



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 13, 2017 – 07:49 PM EDT

PDB ID : 5UAC
Title : Escherichia coli RNA polymerase and Rifampin complex, wild-type
Authors : Molodtsov, V.; Scharf, N.T.; Stefan, M.A.; Garcia, G.A.; Murakami, K.S.
Deposited on : unknown
Resolution : 3.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
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)	:	rb-20029824

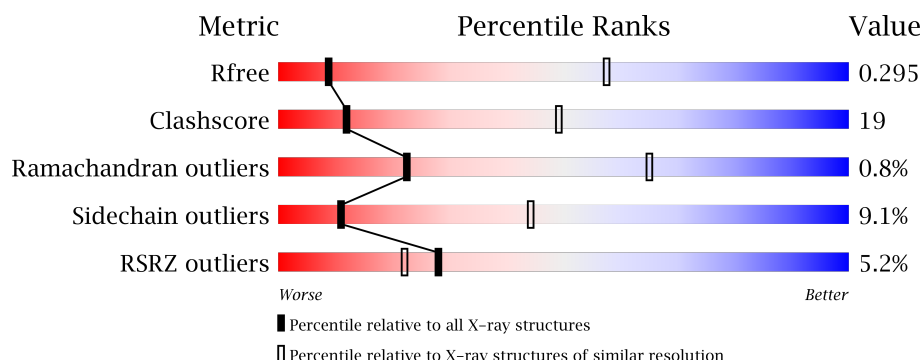
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	1019 (4.08-3.52)
Clashscore	112137	1030 (4.04-3.56)
Ramachandran outliers	110173	1011 (4.06-3.54)
Sidechain outliers	110143	1005 (4.06-3.54)
RSRZ outliers	101464	1032 (4.08-3.52)

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	329	<div> <div>0.1%</div> <div> <div>40%</div> <div>26%</div> <div>•</div> <div>31%</div> </div> </div>
1	B	329	<div> <div>2%</div> <div> <div>36%</div> <div>27%</div> <div>•</div> <div>35%</div> </div> </div>
1	G	329	<div> <div>39%</div> <div>25%</div> <div>•</div> <div>32%</div> </div>
1	H	329	<div> <div>3%</div> <div> <div>31%</div> <div>32%</div> <div>•</div> <div>35%</div> </div> </div>
2	C	1342	<div> <div>4%</div> <div> <div>58%</div> <div>36%</div> <div>6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	I	1342	
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
8	ZN	D	1503	-	-	X	-
8	ZN	J	1503	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 55049 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	227	Total	C	N	O	S	0	0	0
			1753	1091	311	345	6			
1	B	214	Total	C	N	O	S	0	0	0
			1649	1029	290	324	6			
1	G	224	Total	C	N	O	S	0	0	0
			1730	1076	308	340	6			
1	H	215	Total	C	N	O	S	0	0	0
			1659	1037	291	325	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1342	Total	C	N	O	S	0	0	0
			10585	6641	1843	2057	44			
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
			9089	5714	1627	1702	46			
3	J	1155	Total	C	N	O	S	0	0	0
			9001	5659	1612	1684	46			

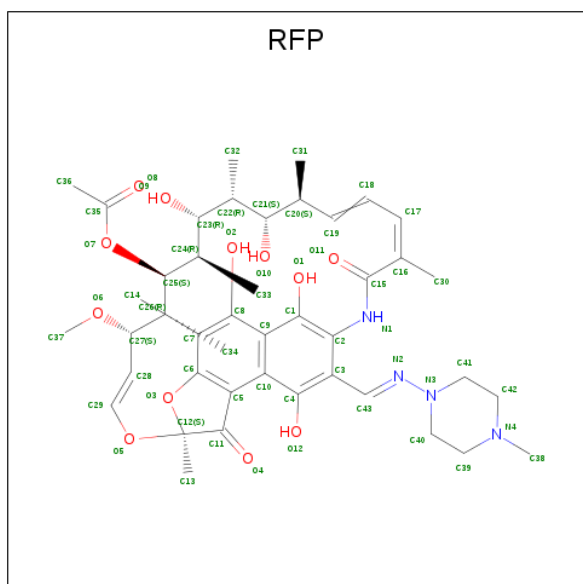
- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

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	468	Total	C	N	O	S	0	0	0
			3813	2389	678	723	23			
5	L	469	Total	C	N	O	S	0	0	0
			3821	2393	679	726	23			

- Molecule 6 is RIFAMPICIN (three-letter code: RFP) (formula: $C_{43}H_{58}N_4O_{12}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			59	43	4	12		

- 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		

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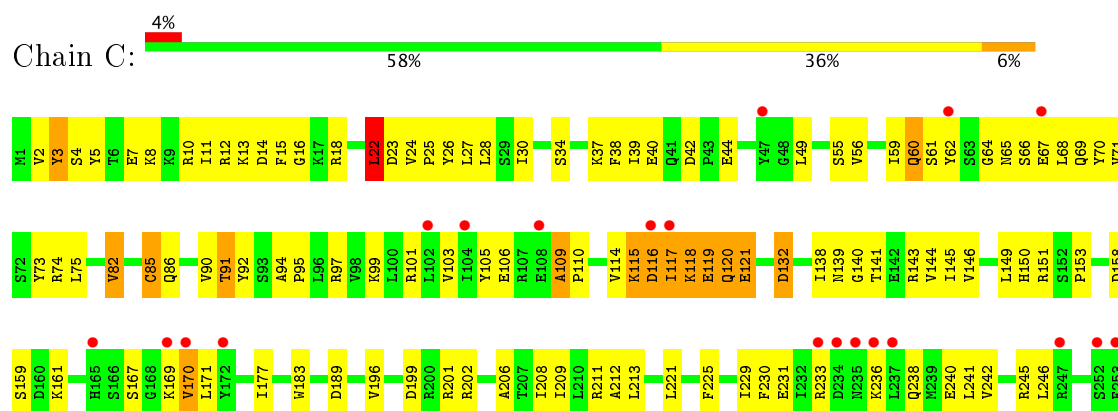
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	2	Total	Zn	0	0
			2	2		

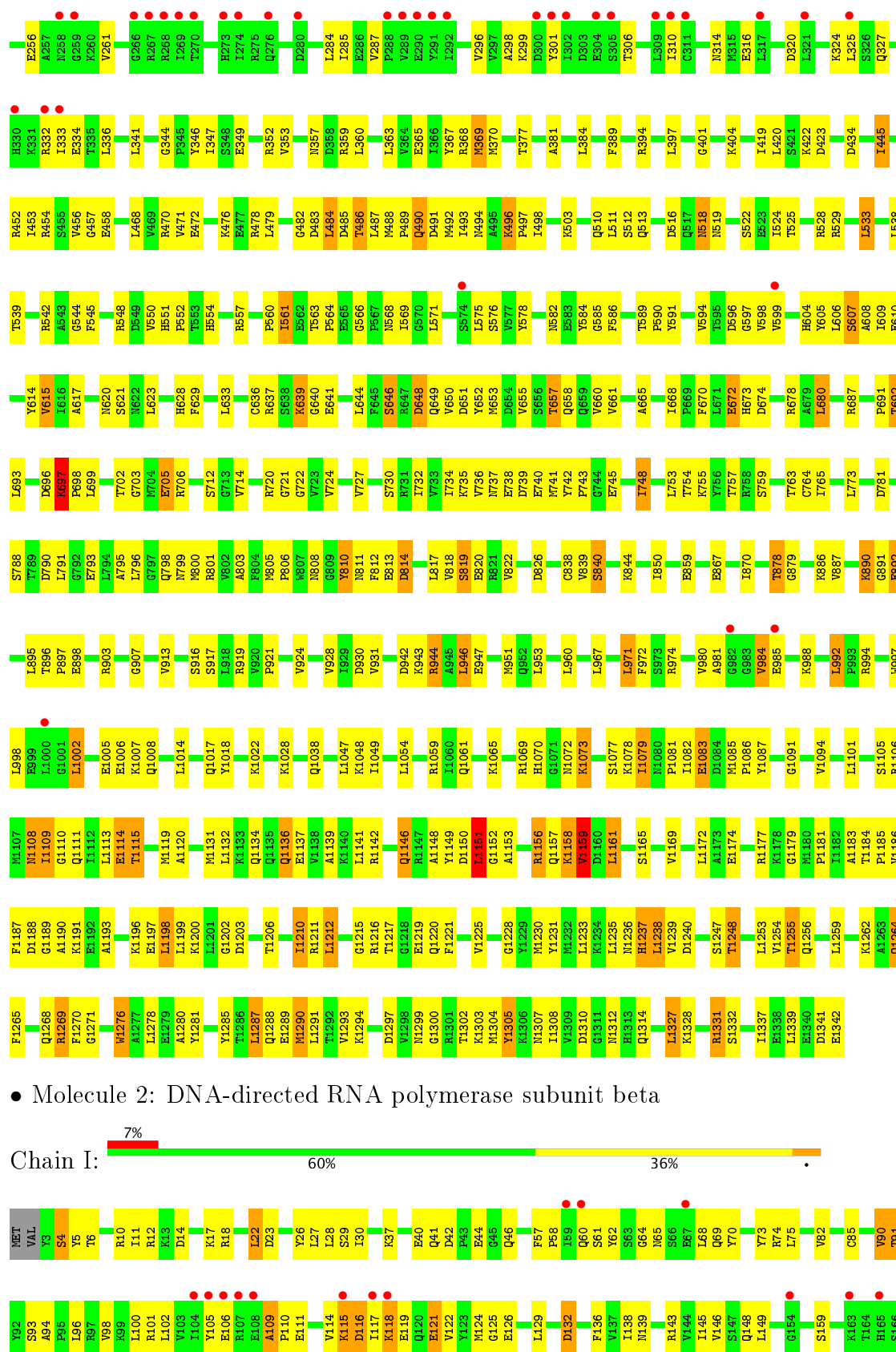
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

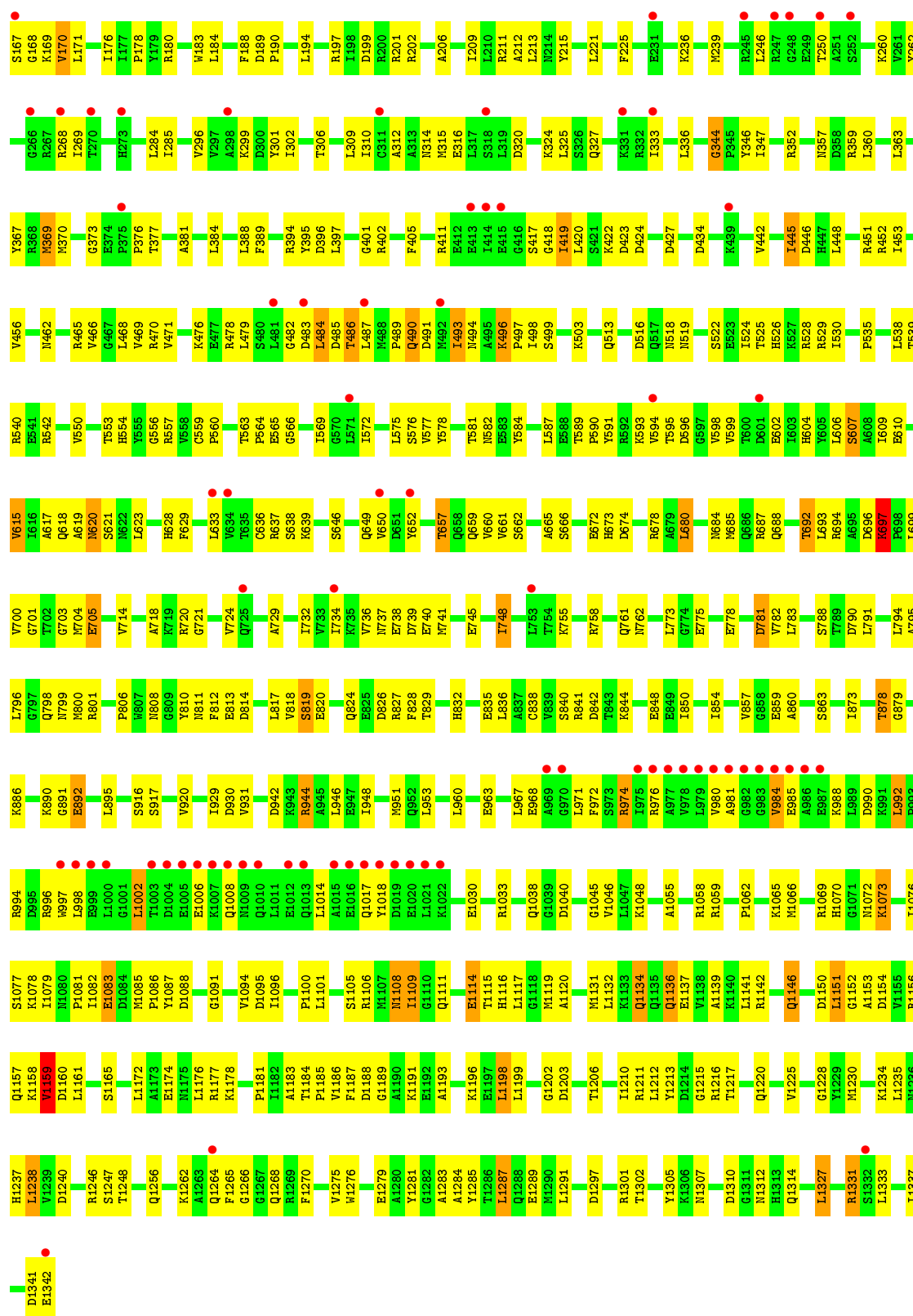
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PROTEIN DATA BANK



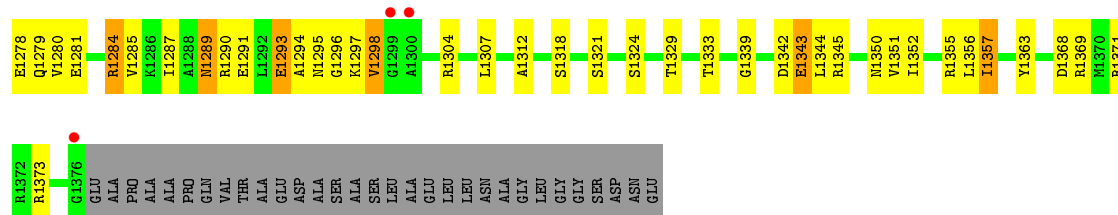




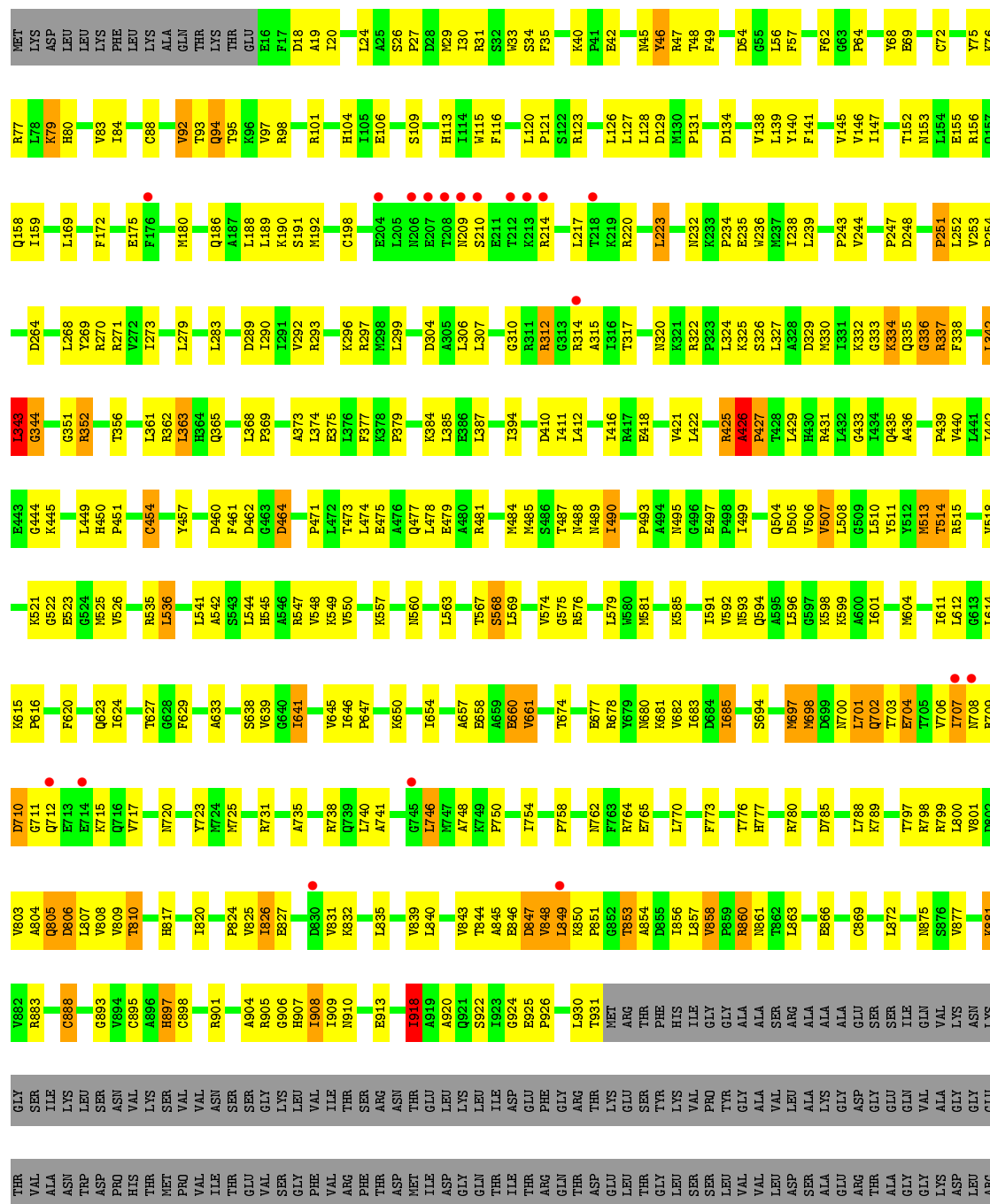
● Molecule 3: DNA-directed RNA polymerase subunit beta'

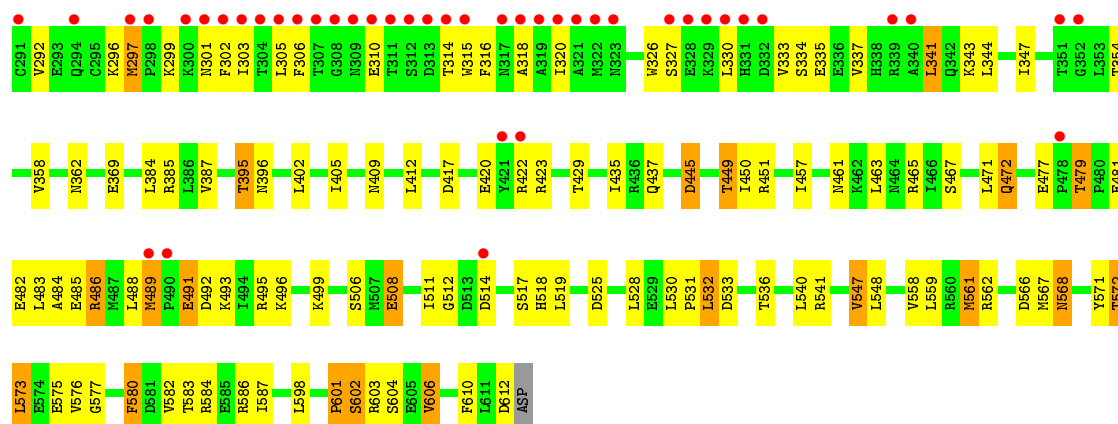




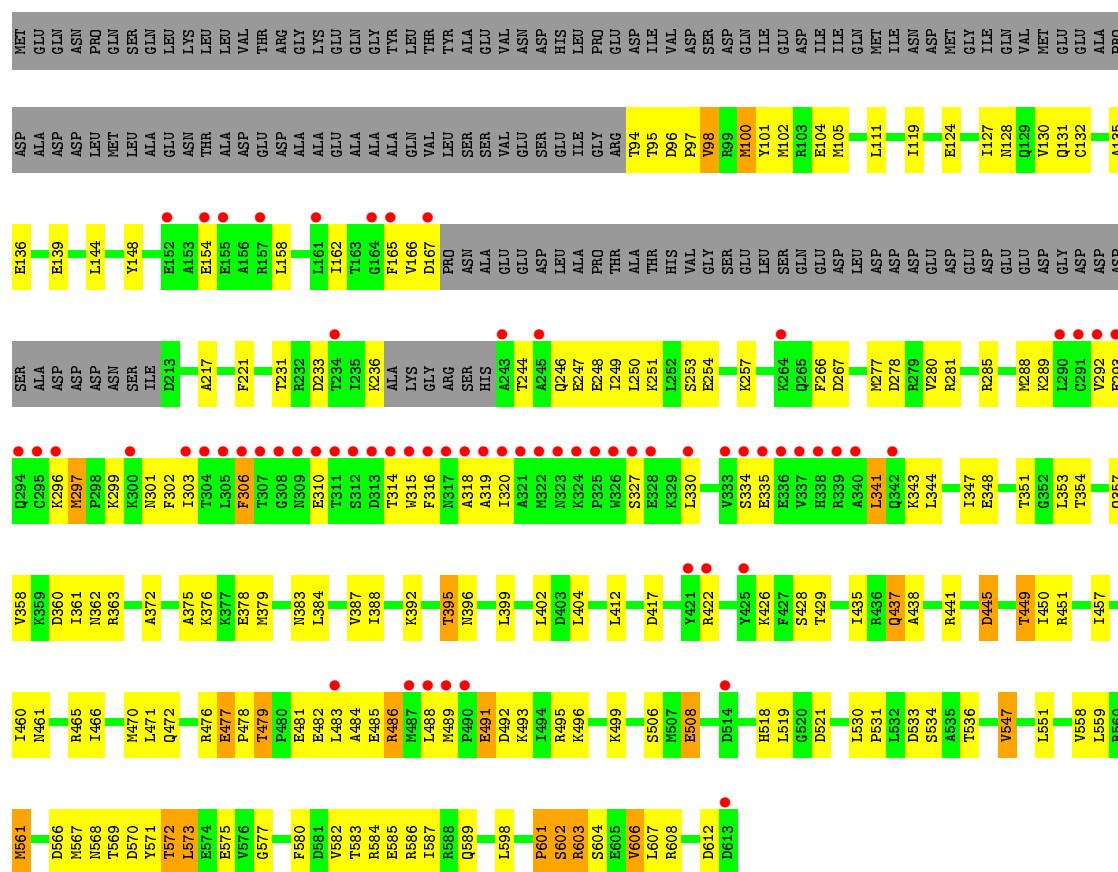


• Molecule 3: DNA-directed RNA polymerase subunit beta'





• Molecule 5: RNA polymerase sigma factor RpoD



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	188.96Å 204.43Å 313.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 3.80 29.98 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.98-3.80) 99.8 (29.98-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 3.75Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.248 , 0.295 0.245 , 0.295	Depositor DCC
R_{free} test set	1994 reflections (1.67%)	DCC
Wilson B-factor (Å ²)	159.8	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 102.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	55049	wwPDB-VP
Average B, all atoms (Å ²)	188.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% 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, RFP, 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	0.73	2/1774 (0.1%)	0.86	2/2405 (0.1%)
1	B	0.66	0/1668	0.91	1/2260 (0.0%)
1	G	0.54	0/1751	0.77	1/2373 (0.0%)
1	H	0.53	0/1678	0.85	2/2274 (0.1%)
2	C	0.89	12/10754 (0.1%)	0.92	25/14509 (0.2%)
2	I	0.58	4/10735 (0.0%)	0.71	2/14484 (0.0%)
3	D	0.96	20/9229 (0.2%)	0.98	27/12459 (0.2%)
3	J	0.74	4/9140 (0.0%)	0.86	14/12341 (0.1%)
4	E	0.69	0/693	0.81	1/935 (0.1%)
4	K	0.31	0/629	0.55	0/847
5	F	0.50	0/3864	0.69	3/5194 (0.1%)
5	L	0.46	0/3872	0.63	1/5205 (0.0%)
All	All	0.74	42/55787 (0.1%)	0.84	79/75286 (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
2	C	0	6
2	I	0	2
3	D	0	6
3	J	0	2
4	E	0	1
5	F	0	1
5	L	0	1
All	All	0	20

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	764	CYS	CB-SG	-11.76	1.62	1.82
3	D	454	CYS	CB-SG	-8.90	1.67	1.82
2	C	636	CYS	CB-SG	-8.85	1.67	1.82
3	J	888	CYS	CB-SG	-8.72	1.67	1.82
2	C	838	CYS	CB-SG	-8.60	1.67	1.82

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	343	LEU	CA-CB-CG	-8.74	95.19	115.30
3	D	807	LEU	CB-CG-CD2	-8.46	96.62	111.00
3	J	327	LEU	CB-CG-CD2	-8.45	96.64	111.00
3	D	888	CYS	CA-CB-SG	-8.38	98.92	114.00
3	J	426	ALA	C-N-CD	-8.01	102.98	120.60

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	29	GLU	Peptide
2	C	109	ALA	Peptide
2	C	1239	VAL	Mainchain
2	C	236	LYS	Peptide
2	C	646	SER	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	1753	0	1780	90	0
1	B	1649	0	1674	101	0
1	G	1730	0	1756	82	0
1	H	1659	0	1692	91	0
2	C	10585	0	10603	425	0
2	I	10566	0	10576	385	0
3	D	9089	0	9264	449	0
3	J	9001	0	9170	378	0
4	E	691	0	695	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	627	0	634	24	0
5	F	3813	0	3880	132	0
5	L	3821	0	3884	134	0
6	C	59	0	54	14	0
7	D	1	0	0	0	0
7	J	1	0	0	0	0
8	D	2	0	0	2	0
8	J	2	0	0	1	0
All	All	55049	0	55662	2119	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 19.

The worst 5 of 2119 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:343:LEU:CG	3:J:343:LEU:CD2	1.79	1.59
3:D:426:ALA:CB	3:D:427:PRO:CD	2.12	1.26
3:J:426:ALA:CB	3:J:427:PRO:HD3	1.69	1.19
3:D:343:LEU:HD22	3:D:344:GLY:HA3	1.16	1.16
3:D:426:ALA:HB3	3:D:427:PRO:CD	1.70	1.13

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	225/329 (68%)	196 (87%)	25 (11%)	4 (2%)	10	50
1	B	210/329 (64%)	183 (87%)	22 (10%)	5 (2%)	7	45
1	G	222/329 (68%)	193 (87%)	25 (11%)	4 (2%)	10	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	211/329 (64%)	187 (89%)	17 (8%)	7 (3%)	4	39
2	C	1340/1342 (100%)	1233 (92%)	100 (8%)	7 (0%)	32	73
2	I	1338/1342 (100%)	1232 (92%)	101 (8%)	5 (0%)	38	77
3	D	1162/1407 (83%)	1072 (92%)	81 (7%)	9 (1%)	22	65
3	J	1151/1407 (82%)	1056 (92%)	80 (7%)	15 (1%)	14	56
4	E	87/91 (96%)	82 (94%)	5 (6%)	0	100	100
4	K	77/91 (85%)	74 (96%)	3 (4%)	0	100	100
5	F	462/613 (75%)	422 (91%)	39 (8%)	1 (0%)	51	85
5	L	463/613 (76%)	424 (92%)	38 (8%)	1 (0%)	51	85
All	All	6948/8222 (84%)	6354 (92%)	536 (8%)	58 (1%)	22	65

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	GLU
1	A	167	PRO
1	B	13	LEU
2	C	1159	VAL
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	194/286 (68%)	182 (94%)	12 (6%)	21	59
1	B	182/286 (64%)	172 (94%)	10 (6%)	25	63
1	G	191/286 (67%)	179 (94%)	12 (6%)	21	58
1	H	184/286 (64%)	177 (96%)	7 (4%)	38	70
2	C	1157/1157 (100%)	1051 (91%)	106 (9%)	11	43
2	I	1154/1157 (100%)	1050 (91%)	104 (9%)	11	45
3	D	970/1168 (83%)	873 (90%)	97 (10%)	9	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	J	960/1168 (82%)	860 (90%)	100 (10%)	8	38
4	E	72/75 (96%)	64 (89%)	8 (11%)	7	35
4	K	67/75 (89%)	63 (94%)	4 (6%)	22	60
5	F	417/540 (77%)	376 (90%)	41 (10%)	9	40
5	L	418/540 (77%)	376 (90%)	42 (10%)	9	39
All	All	5966/7024 (85%)	5423 (91%)	543 (9%)	11	44

5 of 543 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	395	THR
2	I	116	ASP
5	L	98	VAL
5	F	450	ILE
1	G	13	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	362	ASN
2	I	69	GLN
5	L	131	GLN
5	F	383	ASN
5	F	472	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 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	RFP	C	3001	-	62,63,63	2.40	19 (30%)	91,94,94	2.49	32 (35%)

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	RFP	C	3001	-	-	0/60/85/85	0/1/5/5

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	3001	RFP	O7-C25	-8.04	1.32	1.44
6	C	3001	RFP	C12-C11	-4.48	1.32	1.54
6	C	3001	RFP	C6-C7	-3.20	1.34	1.39
6	C	3001	RFP	O6-C27	-3.11	1.34	1.43
6	C	3001	RFP	O9-C23	-3.01	1.36	1.43

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	3001	RFP	C32-C22-C23	-6.95	96.82	111.28
6	C	3001	RFP	C33-C24-C23	-6.65	97.45	111.28
6	C	3001	RFP	O7-C25-C26	-6.07	92.21	107.56
6	C	3001	RFP	C34-C26-C25	-5.19	101.87	111.43
6	C	3001	RFP	C31-C20-C19	-4.93	97.59	110.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	3001	RFP	14	0

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	227/329 (68%)	-0.20	3 (1%) 77 69	128, 159, 207, 262	0
1	B	214/329 (65%)	0.11	7 (3%) 47 37	115, 179, 246, 259	0
1	G	224/329 (68%)	-0.20	1 (0%) 92 88	162, 193, 225, 245	0
1	H	215/329 (65%)	0.10	10 (4%) 32 25	165, 218, 246, 265	0
2	C	1342/1342 (100%)	-0.04	55 (4%) 38 30	96, 152, 303, 368	0
2	I	1340/1342 (99%)	0.23	89 (6%) 19 14	129, 200, 287, 371	0
3	D	1166/1407 (82%)	-0.14	25 (2%) 64 54	94, 140, 215, 278	0
3	J	1155/1407 (82%)	-0.07	28 (2%) 59 49	118, 164, 225, 300	0
4	E	89/91 (97%)	-0.16	0 100 100	131, 170, 200, 214	0
4	K	79/91 (86%)	1.00	18 (22%) 1 1	221, 276, 310, 318	0
5	F	468/613 (76%)	0.49	62 (13%) 4 4	139, 216, 432, 522	0
5	L	469/613 (76%)	0.71	66 (14%) 3 4	144, 239, 458, 518	0
All	All	6988/8222 (84%)	0.09	364 (5%) 28 22	94, 176, 295, 522	0

The worst 5 of 364 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	L	318	ALA	14.6
5	L	321	ALA	13.9
5	L	319	ALA	13.9
5	F	312	SER	13.4
5	L	327	SER	12.4

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 [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
8	ZN	J	1503	1/1	0.86	0.42	3.25	281,281,281,281	0
8	ZN	D	1503	1/1	0.71	0.37	1.35	274,274,274,274	0
8	ZN	D	1502	1/1	0.58	0.25	0.23	324,324,324,324	0
6	RFP	C	3001	59/59	0.92	0.22	-0.50	88,136,160,162	0
8	ZN	J	1502	1/1	0.61	0.18	-0.94	322,322,322,322	0
7	MG	D	1501	1/1	0.80	0.41	-	264,264,264,264	0
7	MG	J	1501	1/1	0.52	0.51	-	290,290,290,290	0

6.5 Other polymers [i](#)

There are no such residues in this entry.