wwPDB X-ray Structure Validation Summary Report (i)

Jan 13, 2025 – 06:09 PM EST

PDB ID	:	5VI8
Title	:	Structure of a mycobacterium smegmatis transcription initiation complex with an upstream-fork promoter fragment
Authors	:	Hubin, E.A.; Campbell, E.A.; Darst, S.A.
Deposited on	:	2017-04-14
Resolution	:	2.76 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 (i) 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 (i)) were used in the production of this report:

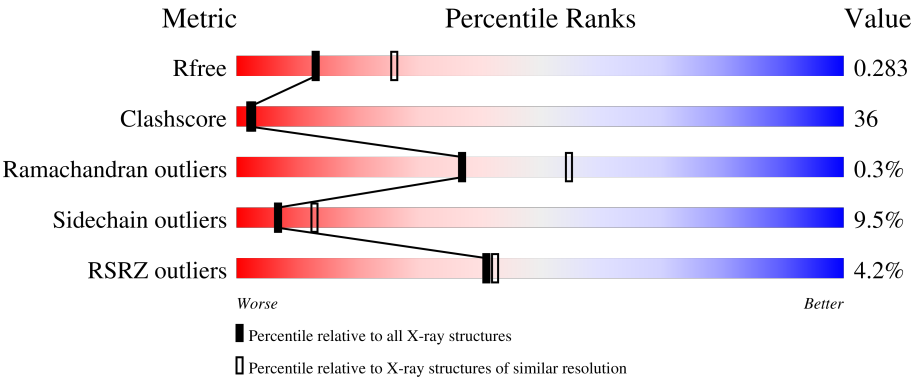
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 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}	164625	1606 (2.78-2.74)
Clashscore	180529	1689 (2.78-2.74)
Ramachandran outliers	177936	1665 (2.78-2.74)
Sidechain outliers	177891	1665 (2.78-2.74)
RSRZ outliers	164620	1606 (2.78-2.74)

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 <=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	J	114	3% 35% 32% 5% 27%
2	A	350	2% 23% 36% • 38%
2	B	350	9% 25% 36% 6% 33%
3	C	1169	4% 44% 44% 6% 6%
4	D	1317	2% 50% 41% • 5%

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Mol	Chain	Length	Quality of chain
5	E	107	2% 33% 28% 9% 29%
6	F	466	2% 41% 24% 32%
7	O	31	39% 61%
8	P	26	62% 38%
9	T	100	13% 29% 21% 47%

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
10	SO4	C	1203	-	-	X	-
10	SO4	D	2005	-	-	X	-

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 26631 atoms, of which 36 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 RNA polymerase-binding protein RbpA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	J	83	Total	C	N	O	S	0	0	0
			667	419	118	128	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	218	Total	C	N	O	S	0	0	0
			1617	1020	276	318	3			
2	B	233	Total	C	N	O	S	0	0	0
			1667	1054	289	322	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	1099	Total	C	N	O	S	0	0	0
			8250	5164	1448	1603	35			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	1248	Total	C	N	O	S	0	0	0
			9588	6016	1727	1805	40			

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	76	Total	C	N	O	0	0	0
			592	378	100	114			

- Molecule 6 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	319	Total	C	N	O	S	0	0	0
			2481	1553	450	471	7			

- Molecule 7 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	O	31	Total	C	N	O	P	0	0	0
			634	305	114	185	30			

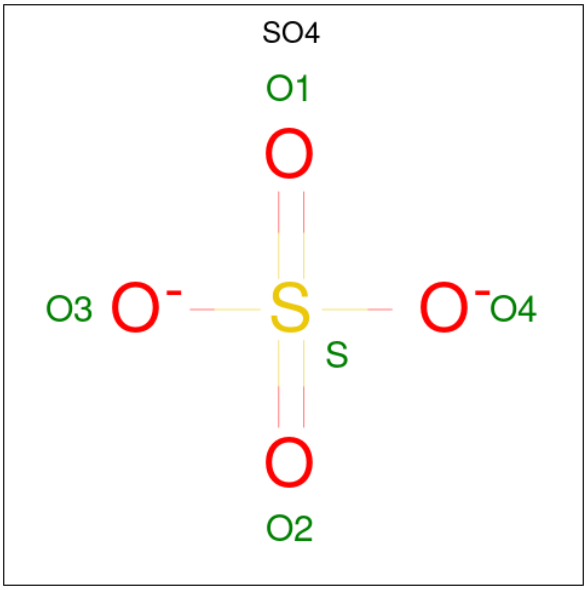
- Molecule 8 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	P	26	Total	C	N	O	P	0	0	0
			526	254	94	153	25			

- Molecule 9 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	T	53	Total	C	N	O	S	0	0	0
			377	237	66	73	1			

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	O	S	0	0
			5	4	1		

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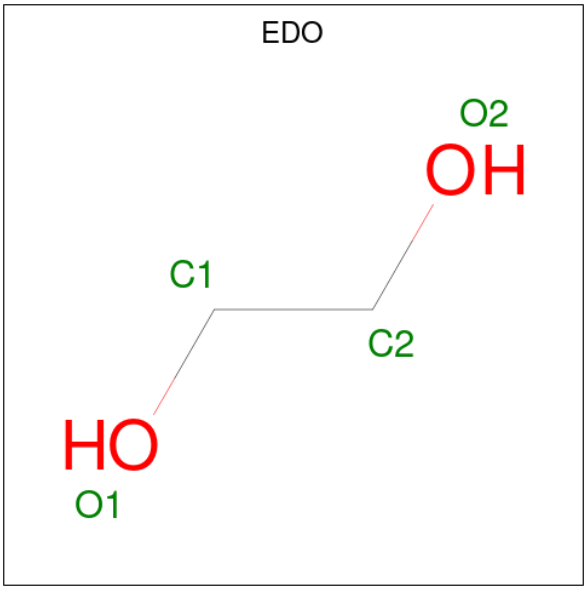
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	1	Total O S 5 4 1	0	0
10	C	1	Total O S 5 4 1	0	0
10	D	1	Total O S 5 4 1	0	0
10	D	1	Total O S 5 4 1	0	0
10	D	1	Total O S 5 4 1	0	0
10	D	1	Total O S 5 4 1	0	0
10	F	1	Total O S 5 4 1	0	0
10	F	1	Total O S 5 4 1	0	0
10	F	1	Total O S 5 4 1	0	0
10	F	1	Total O S 5 4 1	0	0
10	F	1	Total O S 5 4 1	0	0

- Molecule 11 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	C	1	Total C H O 10 2 6 2	0	0
11	C	1	Total C H O 10 2 6 2	0	0
11	D	1	Total C H O 10 2 6 2	0	0
11	D	1	Total C H O 10 2 6 2	0	0
11	D	1	Total C H O 10 2 6 2	0	0
11	F	1	Total C H O 10 2 6 2	0	0

- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 13 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	D	1	Total Mg 1 1	0	0

- Molecule 14 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	J	1	Total O 1 1	0	0
14	A	3	Total O 3 3	0	0
14	B	1	Total O 1 1	0	0
14	C	17	Total O 17 17	0	0
14	D	51	Total O 51 51	0	0
14	E	2	Total O 2 2	0	0
14	F	16	Total O 16 16	0	0

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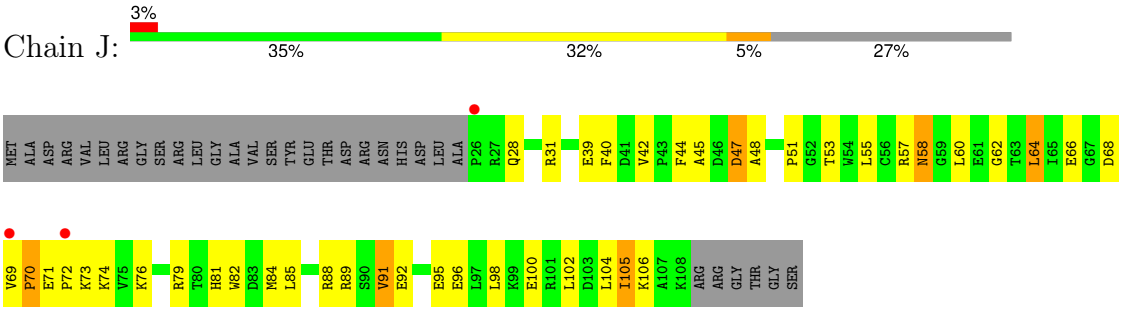
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	O	13	Total O 13 13	0	0
14	P	4	Total O 4 4	0	0
14	T	1	Total O 1 1	0	0

3 Residue-property plots (i)

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.

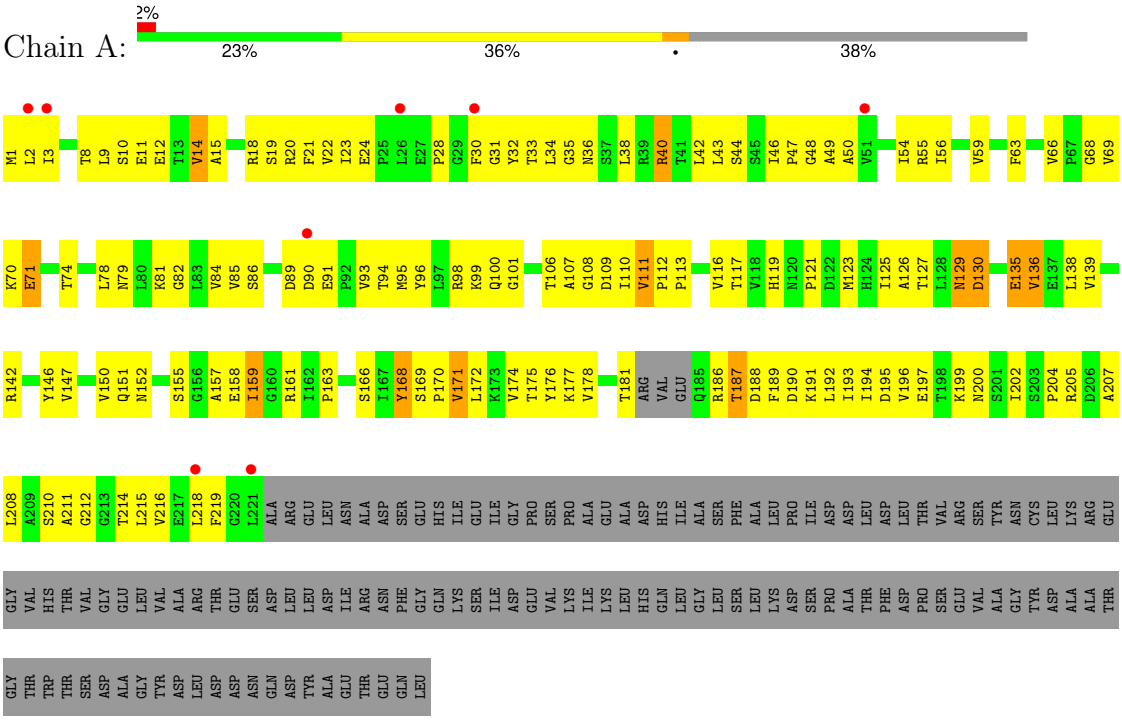
• Molecule 1: RNA polymerase-binding protein RbpA

Chain J:



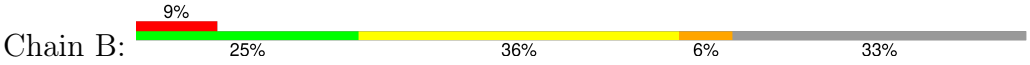
• Molecule 2: DNA-directed RNA polymerase subunit alpha

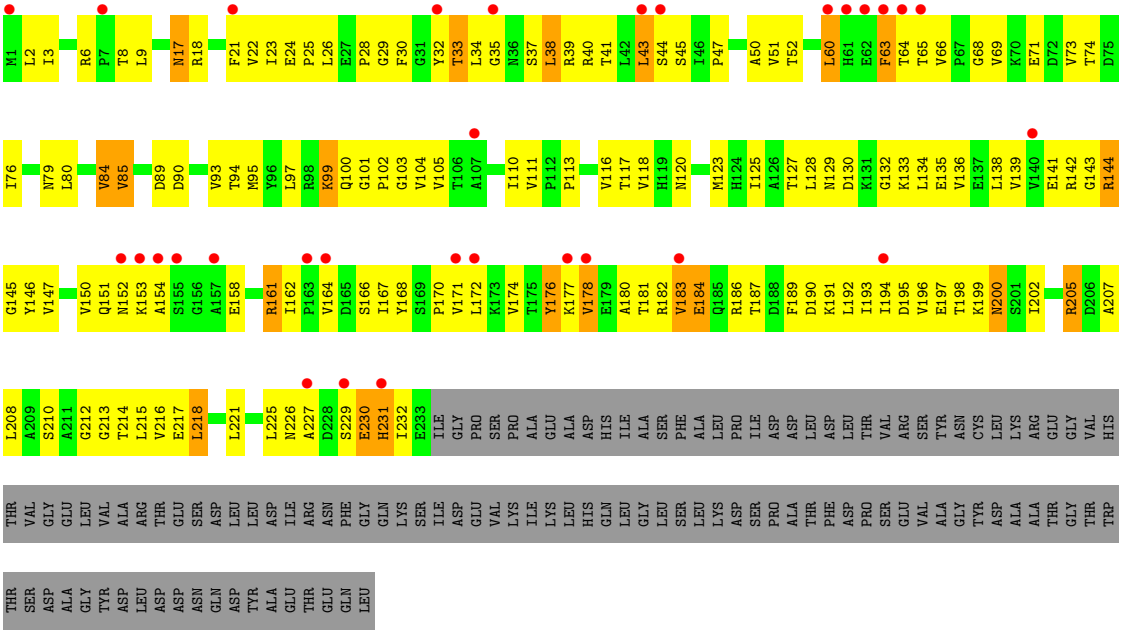
Chain A:



• Molecule 2: DNA-directed RNA polymerase subunit alpha

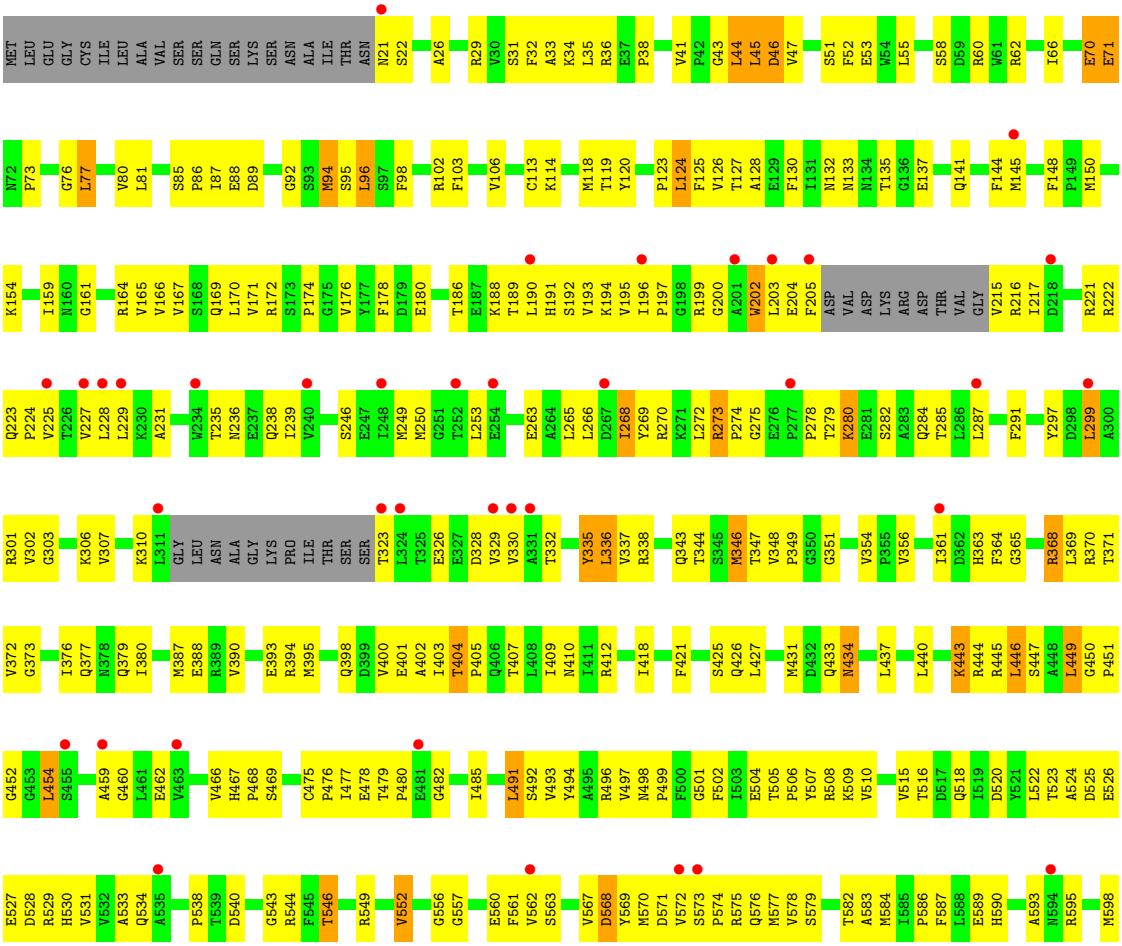
Chain B:

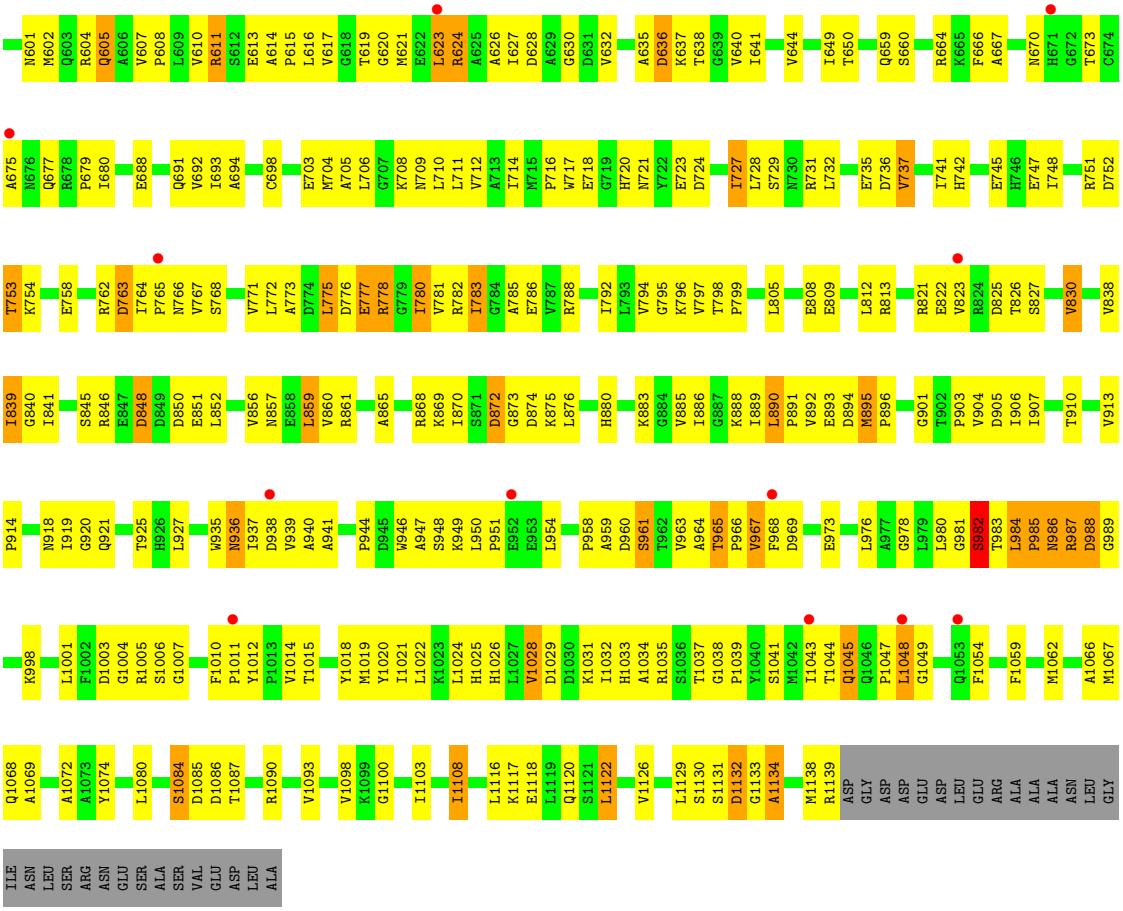




• Molecule 3: DNA-directed RNA polymerase subunit beta

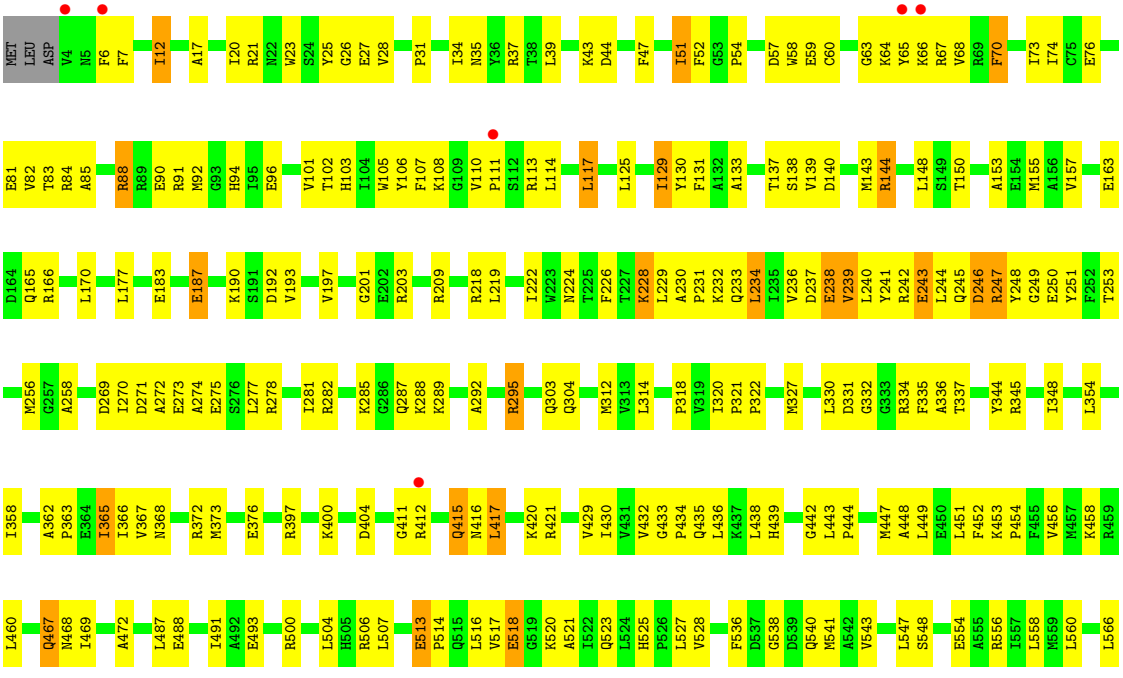
Chain C:

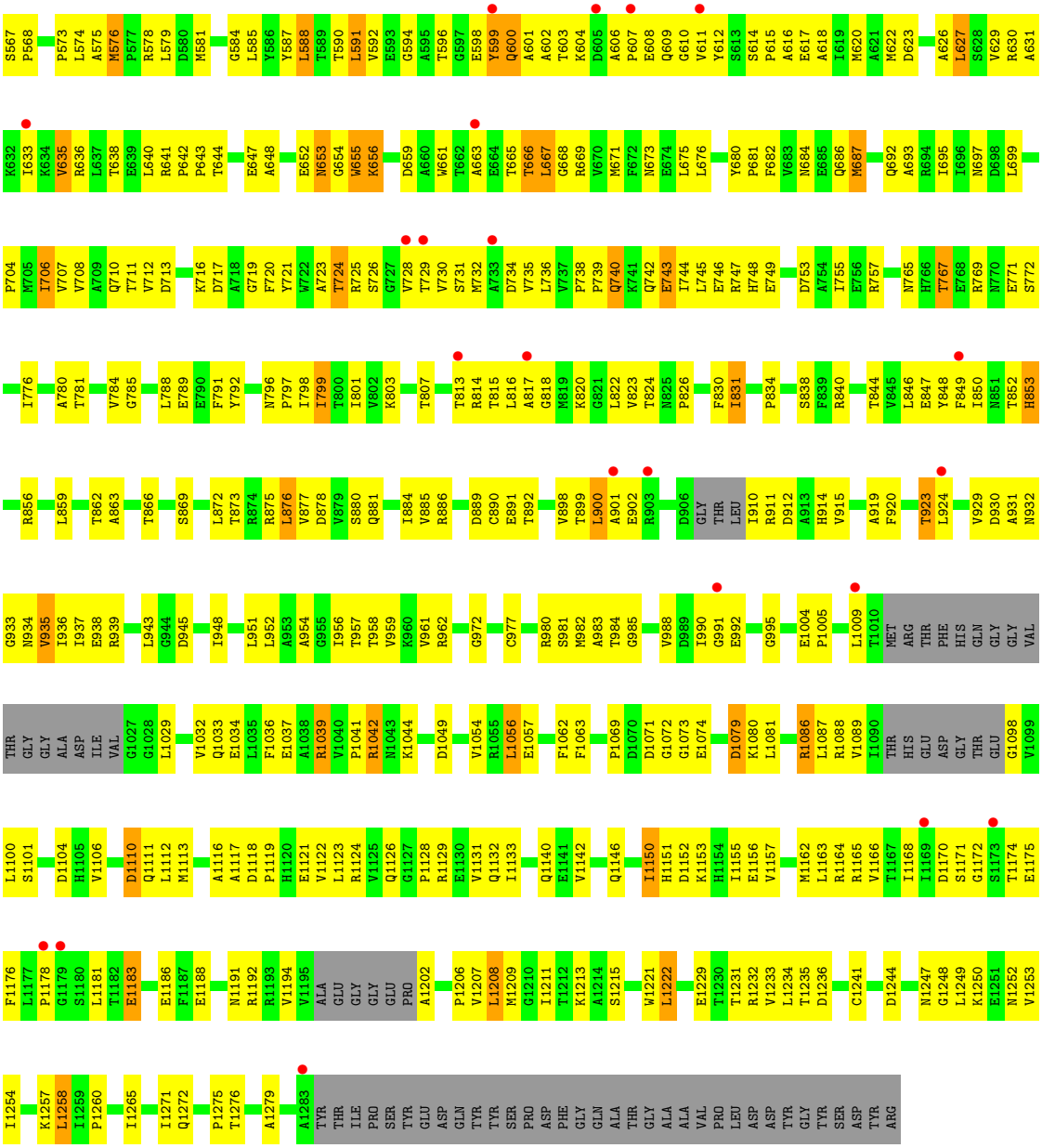




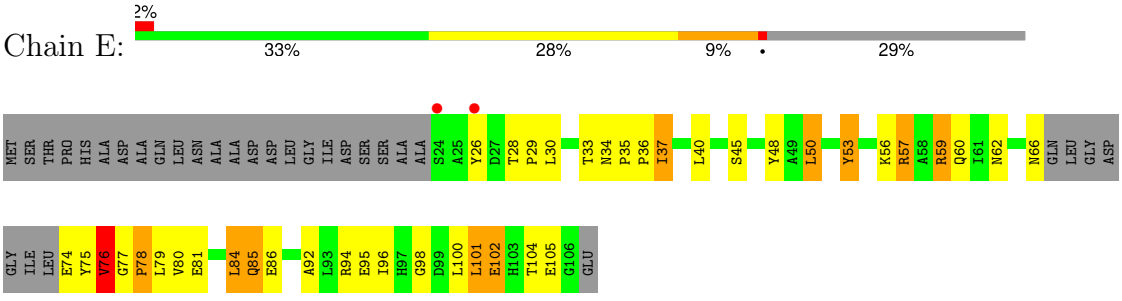
• Molecule 4: DNA-directed RNA polymerase subunit beta'

Chain D:

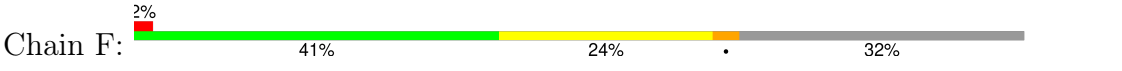


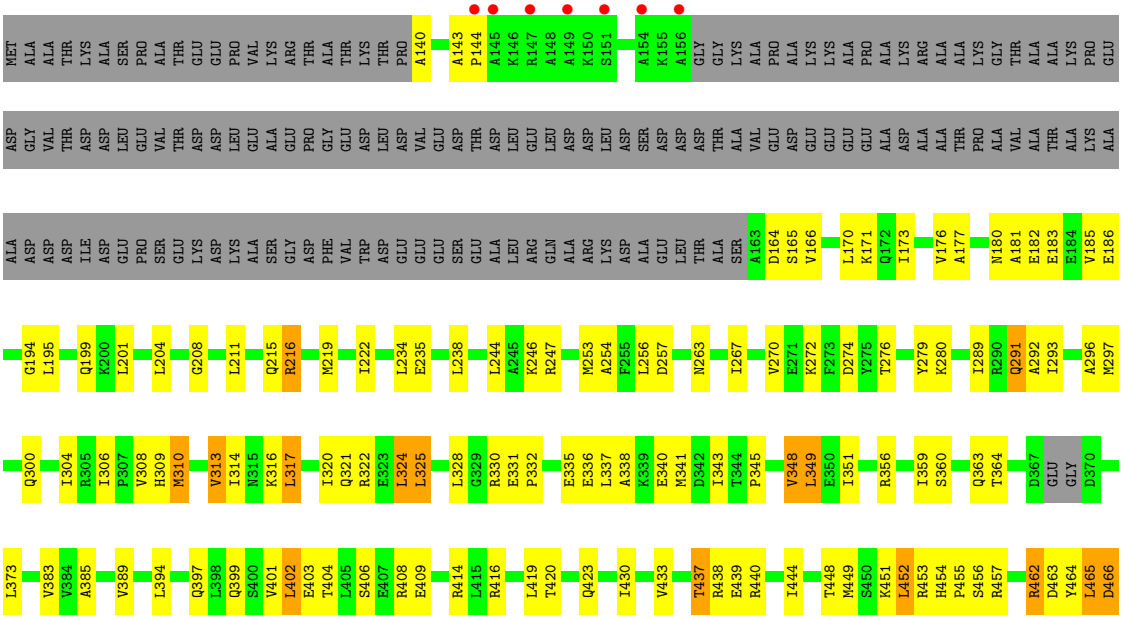


• Molecule 5: DNA-directed RNA polymerase subunit omega



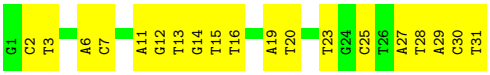
• Molecule 6: RNA polymerase sigma factor SigA





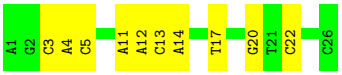
• Molecule 7: DNA (31-MER)

Chain O:



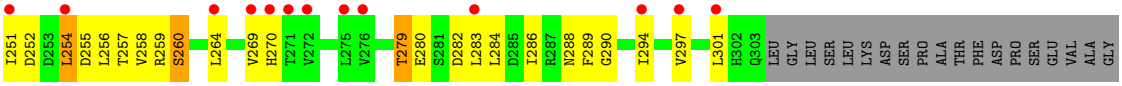
• Molecule 8: DNA (26-MER)

Chain P:



• Molecule 9: DNA-directed RNA polymerase subunit alpha

Chain T:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	133.01Å 161.63Å 139.21Å 90.00° 107.72° 90.00°	Depositor
Resolution (Å)	51.99 – 2.76 51.99 – 2.76	Depositor EDS
% Data completeness (in resolution range)	99.5 (51.99-2.76) 99.5 (51.99-2.76)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.240 , 0.281 0.245 , 0.283	Depositor DCC
R_{free} test set	141860 reflections (1.38%)	wwPDB-VP
Wilson B-factor (Å^2)	78.4	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 46.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.003 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	26631	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: EDO, ZN, SO4, 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	J	0.24	0/681	0.45	0/923
2	A	0.24	0/1641	0.48	0/2236
2	B	0.24	0/1693	0.48	0/2316
3	C	0.25	0/8394	0.47	1/11410 (0.0%)
4	D	0.25	0/9742	0.45	0/13189
5	E	0.24	0/604	0.45	0/822
6	F	0.23	0/2510	0.42	1/3389 (0.0%)
7	O	0.54	0/710	0.96	0/1095
8	P	0.56	0/589	0.95	0/906
9	T	0.24	0/379	0.39	0/515
All	All	0.27	0/26943	0.50	2/36801 (0.0%)

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	J	0	1
3	C	0	5
All	All	0	6

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	144	PRO	N-CA-CB	5.81	110.27	103.30
3	C	890	LEU	CA-CB-CG	5.20	127.26	115.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	368	ARG	Peptide
3	C	433	GLN	Peptide
3	C	982	SER	Peptide
3	C	985	PRO	Peptide
1	J	70	PRO	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	J	667	0	649	48	0
2	A	1617	0	1636	178	0
2	B	1667	0	1636	198	0
3	C	8250	0	7989	690	1
4	D	9588	0	9552	634	1
5	E	592	0	583	54	0
6	F	2481	0	2481	137	0
7	O	634	0	350	34	0
8	P	526	0	296	16	0
9	T	377	0	348	30	0
10	C	15	0	0	2	0
10	D	20	0	0	2	0
10	F	25	0	0	1	0
11	C	8	12	12	1	0
11	D	12	18	18	3	0
11	F	4	6	6	1	0
12	D	2	0	0	0	0
13	D	1	0	0	0	0
14	A	3	0	0	1	0
14	B	1	0	0	1	0
14	C	17	0	0	8	0
14	D	51	0	0	7	0
14	E	2	0	0	0	0
14	F	16	0	0	2	0
14	J	1	0	0	0	0
14	O	13	0	0	4	0
14	P	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	T	1	0	0	1	0
All	All	26595	36	25556	1848	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 36.

The worst 5 of 1848 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:B:184:GLU:HA	2:B:187:THR:HG22	1.28	1.16
3:C:940:ALA:HB1	3:C:941:ALA:HA	1.27	1.14
3:C:228:LEU:HD21	3:C:268:ILE:HG12	1.33	1.08
3:C:540:ASP:HB2	3:C:546:THR:HG23	1.30	1.08
3:C:176:VAL:HG12	3:C:195:VAL:HG22	1.36	1.06

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)
3:C:777:GLU:OE2	4:D:209:ARG:NH1[2_356]	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	J	81/114 (71%)	75 (93%)	6 (7%)	0	100	100
2	A	214/350 (61%)	201 (94%)	13 (6%)	0	100	100
2	B	231/350 (66%)	216 (94%)	13 (6%)	2 (1%)	14	26
3	C	1093/1169 (94%)	1039 (95%)	50 (5%)	4 (0%)	30	47
4	D	1238/1317 (94%)	1190 (96%)	45 (4%)	3 (0%)	44	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	E	72/107 (67%)	65 (90%)	5 (7%)	2 (3%)	4 6
6	F	313/466 (67%)	307 (98%)	6 (2%)	0	100 100
9	T	51/100 (51%)	51 (100%)	0	0	100 100
All	All	3293/3973 (83%)	3144 (96%)	138 (4%)	11 (0%)	37 55

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	76	VAL
3	C	982	SER
3	C	544	ARG
3	C	1134	ALA
4	D	902	GLU

5.3.2 Protein sidechains (i)

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	J	71/98 (72%)	65 (92%)	6 (8%)	8 16
2	A	178/297 (60%)	161 (90%)	17 (10%)	7 12
2	B	171/297 (58%)	152 (89%)	19 (11%)	5 8
3	C	857/984 (87%)	780 (91%)	77 (9%)	8 14
4	D	994/1095 (91%)	904 (91%)	90 (9%)	7 13
5	E	62/86 (72%)	50 (81%)	12 (19%)	1 1
6	F	252/379 (66%)	232 (92%)	20 (8%)	10 18
9	T	36/86 (42%)	29 (81%)	7 (19%)	1 1
All	All	2621/3322 (79%)	2373 (90%)	248 (10%)	7 13

5 of 248 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	1108	ILE

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Mol	Chain	Res	Type
6	F	182	GLU
4	D	304	GLN
5	E	102	GLU
6	F	437	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	684	ASN
4	D	1085	GLN
4	D	740	GLN
4	D	796	ASN
4	D	1140	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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 21 ligands modelled in this entry, 3 are monoatomic - leaving 18 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	$\#\|Z\|>2$
10	SO4	D	2006	-	4,4,4	0.24	0	6,6,6	0.07	0
10	SO4	F	504	-	4,4,4	0.24	0	6,6,6	0.08	0
11	EDO	C	1204	-	3,3,3	0.42	0	2,2,2	0.38	0
10	SO4	D	2005	-	4,4,4	0.23	0	6,6,6	0.07	0
10	SO4	F	503	-	4,4,4	0.24	0	6,6,6	0.09	0
11	EDO	D	2008	-	3,3,3	0.43	0	2,2,2	0.33	0
10	SO4	F	502	-	4,4,4	0.23	0	6,6,6	0.10	0
10	SO4	C	1202	-	4,4,4	0.24	0	6,6,6	0.11	0
10	SO4	D	2004	-	4,4,4	0.24	0	6,6,6	0.10	0
10	SO4	D	2007	-	4,4,4	0.24	0	6,6,6	0.09	0
11	EDO	D	2010	-	3,3,3	0.43	0	2,2,2	0.23	0
10	SO4	F	501	-	4,4,4	0.23	0	6,6,6	0.09	0
11	EDO	C	1205	-	3,3,3	0.43	0	2,2,2	0.33	0
10	SO4	C	1201	-	4,4,4	0.23	0	6,6,6	0.07	0
10	SO4	F	505	-	4,4,4	0.23	0	6,6,6	0.07	0
11	EDO	D	2009	-	3,3,3	0.42	0	2,2,2	0.35	0
10	SO4	C	1203	-	4,4,4	0.23	0	6,6,6	0.05	0
11	EDO	F	506	-	3,3,3	0.43	0	2,2,2	0.31	0

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
11	EDO	C	1204	-	-	1/1/1/1	-
11	EDO	D	2008	-	-	1/1/1/1	-
11	EDO	D	2010	-	-	0/1/1/1	-
11	EDO	C	1205	-	-	1/1/1/1	-
11	EDO	D	2009	-	-	0/1/1/1	-
11	EDO	F	506	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	1204	EDO	O1-C1-C2-O2
11	D	2008	EDO	O1-C1-C2-O2
11	C	1205	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
11	F	506	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	2005	SO4	2	0
11	D	2008	EDO	3	0
10	F	502	SO4	1	0
11	C	1205	EDO	1	0
10	C	1203	SO4	2	0
11	F	506	EDO	1	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, 95^{th} 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	J	83/114 (72%)	0.38	3 (3%) 46 48	65, 98, 141, 159	0
2	A	218/350 (62%)	0.45	8 (3%) 45 47	60, 88, 120, 139	0
2	B	233/350 (66%)	0.93	31 (13%) 8 10	82, 112, 136, 148	0
3	C	1099/1169 (94%)	0.38	49 (4%) 39 40	43, 86, 149, 168	0
4	D	1248/1317 (94%)	0.12	28 (2%) 62 62	39, 74, 127, 157	0
5	E	76/107 (71%)	0.20	2 (2%) 57 58	52, 79, 113, 118	0
6	F	319/466 (68%)	0.00	7 (2%) 62 62	40, 74, 136, 159	0
7	O	31/31 (100%)	-0.70	0 100 100	52, 65, 85, 90	0
8	P	26/26 (100%)	-0.63	0 100 100	60, 70, 84, 94	0
9	T	53/100 (53%)	1.22	13 (24%) 2 3	115, 149, 167, 170	0
All	All	3386/4030 (84%)	0.28	141 (4%) 41 42	39, 83, 143, 170	0

The worst 5 of 141 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	155	SER	5.9
9	T	275	LEU	5.7
3	C	228	LEU	4.9
3	C	229	LEU	4.3
2	B	157	ALA	4.0

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 monosaccharides 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, 95^{th} 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(Å^2)	Q<0.9
10	SO4	D	2007	5/5	0.71	0.08	95,100,113,141	0
10	SO4	F	504	5/5	0.72	0.07	115,115,118,128	0
10	SO4	C	1203	5/5	0.73	0.08	106,115,140,197	0
10	SO4	C	1202	5/5	0.75	0.08	108,111,116,178	0
13	MG	D	2003	1/1	0.78	0.29	79,79,79,79	0
10	SO4	C	1201	5/5	0.79	0.07	113,115,126,138	0
11	EDO	D	2009	4/4	0.80	0.12	74,89,104,104	0
11	EDO	C	1205	4/4	0.80	0.15	74,94,102,113	0
11	EDO	F	506	4/4	0.83	0.12	74,88,95,95	0
11	EDO	C	1204	4/4	0.85	0.11	52,66,79,80	0
11	EDO	D	2008	4/4	0.87	0.10	73,90,108,108	0
10	SO4	D	2006	5/5	0.87	0.10	85,104,119,125	0
10	SO4	F	501	5/5	0.87	0.06	100,100,118,124	0
10	SO4	F	502	5/5	0.87	0.09	88,88,104,107	0
10	SO4	D	2004	5/5	0.89	0.11	70,77,85,88	0
10	SO4	F	505	5/5	0.90	0.10	79,86,117,167	0
10	SO4	F	503	5/5	0.91	0.10	86,95,99,116	0
11	EDO	D	2010	4/4	0.92	0.21	63,76,77,90	0
10	SO4	D	2005	5/5	0.93	0.14	86,87,98,125	0
12	ZN	D	2002	1/1	0.95	0.16	222,222,222,222	0
12	ZN	D	2001	1/1	1.00	0.08	78,78,78,78	0

6.5 Other polymers (i)

There are no such residues in this entry.