



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 08:09 am GMT

PDB ID : 4LJZ
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

<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
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

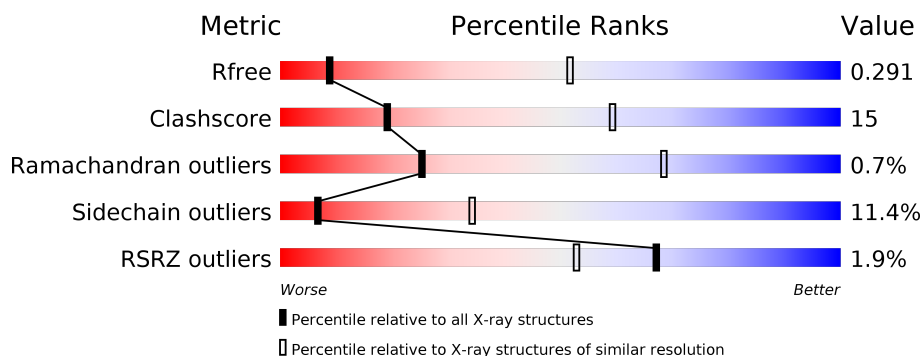
1 Overall quality at a glance

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}	100719	1009 (3.70-3.46)
Clashscore	112137	1128 (3.70-3.46)
Ramachandran outliers	110173	1088 (3.70-3.46)
Sidechain outliers	110143	1088 (3.70-3.46)
RSRZ outliers	101464	1034 (3.70-3.46)

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>60%</div> <div>29%</div> <div>• 6%</div> </div>
1	B	239	<div>4%</div> <div>50%</div> <div>38%</div> <div>• 8%</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	522	
5	L	522	

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
7	ZN	J	1503	-	-	-	X

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 (three-letter code: MG) (formula: Mg).

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

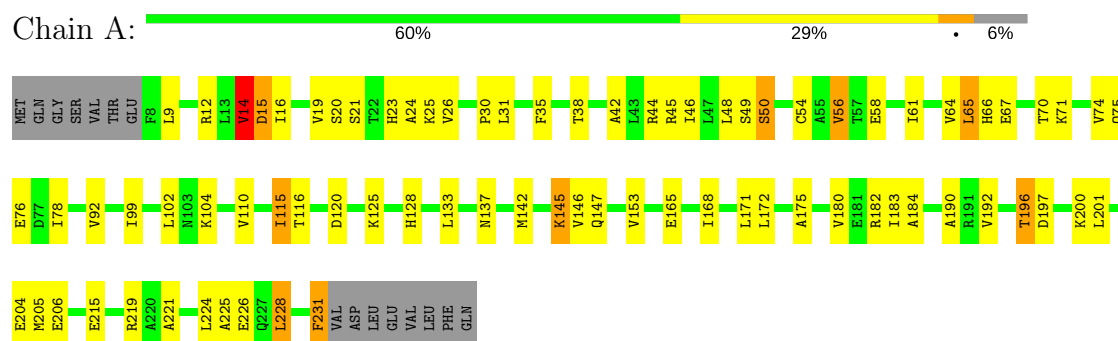
- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

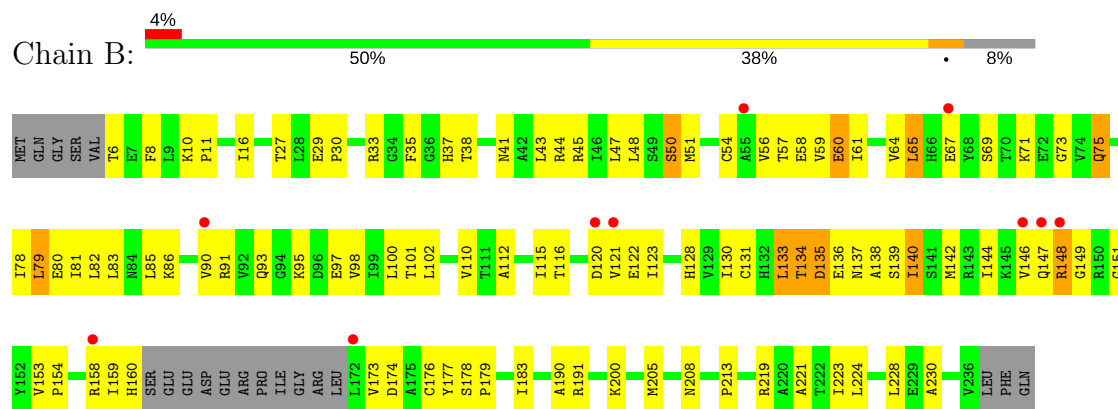
3 Residue-property plots [i](#)

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.

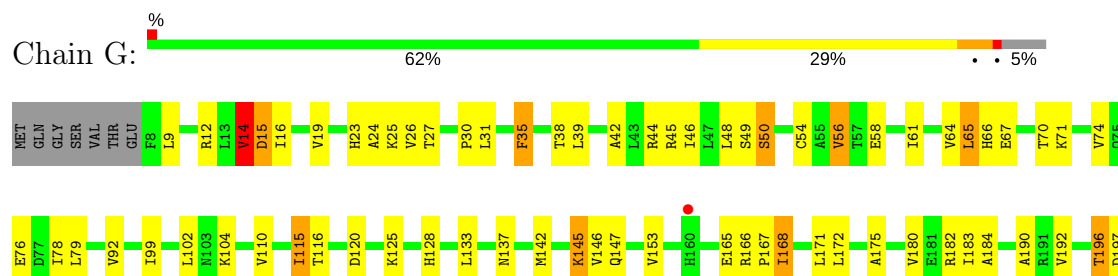
• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 1: DNA-directed RNA polymerase subunit alpha

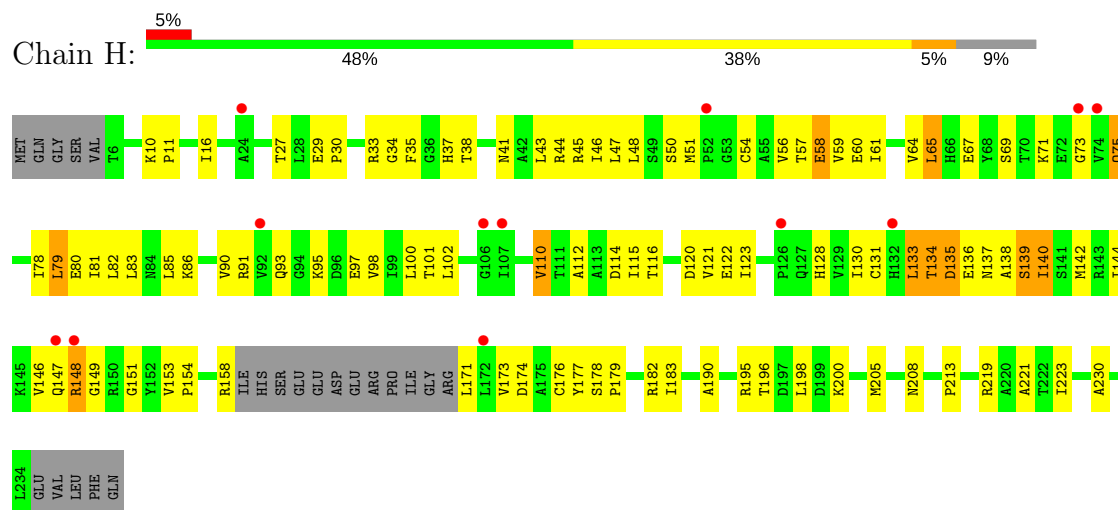


• Molecule 1: DNA-directed RNA polymerase subunit alpha

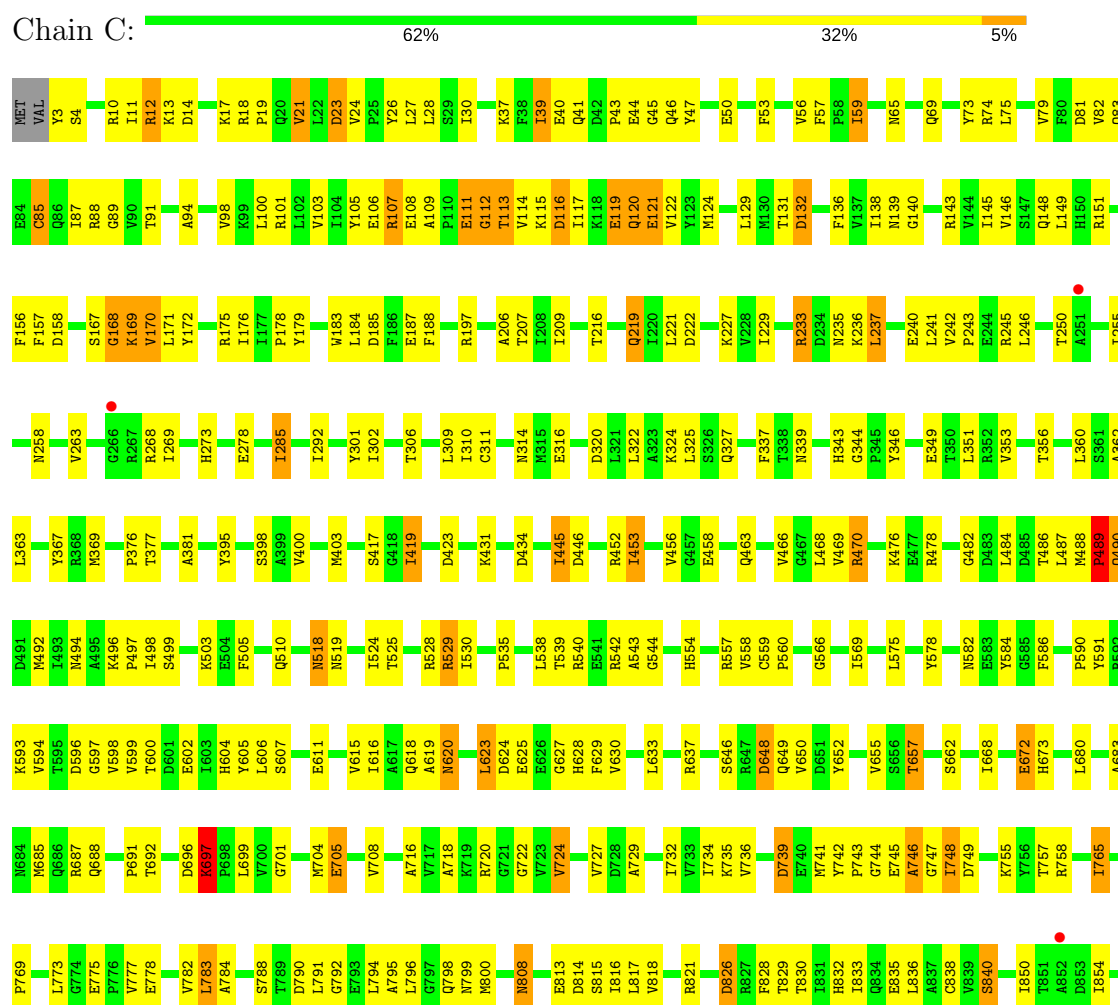


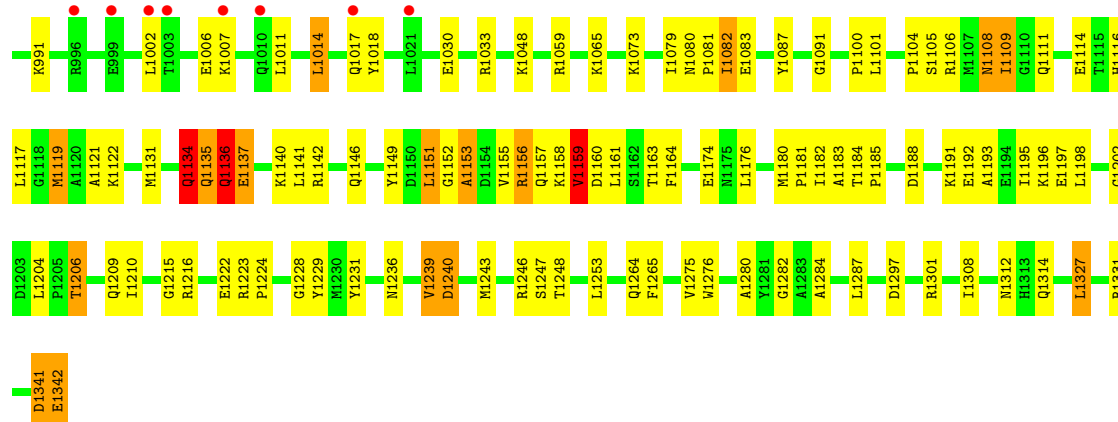


• Molecule 1: DNA-directed RNA polymerase subunit alpha

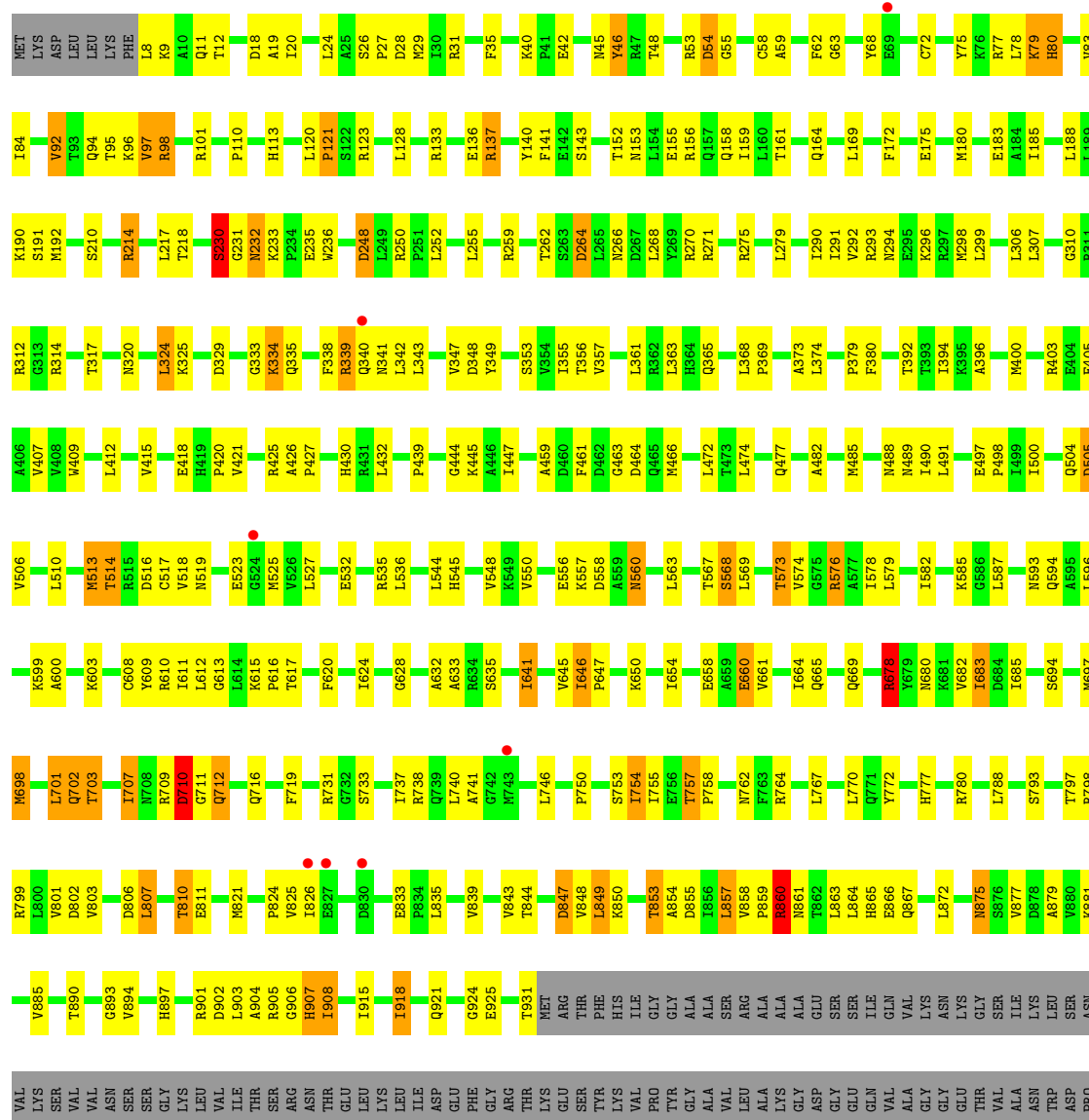


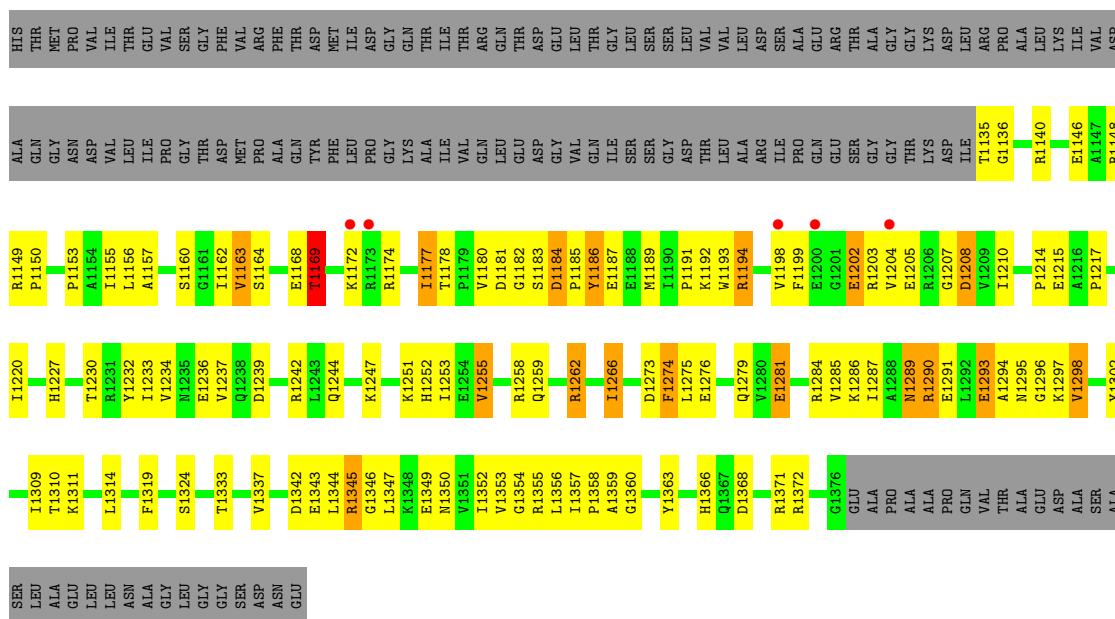
• Molecule 2: DNA-directed RNA polymerase subunit beta



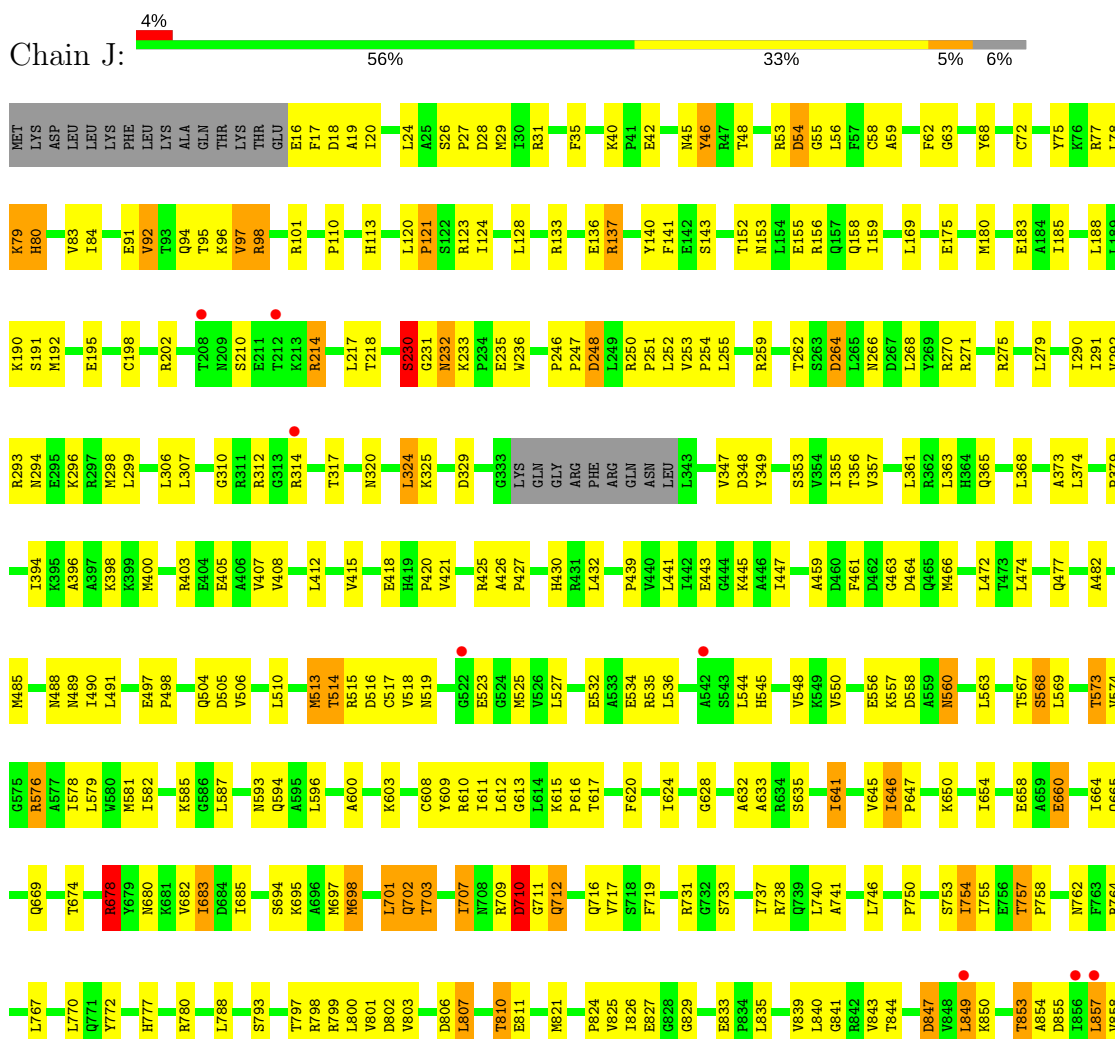


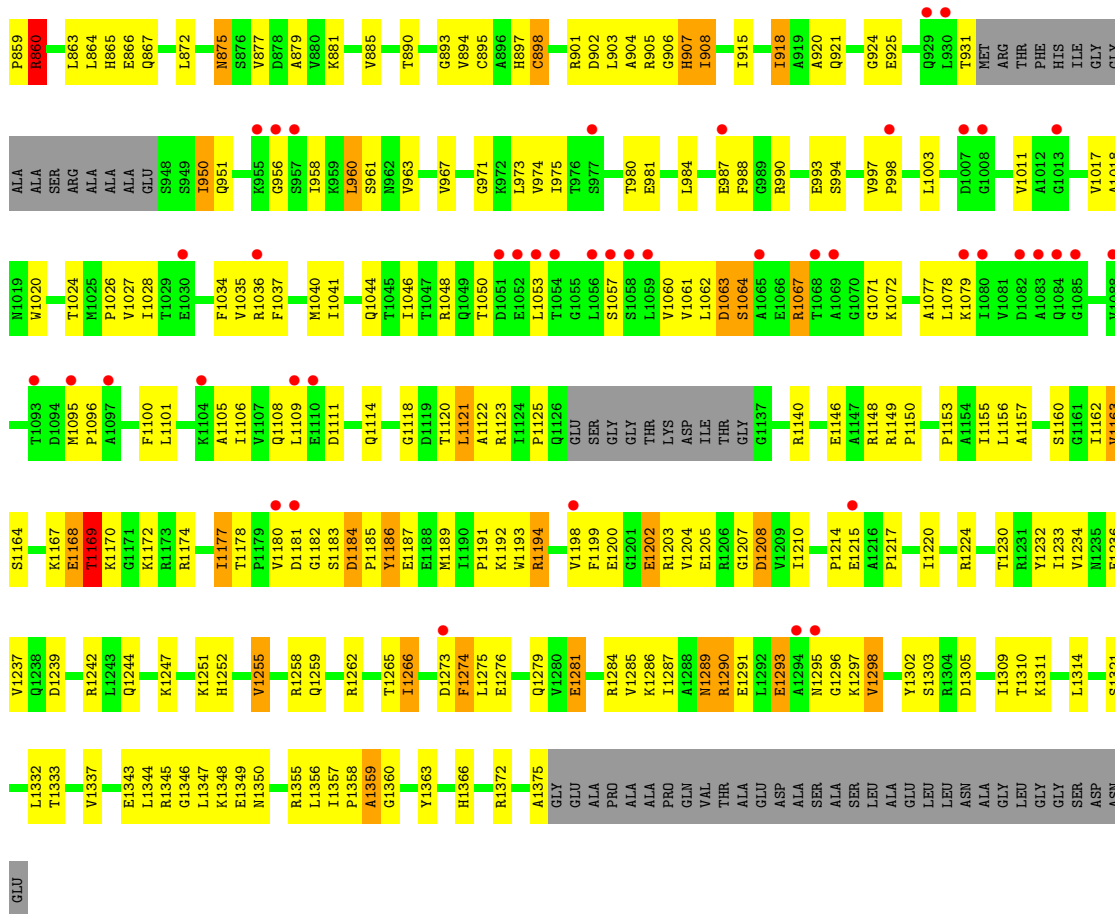
• Molecule 3: DNA-directed RNA polymerase subunit beta'



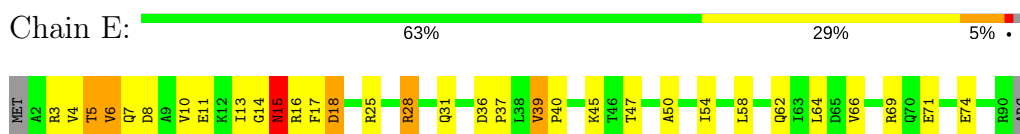


- Molecule 3: DNA-directed RNA polymerase subunit beta'

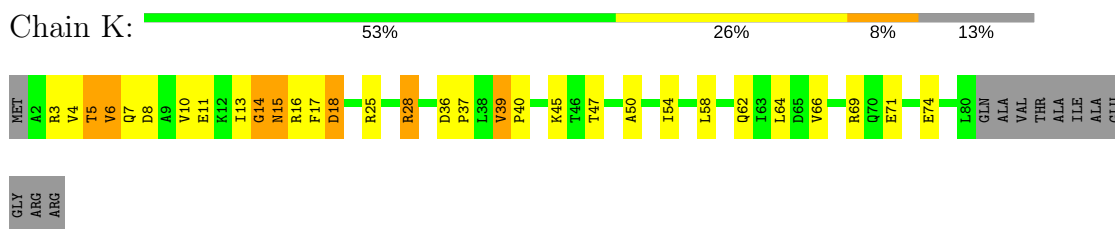




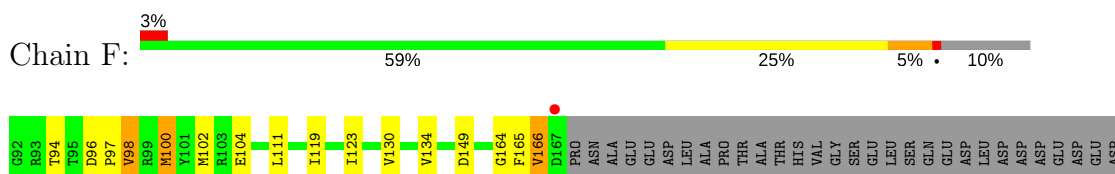
- Molecule 4: DNA-directed RNA polymerase subunit omega

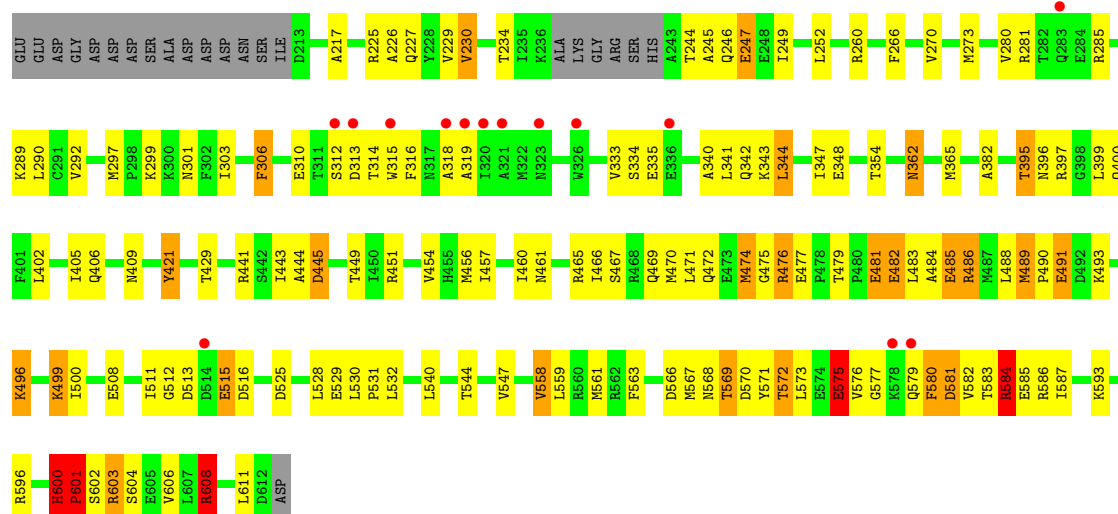


- Molecule 4: DNA-directed RNA polymerase subunit omega

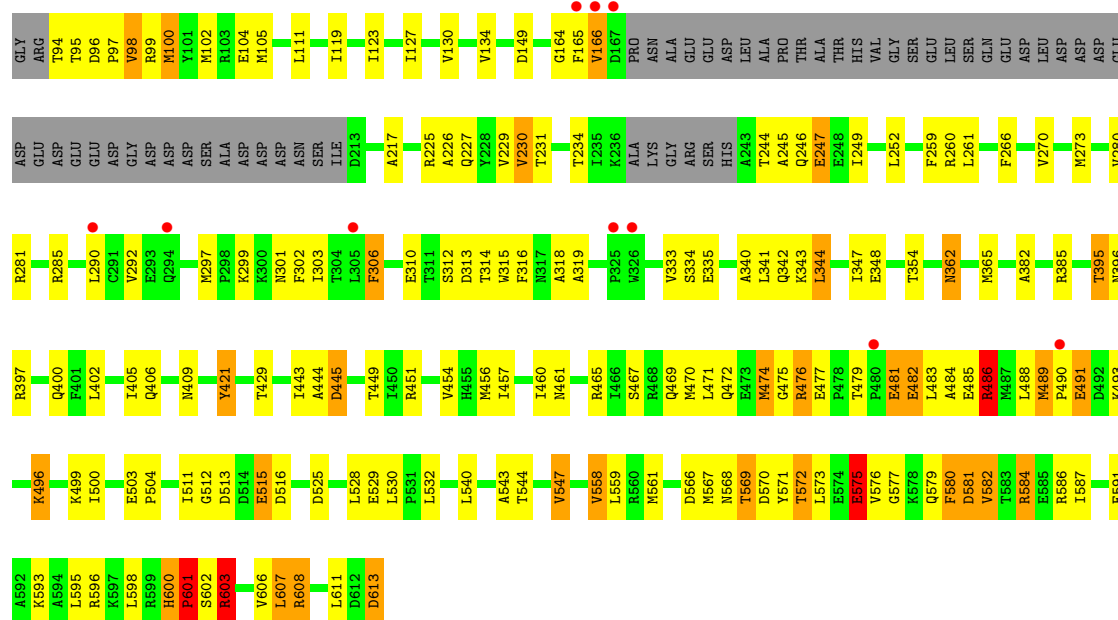


- Molecule 5: RNA polymerase sigma factor RpoD





• 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	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) 99.3 (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 (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.246 , 0.288 0.246 , 0.291	Depositor DCC
R_{free} test set	6970 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	122.5	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 48.3	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: 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	0.28	0/1751	0.59	1/2373 (0.0%)
1	B	0.28	0/1707	0.58	1/2314 (0.0%)
1	G	0.30	0/1771	0.61	2/2401 (0.1%)
1	H	0.28	0/1686	0.59	1/2285 (0.0%)
2	C	0.30	0/10739	0.59	6/14489 (0.0%)
2	I	0.30	0/10735	0.58	7/14484 (0.0%)
3	D	0.28	0/9246	0.59	5/12478 (0.0%)
3	J	0.28	0/10450	0.56	2/14112 (0.0%)
4	E	0.27	0/693	0.58	1/935 (0.1%)
4	K	0.28	0/629	0.54	0/847
5	F	0.36	1/3873 (0.0%)	0.62	7/5206 (0.1%)
5	L	0.35	0/3872	0.63	6/5205 (0.1%)
All	All	0.30	1/57152 (0.0%)	0.59	39/77129 (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
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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	600	HIS	N-CA	5.34	1.57	1.46

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	747	GLY	N-CA-C	14.60	149.61	113.10
2	I	747	GLY	N-CA-C	11.86	142.76	113.10
3	D	1262	ARG	NE-CZ-NH1	-7.19	116.70	120.30
2	I	112	GLY	N-CA-C	6.85	130.22	113.10
3	D	860	ARG	NE-CZ-NH1	6.80	123.70	120.30

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 ⓘ

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	54	0
1	B	1687	0	1700	70	0
1	G	1750	0	1764	52	0
1	H	1667	0	1689	71	0
2	C	10570	0	10582	305	1
2	I	10566	0	10576	284	1
3	D	9107	0	9308	331	0
3	J	10295	0	10511	386	0
4	E	691	0	695	21	0
4	K	627	0	634	18	0
5	F	3822	0	3885	98	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	3821	0	3884	106	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	1652	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 1652 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:HH11	3:J:98:ARG:HG2	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%)	32	73
1	B	216/239 (90%)	192 (89%)	23 (11%)	1 (0%)	32	73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	226/239 (95%)	197 (87%)	27 (12%)	2 (1%)	20	64
1	H	213/239 (89%)	191 (90%)	21 (10%)	1 (0%)	32	73
2	C	1338/1342 (100%)	1224 (92%)	100 (8%)	14 (1%)	18	62
2	I	1338/1342 (100%)	1228 (92%)	97 (7%)	13 (1%)	18	62
3	D	1162/1407 (83%)	1078 (93%)	78 (7%)	6 (0%)	32	73
3	J	1317/1407 (94%)	1225 (93%)	87 (7%)	5 (0%)	38	76
4	E	87/91 (96%)	76 (87%)	10 (12%)	1 (1%)	17	61
4	K	77/91 (85%)	72 (94%)	4 (5%)	1 (1%)	14	57
5	F	464/522 (89%)	420 (90%)	41 (9%)	3 (1%)	28	70
5	L	463/522 (89%)	422 (91%)	36 (8%)	5 (1%)	17	61
All	All	7123/7680 (93%)	6520 (92%)	550 (8%)	53 (1%)	25	68

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%)	169 (88%)	22 (12%)	6	34
1	B	184/206 (89%)	161 (88%)	23 (12%)	5	30
1	G	191/206 (93%)	169 (88%)	22 (12%)	6	34
1	H	183/206 (89%)	164 (90%)	19 (10%)	8	39
2	C	1155/1157 (100%)	1025 (89%)	130 (11%)	7	35
2	I	1154/1157 (100%)	1022 (89%)	132 (11%)	7	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	975/1168 (84%)	870 (89%)	105 (11%)	7	37
3	J	1110/1168 (95%)	996 (90%)	114 (10%)	8	39
4	E	72/75 (96%)	63 (88%)	9 (12%)	5	30
4	K	67/75 (89%)	58 (87%)	9 (13%)	4	27
5	F	417/462 (90%)	361 (87%)	56 (13%)	4	27
5	L	418/462 (90%)	359 (86%)	59 (14%)	4	26
All	All	6117/6548 (93%)	5417 (89%)	700 (11%)	7	34

5 of 700 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	476	ARG
2	I	23	ASP
5	L	246	GLN
5	F	515	GLU
1	G	64	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	406	GLN
2	I	628	HIS
5	L	396	ASN
5	F	579	GLN
1	H	66	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 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

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%)	-0.35	0 100 100	59, 91, 130, 167	0
1	B	220/239 (92%)	0.12	10 (4%) 34 24	63, 125, 155, 166	0
1	G	228/239 (95%)	-0.15	2 (0%) 84 72	85, 121, 148, 164	0
1	H	217/239 (90%)	0.13	12 (5%) 26 18	90, 130, 156, 165	0
2	C	1340/1342 (99%)	-0.35	5 (0%) 92 86	33, 84, 134, 170	0
2	I	1340/1342 (99%)	-0.17	21 (1%) 72 58	48, 101, 149, 179	0
3	D	1166/1407 (82%)	-0.26	12 (1%) 82 70	28, 77, 137, 168	0
3	J	1325/1407 (94%)	-0.05	52 (3%) 40 28	40, 96, 152, 176	0
4	E	89/91 (97%)	-0.51	0 100 100	44, 84, 114, 133	0
4	K	79/91 (86%)	-0.31	0 100 100	63, 97, 136, 150	0
5	F	470/522 (90%)	-0.08	15 (3%) 48 35	53, 119, 159, 181	0
5	L	469/522 (89%)	-0.12	10 (2%) 64 49	61, 117, 159, 173	0
All	All	7167/7680 (93%)	-0.18	139 (1%) 67 53	28, 97, 150, 181	0

The worst 5 of 139 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	167	ASP	9.2
1	B	172	LEU	7.5
5	L	167	ASP	7.2
2	I	999	GLU	5.9
3	J	1054	THR	5.8

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
7	ZN	J	1503	1/1	0.41	0.43	4.33	316,316,316,316	0
7	ZN	J	1502	1/1	0.91	0.30	0.93	314,314,314,314	0
7	ZN	D	1503	1/1	0.88	0.28	0.64	114,114,114,114	0
7	ZN	D	1502	1/1	0.95	0.21	-0.53	198,198,198,198	0
6	MG	J	1501	1/1	0.87	0.22	-	89,89,89,89	0
6	MG	D	1501	1/1	0.83	0.41	-	78,78,78,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.