



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 11:25 PM UTC

PDB ID : 6KQL / pdb_00006kql
Title : Thermus thermophilus initial transcription complex comprising sigma A and 5'-triphosphate RNA of 4 nt
Authors : Zhang, Y.; Li, L.; Ebright, R.H.
Deposited on : 2019-08-18
Resolution : 2.89 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
Mogul : 2022.3.0, CSD as543be (2022)
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

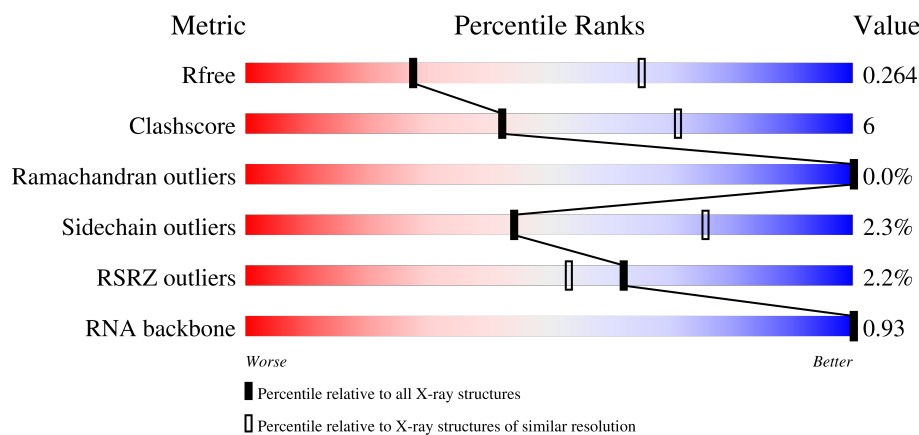
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)
RNA backbone	3983	1120 (3.10-2.70)

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	315	
1	B	315	
2	C	1119	
3	D	1524	

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Mol	Chain	Length	Quality of chain
4	E	99	% 88% 6% • 5%
5	F	443	3% 66% 11% • 22%
6	G	21	5% 62% 19% 19%
7	H	26	4% 46% 46% 8%
8	I	4	50% 50%

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 28900 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	231	Total	C	N	O	S	0	0	0
			1809	1155	315	337	2			
1	B	227	Total	C	N	O	S	0	0	0
			1789	1143	310	334	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1112	Total	C	N	O	S	0	0	0
			8762	5544	1559	1635	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1486	Total	C	N	O	S	0	1	0
			11746	7446	2070	2195	35			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	94	Total	C	N	O	S	0	0	0
			759	484	132	139	4			

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	346	Total	C	N	O	S	0	0	0
			2807	1770	509	524	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	initiating methionine	UNP Q5SKW1
F	-18	GLY	-	expression tag	UNP Q5SKW1
F	-17	SER	-	expression tag	UNP Q5SKW1
F	-16	SER	-	expression tag	UNP Q5SKW1
F	-15	HIS	-	expression tag	UNP Q5SKW1
F	-14	HIS	-	expression tag	UNP Q5SKW1
F	-13	HIS	-	expression tag	UNP Q5SKW1
F	-12	HIS	-	expression tag	UNP Q5SKW1
F	-11	HIS	-	expression tag	UNP Q5SKW1
F	-10	HIS	-	expression tag	UNP Q5SKW1
F	-9	SER	-	expression tag	UNP Q5SKW1
F	-8	SER	-	expression tag	UNP Q5SKW1
F	-7	GLY	-	expression tag	UNP Q5SKW1
F	-6	LEU	-	expression tag	UNP Q5SKW1
F	-5	VAL	-	expression tag	UNP Q5SKW1
F	-4	PRO	-	expression tag	UNP Q5SKW1
F	-3	ARG	-	expression tag	UNP Q5SKW1
F	-2	GLY	-	expression tag	UNP Q5SKW1
F	-1	SER	-	expression tag	UNP Q5SKW1
F	0	HIS	-	expression tag	UNP Q5SKW1

- Molecule 6 is a DNA chain called DNA (5'-D(*CP*CP*T*GP*CP*AP*TP*CP*CP*GP*T
P*GP*AP*GP*TP*CP*GP*AP*GP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	17	Total	C	N	O	P	0	0	0
			350	166	68	100	16			

- Molecule 7 is a DNA chain called DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*
GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*AP*G*)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	24	Total	C	N	O	P	0	0	0
			495	236	94	142	23			

- Molecule 8 is a RNA chain called RNA (5'-R(*(UTP))-R(P*CP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	4	Total	C	N	O	P	0	0	0
			86	38	15	29	4			

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	3	Total	Mg	0	0
			3	3		
10	F	1	Total	Mg	0	0
			1	1		

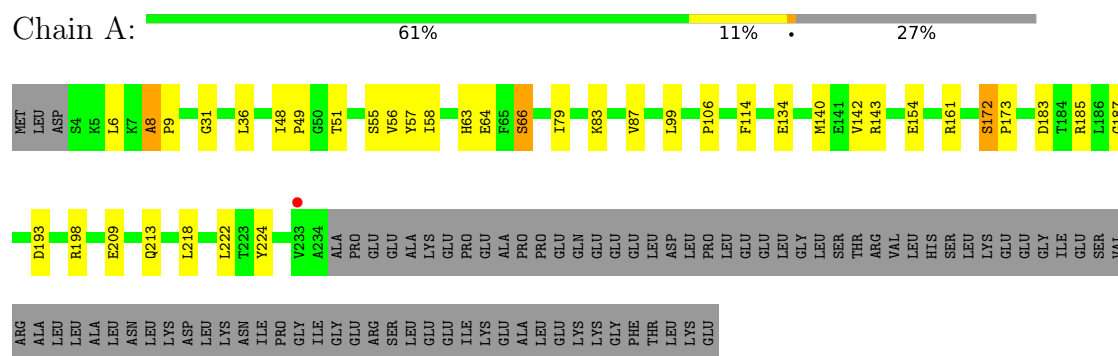
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	11	Total	O	0	0
			11	11		
11	B	8	Total	O	0	0
			8	8		
11	C	96	Total	O	0	0
			96	96		
11	D	128	Total	O	0	0
			128	128		
11	E	8	Total	O	0	0
			8	8		
11	F	26	Total	O	0	0
			26	26		
11	G	10	Total	O	0	0
			10	10		
11	I	4	Total	O	0	0
			4	4		

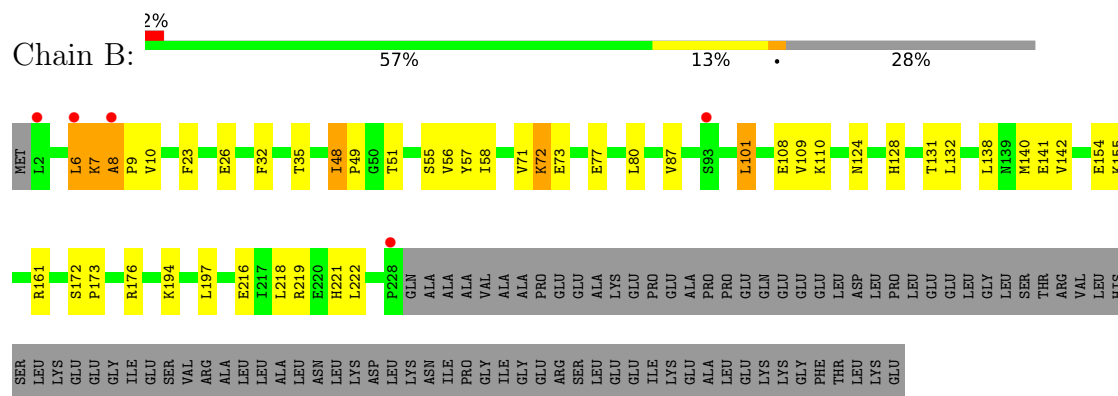
3 Residue-property plots [i](#)

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.

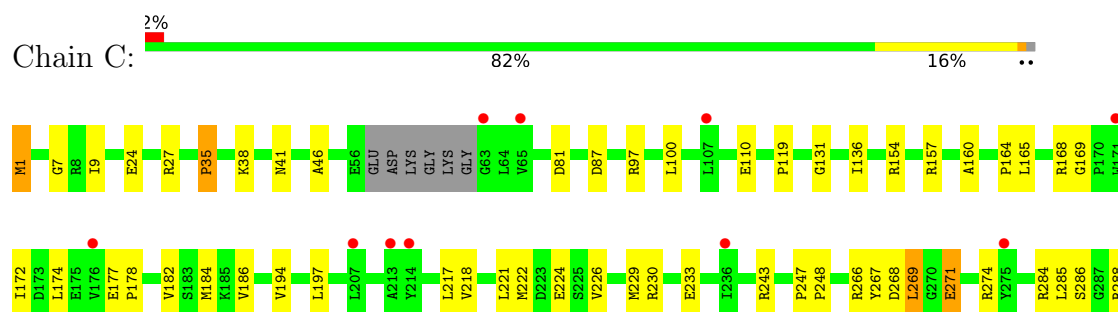
• Molecule 1: DNA-directed RNA polymerase subunit alpha

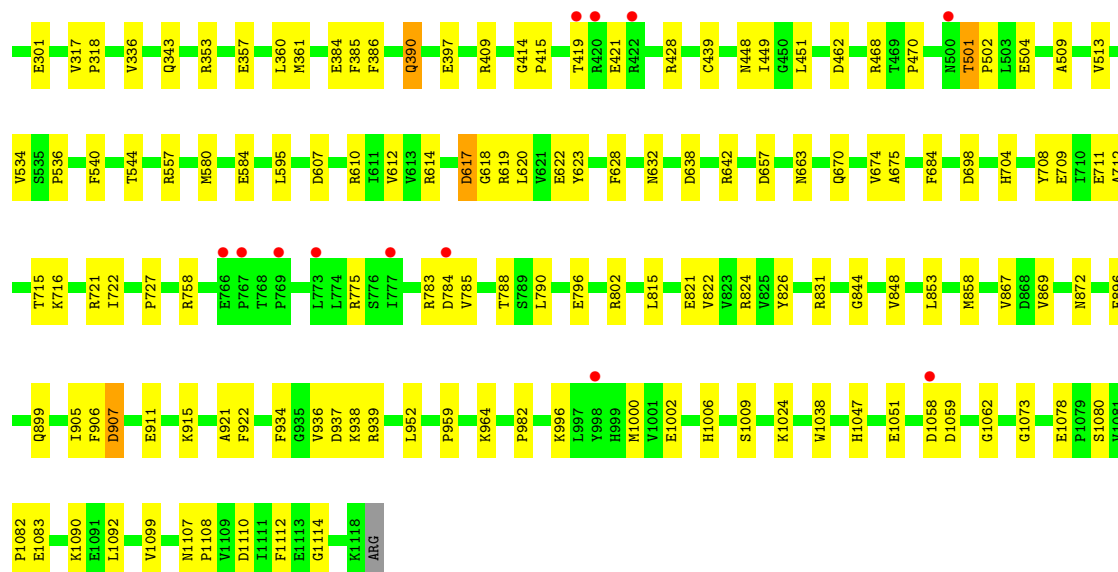


• Molecule 1: DNA-directed RNA polymerase subunit alpha

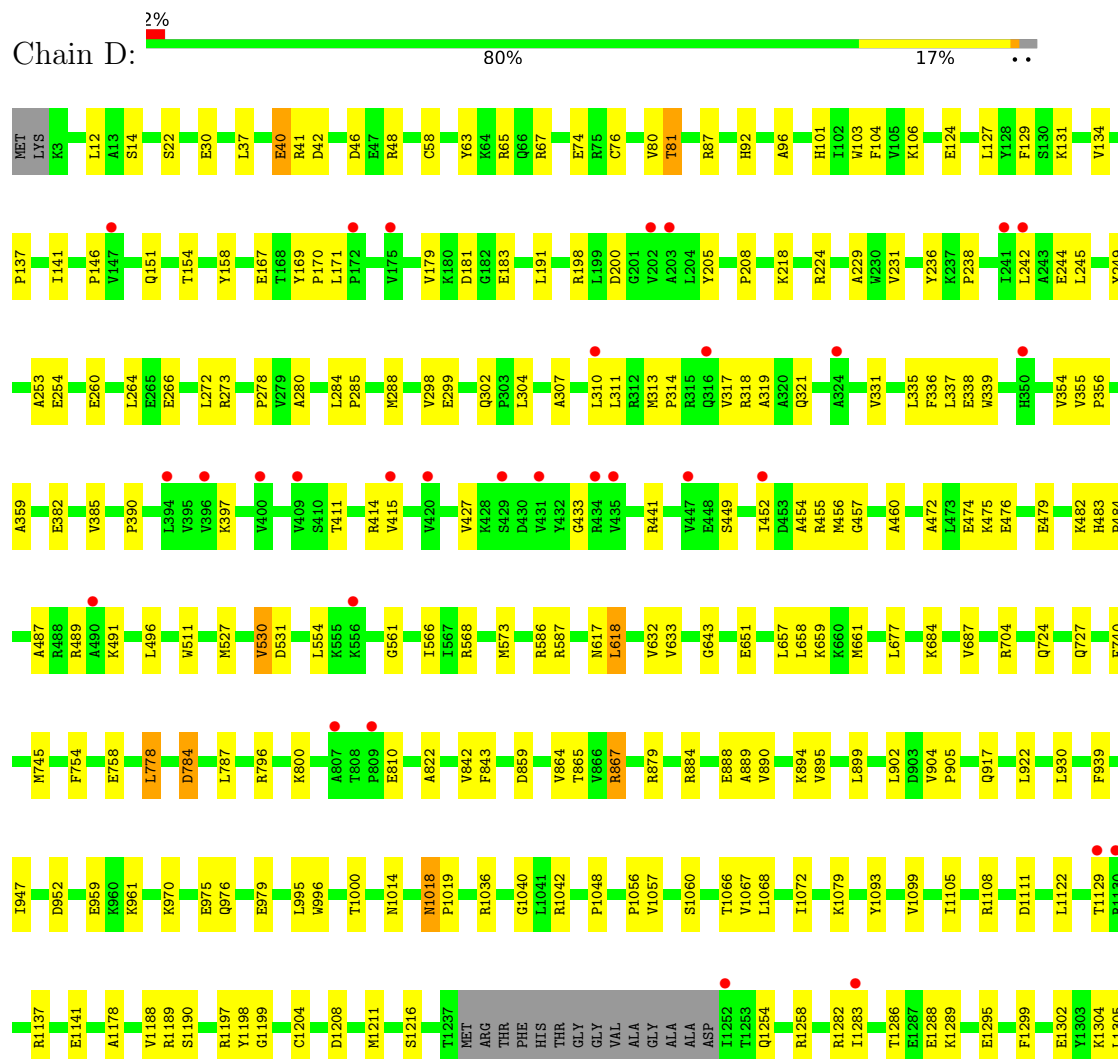


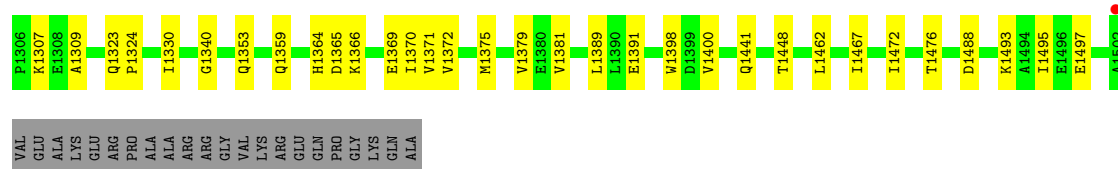
• Molecule 2: DNA-directed RNA polymerase subunit beta



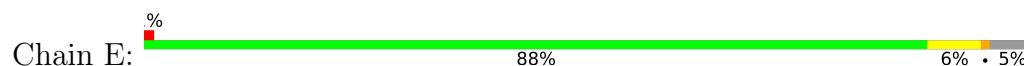


• Molecule 3: DNA-directed RNA polymerase subunit beta'

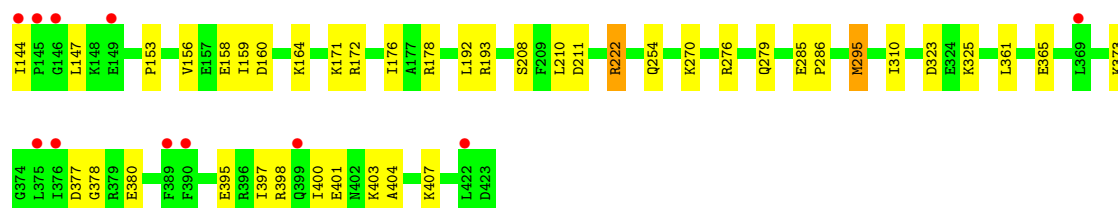
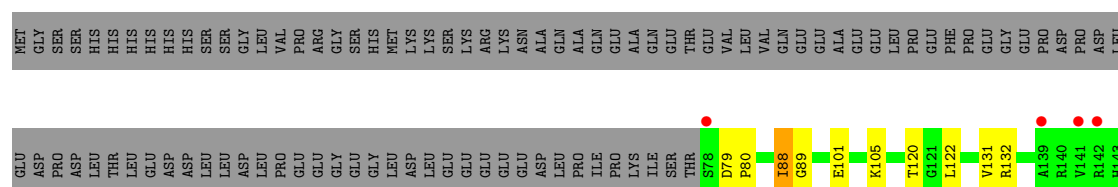




- Molecule 4: DNA-directed RNA polymerase subunit omega



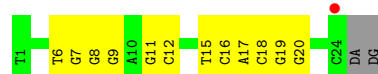
- Molecule 5: RNA polymerase sigma factor SigA



- Molecule 6: DNA (5'-D(*CP*CP*T*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*GP*AP*GP*GP*G)-3')



- Molecule 7: DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*AP*G)-3')



- Molecule 8: RNA (5'-R*(UTP))-R(P*CP*GP*A)-3')



UTP4	CS	GS	A7
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	183.80Å 103.17Å 295.56Å 90.00° 99.12° 90.00°	Depositor
Resolution (Å)	44.84 – 2.89 44.84 – 2.89	Depositor EDS
% Data completeness (in resolution range)	98.9 (44.84-2.89) 99.0 (44.84-2.89)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.207 , 0.246 (Not available) , 0.264	Depositor DCC
R_{free} test set	2680 reflections (2.19%)	wwPDB-VP
Wilson B-factor (Å ²)	67.8	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 38.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for $1/2^*h-3/2^*k,-1/2^*h-1/2^*k,-1/2^*h+1/2^*k-l$ 0.011 for $1/2^*h+3/2^*k,1/2^*h-1/2^*k,-1/2^*h-1/2^*k-l$	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28900	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, UTP, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.31	0/1841	0.83	4/2504 (0.2%)
1	B	0.33	0/1821	0.83	2/2476 (0.1%)
2	C	0.33	0/8929	0.77	10/12078 (0.1%)
3	D	0.32	0/11955	0.77	10/16163 (0.1%)
4	E	0.29	0/773	0.74	0/1042
5	F	0.29	0/2852	0.74	1/3837 (0.0%)
6	G	0.17	0/393	0.48	0/606
7	H	0.16	0/556	0.52	0/858
8	I	0.14	0/72	0.26	0/110
All	All	0.32	0/29192	0.77	27/39674 (0.1%)

There are no bond length outliers.

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	SER	CA-C-N	7.10	126.73	119.56
1	A	172	SER	C-N-CA	7.10	126.73	119.56
3	D	433	GLY	N-CA-C	6.90	119.87	110.69
3	D	1340	GLY	CA-C-N	6.86	126.10	118.97
3	D	1340	GLY	C-N-CA	6.86	126.10	118.97

There are no chirality outliers.

There are no planarity outliers.

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	1809	0	1863	24	0
1	B	1789	0	1841	30	0
2	C	8762	0	8855	120	0
3	D	11746	0	11984	160	0
4	E	759	0	771	6	0
5	F	2807	0	2882	35	0
6	G	350	0	192	3	0
7	H	495	0	272	20	0
8	I	86	0	42	3	0
9	D	2	0	0	0	0
10	D	3	0	0	0	0
10	F	1	0	0	0	0
11	A	11	0	0	0	0
11	B	8	0	0	0	0
11	C	96	0	0	1	0
11	D	128	0	0	2	0
11	E	8	0	0	1	0
11	F	26	0	0	1	0
11	G	10	0	0	0	0
11	I	4	0	0	0	0
All	All	28900	0	28702	356	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 6.

The worst 5 of 356 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)
7:H:16:DC:H2''	7:H:17:DA:C8	1.73	1.23
2:C:7:GLY:CA	2:C:907:ASP:OD1	2.23	0.87
2:C:628:PHE:H	2:C:638:ASP:HB3	1.45	0.82
7:H:16:DC:H2''	7:H:17:DA:H8	1.38	0.78
7:H:19:DG:H1'	7:H:20:DG:H5'	1.70	0.74

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	229/315 (73%)	226 (99%)	3 (1%)	0	100	100
1	B	225/315 (71%)	221 (98%)	3 (1%)	1 (0%)	30	59
2	C	1108/1119 (99%)	1085 (98%)	23 (2%)	0	100	100
3	D	1483/1524 (97%)	1448 (98%)	35 (2%)	0	100	100
4	E	92/99 (93%)	91 (99%)	1 (1%)	0	100	100
5	F	344/443 (78%)	340 (99%)	4 (1%)	0	100	100
All	All	3481/3815 (91%)	3411 (98%)	69 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	8	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	200/273 (73%)	198 (99%)	2 (1%)	68	89
1	B	200/273 (73%)	193 (96%)	7 (4%)	32	66
2	C	934/941 (99%)	911 (98%)	23 (2%)	42	74
3	D	1254/1279 (98%)	1227 (98%)	27 (2%)	45	77
4	E	82/88 (93%)	81 (99%)	1 (1%)	63	86
5	F	301/388 (78%)	293 (97%)	8 (3%)	39	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2971/3242 (92%)	2903 (98%)	68 (2%)	44 76

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	1307	LYS
4	E	50	THR
5	F	325	LYS
2	C	722	ILE
2	C	715	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	703	ASN
3	D	1442	ASN
3	D	724	GLN
4	E	49	GLN
3	D	1124	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	2/4 (50%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 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	231/315 (73%)	0.03	1 (0%) 88 85	56, 75, 103, 157	0
1	B	227/315 (72%)	0.22	5 (2%) 62 53	58, 85, 120, 151	0
2	C	1112/1119 (99%)	-0.02	22 (1%) 65 56	38, 70, 137, 161	0
3	D	1486/1524 (97%)	0.11	32 (2%) 62 53	36, 70, 140, 167	1 (0%)
4	E	94/99 (94%)	0.12	1 (1%) 78 71	47, 73, 114, 125	0
5	F	346/443 (78%)	0.35	15 (4%) 40 31	46, 88, 145, 172	0
6	G	17/21 (80%)	0.20	1 (5%) 28 22	49, 86, 175, 182	0
7	H	24/26 (92%)	0.34	1 (4%) 40 32	75, 114, 160, 180	0
8	I	3/4 (75%)	-0.86	0 100 100	51, 51, 55, 66	0
All	All	3540/3866 (91%)	0.10	78 (2%) 62 53	36, 75, 138, 182	1 (0%)

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	420	VAL	4.0
5	F	422	LEU	3.8
3	D	431	VAL	3.5
5	F	141	VAL	3.4
3	D	203	ALA	3.4

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
10	MG	D	2004	1/1	0.77	0.33	72,72,72,72	0
10	MG	D	2005	1/1	0.80	0.12	74,74,74,74	0
10	MG	F	2001	1/1	0.92	0.08	71,71,71,71	0
10	MG	D	2003	1/1	0.99	0.03	41,41,41,41	0
9	ZN	D	2002	1/1	0.99	0.03	103,103,103,103	0
9	ZN	D	2001	1/1	1.00	0.04	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.