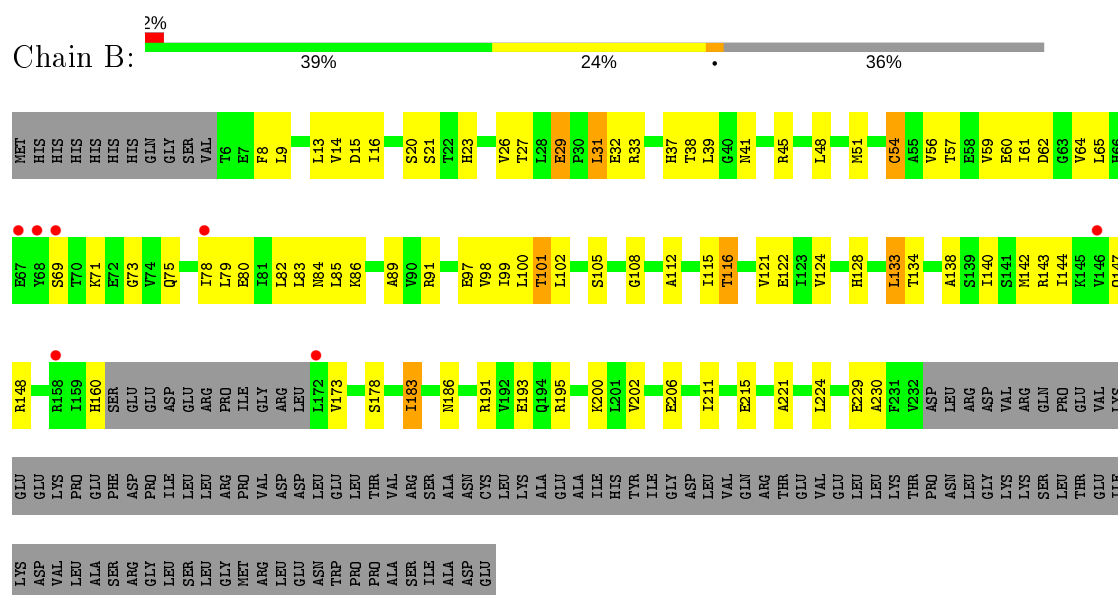
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

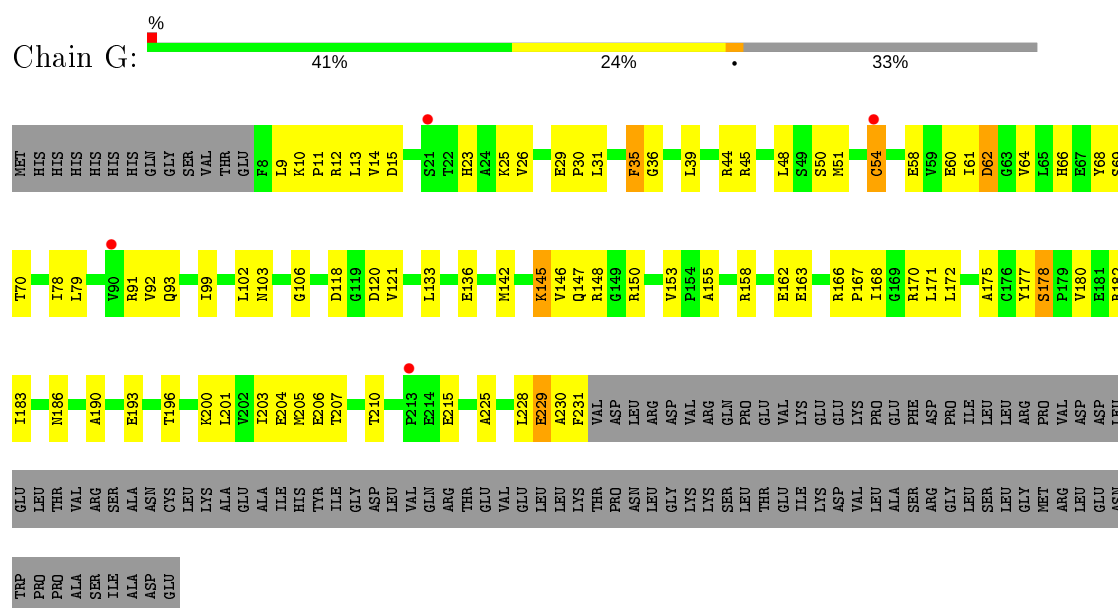
• Molecule 1: DNA-directed RNA polymerase subunit alpha



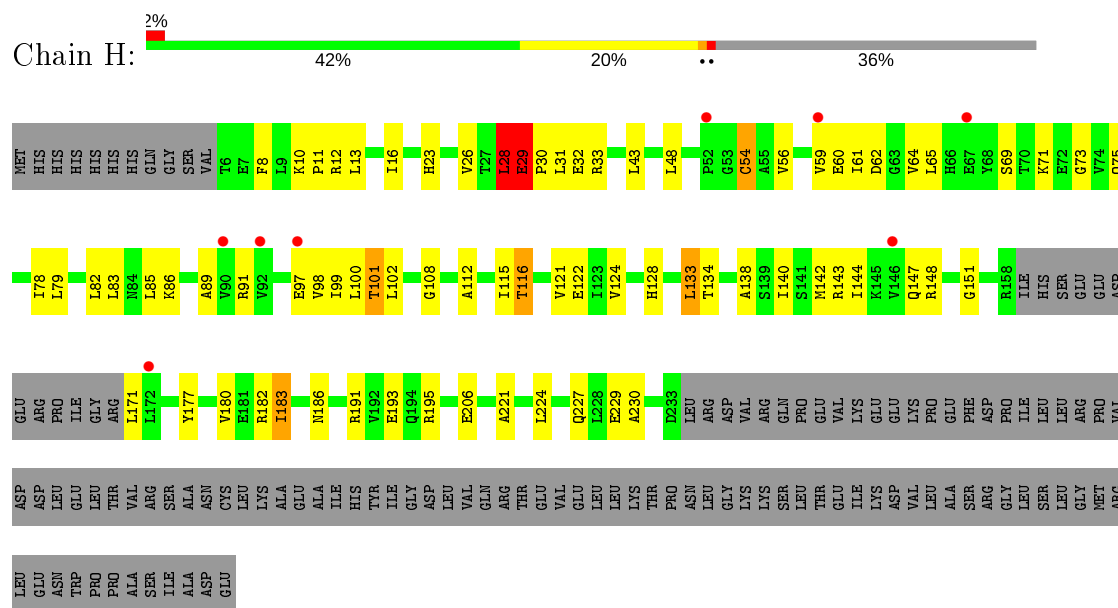
• Molecule 1: DNA-directed RNA polymerase subunit alpha



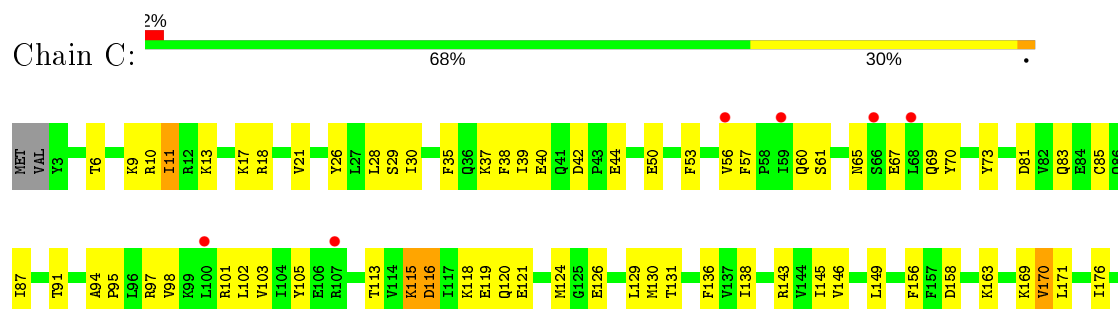
• Molecule 1: DNA-directed RNA polymerase subunit alpha

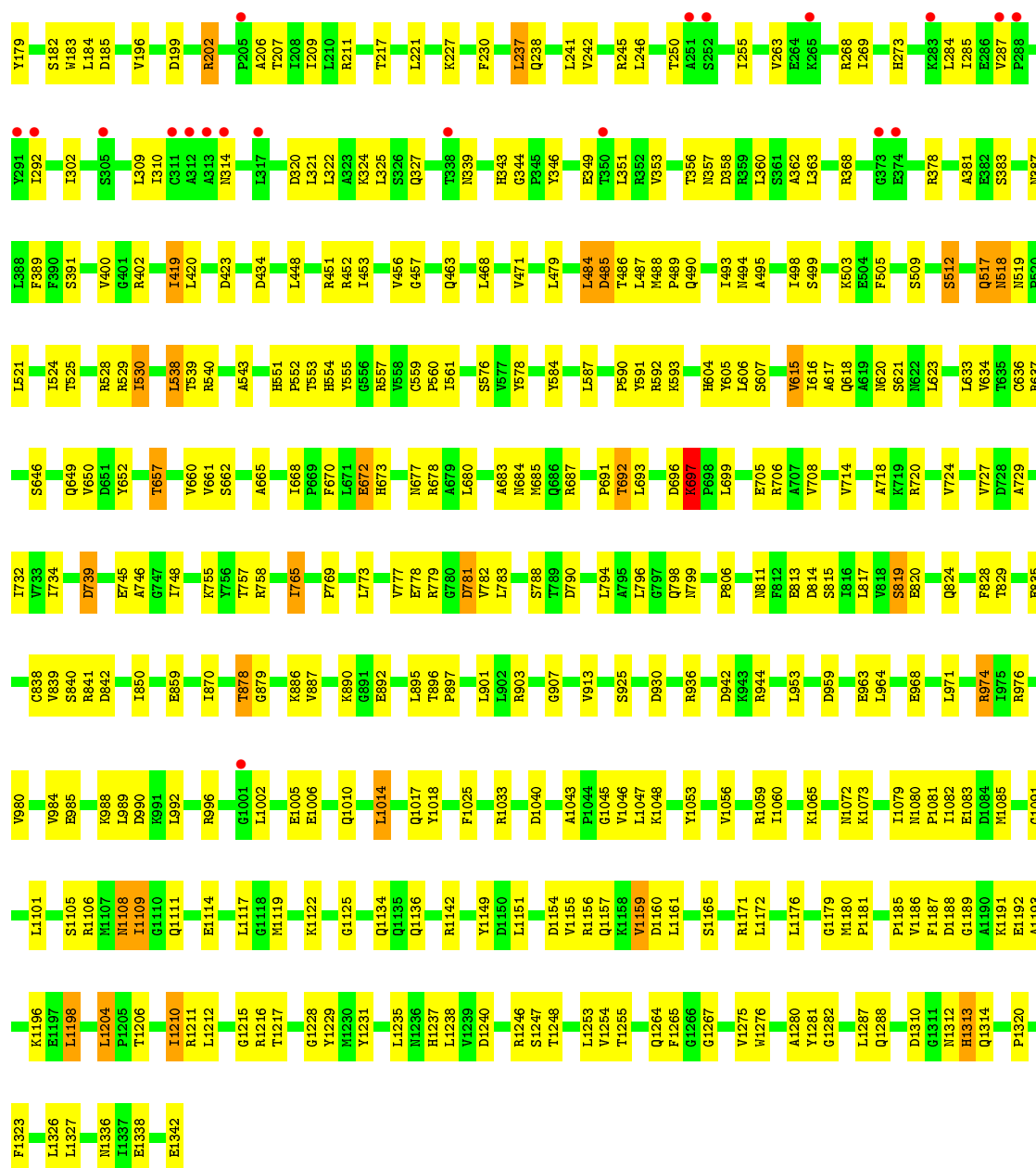


• Molecule 1: DNA-directed RNA polymerase subunit alpha

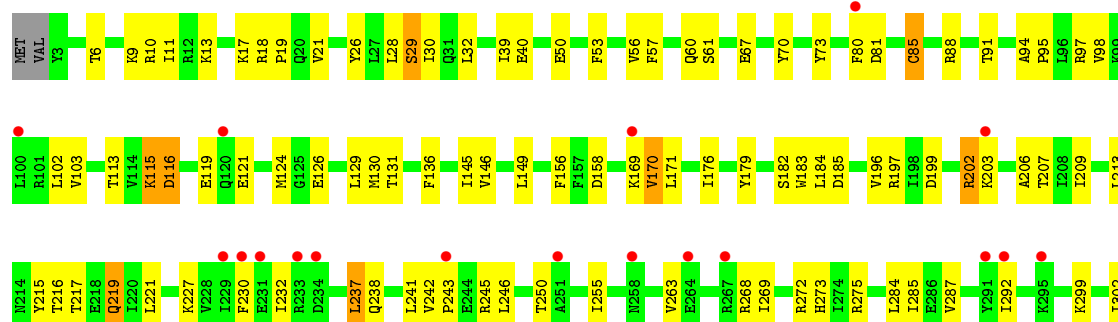


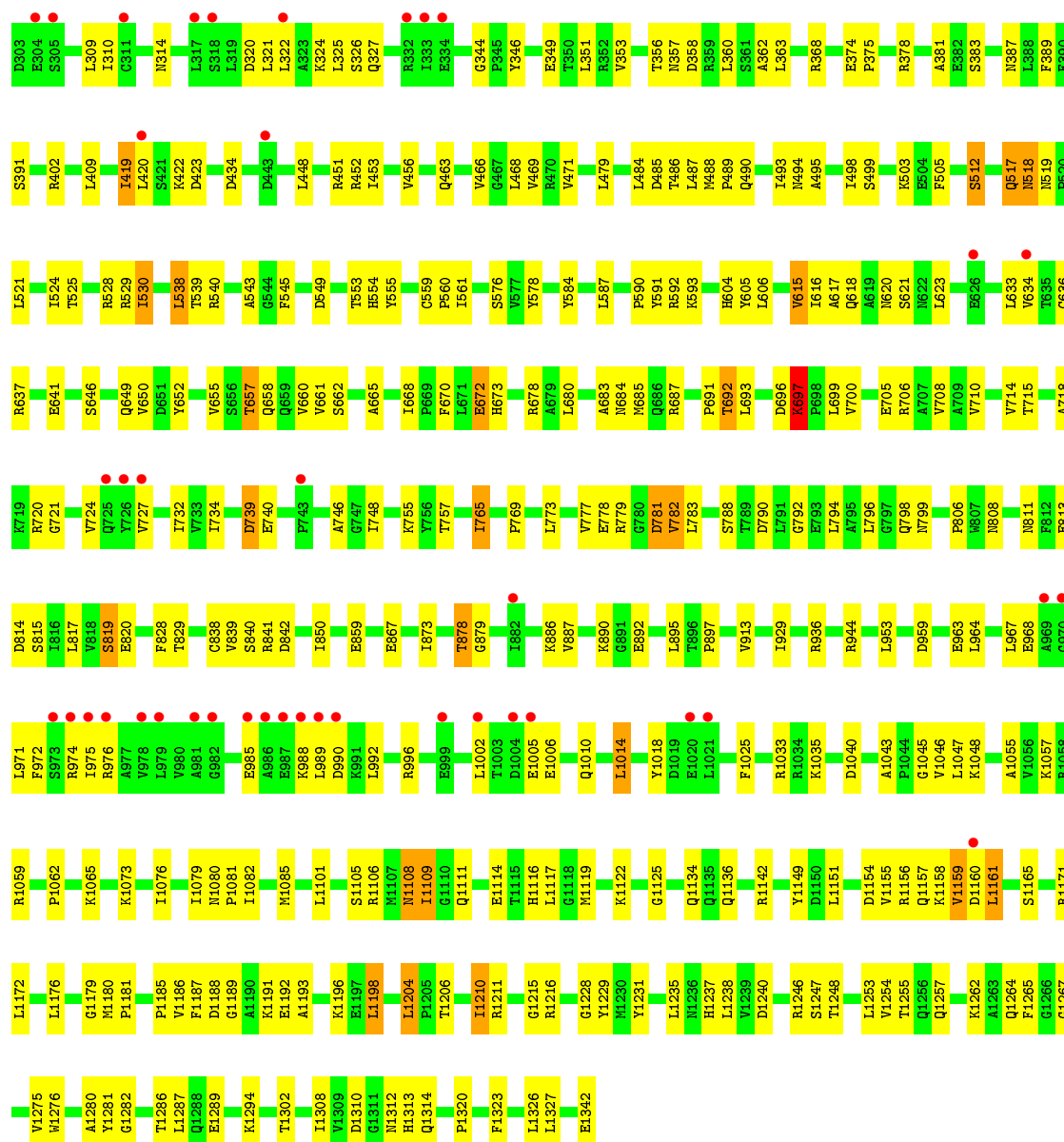
• Molecule 2: DNA-directed RNA polymerase subunit beta



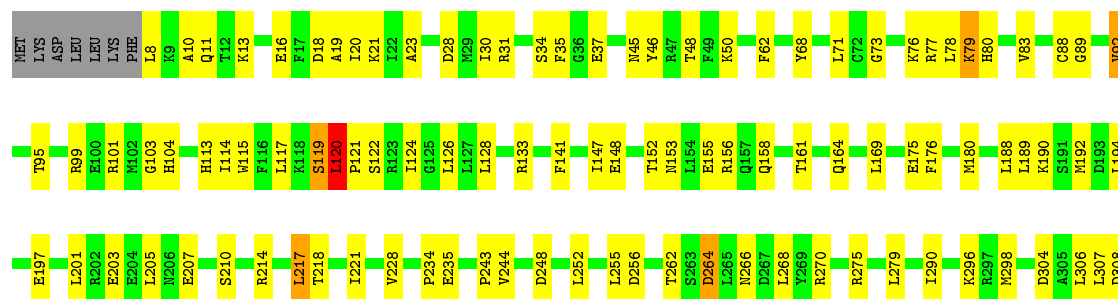


• Molecule 2: DNA-directed RNA polymerase subunit beta

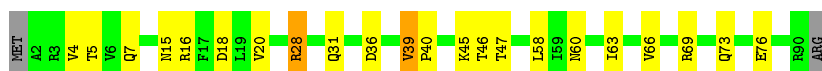




● Molecule 3: DNA-directed RNA polymerase subunit beta'







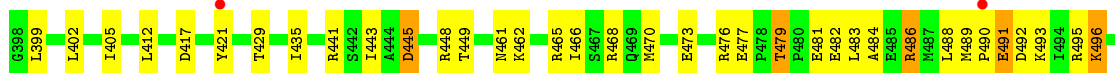
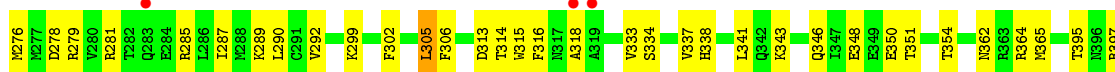
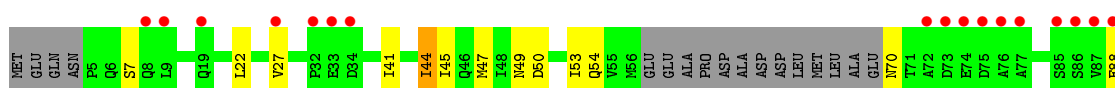
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain K: 63% 22% 13%



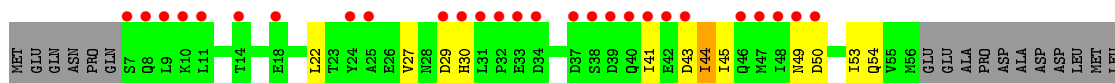
- Molecule 5: RNA polymerase sigma factor RpoD

Chain F: 6% 64% 22% 12%



- Molecule 5: RNA polymerase sigma factor RpoD

Chain L: 6% 62% 24% 12%





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	185.79 Å 205.83 Å 307.46 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.76 – 4.20 49.75 – 4.20	Depositor EDS
% Data completeness (in resolution range)	94.5 (49.76-4.20) 93.8 (49.75-4.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 4.14 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.266 , 0.288 0.267 , 0.290	Depositor DCC
R_{free} test set	2581 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	152.4	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 99.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	57763	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: 4OB, 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 >5	RMSZ	# Z >5
1	A	0.29	0/2358	0.61	1/3197 (0.0%)
1	B	0.33	0/1687	0.64	0/2286
1	G	0.29	0/1751	0.63	0/2373
1	H	0.30	0/1681	0.67	3/2278 (0.1%)
2	C	0.24	0/10739	0.46	0/14489
2	I	0.23	0/10735	0.45	0/14484
3	D	0.25	0/9246	0.47	1/12478 (0.0%)
3	J	0.24	0/10525	0.46	1/14212 (0.0%)
4	E	0.23	0/693	0.45	0/935
4	K	0.22	0/629	0.45	0/847
5	F	0.25	0/4254	0.47	0/5731
5	L	0.25	0/4246	0.47	0/5720
All	All	0.25	0/58544	0.49	6/79030 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	1
3	J	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	317	ARG	NE-CZ-NH1	7.19	123.90	120.30
1	H	29	GLU	C-N-CD	6.85	142.78	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	120	LEU	N-CA-C	5.86	126.83	111.00
3	J	120	LEU	N-CA-C	5.66	126.28	111.00
1	H	28	LEU	CA-CB-CG	5.61	128.21	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	120	LEU	Peptide
3	J	120	LEU	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	2328	0	2380	63	0
1	B	1667	0	1692	58	0
1	G	1730	0	1756	68	0
1	H	1662	0	1687	57	0
2	C	10570	0	10582	262	0
2	I	10566	0	10576	270	0
3	D	9107	0	9307	273	0
3	J	10369	0	10588	304	0
4	E	691	0	695	16	0
4	K	627	0	634	14	0
5	F	4204	0	4106	94	0
5	L	4196	0	4103	102	0
6	C	20	0	11	8	0
6	I	20	0	11	8	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	57763	0	58128	1413	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 1413 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:J:660:GLU:HB3	3:J:685:ILE:HD12	1.47	0.97
2:I:1105:SER:HB2	3:J:731:ARG:HG2	1.50	0.93
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.50	0.92
3:D:418:GLU:HG3	4:E:45:LYS:H	1.34	0.92
2:C:555:TYR:HD2	6:C:2001:4OB:H9	1.37	0.90

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	298/335 (89%)	270 (91%)	19 (6%)	9 (3%)	4	32
1	B	212/335 (63%)	190 (90%)	20 (9%)	2 (1%)	17	56
1	G	222/335 (66%)	196 (88%)	20 (9%)	6 (3%)	5	34
1	H	212/335 (63%)	193 (91%)	17 (8%)	2 (1%)	17	56
2	C	1338/1342 (100%)	1234 (92%)	98 (7%)	6 (0%)	34	72
2	I	1338/1342 (100%)	1232 (92%)	100 (8%)	6 (0%)	34	72
3	D	1162/1407 (83%)	1045 (90%)	105 (9%)	12 (1%)	15	54
3	J	1328/1407 (94%)	1195 (90%)	122 (9%)	11 (1%)	19	60
4	E	87/91 (96%)	81 (93%)	6 (7%)	0	100	100
4	K	77/91 (85%)	73 (95%)	4 (5%)	0	100	100
5	F	532/613 (87%)	481 (90%)	50 (9%)	1 (0%)	47	81
5	L	529/613 (86%)	480 (91%)	49 (9%)	0	100	100
All	All	7335/8246 (89%)	6670 (91%)	610 (8%)	55 (1%)	22	62

5 of 55 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	319	GLU
1	A	320	ASN
2	C	237	LEU
3	D	120	LEU
3	D	751	ASP

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	257/292 (88%)	241 (94%)	16 (6%)	18	46
1	B	184/292 (63%)	168 (91%)	16 (9%)	10	34
1	G	191/292 (65%)	182 (95%)	9 (5%)	26	53
1	H	183/292 (63%)	171 (93%)	12 (7%)	16	44
2	C	1155/1157 (100%)	1065 (92%)	90 (8%)	12	39
2	I	1154/1157 (100%)	1060 (92%)	94 (8%)	11	38
3	D	975/1168 (84%)	886 (91%)	89 (9%)	9	32
3	J	1117/1168 (96%)	1019 (91%)	98 (9%)	10	34
4	E	72/75 (96%)	66 (92%)	6 (8%)	11	37
4	K	67/75 (89%)	61 (91%)	6 (9%)	9	33
5	F	426/540 (79%)	392 (92%)	34 (8%)	12	38
5	L	428/540 (79%)	393 (92%)	35 (8%)	11	37
All	All	6209/7048 (88%)	5704 (92%)	505 (8%)	11	38

5 of 505 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	395	THR
2	I	131	THR
4	K	36	ASP
5	F	486	ARG
1	G	145	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	1367	GLN
2	I	343	HIS
3	J	560	ASN
5	F	406	GLN
5	F	600	HIS

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 ⓘ

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	4OB	I	2001	-	21,21,21	2.41	5 (23%)	28,29,29	1.43	5 (17%)
6	4OB	C	2001	-	21,21,21	2.41	5 (23%)	28,29,29	1.43	5 (17%)

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	4OB	I	2001	-	-	1/15/16/16	0/2/2/2
6	4OB	C	2001	-	-	1/15/16/16	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	2001	4OB	CAQ-NAO	-6.57	1.31	1.42
6	C	2001	4OB	CAQ-NAO	-6.56	1.31	1.42
6	I	2001	4OB	CAT-CAS	-5.97	1.37	1.49
6	C	2001	4OB	CAT-CAS	-5.96	1.37	1.49
6	C	2001	4OB	CAR-CAP	-4.53	1.39	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	2001	4OB	CAM-CAS-CAT	3.19	123.89	119.58
6	C	2001	4OB	CAM-CAS-CAT	3.17	123.87	119.58
6	I	2001	4OB	CAL-CAS-CAT	-2.77	115.56	119.97
6	C	2001	4OB	CAL-CAS-CAT	-2.77	115.57	119.97
6	C	2001	4OB	OAA-NAN-CAP	-2.58	113.26	119.49

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	I	2001	4OB	CAR-CAP-NAN-OAA
6	C	2001	4OB	CAR-CAP-NAN-OAA

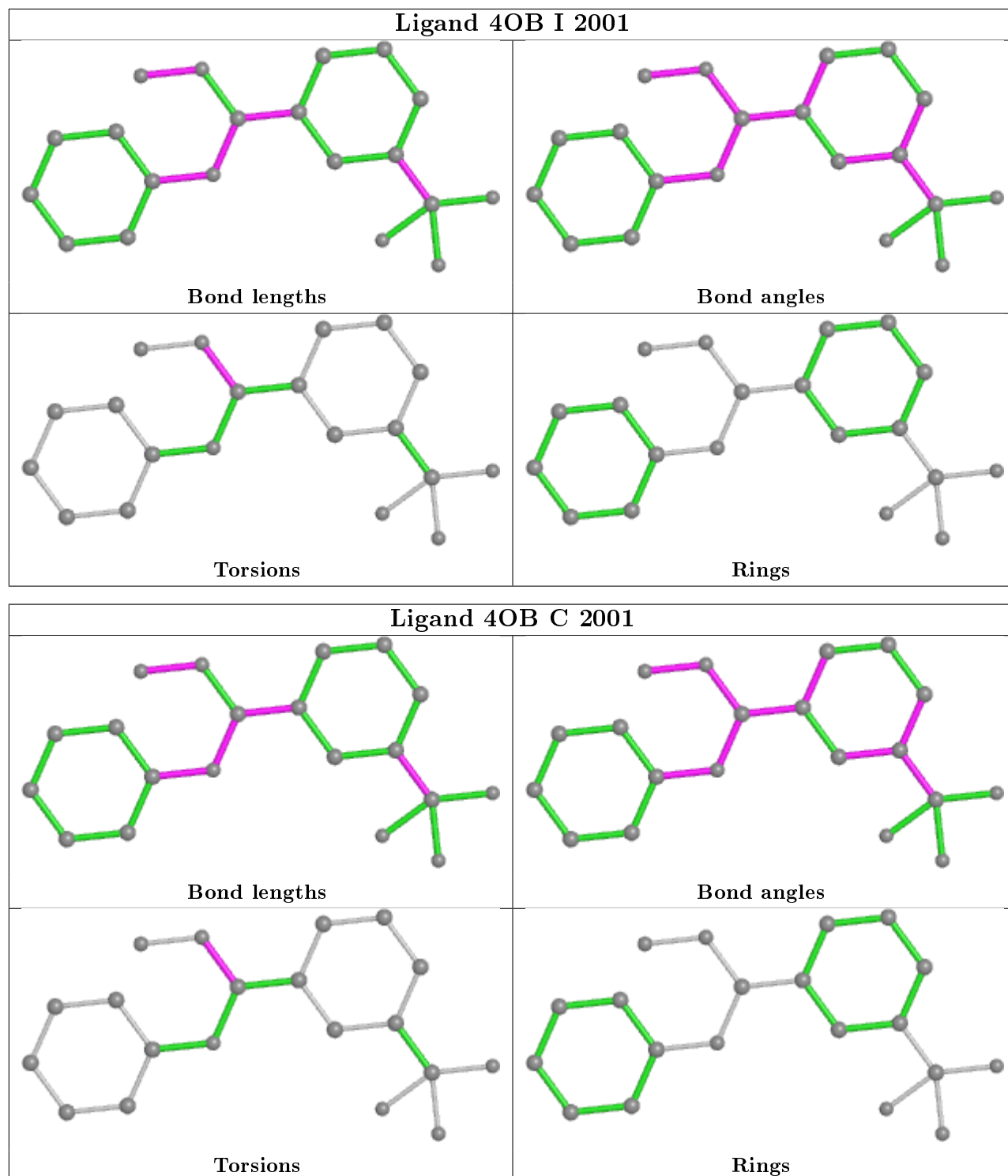
There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	2001	4OB	8	0
6	C	2001	4OB	8	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 than 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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	302/335 (90%)	-0.03	7 (2%) 60 51	28, 105, 237, 409	0
1	B	216/335 (64%)	-0.14	7 (3%) 47 37	28, 127, 210, 290	0
1	G	224/335 (66%)	-0.03	4 (1%) 68 59	59, 127, 200, 244	0
1	H	216/335 (64%)	0.13	8 (3%) 41 33	49, 145, 220, 274	0
2	C	1340/1342 (99%)	-0.13	26 (1%) 66 58	15, 95, 231, 320	0
2	I	1340/1342 (99%)	0.07	59 (4%) 34 28	21, 132, 241, 336	0
3	D	1166/1407 (82%)	-0.18	11 (0%) 84 77	13, 70, 178, 278	0
3	J	1334/1407 (94%)	-0.01	44 (3%) 46 37	16, 95, 214, 287	0
4	E	89/91 (97%)	-0.33	0 100 100	16, 93, 132, 215	0
4	K	79/91 (86%)	-0.13	0 100 100	54, 120, 204, 224	0
5	F	542/613 (88%)	0.18	35 (6%) 18 15	31, 145, 251, 341	0
5	L	539/613 (87%)	0.17	39 (7%) 15 13	34, 147, 248, 314	0
All	All	7387/8246 (89%)	-0.02	240 (3%) 47 37	13, 110, 229, 409	0

The worst 5 of 240 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	74	GLU	10.1
5	L	8	GLN	7.2
5	F	88	GLU	7.1
3	J	1054	THR	7.1
5	F	89	SER	7.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

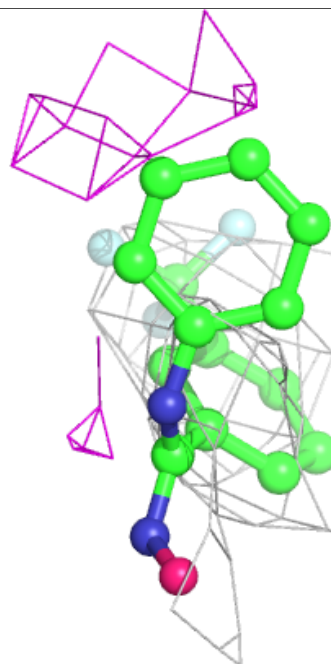
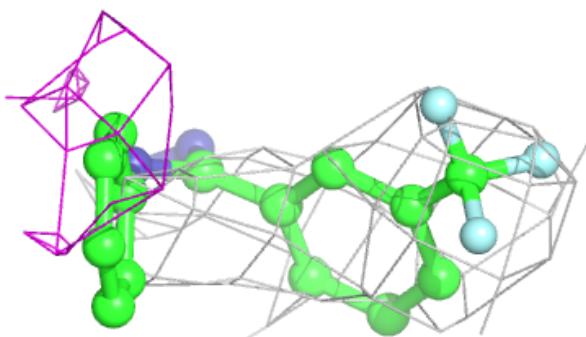
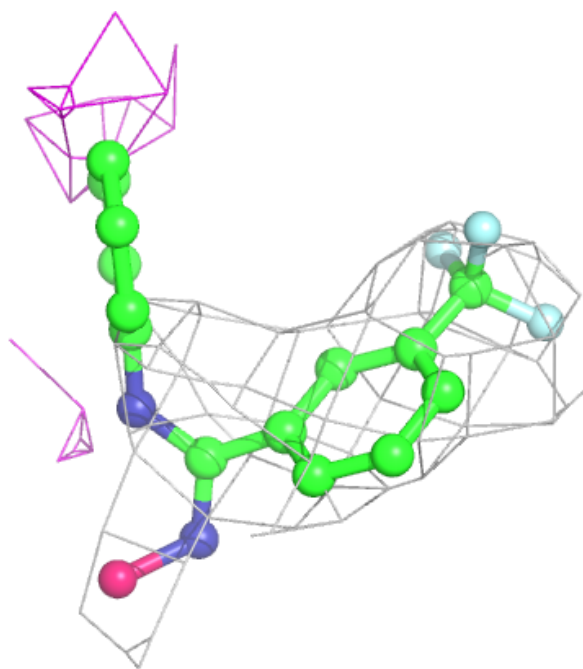
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	4OB	I	2001	20/20	0.74	0.92	90,112,127,136	0
6	4OB	C	2001	20/20	0.83	0.75	50,73,98,99	0
7	MG	D	1501	1/1	0.86	0.80	72,72,72,72	0
8	ZN	D	1502	1/1	0.93	0.10	90,90,90,90	0
8	ZN	D	1503	1/1	0.94	0.39	138,138,138,138	0
8	ZN	J	1502	1/1	0.95	0.13	79,79,79,79	0
7	MG	J	1501	1/1	0.96	0.69	33,33,33,33	0
8	ZN	J	1503	1/1	0.98	0.20	31,31,31,31	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

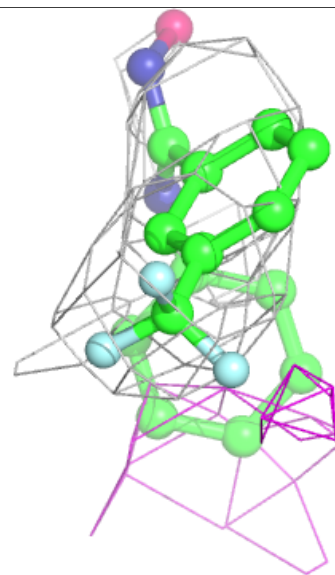
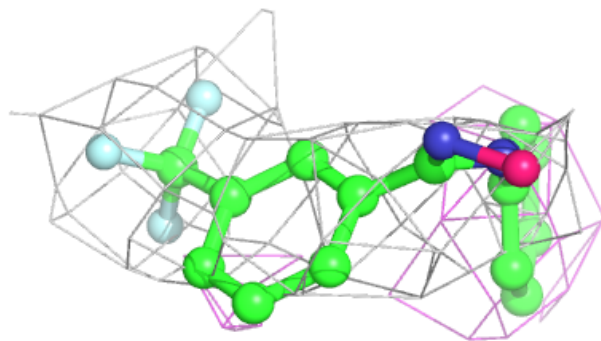
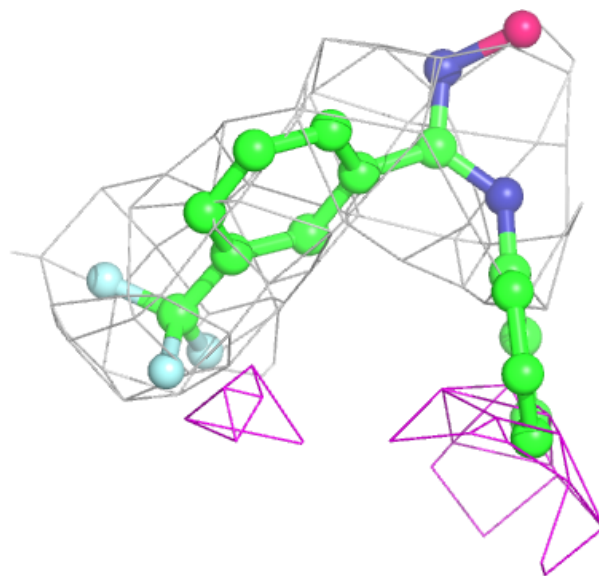
Electron density around 4OB I 2001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 4OB C 2001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.