



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 10:00 AM UTC

PDB ID : 5UAG / pdb_00005uag
Title : Escherichia coli RNA polymerase mutant - RpoB D516V
Authors : Molodtsov, V.; Scharf, N.T.; Stefan, M.A.; Garcia, G.A.; Murakami, K.S.
Deposited on : 2016-12-19
Resolution : 3.40 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

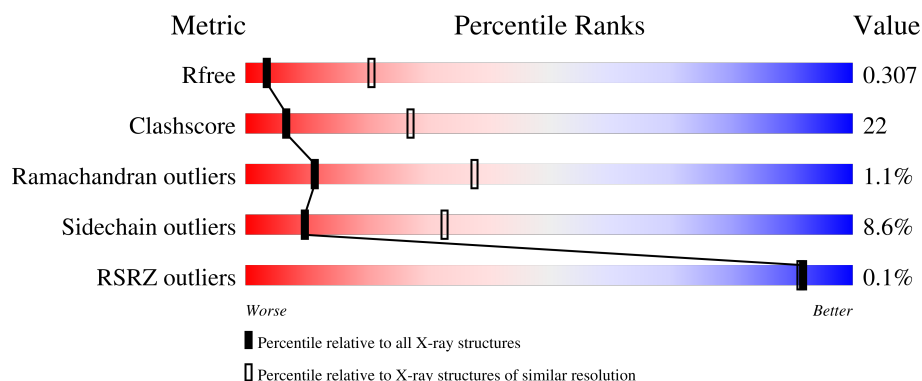
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	320	37% 31% 5% 27%
1	B	320	30% 32% • • 32%
1	G	320	36% 30% • • 29%
1	H	320	32% 33% • 32%
2	C	1342	55% 40% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	I	1342	57% 39%
3	D	1407	46% 32% 5% 17%
3	J	1407	43% 33% 5% 18%
4	E	90	59% 32% 8%
4	K	90	% 54% 27% 6% 12%
5	F	613	43% 29% 24%
5	L	613	44% 28% 23%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 55066 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	233	Total	C	N	O	S	0	0	0
			1812	1127	323	356	6			
1	B	217	Total	C	N	O	S	0	0	0
			1677	1047	295	329	6			
1	G	227	Total	C	N	O	S	0	0	0
			1755	1093	311	345	6			
1	H	216	Total	C	N	O	S	0	0	0
			1662	1038	292	326	6			

- 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
			10569	6632	1841	2053	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10565	6630	1840	2052	43			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	516	VAL	ASP	engineered mutation	UNP P0A8V2
I	516	VAL	ASP	engineered mutation	UNP P0A8V2

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1167	Total	C	N	O	S	0	0	0
			9065	5700	1622	1697	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 MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	2	Total	Mg	0	0
			2	2		
6	I	1	Total	Mg	0	0
			1	1		
6	J	1	Total	Mg	0	0
			1	1		

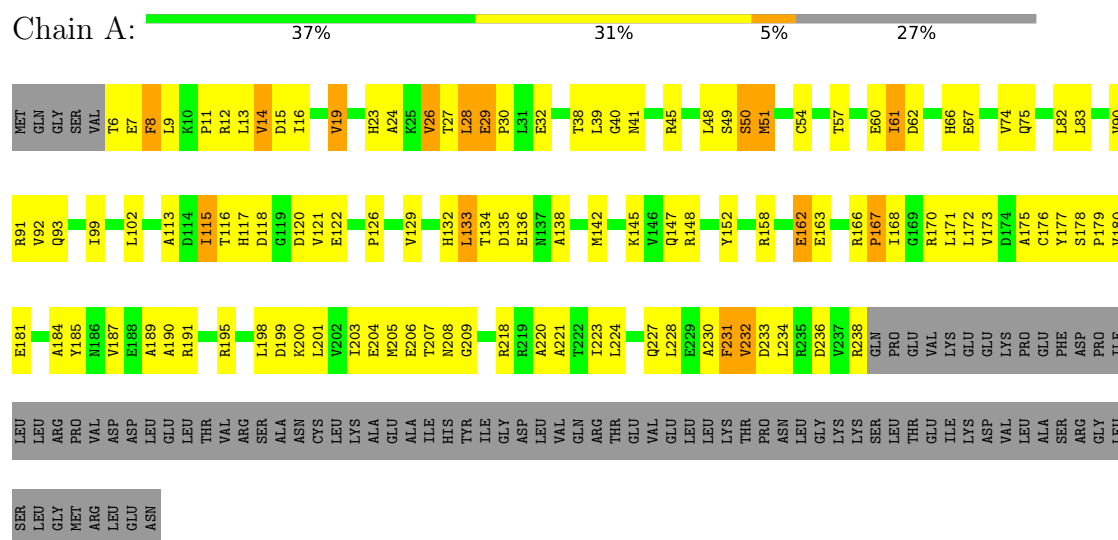
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

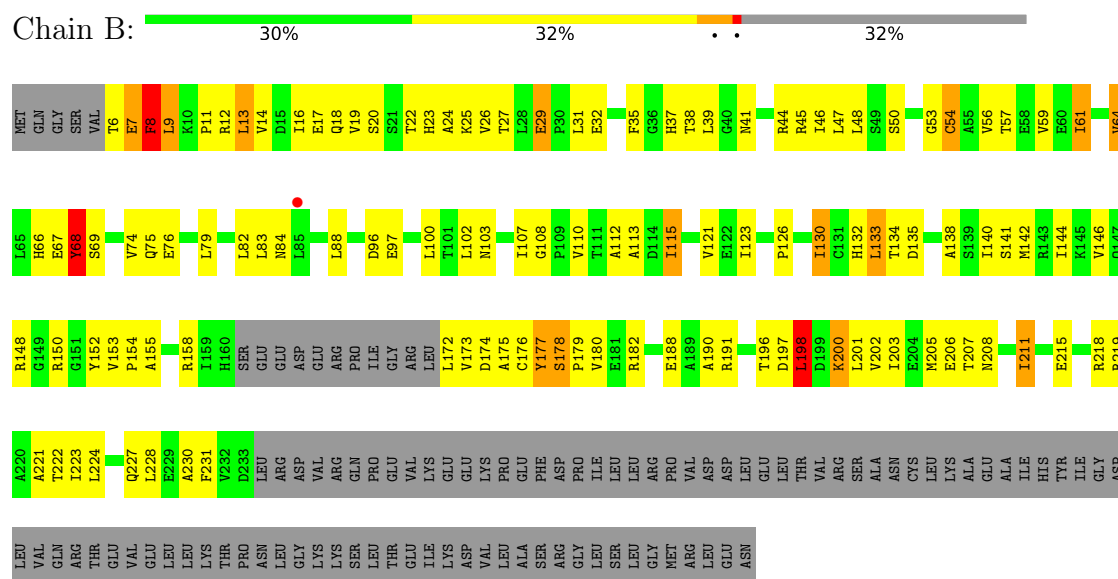
3 Residue-property plots

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

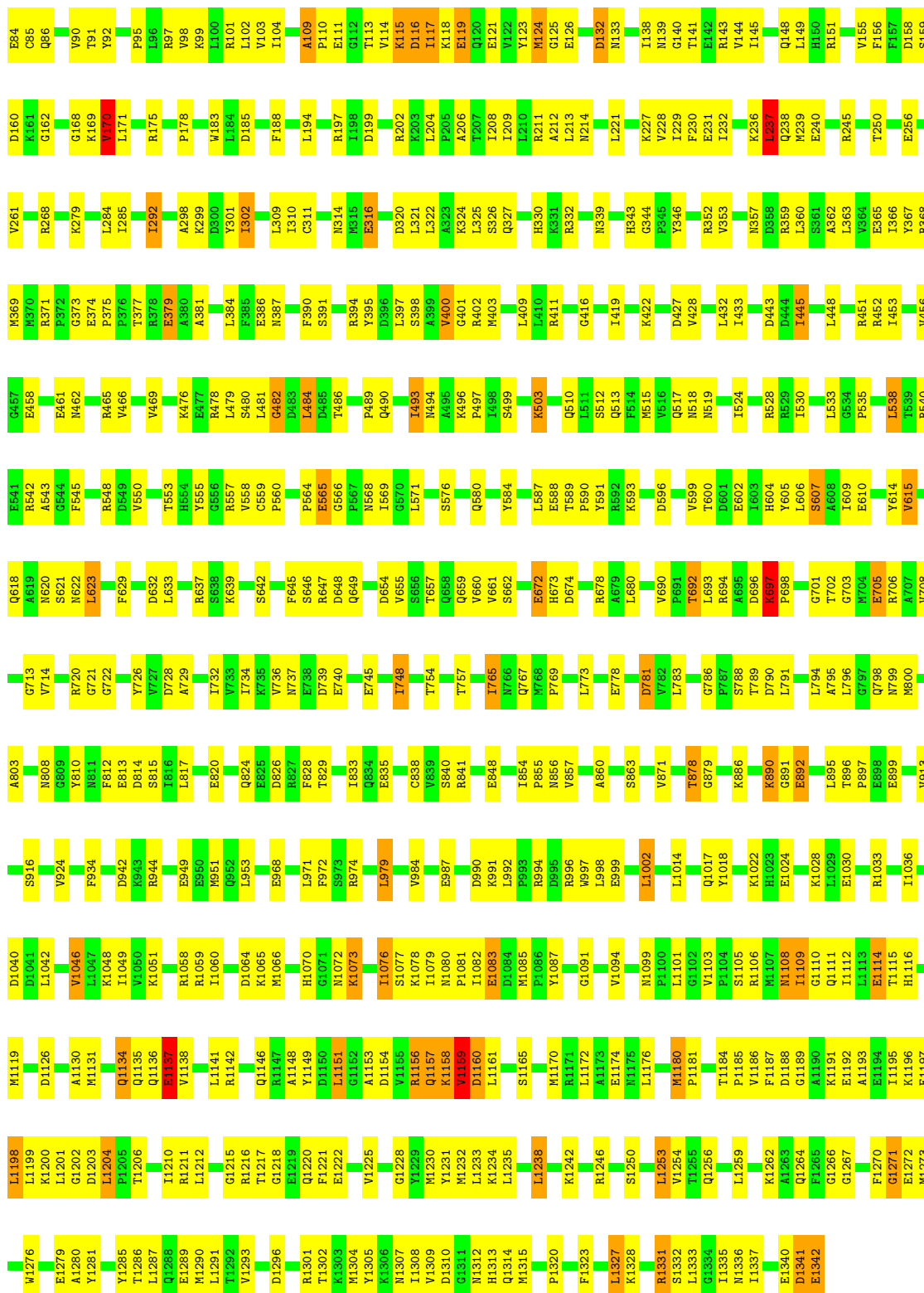


• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 1: DNA-directed RNA polymerase subunit alpha



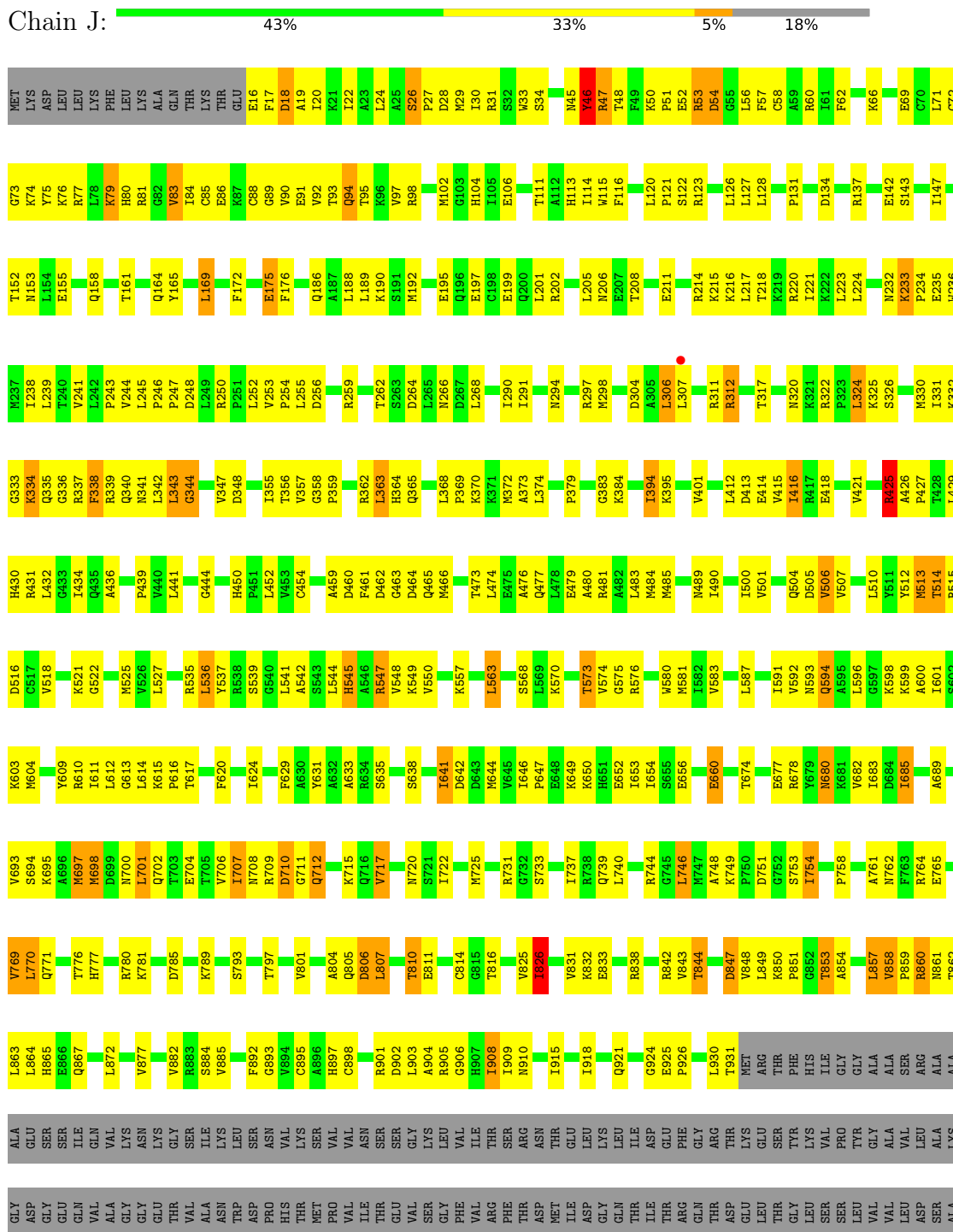


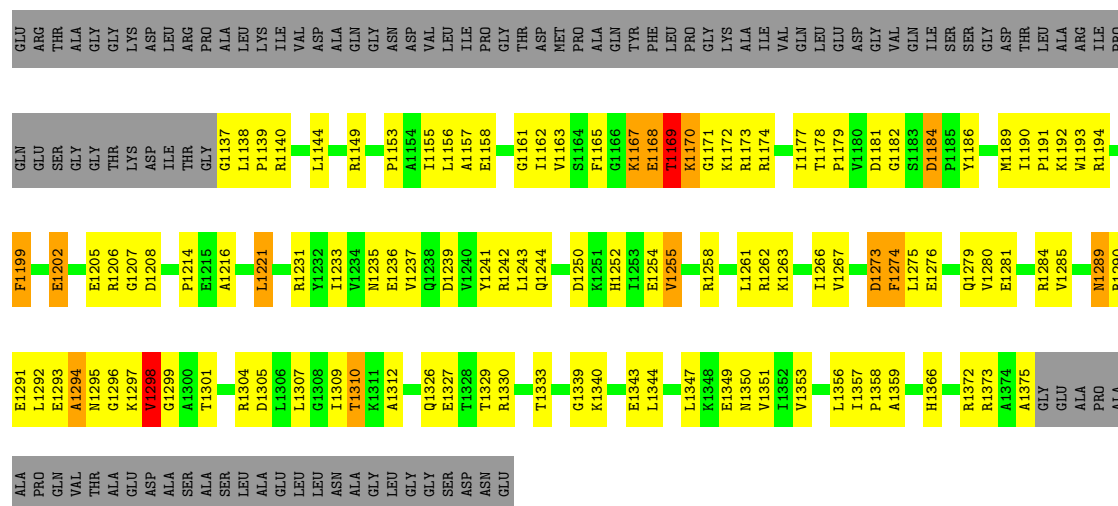
- Molecule 3: DNA-directed RNA polymerase subunit beta'



P1214	V1141	PRO	THR	GLY	V685	Q805	R709	B606	K521	D348	F260	Q158		MET
E1215		ALA	VAL	SER	D889	D806	D710		M525	I442	A261	V83		LYS
I1220	F1145	LEU	ALA	ILE	T890	L807	G712		G526	E443	T262	I84		ASP
L1221		ILE	ASN	LYS	V891	V808	Q711		T356	T355	S263	C85		LEU
		VAL	TRP	LEU	D891	V809			L527	V357	D264	E86		LEU
G1225	R1149	ASP	ASP	SER	F892	T810	K715		E532	G358	L265	K87		LYS
V1226	P1153	ALA	PRO	ASN	G893	E811	Q716		A633	P359	N266	C88		PHE
H1227	A1154	GLN	HIS	VAL	V894		W717		E534	Y360	D267			L8
L1155	I1155	THR	GLN	LYS	C895	C814	W718		E536	H450	L268	V92		R9
L1156	L1156	GLY	MET	SER	A896	G815	F719		L535	C454	Y269	T93		A10
T1230	A1157	ASN	PRO	VAL	H897	T816	W720		R536	L363	L269	Q94		Q11
I1233	E1158	VAL	VAL	VAL	C898	H817	S721		V537	H364	R278	T95		T12
V1234	I1159	LEU	ILE	ASN		T820	I722		R538	A459	L279	K96		K13
V1237	S1160	THR	THR	SER	R901				R539	L368	K280	V97		T14
Q1238	G1161	GLY	GLY	SER	D902		M725		S539	P369	K281	R93		E15
	I1162	THR	VAL	LYS	L903		S728		L541	N372	L188	K101		F17
L1243	V1163	THR	GLY	LEU	A904	L826				A373	S191	M102		D18
Q1244		ASP	PHE	VAL	R905	D642	R731		A546	M192	M192	G103		A19
G1245	K1167	MET	VAL	ILE	H907	T646	G732		R547	E375	L291	H104		I20
V1246	E1168	THR	ARG	THR	I908	F647	S733		V548		E295	L105		K21
K1247	T1169	ALA	PHE	SER	L909	K650	I737		K549	L472	K296	E106		I22
I1248	K1170	GLN	THR	ARG	N910	L835	R738		R551	L374	R297	L107		S26
	G1171	THR	ASP	ASN		R836	Q739			L194	A108	S109		P27
	K1172	PHE	MET	THR	F913		L740				L306			
H1252	R1173	LEU	ILE	GLY	A914	V839	L740		E556	L385	G310	H113		I30
I1253	R1174	PRO	ASP	LEU	I915				K557	T392	R311	I114		R31
E1254	L1175	GLY	GLY	LYS	L918	R842	M743		D558	T393	R312	W115		S32
V1255	V1176	LYS	GLN	LEU	1918	T844	R744		E656	G313	G313	W33		W33
	I1177	ALA	THR	ILE	G824		G745		N560	K395	R314	K118		S34
R1258	P1178	ILE	ILE	ASP	G925	D847	L746		L563	A396	R315	S119		E42
		VAL	THR	GLY	E925	V846	W747				L316	L120		N45
R1262	V1180	GLN	ARG	PHE	P926	V848	A748		S568	V401	T317	P121		Y46
K1263	D1181	LEU	GLN	GLY		L849	K749			L412	K321	L126		R47
I1266	G1182	GLY	THR	ARG	L930	K850	P750			L416	R322	L127		T48
V1267	S1183	ASP	ASP	THR	T931	P851				E414	P323	L128		R53
	D1184	GLY	GLY	LYS	N932		I754			V415	L324	L132		D54
	P1185	VAL	LEU	GLY	ARG	T853				R417	K325	L133		G55
S1272	Y1186	THR	LEU	SER	THR		P758			E418	R326	R133		L56
D1273	E1187	ILE	GLY	TYR	PHE	A854	I759			H419	L327	D134		F57
F1274	E1188	SER	LEU	LYS	HIS	V858				P420	A328	I135		R60
L1275	M1189	SER	SER	VAL	ILE	R860	R764			R425	R332	E136		I61
E1276	I1190	GLY	SER	PRO	GLY	R861				A426	G333	L139		F62
G1277	P1191	ASP	LEU	TYR	GLY	T862	V769			T428	G336	Y140		C70
E1278	K1192	THR	VAL	GLY	ALA		L770			R431	R337	F141		L71
Q1279	W1193	LEU	VAL	ALA	ALA	L863	Q771			P243	R338	E142		C72
V1280	R1194	ALA	LEU	VAL	SER	L864	Y772			V244	Y140	F141		G73
E1281		ARG	ASP	LEU	ARG		H777			P247	R339	E147		K74
	V1198	ILE	SER	ALA	ALA	C869				L429	F338	T152		Y75
R1284	F1199	PRO	GLY	GLY	ALA	L872	D785			H430	R339	N153		K76
V1285	E1200	GLN	GLY	ASP	GLY					Q340	R339	L154		R77
	G1201	GLY	THR	GLY	SER	N875	K789			D248	Q341	E155		L78
M1289	R1203	SER	THR	GLY	SER	S876				P251	L342	R156		K79
A1294	V1204	GLY	GLY	ILE	ILE	V877	T797			L252	R341	L157		
R1295	L1205	THR	GLY	VAL	GLN		R798			P254	L343	L158		
G1296	R1206	LYS	LYS	ALA	VAL	K881				L255	G344	R156		
L1297		ASP	ASP	GLY	LYS	R882	W801			R345	R345	R156		
V1298		ILE	LEU	GLY	ASN	R883	D802			E438	R346	R156		
G1299		ARG	ARG	GLY	LYS	S884				P439	V347	Q157		

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





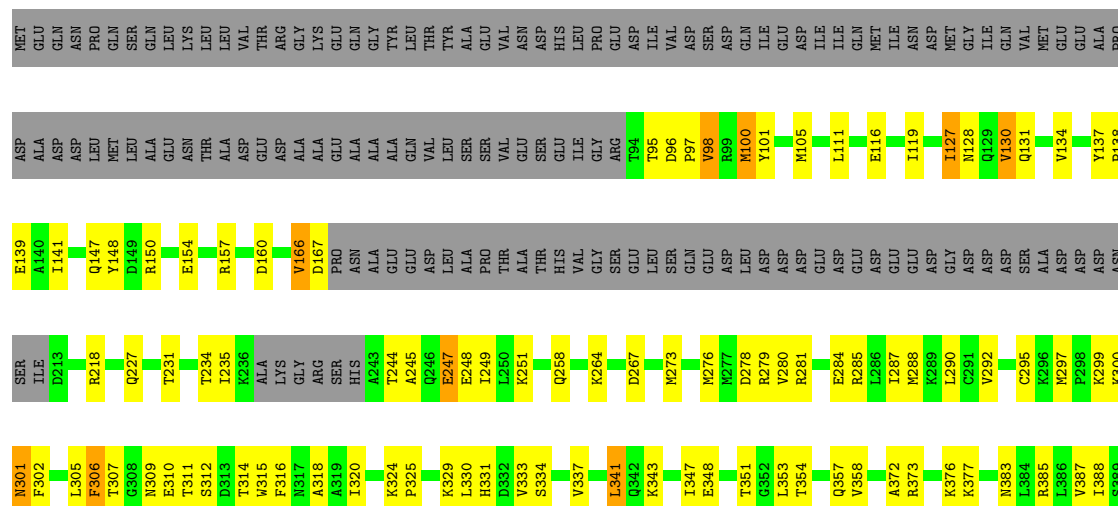
- Molecule 4: DNA-directed RNA polymerase subunit omega

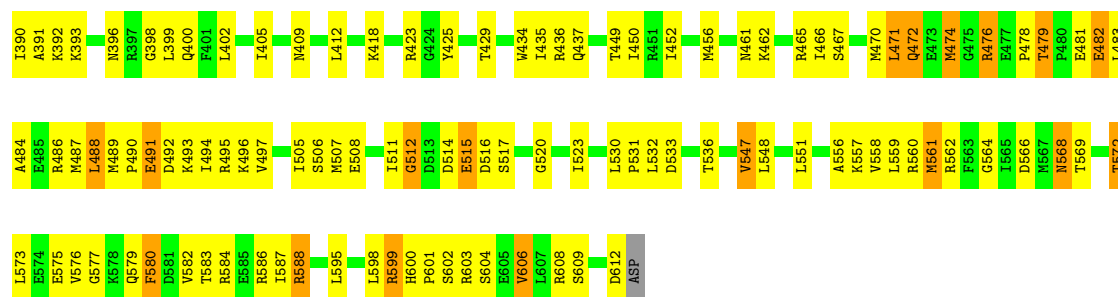


- Molecule 4: DNA-directed RNA polymerase subunit omega



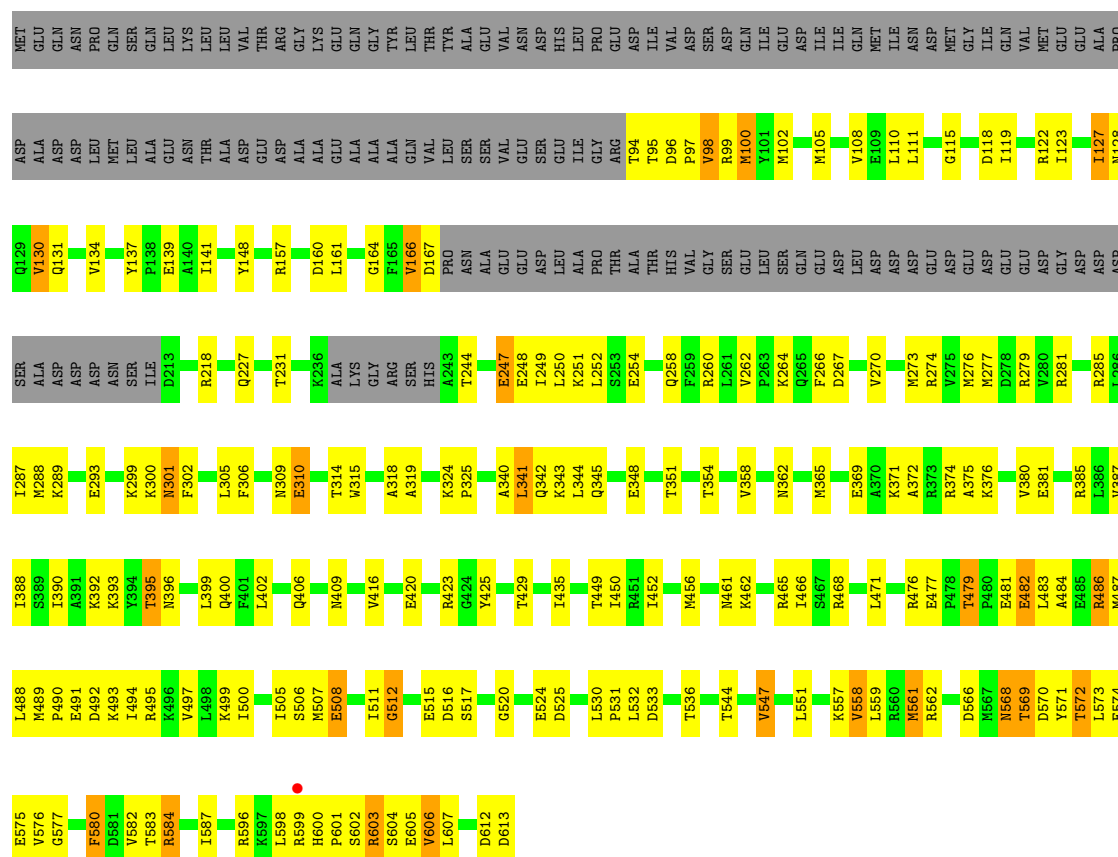
- Molecule 5: RNA polymerase sigma factor RpoD





• Molecule 5: RNA polymerase sigma factor RpoD

Chain L: 44% 28% 23%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	184.83Å 205.04Å 307.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.99 – 3.40 29.99 – 3.40	Depositor EDS
% Data completeness (in resolution range)	89.0 (29.99-3.40) 88.9 (29.99-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 3.39Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.277 , 0.311 0.278 , 0.307	Depositor DCC
R_{free} test set	2000 reflections (1.24%)	wwPDB-VP
Wilson B-factor (Å ²)	135.9	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 101.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	55066	wwPDB-VP
Average B, all atoms (Å ²)	163.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% 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	0.44	1/1834 (0.1%)	1.06	4/2485 (0.2%)
1	B	0.47	0/1697	1.33	17/2300 (0.7%)
1	G	0.49	1/1777 (0.1%)	1.06	3/2408 (0.1%)
1	H	0.44	0/1681	1.27	12/2278 (0.5%)
2	C	0.41	1/10738 (0.0%)	0.99	24/14488 (0.2%)
2	I	0.39	1/10734 (0.0%)	0.98	18/14483 (0.1%)
3	D	0.42	3/9205 (0.0%)	0.99	13/12430 (0.1%)
3	J	0.42	0/9140	1.00	19/12341 (0.2%)
4	E	0.40	0/693	0.92	0/935
4	K	0.40	0/629	0.98	2/847 (0.2%)
5	F	0.42	1/3864 (0.0%)	1.01	8/5194 (0.2%)
5	L	0.40	0/3872	1.02	3/5205 (0.1%)
All	All	0.42	8/55864 (0.0%)	1.02	123/75394 (0.2%)

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	G	0	1
2	C	0	4
2	I	0	2
3	D	0	2
3	J	0	3
4	E	0	1
5	L	0	1
All	All	0	14

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	312	ARG	CA-C	8.91	1.56	1.52
2	I	373	GLY	C-N	8.24	1.50	1.33
1	G	29	GLU	C-N	7.77	1.52	1.33
5	F	476	ARG	CA-C	-5.83	1.48	1.52
2	C	543	ALA	CA-CB	-5.70	1.45	1.53

The worst 5 of 123 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	53	ARG	N-CA-C	-10.43	93.73	110.20
3	D	53	ARG	N-CA-C	-10.02	94.36	110.20
3	J	425	ARG	NE-CZ-NH2	9.29	127.56	119.20
2	I	111	GLU	CA-C-N	8.05	131.38	120.92
2	I	111	GLU	C-N-CA	8.05	131.38	120.92

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	109	ALA	Peptide
2	C	236	LYS	Peptide
2	C	658	GLN	Sidechain
2	C	985	GLU	Mainchain
3	D	1184	ASP	Peptide

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	1812	0	1839	113	0
1	B	1677	0	1703	130	0
1	G	1755	0	1773	107	0
1	H	1662	0	1687	116	0
2	C	10569	0	10587	460	0
2	I	10565	0	10581	453	0
3	D	9065	0	9210	449	0
3	J	9001	0	9165	479	0
4	E	691	0	695	27	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	627	0	634	26	0
5	F	3813	0	3880	163	0
5	L	3821	0	3884	157	0
6	D	2	0	0	0	0
6	I	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	55066	0	55638	2385	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 22.

The worst 5 of 2385 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:I:1271:GLY:HA2	3:J:343:LEU:HD11	1.25	1.18
2:C:1269:ARG:HG2	3:D:343:LEU:HD12	1.24	1.11
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.35	1.08
3:J:54:ASP:OD2	3:J:60:ARG:NH1	1.89	1.03
2:I:1271:GLY:CA	3:J:343:LEU:HD11	1.87	1.03

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	231/320 (72%)	201 (87%)	25 (11%)	5 (2%)	5	24
1	B	213/320 (67%)	186 (87%)	24 (11%)	3 (1%)	9	31
1	G	225/320 (70%)	193 (86%)	26 (12%)	6 (3%)	4	20

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	212/320 (66%)	189 (89%)	19 (9%)	4 (2%)	6	26
2	C	1338/1342 (100%)	1229 (92%)	99 (7%)	10 (1%)	18	47
2	I	1338/1342 (100%)	1227 (92%)	100 (8%)	11 (1%)	16	44
3	D	1163/1407 (83%)	1067 (92%)	86 (7%)	10 (1%)	14	42
3	J	1151/1407 (82%)	1054 (92%)	81 (7%)	16 (1%)	9	31
4	E	87/90 (97%)	82 (94%)	5 (6%)	0	100	100
4	K	77/90 (86%)	72 (94%)	3 (4%)	2 (3%)	4	21
5	F	462/613 (75%)	421 (91%)	36 (8%)	5 (1%)	11	38
5	L	463/613 (76%)	422 (91%)	39 (8%)	2 (0%)	30	59
All	All	6960/8184 (85%)	6343 (91%)	543 (8%)	74 (1%)	11	38

5 of 74 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	GLU
1	A	232	VAL
2	C	170	VAL
2	C	484	LEU
2	C	1137	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	201/279 (72%)	190 (94%)	11 (6%)	19	46
1	B	186/279 (67%)	172 (92%)	14 (8%)	12	38
1	G	193/279 (69%)	177 (92%)	16 (8%)	10	35
1	H	183/279 (66%)	174 (95%)	9 (5%)	22	49
2	C	1155/1157 (100%)	1057 (92%)	98 (8%)	10	33
2	I	1154/1157 (100%)	1052 (91%)	102 (9%)	9	31
3	D	962/1168 (82%)	876 (91%)	86 (9%)	9	31

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	J	960/1168 (82%)	871 (91%)	89 (9%)	8	29
4	E	72/74 (97%)	64 (89%)	8 (11%)	6	21
4	K	67/74 (90%)	62 (92%)	5 (8%)	12	38
5	F	417/540 (77%)	378 (91%)	39 (9%)	8	29
5	L	418/540 (77%)	383 (92%)	35 (8%)	10	34
All	All	5968/6994 (85%)	5456 (91%)	512 (9%)	10	33

5 of 512 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	1273	ASP
4	K	58	LEU
3	J	1255	VAL
3	D	860	ARG
3	D	844	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 115 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	69	GLN
5	L	446	GLN
2	I	1017	GLN
5	L	406	GLN
3	J	1244	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 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	233/320 (72%)	-0.53	0 100 100	105, 144, 198, 236	0
1	B	217/320 (67%)	-0.39	1 (0%) 87 78	121, 192, 243, 265	0
1	G	227/320 (70%)	-0.41	0 100 100	162, 195, 234, 271	0
1	H	216/320 (67%)	-0.26	1 (0%) 87 78	175, 215, 240, 264	0
2	C	1340/1342 (99%)	-0.50	1 (0%) 92 91	78, 133, 242, 297	0
2	I	1340/1342 (99%)	-0.44	0 100 100	104, 171, 269, 334	0
3	D	1167/1407 (82%)	-0.52	1 (0%) 92 91	83, 120, 204, 261	0
3	J	1155/1407 (82%)	-0.47	1 (0%) 92 91	99, 146, 228, 277	0
4	E	89/90 (98%)	-0.64	0 100 100	118, 156, 179, 198	0
4	K	79/90 (87%)	-0.47	1 (1%) 75 61	211, 251, 298, 305	0
5	F	468/613 (76%)	-0.48	0 100 100	115, 167, 295, 326	0
5	L	469/613 (76%)	-0.51	1 (0%) 91 87	130, 181, 301, 320	0
All	All	7000/8184 (85%)	-0.47	7 (0%) 92 91	78, 156, 252, 334	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	45	GLY	2.6
1	B	85	LEU	2.3
3	J	307	LEU	2.2
4	K	16	ARG	2.2
1	H	220	ALA	2.1

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	2002	1/1	0.25	0.21	189,189,189,189	0
6	MG	I	1401	1/1	0.30	0.09	189,189,189,189	0
6	MG	J	2001	1/1	0.50	0.10	189,189,189,189	0
6	MG	D	2001	1/1	0.59	0.12	189,189,189,189	0
7	ZN	D	2003	1/1	0.91	0.11	189,189,189,189	0
7	ZN	D	2004	1/1	0.92	0.13	189,189,189,189	0
7	ZN	J	2003	1/1	0.95	0.07	189,189,189,189	0
7	ZN	J	2002	1/1	0.97	0.06	310,310,310,310	0

6.5 Other polymers [i](#)

There are no such residues in this entry.