



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 07:31 PM BST

PDB ID : 6KQE
Title : Thermus thermophilus initial transcription complex comprising sigma A and 5'-OH RNA of 4 nt
Authors : Zhang, Y.; Li, L.; Ebright, R.H.
Deposited on : 2019-08-17
Resolution : 3.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
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)	:	2.13.1

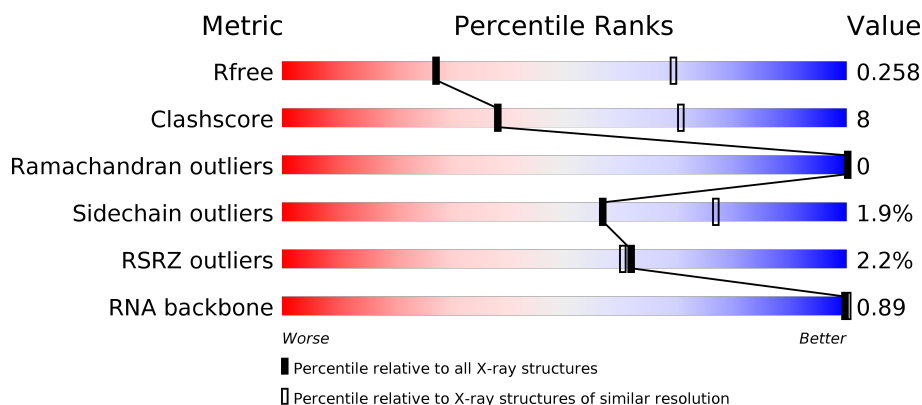
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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.




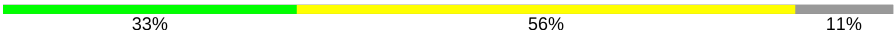

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

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 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	<div> <div>0%</div> <div>60% 13% 27%</div> </div>
1	B	315	<div> <div>58% 13% 28%</div> </div>
2	C	1119	<div> <div>2%</div> <div>82% 16% ..</div> </div>
3	D	1524	<div> <div>3%</div> <div>79% 18% .</div> </div>

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Mol	Chain	Length	Quality of chain
4	E	99	 80% 15% 5%
5	F	443	%  65% 13% 22%
6	G	21	 48% 33% 19%
7	H	27	 33% 56% 11%
8	I	4	 100%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 28688 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
			1784	1140	309	333	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	2	0
			11751	7450	2070	2195	36			

- 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
			2801	1767	506	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*GP*G*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(*UP*CP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	4	Total	C	N	O	P	0	0	0
			82	38	15	26	3			

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

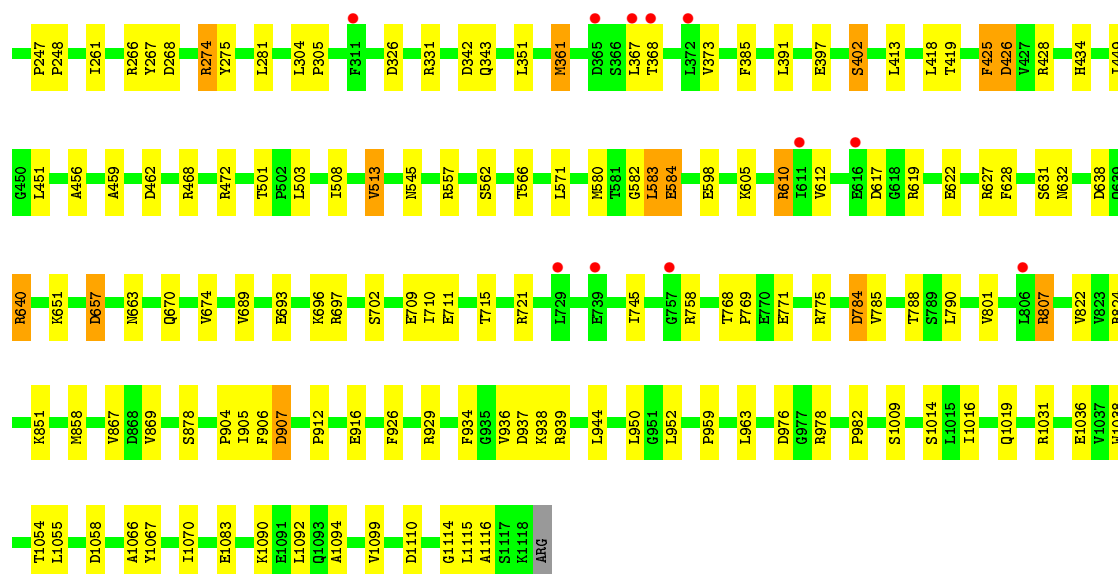
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Mg 1 1	0	0
9	D	2	Total Mg 2 2	0	0

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

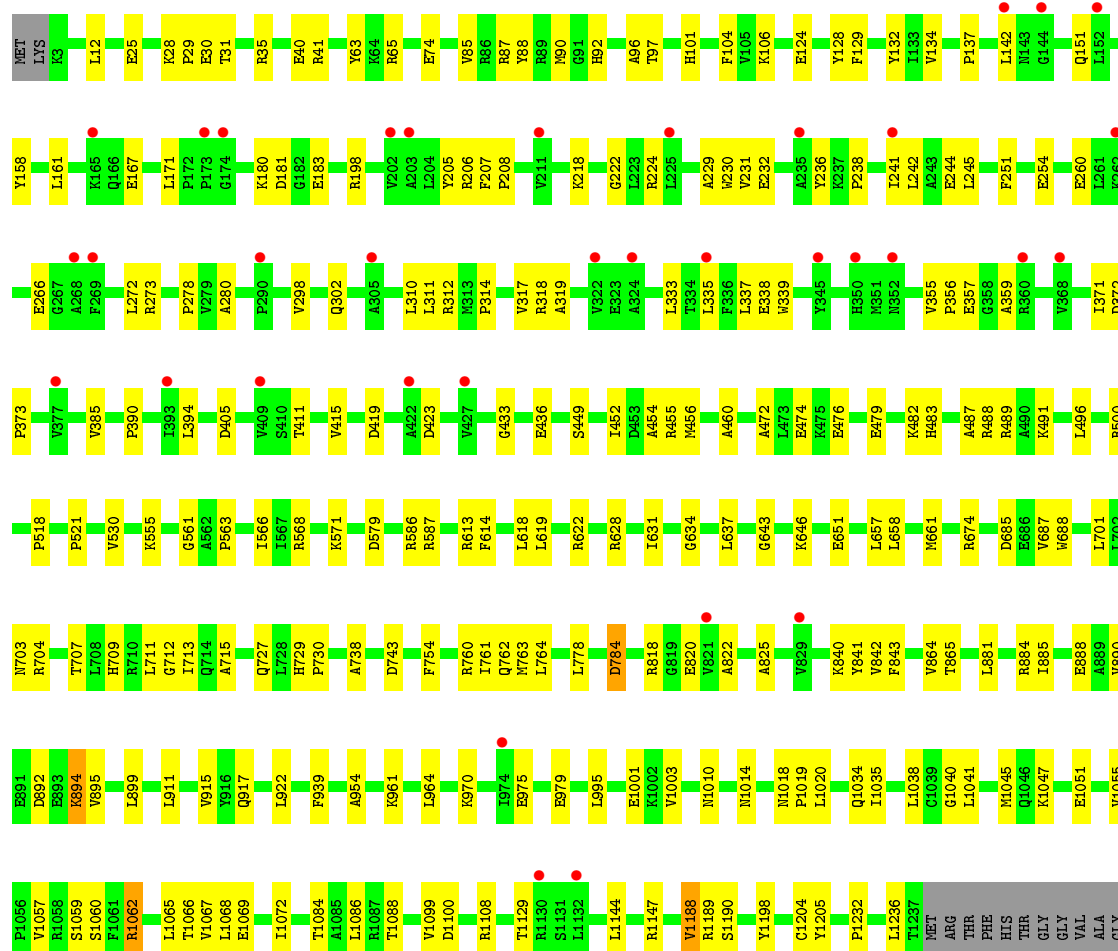
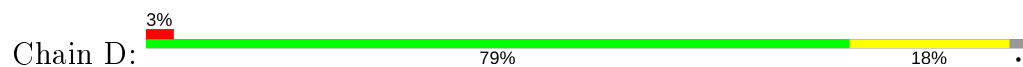
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	2	Total Zn 2 2	0	0

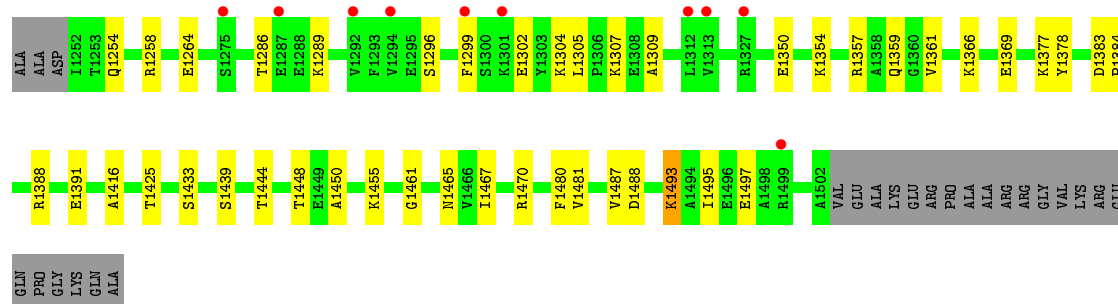
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	8	Total O 8 8	0	0
11	B	4	Total O 4 4	0	0
11	C	23	Total O 23 23	0	0
11	D	39	Total O 39 39	0	0
11	E	2	Total O 2 2	0	0
11	F	9	Total O 9 9	0	0
11	G	3	Total O 3 3	0	0
11	H	1	Total O 1 1	0	0
11	I	1	Total O 1 1	0	0



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

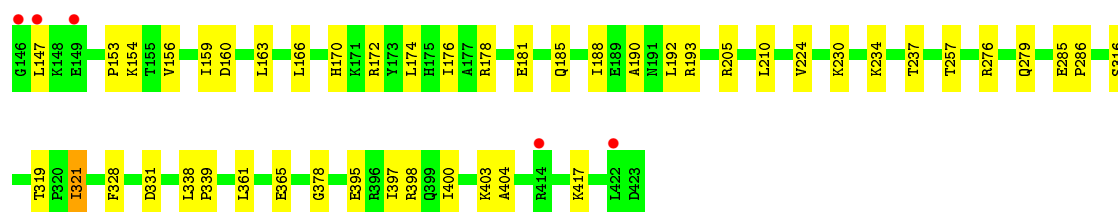
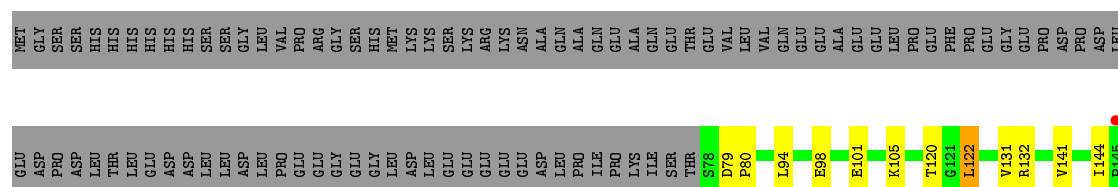




- Molecule 4: DNA-directed RNA polymerase subunit omega



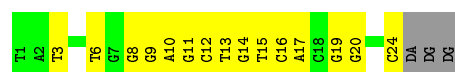
- Molecule 5: RNA polymerase sigma factor SigA



- 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*GP*G*G)-3')



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

Chain I:  100%

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	184.57Å 103.76Å 295.98Å 90.00° 98.70° 90.00°	Depositor
Resolution (Å)	48.95 – 3.30 48.95 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.95-3.30) 99.9 (48.95-3.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.217 , 0.258 0.217 , 0.258	Depositor DCC
R_{free} test set	4156 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	85.9	Xtriage
Anisotropy	0.523	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	28688	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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: 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	0.25	0/1841	0.46	0/2504
1	B	0.26	0/1816	0.48	1/2469 (0.0%)
2	C	0.27	0/8929	0.46	0/12078
3	D	0.24	0/11963	0.45	0/16173
4	E	0.24	0/773	0.42	0/1042
5	F	0.24	0/2846	0.41	0/3830
6	G	0.42	0/393	0.91	0/606
7	H	0.39	0/556	0.94	0/858
8	I	0.23	0/91	0.63	0/140
All	All	0.26	0/29208	0.48	1/39700 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	8	ALA	C-N-CD	5.15	139.21	128.40

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	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1784	0	1830	38	0
2	C	8762	0	8855	135	0
3	D	11751	0	11993	187	0
4	E	759	0	771	10	0
5	F	2801	0	2871	35	0
6	G	350	0	192	16	0
7	H	495	0	272	41	0
8	I	82	0	44	0	0
9	B	1	0	0	0	0
9	D	2	0	0	0	0
10	D	2	0	0	0	0
11	A	8	0	0	1	0
11	B	4	0	0	0	0
11	C	23	0	0	1	0
11	D	39	0	0	1	0
11	E	2	0	0	1	0
11	F	9	0	0	0	0
11	G	3	0	0	0	0
11	H	1	0	0	0	0
11	I	1	0	0	0	0
All	All	28688	0	28691	433	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 8.

The worst 5 of 433 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:C:425:PHE:CE1	3:D:1086:LEU:HD12	1.74	1.23
7:H:16:DC:H2"	7:H:17:DA:C8	1.78	1.18
7:H:19:DG:H2"	7:H:20:DG:C8	1.80	1.16
6:G:4:DG:H2"	6:G:5:DC:C6	1.82	1.13
6:G:4:DG:H2"	6:G:5:DC:C5	1.82	1.13

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%)	218 (97%)	7 (3%)	0	100	100
2	C	1108/1119 (99%)	1077 (97%)	31 (3%)	0	100	100
3	D	1484/1524 (97%)	1447 (98%)	37 (2%)	0	100	100
4	E	92/99 (93%)	88 (96%)	4 (4%)	0	100	100
5	F	344/443 (78%)	339 (98%)	5 (2%)	0	100	100
All	All	3482/3815 (91%)	3395 (98%)	87 (2%)	0	100	100

There are no Ramachandran outliers to report.

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%)	76	86
1	B	198/273 (72%)	195 (98%)	3 (2%)	65	81
2	C	934/941 (99%)	910 (97%)	24 (3%)	46	71
3	D	1255/1279 (98%)	1236 (98%)	19 (2%)	65	81
4	E	82/88 (93%)	79 (96%)	3 (4%)	34	63
5	F	300/388 (77%)	294 (98%)	6 (2%)	55	76
All	All	2969/3242 (92%)	2912 (98%)	57 (2%)	57	77

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	784	ASP
3	D	530	VAL
5	F	141	VAL
2	C	807	ARG
2	C	1014	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	714	GLN
3	D	1334	GLN
3	D	855	HIS
2	C	498	GLN
3	D	976	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	3/4 (75%)	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 5 ligands modelled in this entry, 5 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%)	-0.04	4 (1%) 70 68	63, 91, 117, 162	0
1	B	227/315 (72%)	-0.11	1 (0%) 92 93	63, 95, 124, 155	0
2	C	1112/1119 (99%)	0.02	23 (2%) 63 62	45, 88, 139, 167	0
3	D	1486/1524 (97%)	0.09	45 (3%) 50 49	46, 86, 145, 169	1 (0%)
4	E	94/99 (94%)	-0.22	0 100 100	65, 97, 135, 142	0
5	F	346/443 (78%)	-0.02	6 (1%) 70 68	65, 103, 147, 164	0
6	G	17/21 (80%)	-0.33	0 100 100	70, 105, 177, 184	0
7	H	24/27 (88%)	-0.46	0 100 100	96, 126, 177, 188	0
8	I	4/4 (100%)	-0.13	0 100 100	69, 72, 79, 89	0
All	All	3541/3867 (91%)	0.02	79 (2%) 62 60	45, 91, 142, 188	1 (0%)

The worst 5 of 79 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	63	GLY	9.0
1	A	232	ALA	4.6
3	D	322	VAL	4.4
3	D	203	ALA	4.3
3	D	173	PRO	4.2

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(\AA^2)	Q<0.9
9	MG	B	2001	1/1	0.88	0.25	95,95,95,95	0
9	MG	D	2003	1/1	0.90	0.18	52,52,52,52	0
9	MG	D	2004	1/1	0.95	0.47	63,63,63,63	0
10	ZN	D	2002	1/1	0.97	0.07	111,111,111,111	0
10	ZN	D	2001	1/1	0.99	0.21	71,71,71,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.