



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 09:54 PM UTC

PDB ID : 4ZH3 / pdb_00004zh3
Title : Crystal structure of Escherichia coli RNA polymerase in complex with CBRH16-Br
Authors : Feng, Y.; Ebright, R.H.
Deposited on : 2015-04-24
Resolution : 4.08 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

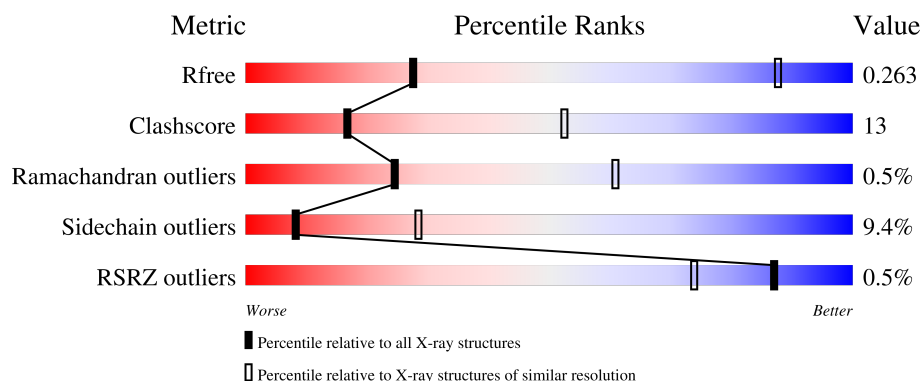
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.08 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}	180053	1200 (4.36-3.80)
Clashscore	190562	1249 (4.36-3.80)
Ramachandran outliers	187476	1169 (4.36-3.80)
Sidechain outliers	187428	1158 (4.36-3.80)
RSRZ outliers	180081	1199 (4.36-3.80)

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 $\leq 5\%$. 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	% 57% 28% • 10%
1	B	335	38% 22% • 36%
1	G	335	% 39% 25% • 33%
1	H	335	38% 22% • • 36%
2	C	1342	66% 30% •

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Mol	Chain	Length	Quality of chain
2	I	1342	67%29%.
3	D	1407	52%26%.18%
3	J	1407	61%29%.6%
4	E	91	71%24%. .
4	K	91	58%25%.13%
5	F	613	%61%24%.12%
5	L	613	59%25%.12%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 57537 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	1151	Total	C	N	O	S	0	0	0
			8992	5653	1608	1686	45			
3	J	1319	Total	C	N	O	S	0	0	0
			10254	6443	1824	1939	48			

- 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			

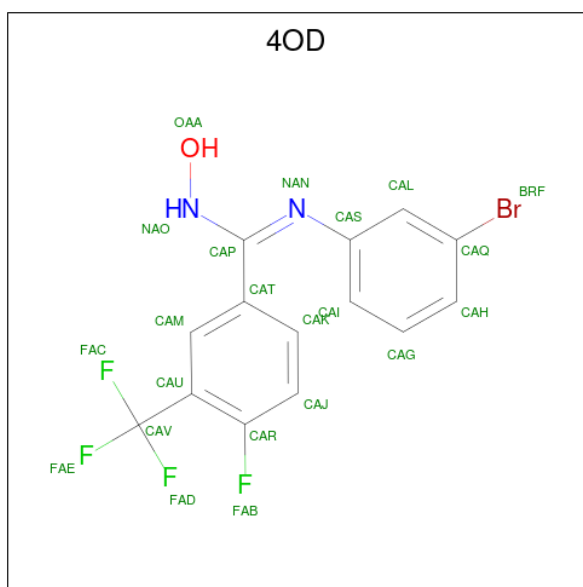
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 8 is N'-(3-bromophenyl)-4-fluoro-N-hydroxy-3-(trifluoromethyl)benzenecarboximide (CCD ID: 4OD) (formula: C₁₄H₉BrF₄N₂O).

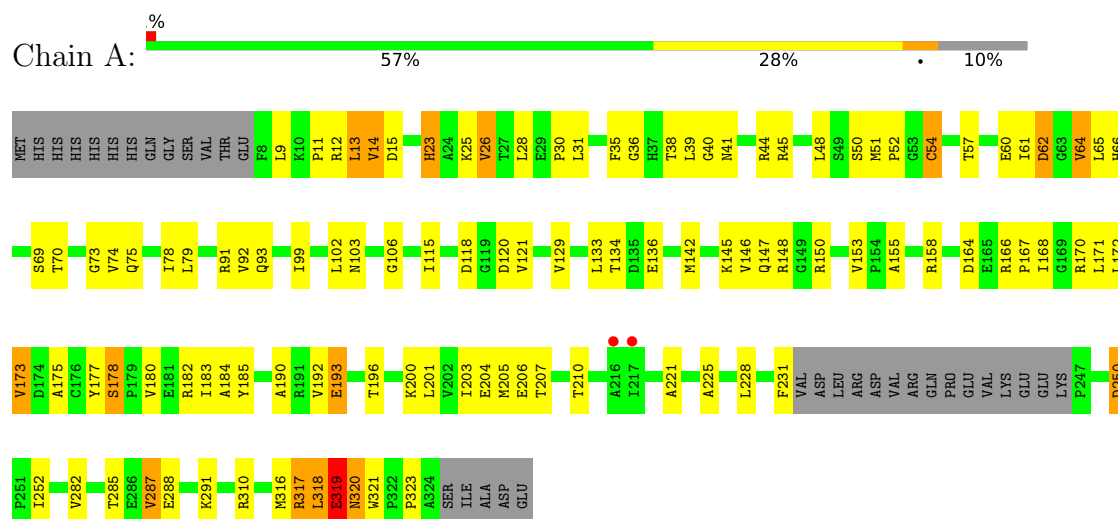


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	D	1	Total	Br	C	F	N	O	0	0
			22	1	14	4	2	1		
8	J	1	Total	Br	C	F	N	O	0	0
			22	1	14	4	2	1		

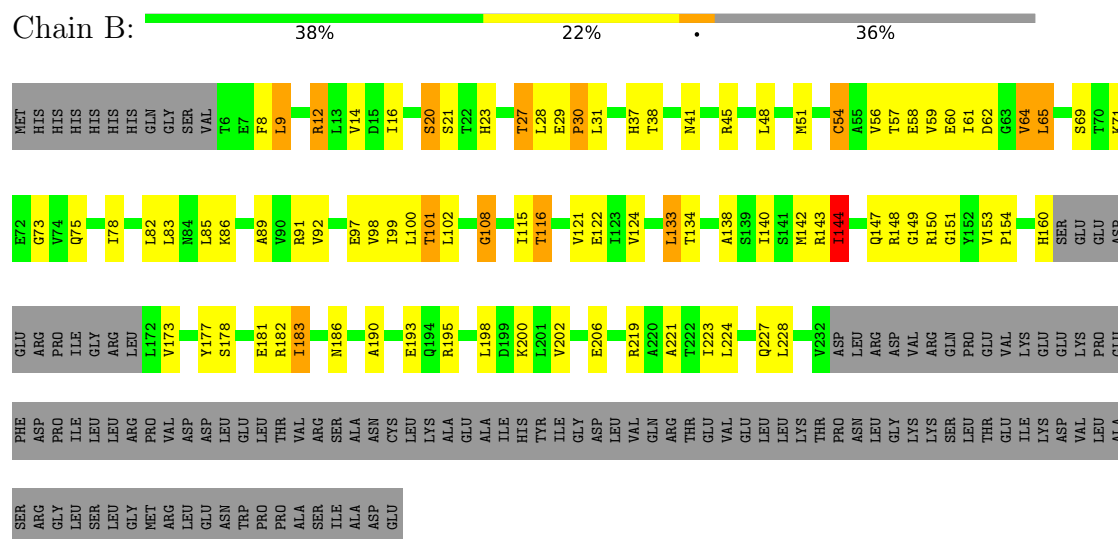
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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

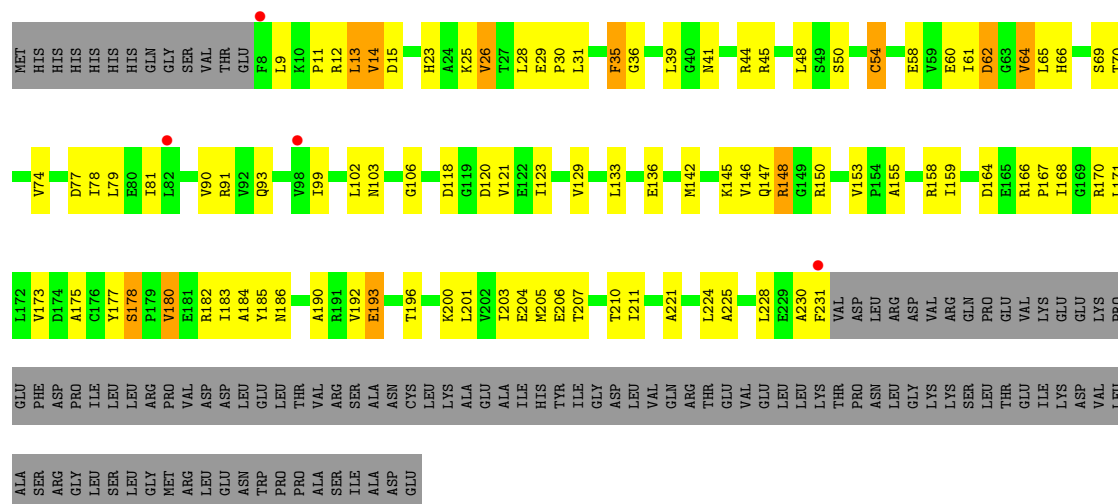


• Molecule 1: DNA-directed RNA polymerase subunit alpha



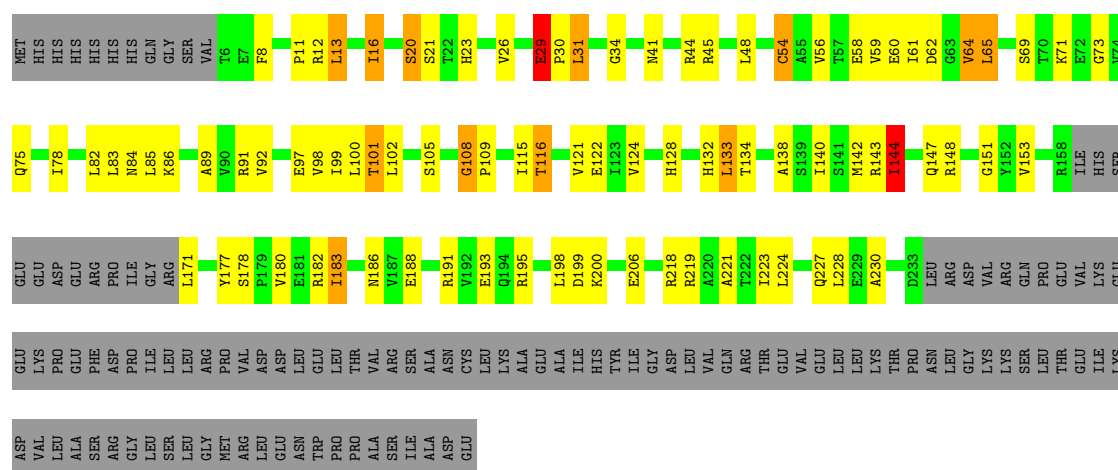
• Molecule 1: DNA-directed RNA polymerase subunit alpha





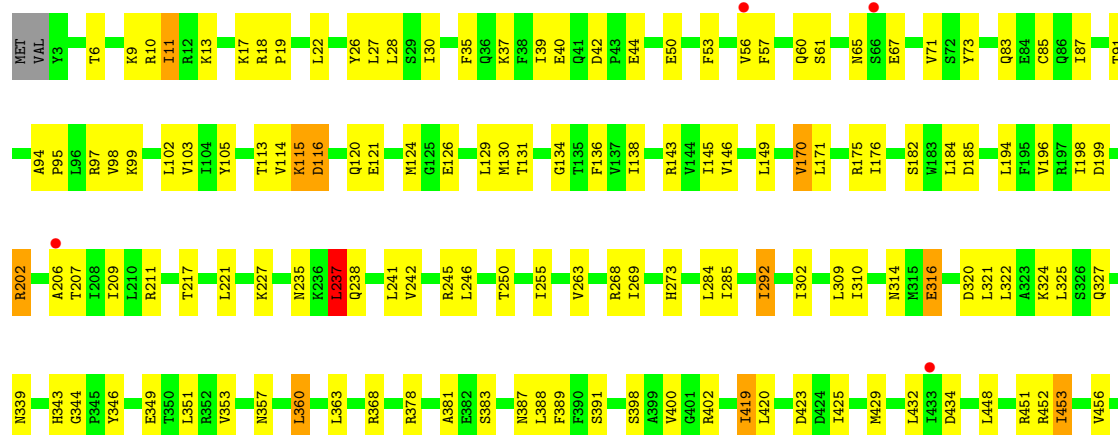
• Molecule 1: DNA-directed RNA polymerase subunit alpha

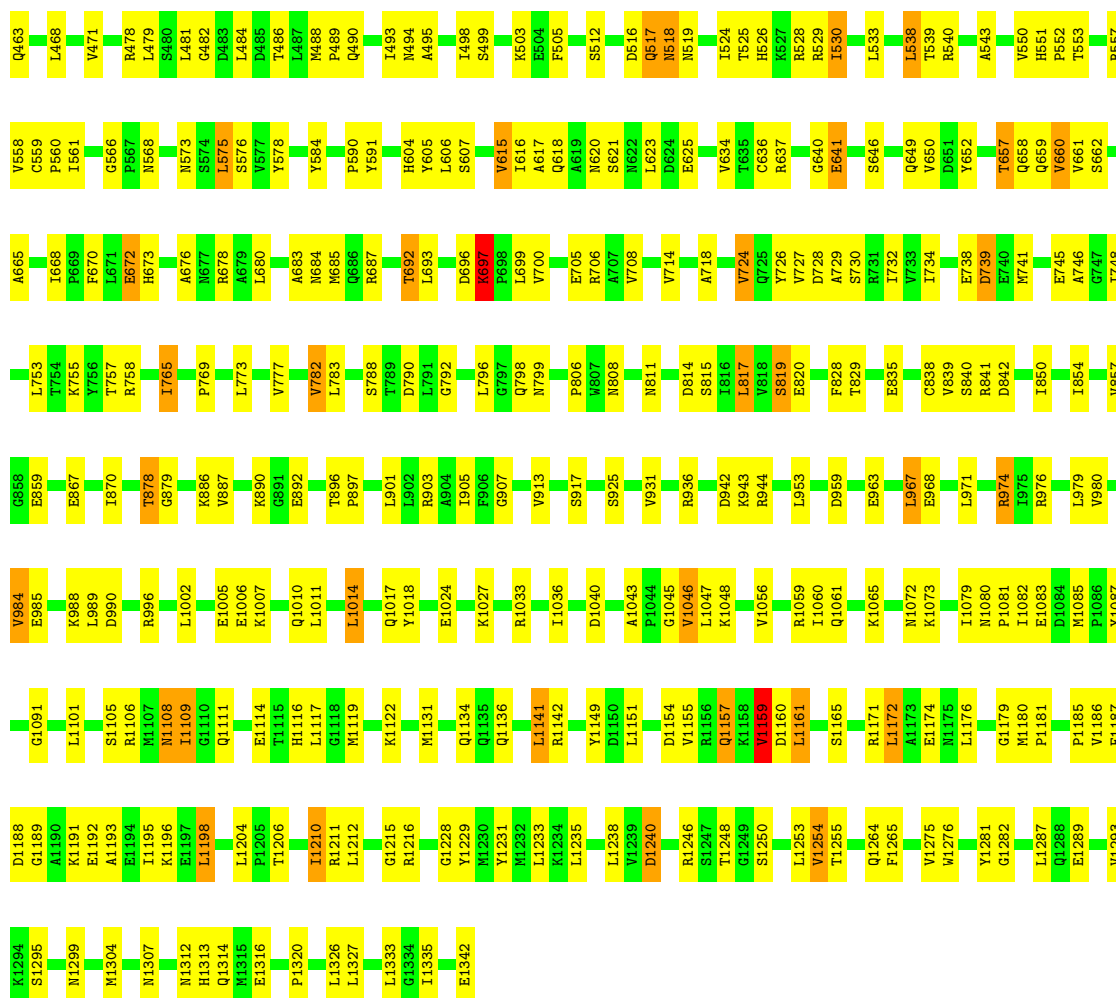
Chain H: 38% 22% 36%



• Molecule 2: DNA-directed RNA polymerase subunit beta

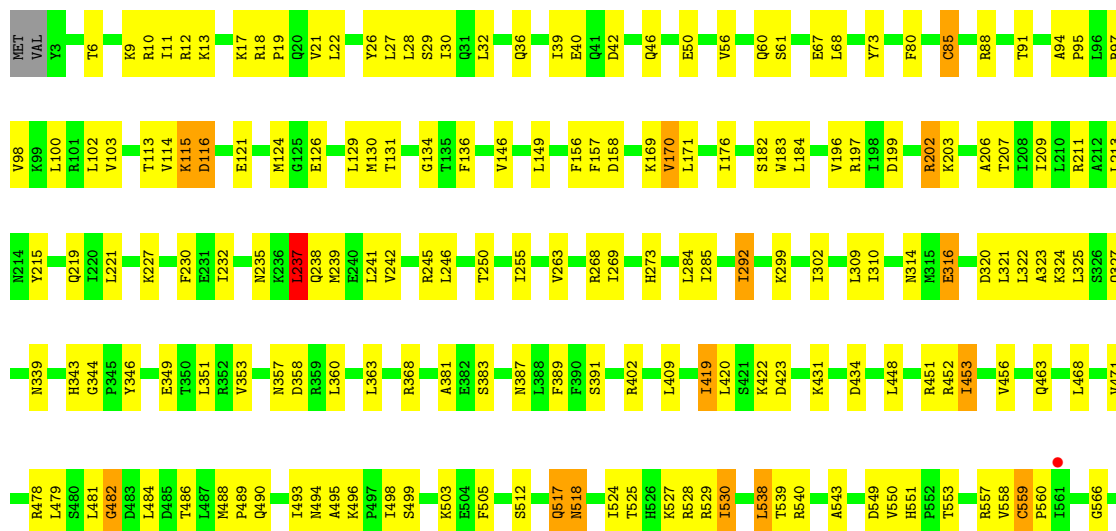
Chain C: 66% 30%

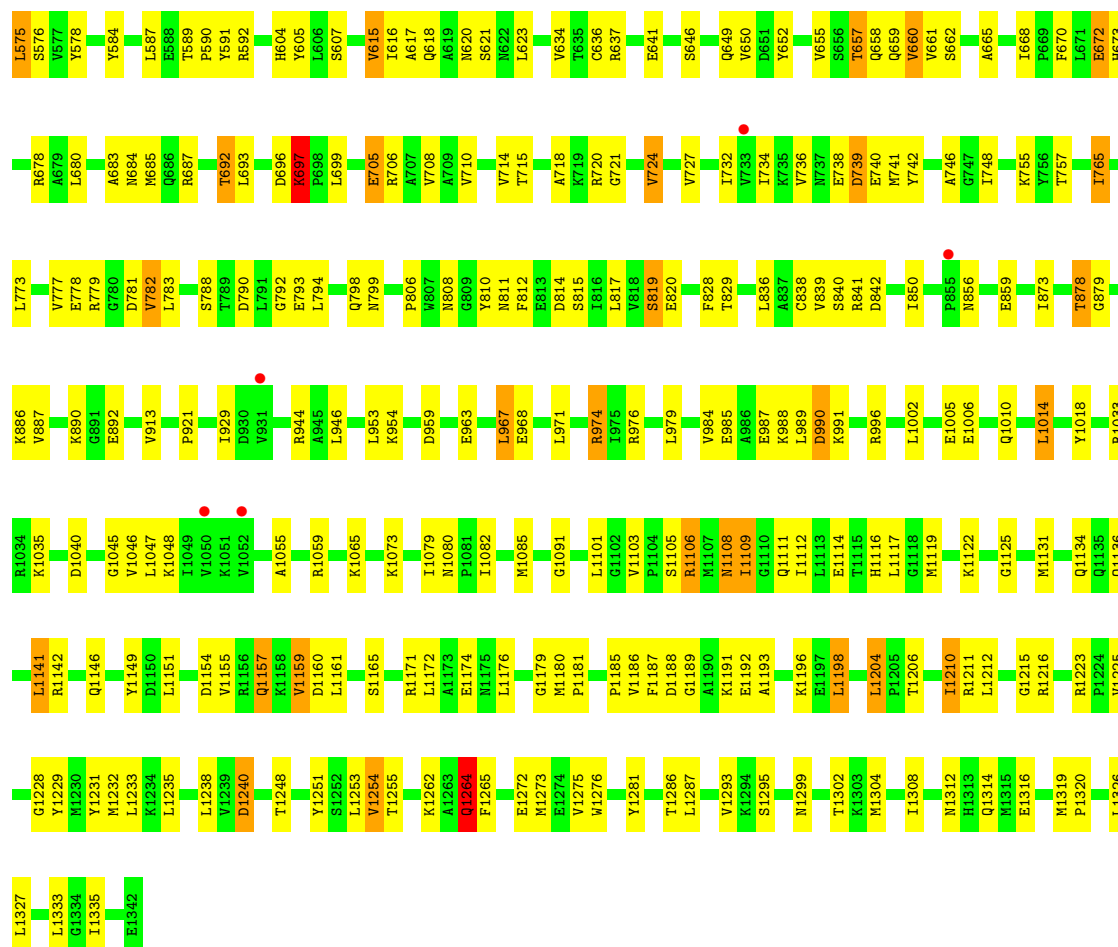




• Molecule 2: DNA-directed RNA polymerase subunit beta

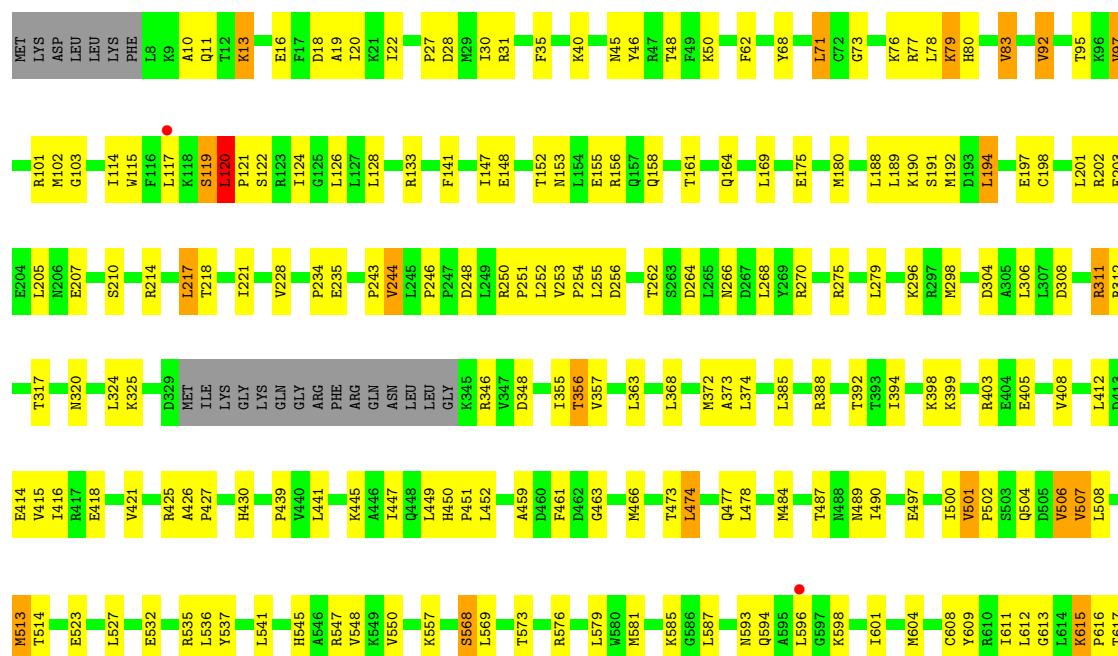
Chain I: 67% 29%

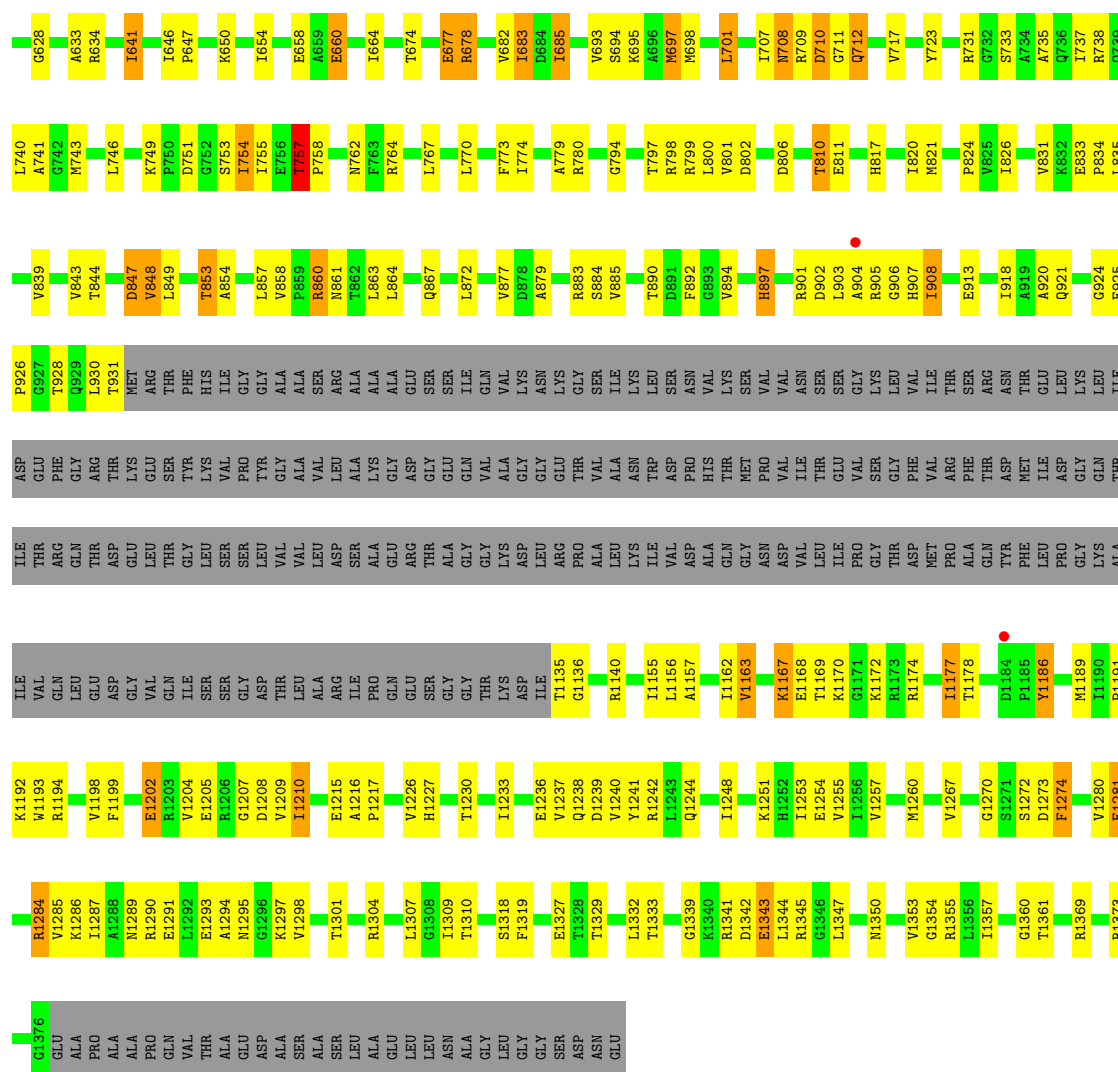




• Molecule 3: DNA-directed RNA polymerase subunit beta'

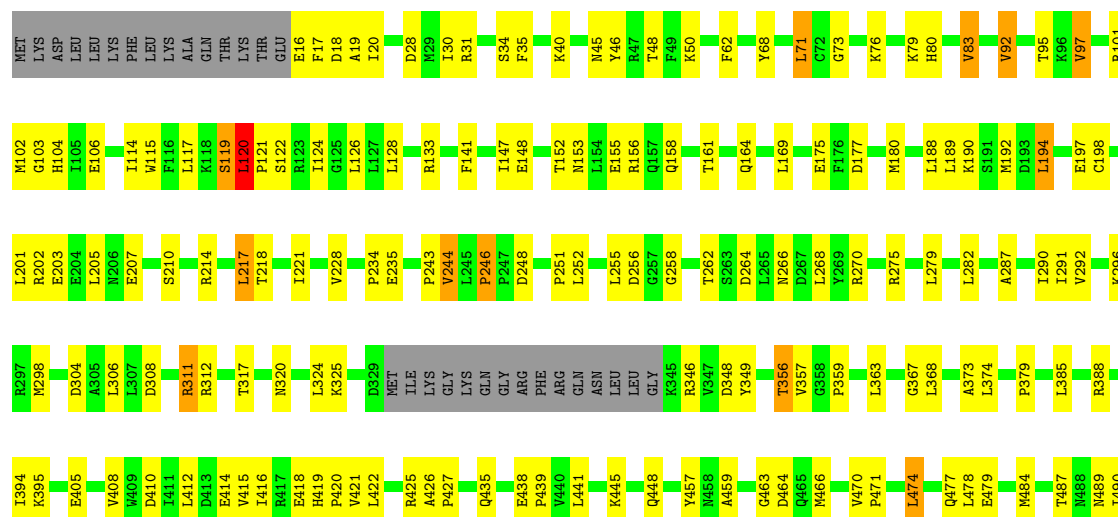
Chain D: 52% 26% 18%

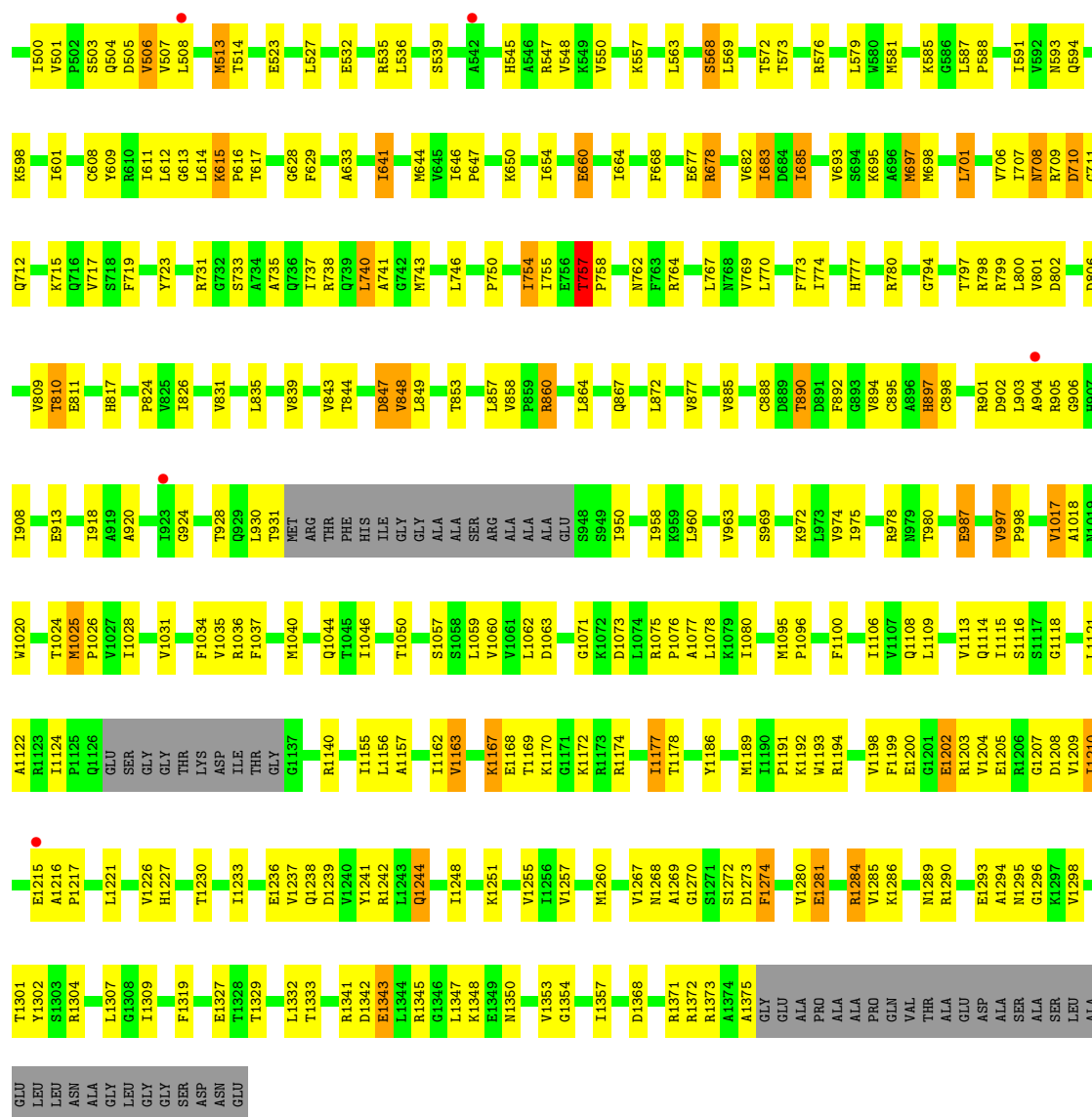




• Molecule 3: DNA-directed RNA polymerase subunit beta'

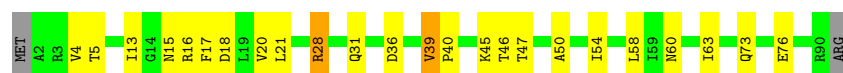
Chain J: 61% 29% 6%





- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 71% 24% . .



- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain K: 58% 25% . 13%



[illegible][illegible]

L598	R599	H600	P601	S602	E605	V606	D613
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	186.34Å 205.79Å 307.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.75 – 4.08 49.75 – 4.08	Depositor EDS
% Data completeness (in resolution range)	93.2 (49.75-4.08) 92.6 (49.75-4.08)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 4.14Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.237 , 0.267 0.238 , 0.263	Depositor DCC
R_{free} test set	1879 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	143.4	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 138.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	57537	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.72% 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: MG, ZN, 4OD

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	0.52	3/2358 (0.1%)	0.97	5/3197 (0.2%)
1	B	0.53	0/1687	1.03	8/2286 (0.3%)
1	G	0.46	0/1751	1.01	3/2373 (0.1%)
1	H	0.49	0/1681	1.14	9/2278 (0.4%)
2	C	0.36	0/10739	0.80	11/14489 (0.1%)
2	I	0.34	0/10735	0.79	12/14484 (0.1%)
3	D	0.38	0/9130	0.84	15/12325 (0.1%)
3	J	0.36	0/10409	0.83	12/14059 (0.1%)
4	E	0.37	0/693	0.82	0/935
4	K	0.38	0/629	0.85	0/847
5	F	0.38	0/4254	0.83	3/5731 (0.1%)
5	L	0.38	0/4246	0.82	4/5720 (0.1%)
All	All	0.38	3/58312 (0.0%)	0.85	82/78724 (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
3	D	0	1
3	J	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	317	ARG	CZ-NH2	-5.68	1.26	1.33
1	A	250	ASP	C-O	-5.11	1.17	1.24
1	A	250	ASP	CB-CG	-5.06	1.39	1.52

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	29	GLU	CA-C-N	-16.58	104.06	120.31
1	H	29	GLU	C-N-CA	-16.58	104.06	120.31
3	J	120	LEU	CA-C-N	-11.91	104.96	119.84
3	J	120	LEU	C-N-CA	-11.91	104.96	119.84
3	D	120	LEU	CA-C-N	-9.86	107.51	119.84

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	79	0
1	B	1667	0	1692	60	0
1	G	1730	0	1756	72	0
1	H	1662	0	1687	62	0
2	C	10570	0	10582	272	0
2	I	10566	0	10576	263	0
3	D	8992	0	9180	268	0
3	J	10254	0	10462	286	0
4	E	691	0	695	17	0
4	K	627	0	634	14	0
5	F	4204	0	4106	104	0
5	L	4196	0	4103	118	0
6	D	1	0	0	0	0
6	J	1	0	0	0	0
7	D	2	0	0	0	0
7	J	2	0	0	0	0
8	D	22	0	9	3	0
8	J	22	0	9	4	0
All	All	57537	0	57871	1475	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 13.

The worst 5 of 1475 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	1.37	1.04
3:J:660:GLU:HB3	3:J:685:ILE:HD12	1.46	0.97
1:B:29:GLU:HB3	1:B:30:PRO:HD3	1.49	0.92
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.57	0.87
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.57	0.86

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	3	26
1	B	212/335 (63%)	194 (92%)	16 (8%)	2 (1%)	14	49
1	G	222/335 (66%)	202 (91%)	14 (6%)	6 (3%)	4	28
1	H	212/335 (63%)	195 (92%)	15 (7%)	2 (1%)	14	49
2	C	1338/1342 (100%)	1235 (92%)	96 (7%)	7 (0%)	24	61
2	I	1338/1342 (100%)	1235 (92%)	97 (7%)	6 (0%)	30	65
3	D	1145/1407 (81%)	1052 (92%)	89 (8%)	4 (0%)	36	70
3	J	1311/1407 (93%)	1200 (92%)	108 (8%)	3 (0%)	43	75
4	E	87/91 (96%)	79 (91%)	8 (9%)	0	100	100
4	K	77/91 (85%)	73 (95%)	4 (5%)	0	100	100
5	F	532/613 (87%)	482 (91%)	49 (9%)	1 (0%)	43	75
5	L	529/613 (86%)	480 (91%)	49 (9%)	0	100	100
All	All	7301/8246 (88%)	6697 (92%)	564 (8%)	40 (0%)	24	61

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	GLU
1	A	319	GLU
1	A	320	ASN
2	C	237	LEU
3	D	10	ALA

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%)	238 (93%)	19 (7%)	13	36
1	B	184/292 (63%)	162 (88%)	22 (12%)	5	21
1	G	191/292 (65%)	177 (93%)	14 (7%)	13	36
1	H	183/292 (63%)	165 (90%)	18 (10%)	7	27
2	C	1155/1157 (100%)	1054 (91%)	101 (9%)	9	32
2	I	1154/1157 (100%)	1053 (91%)	101 (9%)	9	31
3	D	964/1168 (82%)	865 (90%)	99 (10%)	7	25
3	J	1106/1168 (95%)	999 (90%)	107 (10%)	8	27
4	E	72/75 (96%)	65 (90%)	7 (10%)	8	27
4	K	67/75 (89%)	59 (88%)	8 (12%)	5	21
5	F	426/540 (79%)	384 (90%)	42 (10%)	7	26
5	L	428/540 (79%)	386 (90%)	42 (10%)	7	27
All	All	6187/7048 (88%)	5607 (91%)	580 (9%)	8	28

5 of 580 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	660	GLU
5	L	572	THR
3	J	740	LEU
3	J	641	ILE

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Mol	Chain	Res	Type
3	J	1274	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
3	J	667	GLN
3	J	897	HIS
5	L	345	GLN
3	D	593	ASN
3	D	560	ASN

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 oligosaccharides 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
8	4OD	J	1504	-	23,23,23	2.94	6 (26%)	32,33,33	1.38	6 (18%)
8	4OD	D	1504	-	23,23,23	2.94	6 (26%)	32,33,33	1.38	6 (18%)

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
8	4OD	J	1504	-	-	3/15/16/16	0/2/2/2
8	4OD	D	1504	-	-	3/15/16/16	0/2/2/2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	1504	4OD	BRF-CAQ	-6.84	1.76	1.90
8	D	1504	4OD	BRF-CAQ	-6.83	1.76	1.90
8	D	1504	4OD	CAS-NAN	-6.57	1.31	1.42
8	J	1504	4OD	CAS-NAN	-6.55	1.31	1.42
8	D	1504	4OD	FAB-CAR	-6.51	1.18	1.35

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	1504	4OD	CAK-CAT-CAP	-2.87	115.73	120.83
8	J	1504	4OD	CAK-CAT-CAP	-2.85	115.76	120.83
8	D	1504	4OD	FAC-CAV-CAU	-2.83	107.62	112.65
8	D	1504	4OD	CAS-NAN-CAP	2.82	126.64	120.49
8	J	1504	4OD	CAS-NAN-CAP	2.81	126.61	120.49

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

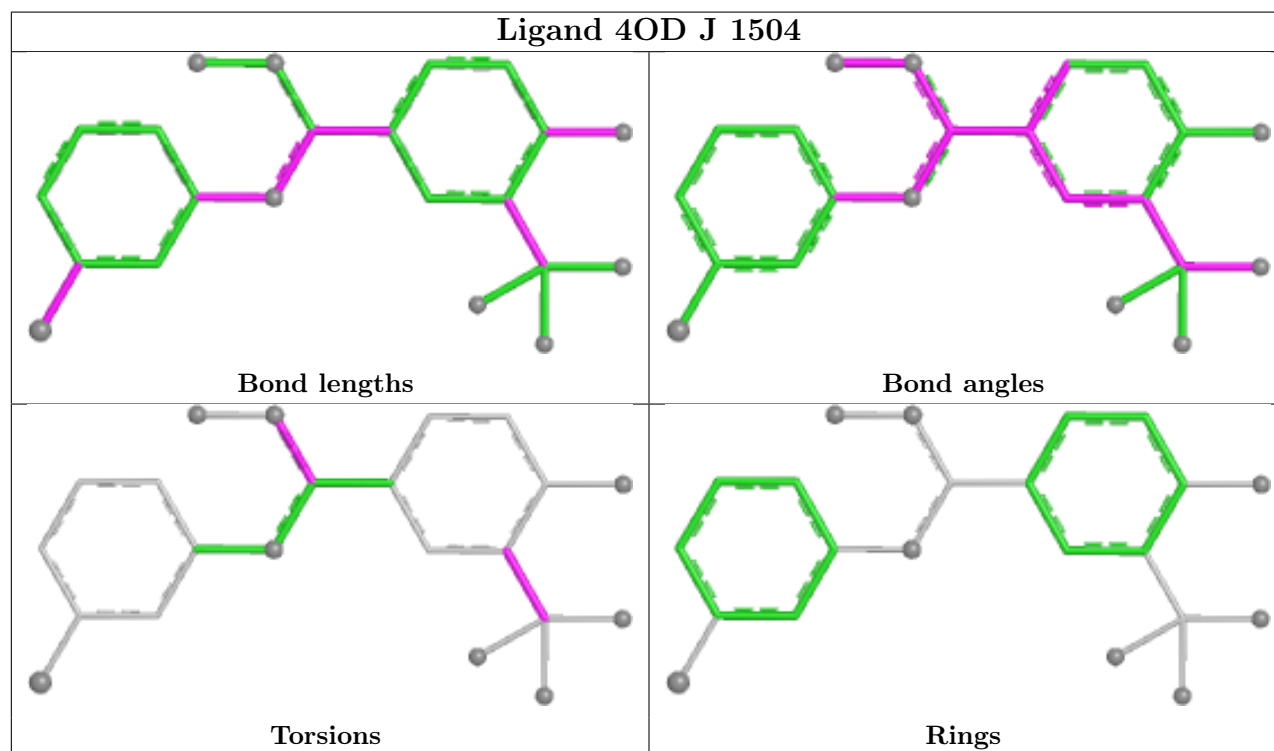
Mol	Chain	Res	Type	Atoms
8	D	1504	4OD	CAT-CAP-NAO-OAA
8	J	1504	4OD	CAT-CAP-NAO-OAA
8	D	1504	4OD	CAR-CAU-CAV-FAD
8	D	1504	4OD	CAR-CAU-CAV-FAE
8	J	1504	4OD	CAR-CAU-CAV-FAD

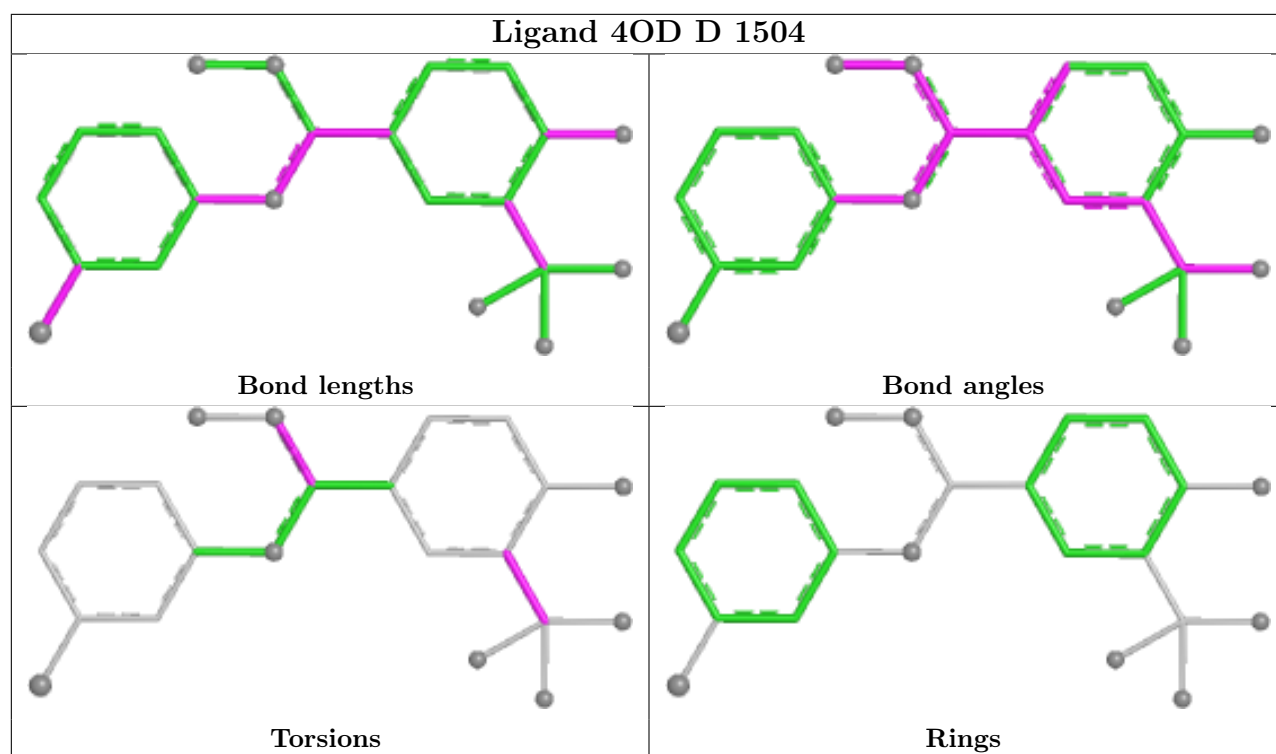
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	J	1504	4OD	4	0
8	D	1504	4OD	3	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 [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	302/335 (90%)	-0.34	2 (0%) 84 69	41, 103, 232, 400	0
1	B	216/335 (64%)	-0.18	0 100 100	37, 121, 198, 297	0
1	G	224/335 (66%)	-0.26	4 (1%) 67 51	54, 109, 196, 282	0
1	H	216/335 (64%)	-0.23	0 100 100	65, 135, 230, 280	0
2	C	1340/1342 (99%)	-0.30	4 (0%) 90 79	14, 87, 202, 296	0
2	I	1340/1342 (99%)	-0.30	6 (0%) 88 76	15, 108, 212, 334	0
3	D	1151/1407 (81%)	-0.31	4 (0%) 90 79	13, 73, 170, 292	0
3	J	1319/1407 (93%)	-0.32	5 (0%) 88 76	23, 95, 231, 322	0
4	E	89/91 (97%)	-0.58	0 100 100	33, 77, 139, 160	0
4	K	79/91 (86%)	-0.47	0 100 100	70, 118, 195, 235	0
5	F	542/613 (88%)	-0.24	6 (1%) 78 60	38, 154, 258, 355	0
5	L	539/613 (87%)	-0.36	3 (0%) 85 71	52, 154, 248, 300	0
All	All	7357/8246 (89%)	-0.31	34 (0%) 87 74	13, 103, 222, 400	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	259	PHE	3.7
2	I	561	ILE	3.4
3	D	904	ALA	3.4
1	G	231	PHE	3.4
2	I	1050	VAL	3.2

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

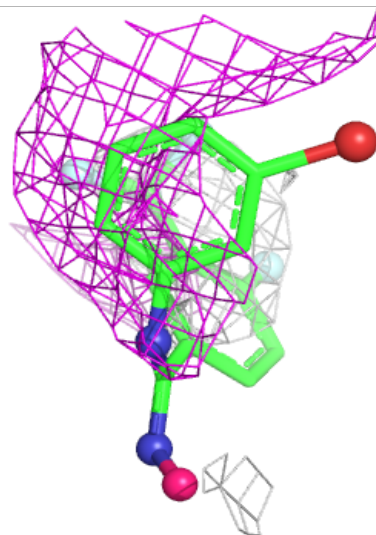
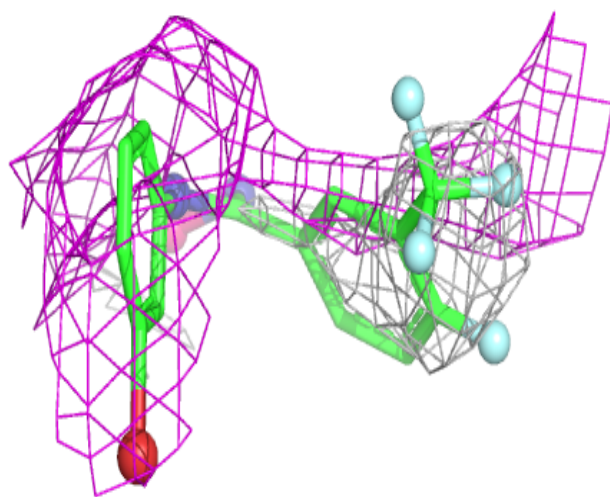
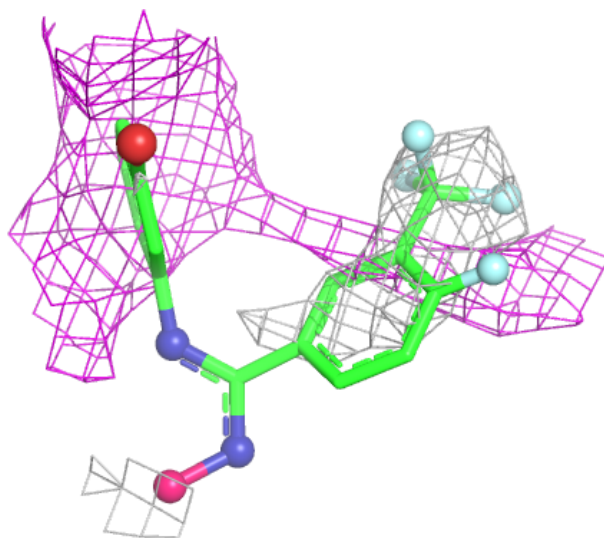
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	4OD	J	1504	22/22	0.60	0.11	100,110,116,133	1
6	MG	J	1501	1/1	0.76	0.22	55,55,55,55	0
8	4OD	D	1504	22/22	0.85	0.08	68,80,89,116	1
6	MG	D	1501	1/1	0.89	0.13	37,37,37,37	0
7	ZN	J	1502	1/1	0.99	0.05	98,98,98,98	0
7	ZN	J	1503	1/1	1.00	0.05	46,46,46,46	0
7	ZN	D	1503	1/1	1.00	0.04	49,49,49,49	0
7	ZN	D	1502	1/1	1.00	0.03	90,90,90,90	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.

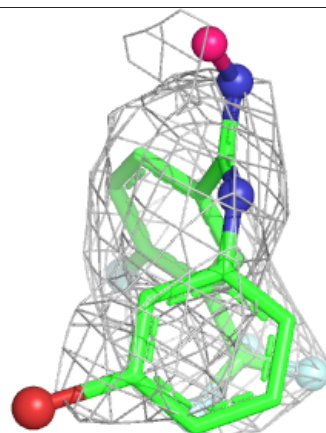
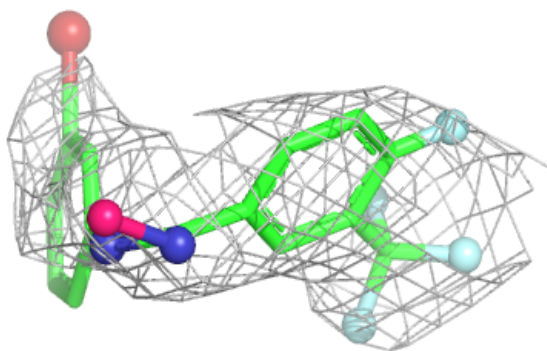
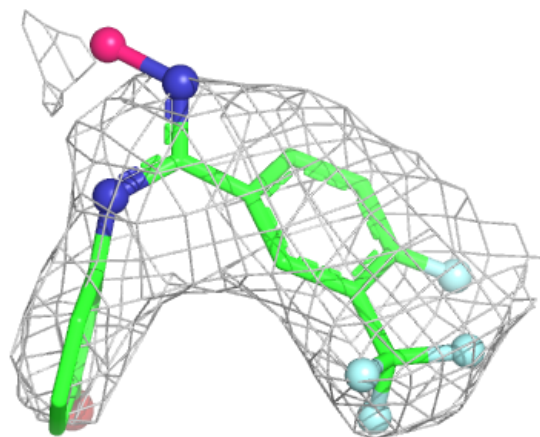
Electron density around 4OD J 1504:

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



Electron density around 4OD D 1504:

$2mF_o-DF_c$ (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.