



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 16, 2024 – 04:25 PM JST

PDB ID : 8W8N
Title : Thermus thermophilus initiation transcription complex in the pre-translocated state
Authors : Li, L.; Zhang, Y.
Deposited on : 2023-09-04
Resolution : 2.69 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

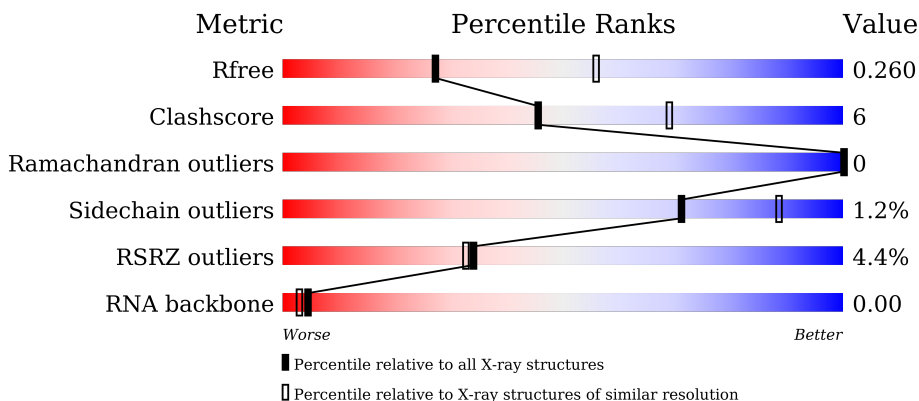
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)
RNA backbone	3102	1159 (3.00-2.40)

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	57% 14% 28%
1	B	315	57% 15% 28%
2	C	1119	81% 18% .
3	D	1524	81% 16% .

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Mol	Chain	Length	Quality of chain
4	E	99	<p>% 81% 14% 5%</p>
5	F	443	<p>2% 67% 11% 22%</p>
6	G	21	<p>38% 38% 24%</p>
7	H	27	<p>7% 44% 41% 15%</p>
8	I	3	<p>100%</p>

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 28636 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
			Total	C	N	O	S			
1	A	227	Total	C	N	O	S	0	0	0
			1787	1141	311	333	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
			Total	C	N	O	S			
2	C	1112	Total	C	N	O	S	0	0	0
			8761	5541	1562	1634	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	1484	Total	C	N	O	S	0	1	0
			11706	7425	2060	2186	35			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
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	-	expression tag	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 (21-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
6	G	16	326	154	62	94	16	0	0	0

- Molecule 7 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
7	H	23	476	227	91	136	22	0	0	0

- Molecule 8 is a RNA chain called RNA (5'-D(*PP*PP*P)-R(*GP*GP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
8	I	3	75	29	12	29	5	0	0	0

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Mg 1 1	0	0
9	D	3	Total Mg 3 3	0	0
9	F	2	Total Mg 2 2	0	0

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

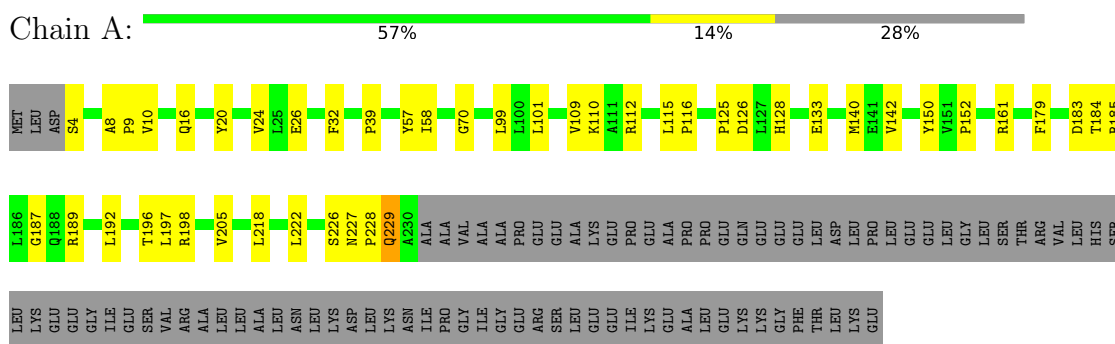
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	3	Total O 3 3	0	0
11	B	4	Total O 4 4	0	0
11	C	47	Total O 47 47	0	0
11	D	72	Total O 72 72	0	0
11	E	2	Total O 2 2	0	0
11	F	6	Total O 6 6	0	0
11	G	5	Total O 5 5	0	0
11	I	1	Total O 1 1	0	0

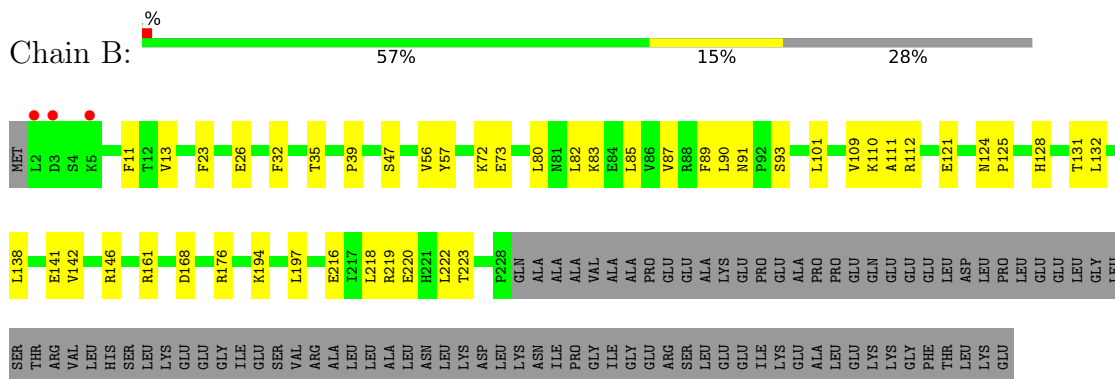
3 Residue-property plots

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.

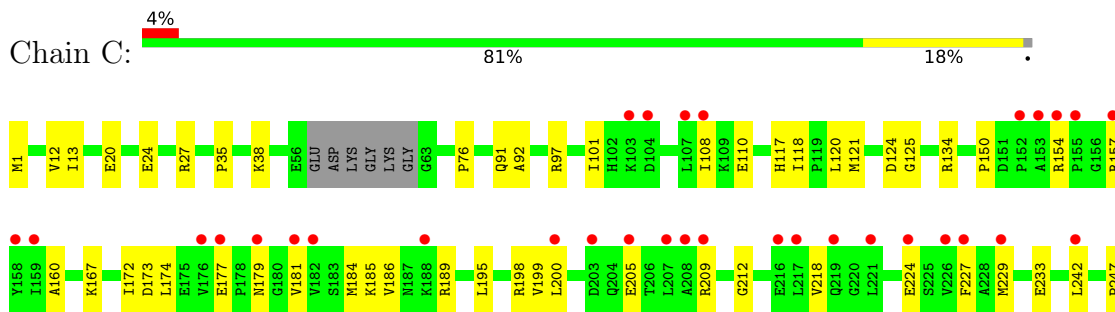
- Molecule 1: DNA-directed RNA polymerase subunit alpha

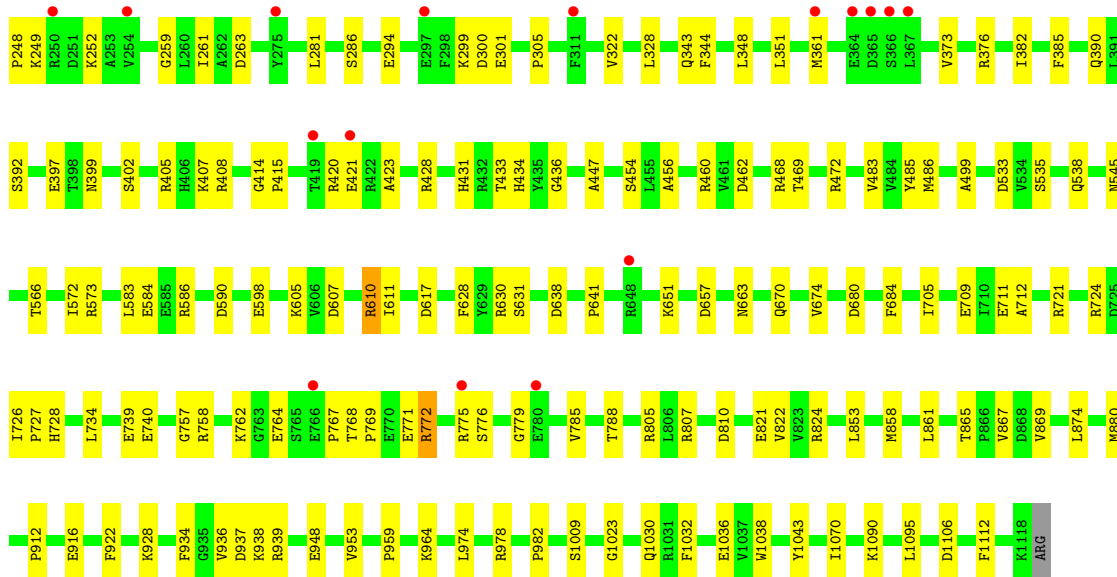


- Molecule 1: DNA-directed RNA polymerase subunit alpha

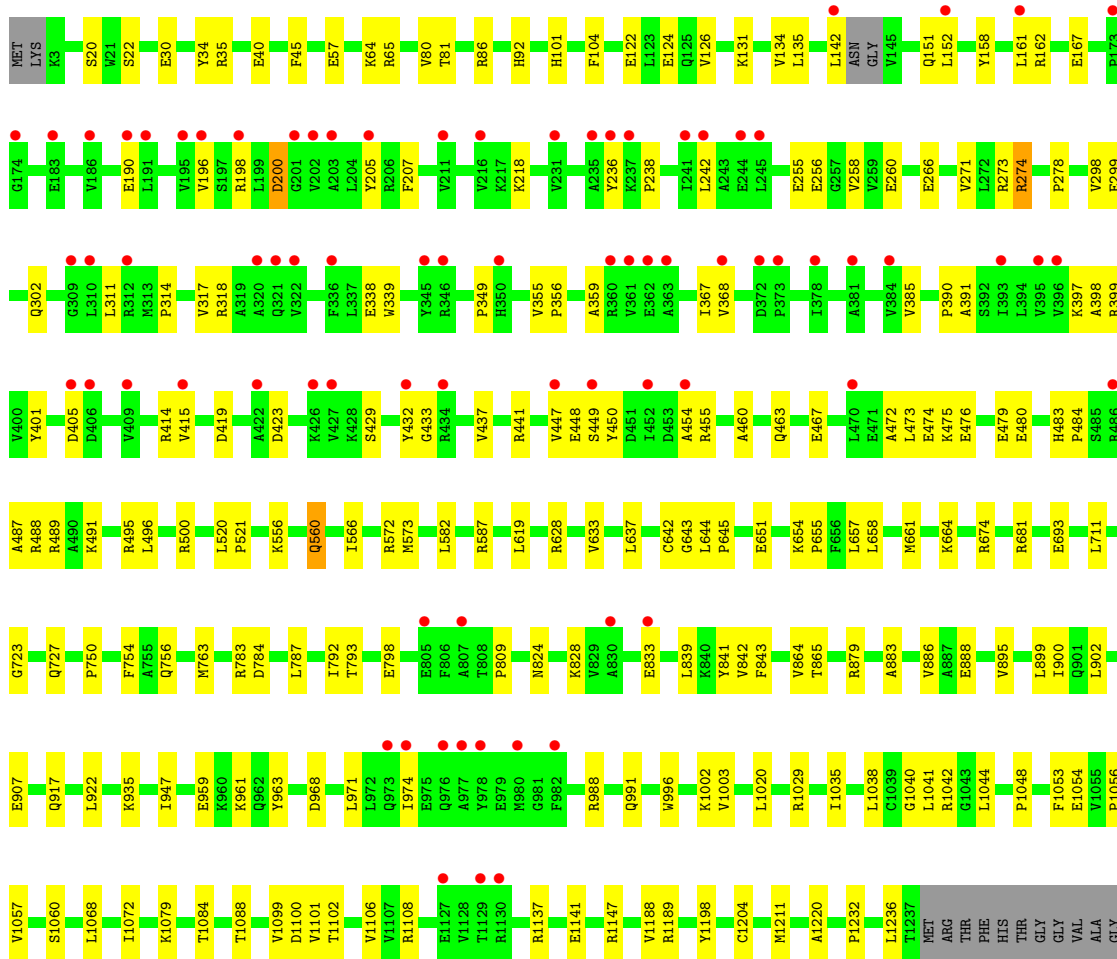


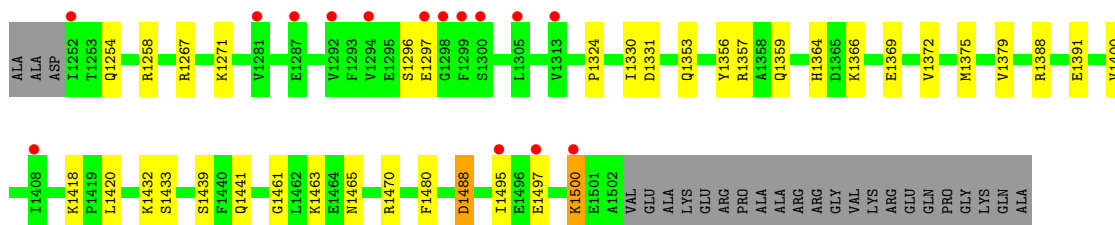
- Molecule 2: DNA-directed RNA polymerase subunit beta



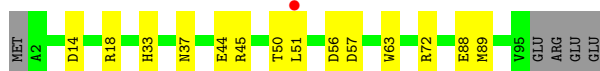
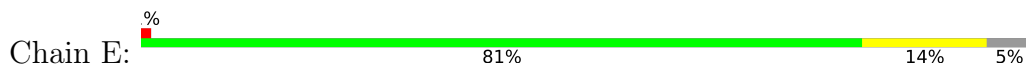


● Molecule 3: DNA-directed RNA polymerase subunit beta'

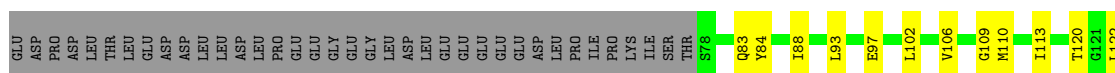
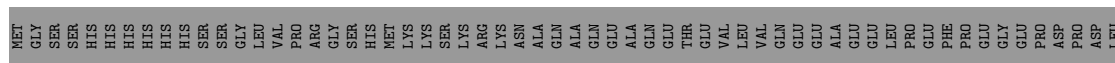




- Molecule 4: DNA-directed RNA polymerase subunit omega



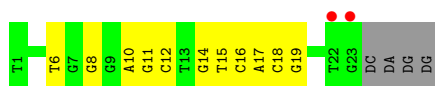
- Molecule 5: RNA polymerase sigma factor SigA



- Molecule 6: DNA (21-MER)



- Molecule 7: DNA (27-MER)



- Molecule 8: RNA (5'-D(*PP*PP*P)-R(*GP*GP*U)-3')



There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	184.42Å 103.70Å 295.44Å 90.00° 98.67° 90.00°	Depositor
Resolution (Å)	48.86 – 2.69 48.86 – 2.69	Depositor EDS
% Data completeness (in resolution range)	74.9 (48.86-2.69) 74.9 (48.86-2.69)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.69Å)	Xtrriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.212 , 0.260 0.212 , 0.260	Depositor DCC
R_{free} test set	2002 reflections (1.75%)	wwPDB-VP
Wilson B-factor (Å ²)	43.7	Xtrriage
Anisotropy	0.079	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	28636	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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: GTP, MG, 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	0.26	0/1819	0.46	0/2473
1	B	0.25	0/1821	0.45	0/2476
2	C	0.26	0/8927	0.44	0/12074
3	D	0.26	0/11914	0.45	0/16111
4	E	0.25	0/775	0.41	0/1045
5	F	0.25	0/2852	0.40	0/3837
6	G	0.52	0/365	0.86	0/560
7	H	0.59	0/535	0.91	0/826
8	I	0.27	0/47	0.81	0/71
All	All	0.27	0/29055	0.47	0/39473

There are no bond length outliers.

There are no bond angle outliers.

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	1787	0	1839	30	0
1	B	1789	0	1841	31	0
2	C	8761	0	8859	127	0
3	D	11706	0	11929	153	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	761	0	778	9	0
5	F	2807	0	2882	33	0
6	G	326	0	179	8	0
7	H	476	0	261	8	0
8	I	75	0	33	0	0
9	B	1	0	0	0	0
9	D	3	0	0	0	0
9	F	2	0	0	0	0
10	D	2	0	0	0	0
11	A	3	0	0	0	0
11	B	4	0	0	0	0
11	C	47	0	0	1	0
11	D	72	0	0	0	0
11	E	2	0	0	0	0
11	F	6	0	0	0	0
11	G	5	0	0	0	0
11	I	1	0	0	0	0
All	All	28636	0	28601	363	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 363 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)
6:G:11:DG:H2'	6:G:12:DA:C8	2.20	0.76
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.68	0.74
5:F:361:LEU:HB3	5:F:365:GLU:HG3	1.69	0.72
3:D:65:ARG:NH1	5:F:378:GLY:O	2.21	0.72
3:D:1254:GLN:HB3	3:D:1258:ARG:HB2	1.70	0.72

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	225/315 (71%)	222 (99%)	3 (1%)	0	100	100
1	B	225/315 (71%)	221 (98%)	4 (2%)	0	100	100
2	C	1108/1119 (99%)	1078 (97%)	30 (3%)	0	100	100
3	D	1479/1524 (97%)	1448 (98%)	31 (2%)	0	100	100
4	E	92/99 (93%)	90 (98%)	2 (2%)	0	100	100
5	F	344/443 (78%)	341 (99%)	3 (1%)	0	100	100
All	All	3473/3815 (91%)	3400 (98%)	73 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	A	199/273 (73%)	197 (99%)	2 (1%)	76	91
1	B	200/273 (73%)	200 (100%)	0	100	100
2	C	934/941 (99%)	921 (99%)	13 (1%)	67	86
3	D	1247/1279 (98%)	1230 (99%)	17 (1%)	67	86
4	E	83/88 (94%)	83 (100%)	0	100	100
5	F	301/388 (78%)	298 (99%)	3 (1%)	76	91
All	All	2964/3242 (91%)	2929 (99%)	35 (1%)	71	88

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	1418	LYS
3	D	1433	SER
5	F	110	MET
2	C	764	GLU
2	C	762	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	ASN
1	B	91	ASN
2	C	538	GLN
3	D	696	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	1/3 (33%)	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 [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

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	227/315 (72%)	-0.29	0 100 100	26, 41, 65, 77	0
1	B	227/315 (72%)	0.01	3 (1%) 77 78	25, 52, 80, 109	0
2	C	1112/1119 (99%)	-0.06	48 (4%) 35 33	7, 36, 97, 122	0
3	D	1484/1524 (97%)	0.08	93 (6%) 20 19	8, 38, 96, 123	0
4	E	94/99 (94%)	-0.32	1 (1%) 80 82	17, 38, 73, 83	0
5	F	346/443 (78%)	0.08	10 (2%) 51 52	17, 55, 91, 111	0
6	G	16/21 (76%)	-0.22	0 100 100	29, 49, 123, 131	0
7	H	23/27 (85%)	0.02	2 (8%) 10 8	52, 72, 120, 136	0
8	I	2/3 (66%)	0.78	0 100 100	37, 37, 37, 43	2 (100%)
All	All	3531/3866 (91%)	-0.00	157 (4%) 34 33	7, 41, 95, 136	2 (0%)

The worst 5 of 157 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	1313	VAL	4.6
3	D	974	ILE	4.5
3	D	173	PRO	4.4
3	D	236	TYR	4.3
5	F	414	ARG	4.3

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 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, 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(Å ²)	Q<0.9
9	MG	D	1605	1/1	0.82	0.09	41,41,41,41	0
9	MG	B	401	1/1	0.84	0.11	60,60,60,60	0
9	MG	F	501	1/1	0.88	0.07	41,41,41,41	0
9	MG	D	1603	1/1	0.97	0.17	18,18,18,18	0
9	MG	D	1604	1/1	0.97	0.28	33,33,33,33	0
9	MG	F	502	1/1	0.98	0.23	43,43,43,43	0
10	ZN	D	1601	1/1	0.99	0.13	23,23,23,23	0
10	ZN	D	1602	1/1	0.99	0.08	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.