



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:28 PM UTC

PDB ID : 4LJZ / pdb_00004ljz
Title : Crystal Structure Analysis of the E.coli holoenzyme
Authors : Bae, B.; Darst, S.A.
Deposited on : 2013-07-05
Resolution : 3.59 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

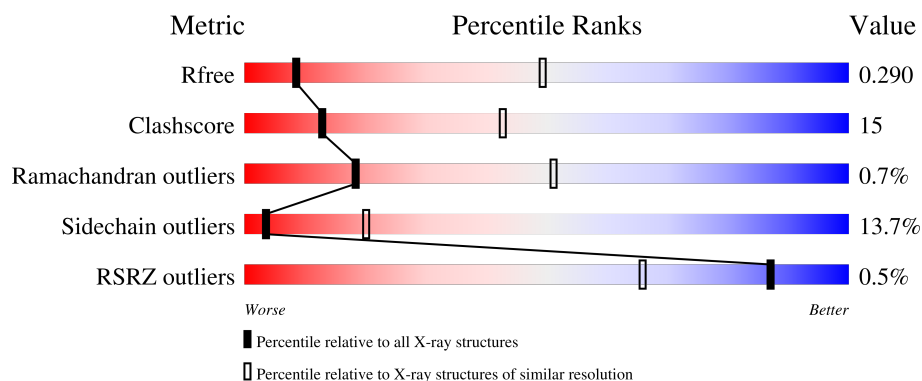
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.59 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	1521 (3.66-3.50)
Clashscore	190562	1595 (3.66-3.50)
Ramachandran outliers	187476	1551 (3.66-3.50)
Sidechain outliers	187428	1551 (3.66-3.50)
RSRZ outliers	180081	1520 (3.66-3.50)

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 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	239	
1	B	239	
1	G	239	
1	H	239	
2	C	1342	

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Mol	Chain	Length	Quality of chain
2	I	1342	% 62%31%6% •
3	D	1407	48%29%6% •17%
3	J	1407	% 54%33%7%6%
4	E	91	60%31%5% ••
4	K	91	52%27%8%13%
5	F	522	% 57%25%6% •10%
5	L	522	56%26%6% •10%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 56339 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	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	-	expression tag	UNP C9QXI7
A	236	VAL	-	expression tag	UNP C9QXI7
A	237	LEU	-	expression tag	UNP C9QXI7
A	238	PHE	-	expression tag	UNP C9QXI7
A	239	GLN	-	expression tag	UNP C9QXI7
B	235	GLU	-	expression tag	UNP C9QXI7
B	236	VAL	-	expression tag	UNP C9QXI7
B	237	LEU	-	expression tag	UNP C9QXI7
B	238	PHE	-	expression tag	UNP C9QXI7
B	239	GLN	-	expression tag	UNP C9QXI7
G	235	GLU	-	expression tag	UNP C9QXI7
G	236	VAL	-	expression tag	UNP C9QXI7
G	237	LEU	-	expression tag	UNP C9QXI7
G	238	PHE	-	expression tag	UNP C9QXI7
G	239	GLN	-	expression tag	UNP C9QXI7
H	235	GLU	-	expression tag	UNP C9QXI7
H	236	VAL	-	expression tag	UNP C9QXI7
H	237	LEU	-	expression tag	UNP C9QXI7
H	238	PHE	-	expression tag	UNP C9QXI7
H	239	GLN	-	expression tag	UNP C9QXI7

- 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	1325	Total	C	N	O	S	0	0	0
			10295	6470	1831	1945	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	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 MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

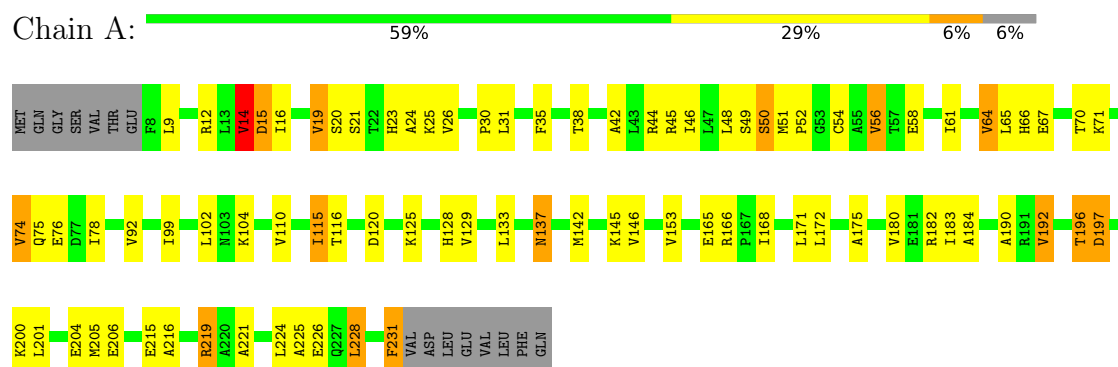
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

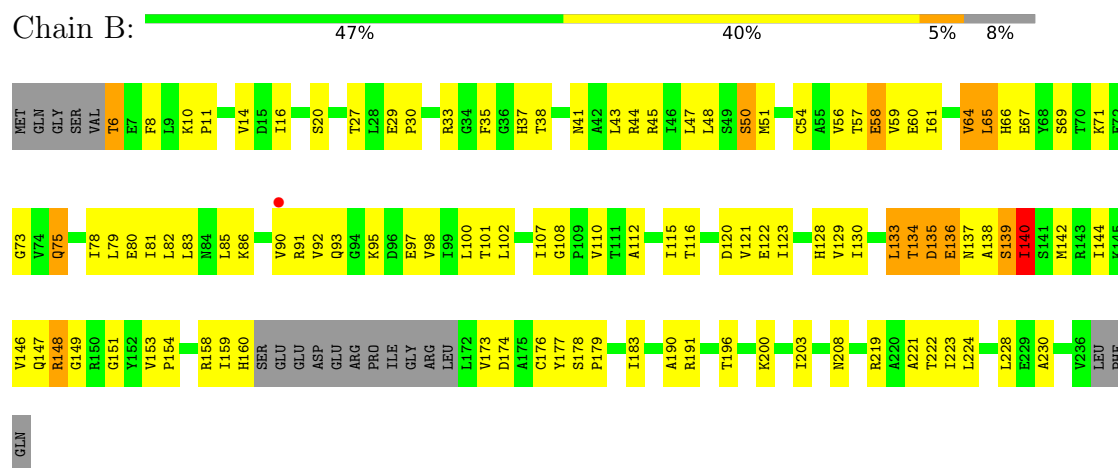
3 Residue-property plots

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.

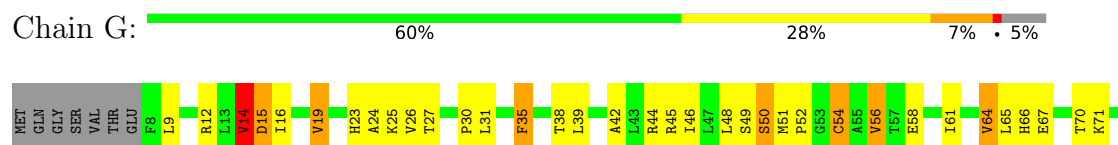
• Molecule 1: DNA-directed RNA polymerase subunit alpha

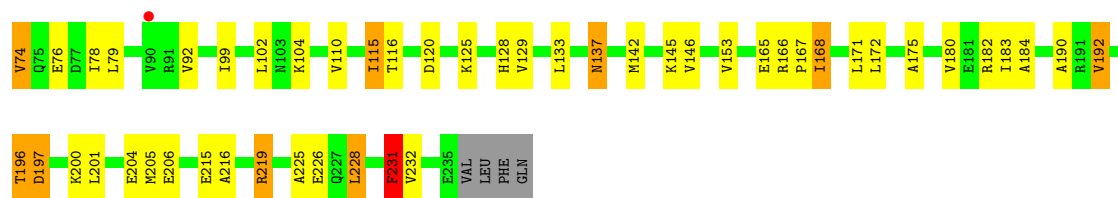


• Molecule 1: DNA-directed RNA polymerase subunit alpha



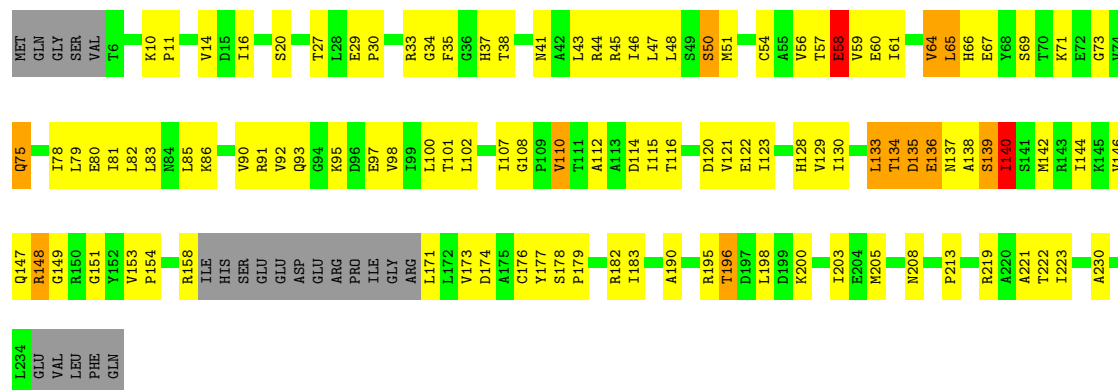
• Molecule 1: DNA-directed RNA polymerase subunit alpha





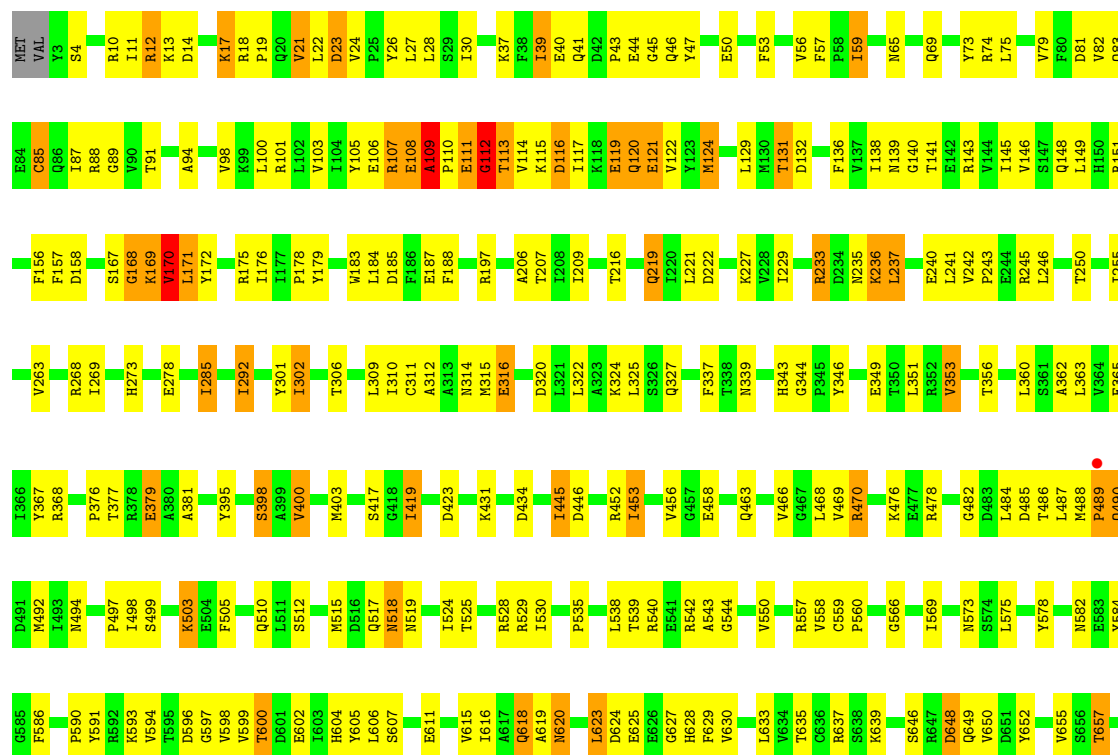
• Molecule 1: DNA-directed RNA polymerase subunit alpha

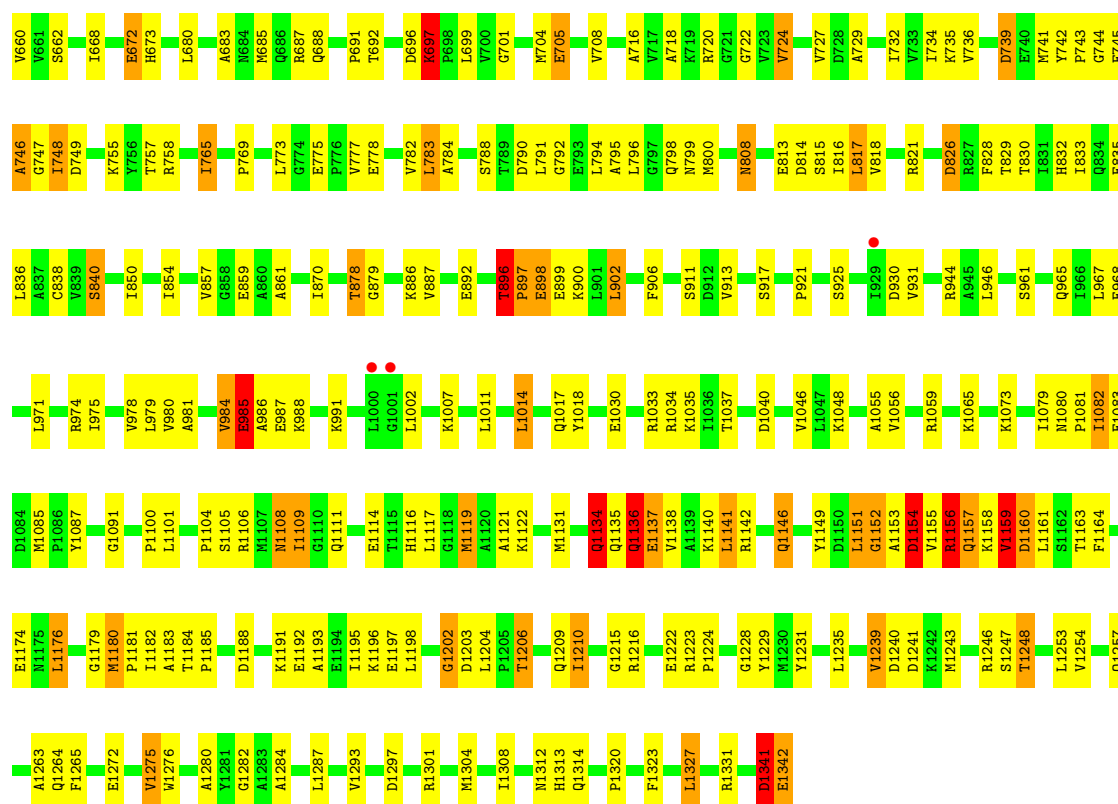
Chain H: 45% 40% 5% 9%



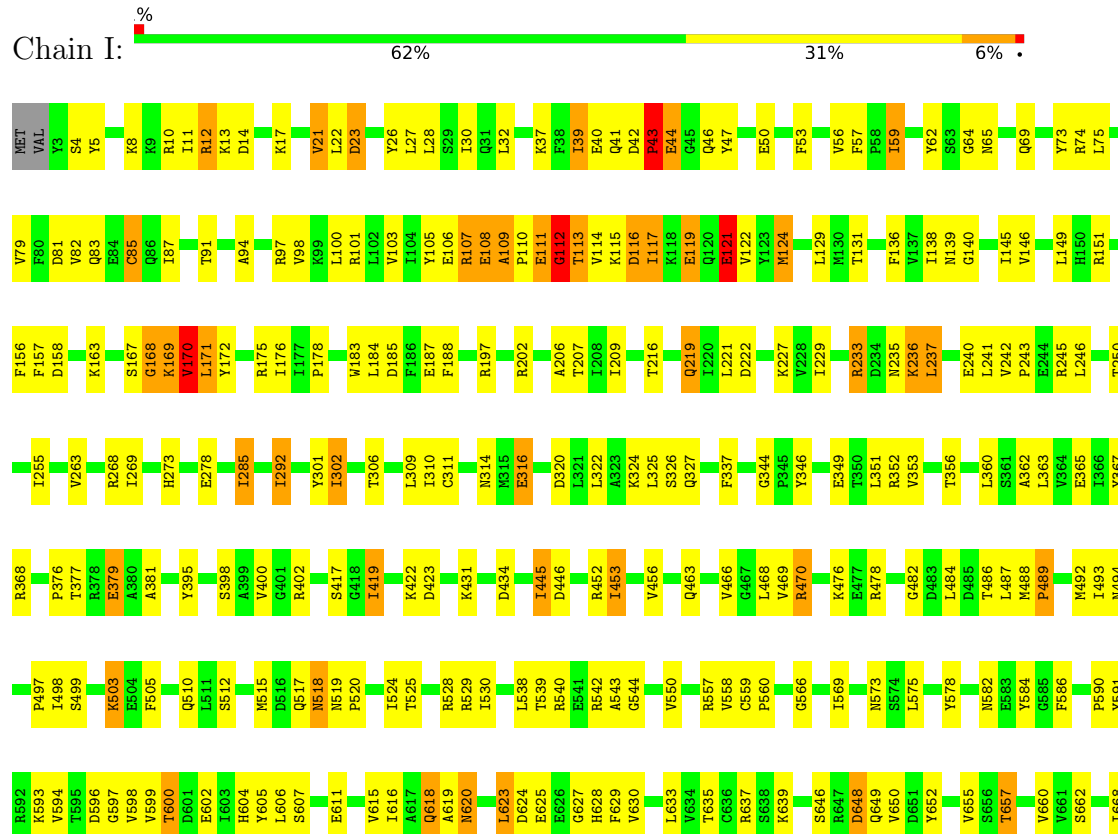
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C: 61% 32% 6%



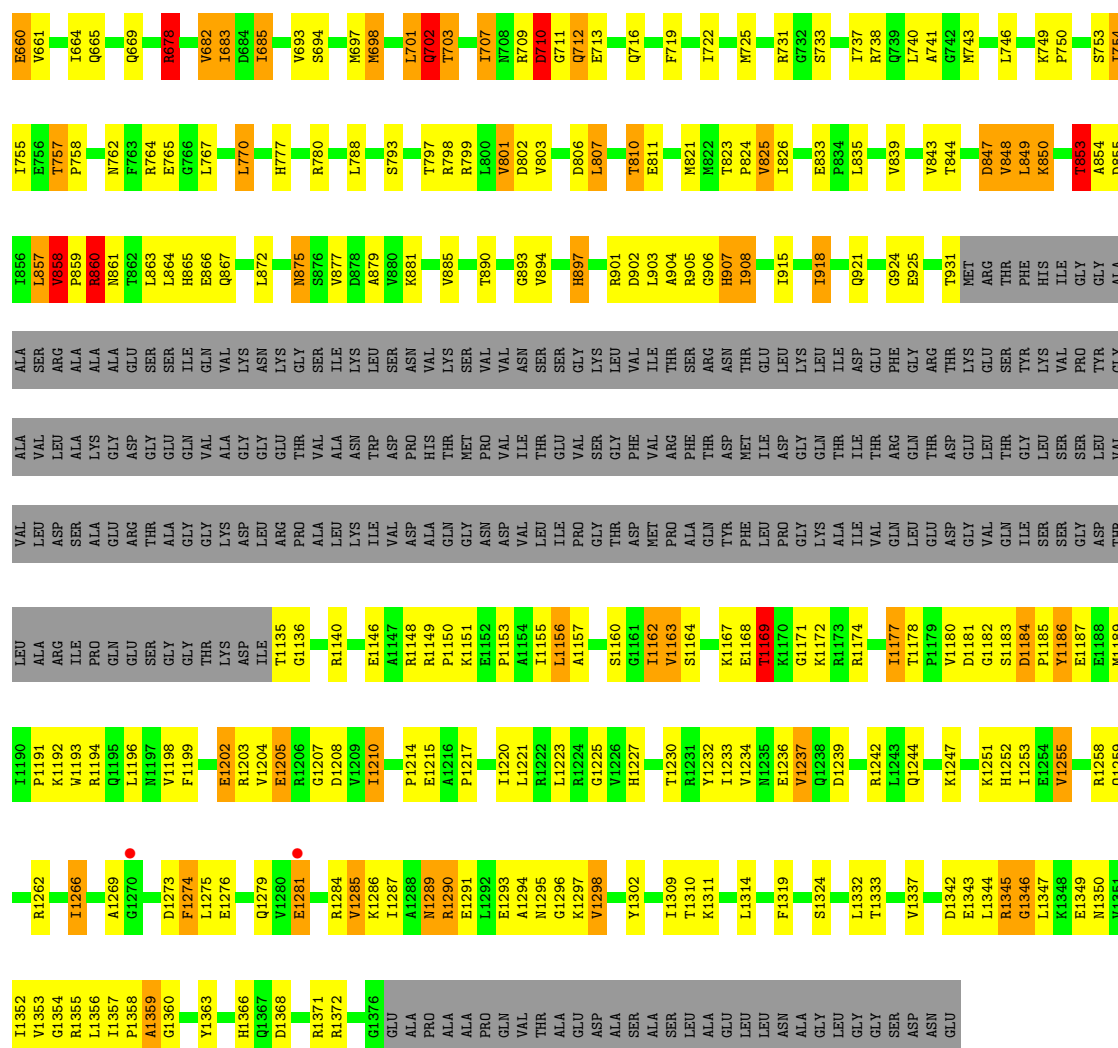


• Molecule 2: DNA-directed RNA polymerase subunit beta

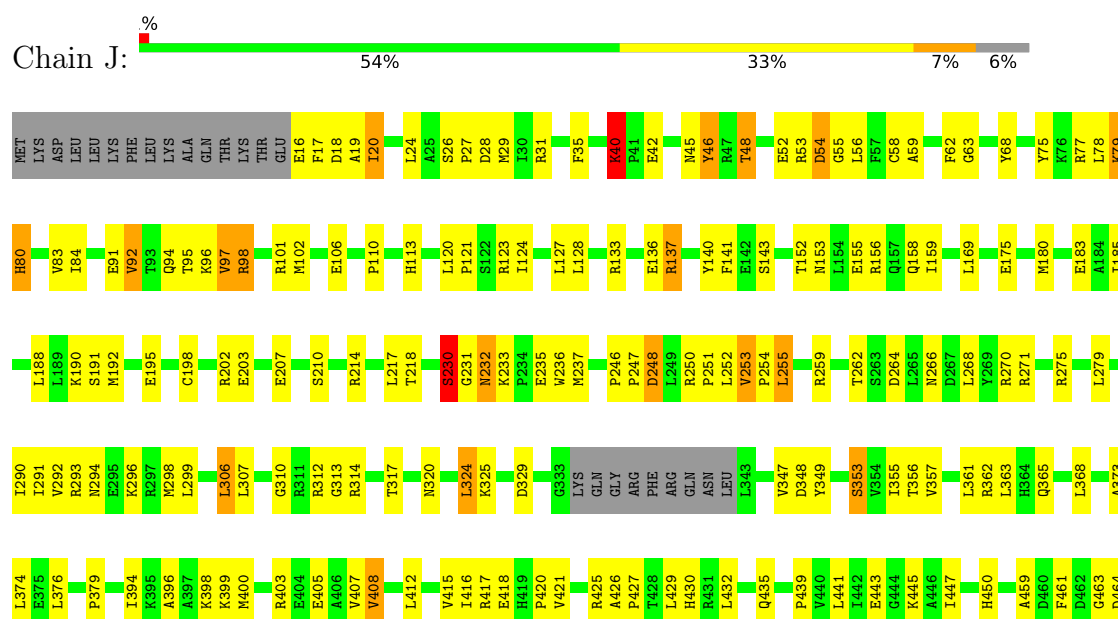




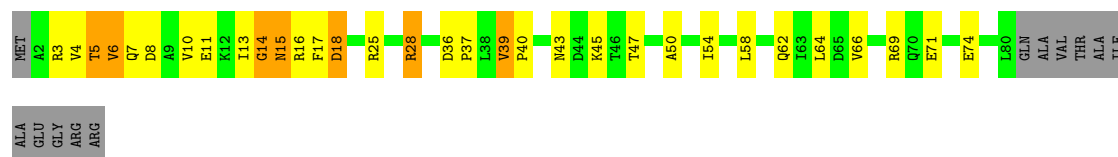
L569	Q477	K296	L188	V92	MET
T573	A452	K297	L189	T93	LYS
V574	L483	K298	K190	Q94	ASP
G575	M484	K395	S191	T95	LEU
R576	M485	L306	M192	K96	LEU
A577		L307	E203	V97	LYS
L578	M488	M400		R98	PHE
L579	M489	G310	E207	R101	L8
	L490	R311		M102	K9
L582	L491	E404	S210		Q11
		E405		E106	T12
K586	E497	A406	R214		
G586	P498	V407		P110	D18
L587	L499	V408	L217		A19
	I500	V409	T218	H113	I20
N593	V501	R320			
Q594		L412	S236	L120	L24
L596	Q504	V415	G231	P121	A25
	V506	D505	S122	R123	S26
K599		R417	R233		P27
A600	M513	E418	P234		D28
	T514	E419	E235	L127	N29
K603	R515	P420	R236	L128	T30
	D516	V421	K237		R31
G608	C517		P246	R133	
V609	V518	R425	P247	E136	F35
R610	M519	R339	R248	R137	
I611		P427	L249		K40
L612	E523	T428	R250	Y140	P41
G613	G524	L429	P251	F141	
K614	M525	H430	L252	E142	
G615	V526	R431	V253	S143	N45
P616	L527	L432	P254	R47	Y46
T617	T528	D348	L255	T152	R47
	G529	Y349		N153	T48
F620			R259		
	E532	S353	L154	E155	E52
I624		V354	T262	R156	R53
	R536	L355	S263	Q157	D54
G628	L536	T356	D264	Q158	G55
		V357	L265	I159	
A632	L544	L447	K266	L160	C58
A633	H545	R361	D267	T161	A59
S635	V548	L268	V269	Q164	
	K549	R363	R270		F62
I641	V550	H364	R271	L169	G63
		D460			Y68
V645		F461			
I646	E556	D462	R275	F172	Y75
P647	K557	G463			K76
	D558	D464	L279	E175	R77
K650	A559	G465			L78
	M560	M466	A373	M180	K79
I654	L563	L472	L374	E183	H80
		E375	L376		
					V63
E558	T567	T473	P379	I185	I84
	V568	L474	R390		



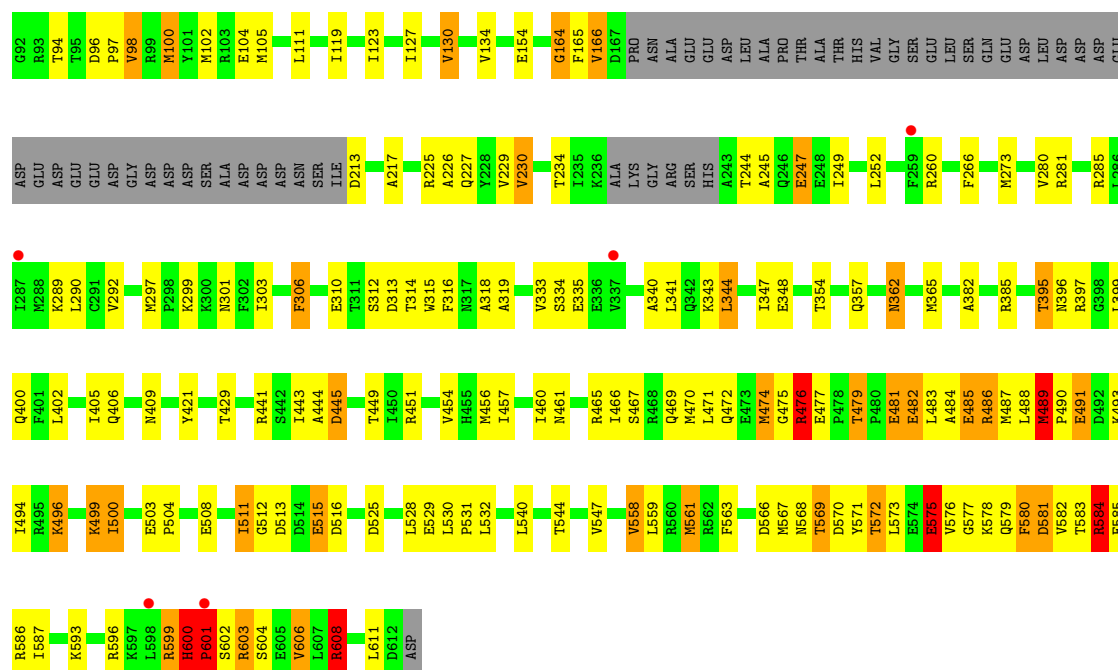
• Molecule 3: DNA-directed RNA polymerase subunit beta'



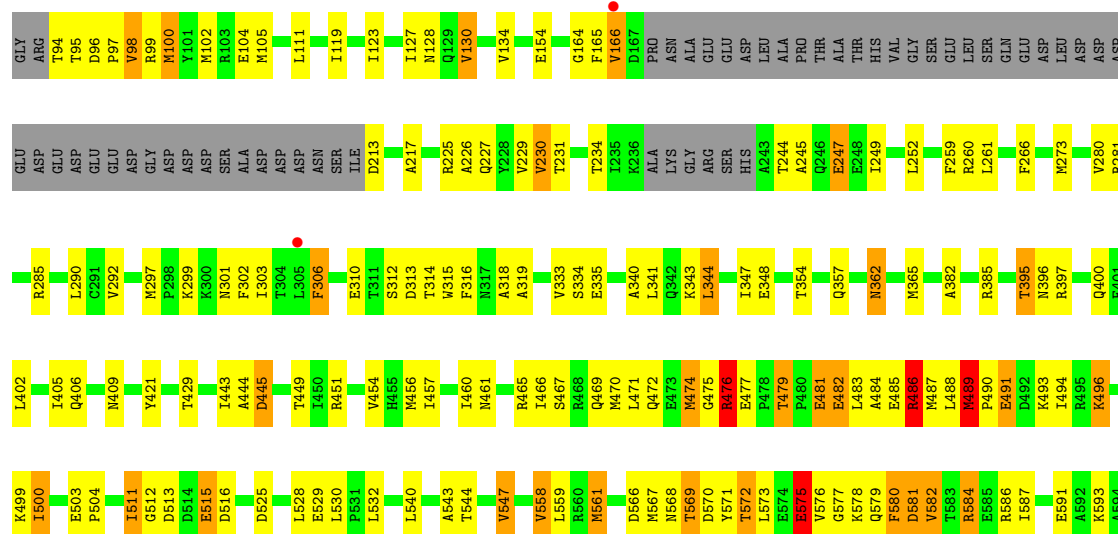




• Molecule 5: RNA polymerase sigma factor RpoD



• Molecule 5: RNA polymerase sigma factor RpoD



L595	R596	R597	L598	R599	H600	R601	S602	R603	V606	L607	R608	L611	D612	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	186.37Å 206.74Å 309.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 3.59 29.88 – 3.59	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.88-3.59) 99.1 (29.88-3.59)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 3.56Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.246 , 0.288 0.244 , 0.290	Depositor DCC
R_{free} test set	6979 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	122.5	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	56339	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.88% 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

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	0.39	0/1751	0.93	4/2373 (0.2%)
1	B	0.39	0/1707	0.93	7/2314 (0.3%)
1	G	0.42	1/1771 (0.1%)	0.94	4/2401 (0.2%)
1	H	0.40	0/1686	0.94	7/2285 (0.3%)
2	C	0.40	0/10739	0.96	42/14489 (0.3%)
2	I	0.40	0/10735	0.94	35/14484 (0.2%)
3	D	0.40	0/9246	0.93	35/12478 (0.3%)
3	J	0.38	0/10450	0.90	29/14112 (0.2%)
4	E	0.38	0/693	0.89	1/935 (0.1%)
4	K	0.39	0/629	0.87	0/847
5	F	0.48	4/3873 (0.1%)	0.97	17/5206 (0.3%)
5	L	0.48	2/3872 (0.1%)	0.97	13/5205 (0.2%)
All	All	0.41	7/57152 (0.0%)	0.94	194/77129 (0.3%)

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
1	B	0	1
1	G	0	1
1	H	0	1
2	C	0	14
2	I	0	15
3	D	0	5
3	J	0	6
4	K	0	1
5	F	0	4
5	L	0	2
All	All	0	50

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	600	HIS	CA-C	7.35	1.62	1.52
5	F	600	HIS	N-CA	6.30	1.57	1.45
1	G	231	PHE	CA-C	5.89	1.60	1.52
5	F	600	HIS	CA-C	5.61	1.61	1.53
5	F	601	PRO	CA-CB	-5.26	1.46	1.53

The worst 5 of 194 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	747	GLY	N-CA-C	21.85	142.76	112.17
2	C	109	ALA	CA-C-N	15.46	136.52	119.83
2	C	109	ALA	C-N-CA	15.46	136.52	119.83
2	C	747	GLY	N-CA-C	15.37	149.61	113.18
2	C	490	GLN	N-CA-C	12.74	128.28	112.23

There are no chirality outliers.

5 of 50 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	140	ILE	Peptide
2	C	109	ALA	Peptide
2	C	111	GLU	Peptide
2	C	112	GLY	Peptide
2	C	43	PRO	Mainchain

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	1730	0	1756	56	0
1	B	1687	0	1700	70	0
1	G	1750	0	1764	54	0
1	H	1667	0	1689	71	0
2	C	10570	0	10582	317	1
2	I	10566	0	10576	297	1
3	D	9107	0	9308	338	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	10295	0	10511	398	0
4	E	691	0	695	23	0
4	K	627	0	634	19	0
5	F	3822	0	3885	104	0
5	L	3821	0	3884	112	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
All	All	56339	0	56984	1715	1

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 15.

The worst 5 of 1715 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:233:ARG:HH11	2:C:233:ARG:HG3	1.24	1.02
3:D:26:SER:HA	3:D:236:TRP:HE1	1.30	0.96
3:J:98:ARG:HG2	3:J:98:ARG:HH11	1.32	0.94
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.51	0.93
3:J:660:GLU:HB3	3:J:685:ILE:HD12	1.51	0.92

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:108:GLU:OE2	2:I:422:LYS:NZ[3_554]	2.19	0.01

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%)	195 (88%)	26 (12%)	1 (0%)	24	57
1	B	216/239 (90%)	192 (89%)	23 (11%)	1 (0%)	24	57
1	G	226/239 (95%)	197 (87%)	27 (12%)	2 (1%)	14	46
1	H	213/239 (89%)	191 (90%)	21 (10%)	1 (0%)	24	57
2	C	1338/1342 (100%)	1224 (92%)	100 (8%)	14 (1%)	12	44
2	I	1338/1342 (100%)	1228 (92%)	97 (7%)	13 (1%)	12	44
3	D	1162/1407 (83%)	1078 (93%)	78 (7%)	6 (0%)	24	57
3	J	1317/1407 (94%)	1225 (93%)	87 (7%)	5 (0%)	30	60
4	E	87/91 (96%)	76 (87%)	10 (12%)	1 (1%)	11	43
4	K	77/91 (85%)	72 (94%)	4 (5%)	1 (1%)	9	39
5	F	464/522 (89%)	420 (90%)	41 (9%)	3 (1%)	21	54
5	L	463/522 (89%)	422 (91%)	36 (8%)	5 (1%)	11	43
All	All	7123/7680 (93%)	6520 (92%)	550 (8%)	53 (1%)	18	51

5 of 53 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	44	GLU
2	C	169	LYS
2	C	697	LYS
2	C	897	PRO
2	C	898	GLU

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%)	164 (86%)	27 (14%)	3	19
1	B	184/206 (89%)	154 (84%)	30 (16%)	2	14
1	G	191/206 (93%)	164 (86%)	27 (14%)	3	19
1	H	183/206 (89%)	156 (85%)	27 (15%)	3	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	1155/1157 (100%)	1007 (87%)	148 (13%)	4	22
2	I	1154/1157 (100%)	1006 (87%)	148 (13%)	4	22
3	D	975/1168 (84%)	842 (86%)	133 (14%)	3	20
3	J	1110/1168 (95%)	961 (87%)	149 (13%)	4	21
4	E	72/75 (96%)	63 (88%)	9 (12%)	4	23
4	K	67/75 (89%)	58 (87%)	9 (13%)	4	21
5	F	417/462 (90%)	352 (84%)	65 (16%)	2	16
5	L	418/462 (90%)	351 (84%)	67 (16%)	2	15
All	All	6117/6548 (93%)	5278 (86%)	839 (14%)	3	20

5 of 839 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	196	THR
2	I	1037	THR
5	L	479	THR
2	I	82	VAL
1	H	183	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 91 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	1017	GLN
3	J	897	HIS
2	I	1136	GLN
3	J	469	HIS
3	J	1049	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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%)	-0.44	0 100 100	59, 91, 130, 167	0
1	B	220/239 (92%)	-0.21	1 (0%) 87 66	63, 125, 155, 166	0
1	G	228/239 (95%)	-0.30	1 (0%) 88 70	85, 121, 148, 164	0
1	H	217/239 (90%)	-0.22	0 100 100	90, 130, 156, 165	0
2	C	1340/1342 (99%)	-0.36	4 (0%) 90 74	33, 84, 134, 170	0
2	I	1340/1342 (99%)	-0.31	9 (0%) 84 60	48, 101, 149, 179	0
3	D	1166/1407 (82%)	-0.40	4 (0%) 90 74	28, 77, 137, 168	0
3	J	1325/1407 (94%)	-0.33	8 (0%) 85 63	40, 96, 152, 176	0
4	E	89/91 (97%)	-0.53	0 100 100	44, 84, 114, 133	0
4	K	79/91 (86%)	-0.38	0 100 100	63, 97, 136, 150	0
5	F	470/522 (90%)	-0.21	5 (1%) 78 51	53, 119, 159, 181	0
5	L	469/522 (89%)	-0.29	2 (0%) 88 70	61, 117, 159, 173	0
All	All	7167/7680 (93%)	-0.33	34 (0%) 87 66	28, 97, 150, 181	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	1017	VAL	3.5
5	F	287	ILE	3.3
3	D	341	ASN	3.3
3	D	340	GLN	3.3
2	C	1000	LEU	3.1

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
6	MG	D	1501	1/1	0.84	0.14	78,78,78,78	0
6	MG	J	1501	1/1	0.87	0.09	89,89,89,89	0
7	ZN	J	1503	1/1	0.90	0.24	316,316,316,316	0
7	ZN	J	1502	1/1	0.95	0.19	314,314,314,314	0
7	ZN	D	1503	1/1	0.97	0.14	114,114,114,114	0
7	ZN	D	1502	1/1	0.98	0.15	198,198,198,198	0

6.5 Other polymers [i](#)

There are no such residues in this entry.