



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 22, 2016 – 09:50 PM EDT

PDB ID : 5E17
Title : T. thermophilus transcription initiation complex having a RRR discriminator sequence and a nontemplate-strand length corresponding to TSS selection at position 7 (RPo-GGG-7)
Authors : Zhang, Y.; Ebright, R.H.
Deposited on : 2015-09-29
Resolution : 3.20 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
<http://wwpdb.org/validation/2016/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
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0122
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

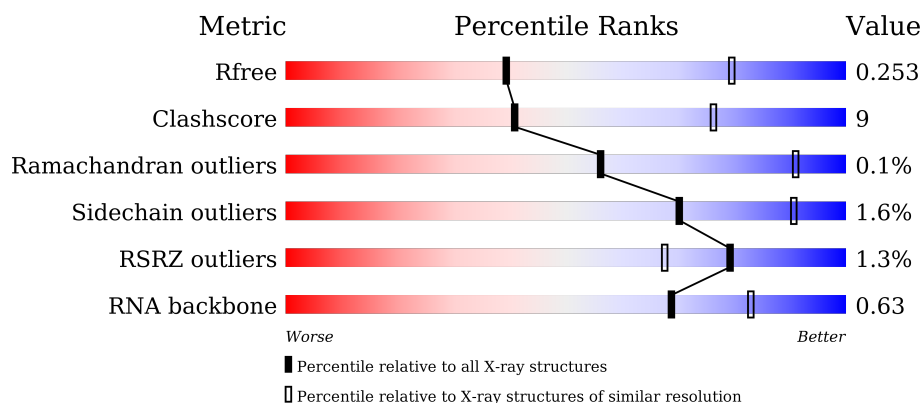
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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.






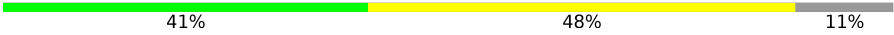

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)
RNA backbone	2183	1079 (3.70-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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>%</div> <div> <div></div> <div>57%</div> <div>16%</div> <div>27%</div> </div> </div>
1	B	315	<div> <div></div> <div>51%</div> <div>19%</div> <div>30%</div> </div>
2	C	1119	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>22%</div> <div>..</div> </div> </div>
3	D	1524	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>20%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	E	99	 83% 12% 5%
5	F	443	 3% 63% 13% 24%
6	G	21	 48% 38% 14%
7	H	27	 41% 48% 11%
8	I	7	 14% 71% 14% 14%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 28784 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	1	0
			1814	1158	316	338	2			
1	B	222	Total	C	N	O	S	0	0	0
			1750	1120	303	325	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	3	0
			8792	5562	1570	1636	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	3	0
			11759	7458	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
			758	483	132	139	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	337	Total	C	N	O	S	0	0	0
			2737	1726	499	508	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	18	Total	C	N	O	P	0	0	0
			372	176	73	106	17			

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

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(*CP*CP*CP*UP*CP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	7	Total	C	N	O	P	0	0	0
			142	65	24	47	6			

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

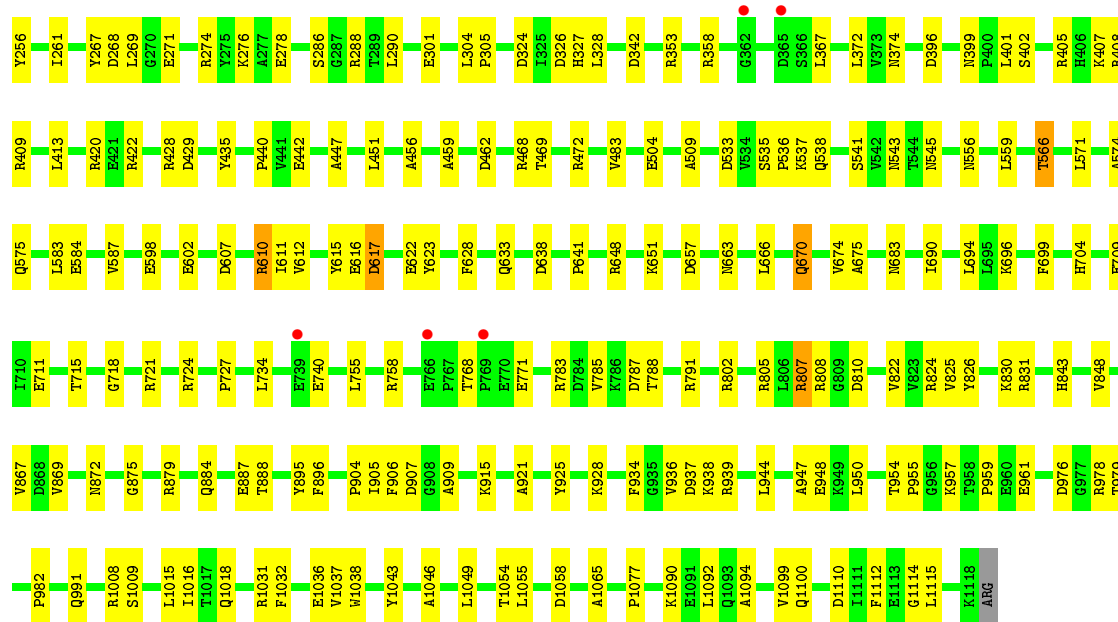
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Mg 1 1	0	0
9	D	2	Total Mg 2 2	0	0
9	F	1	Total Mg 1 1	0	0

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

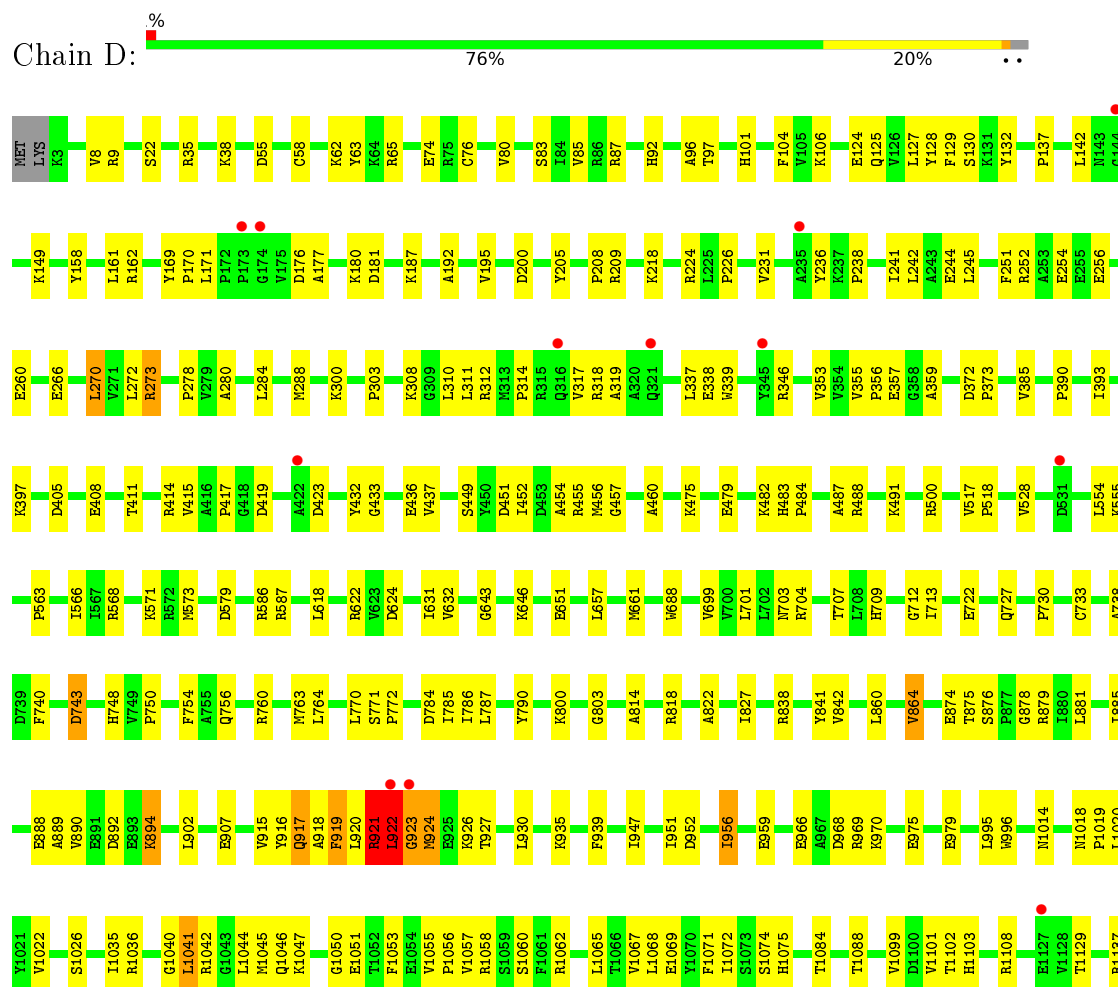
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	2	Total Zn 2 2	0	0

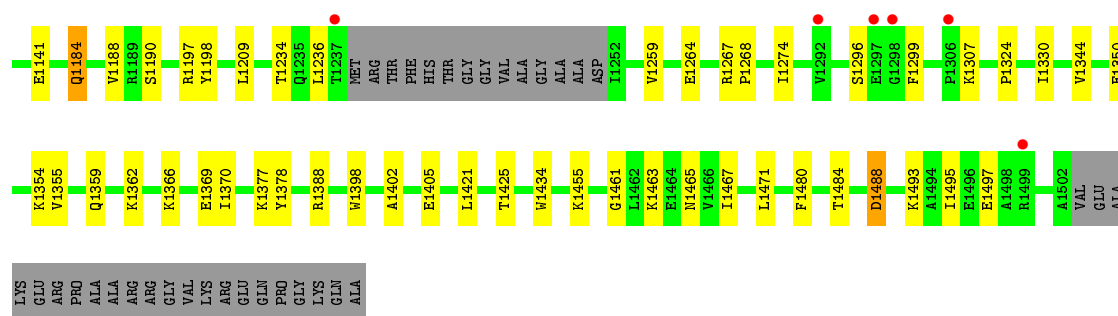
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	12	Total O 12 12	0	0
11	B	12	Total O 12 12	0	0
11	C	49	Total O 49 49	0	0
11	D	62	Total O 62 62	0	0
11	E	5	Total O 5 5	0	0
11	F	8	Total O 8 8	0	0
11	G	5	Total O 5 5	0	0
11	H	4	Total O 4 4	0	0
11	I	2	Total O 2 2	0	0



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





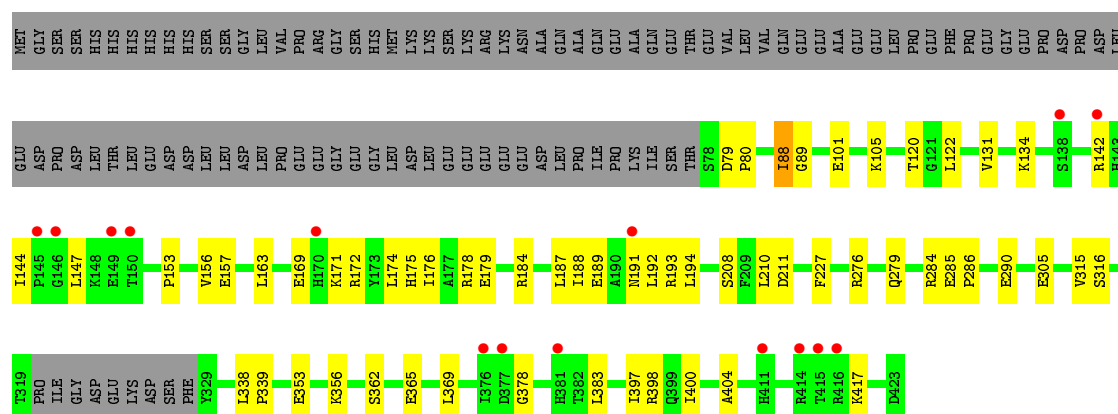
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 83% 12% 5%



- Molecule 5: RNA polymerase sigma factor SigA

Chain F: 3% 63% 13% 24%



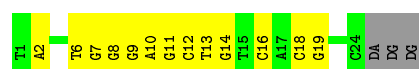
- Molecule 6: DNA (5'-D(*CP*CP*T*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*GP*AP*GP*GP*G)-3')

Chain G: 48% 38% 14%

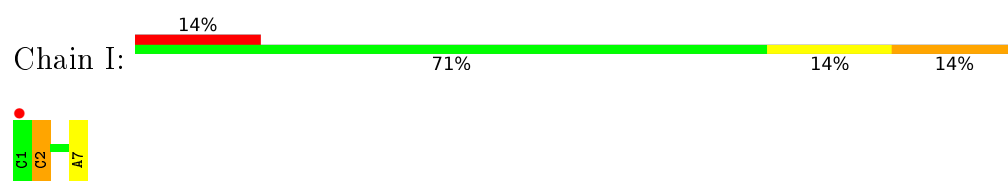


- Molecule 7: DNA (27-MER)

Chain H: 41% 48% 11%



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	183.01Å 103.57Å 294.94Å 90.00° 99.20° 90.00°	Depositor
Resolution (Å)	39.82 – 3.20 39.82 – 3.18	Depositor EDS
% Data completeness (in resolution range)	93.2 (39.82-3.20) 93.2 (39.82-3.18)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 3.18Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.215 , 0.260 0.210 , 0.253	Depositor DCC
R_{free} test set	4211 reflections (4.98%)	DCC
Wilson B-factor (Å ²)	61.3	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 15.0	EDS
Estimated twinning fraction	0.026 for $1/2^*h-3/2^*k,-1/2^*h-1/2^*k,-1/2^*h+1/2^*k-l$ 0.023 for $1/2^*h+3/2^*k,1/2^*h-1/2^*k,-1/2^*h-1/2^*k-l$	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 85558 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	28784	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0/1849	0.46	0/2515
1	B	0.23	0/1781	0.45	0/2420
2	C	0.25	0/8969	0.45	0/12129
3	D	0.31	4/11975 (0.0%)	0.49	7/16189 (0.0%)
4	E	0.24	0/772	0.42	0/1040
5	F	0.30	0/2779	0.44	0/3737
6	G	0.49	0/418	0.83	0/645
7	H	0.53	0/556	0.90	0/858
8	I	0.30	0/157	0.96	0/242
All	All	0.29	4/29256 (0.0%)	0.49	7/39775 (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
3	D	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	921	ARG	C-O	9.12	1.40	1.23
3	D	923	GLY	CA-C	-7.58	1.39	1.51
3	D	917	GLN	C-O	6.03	1.34	1.23
3	D	923	GLY	N-CA	-5.26	1.38	1.46

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	924	MET	C-N-CA	-7.41	103.17	121.70
3	D	923	GLY	C-N-CA	-6.01	106.67	121.70
3	D	922	LEU	N-CA-C	-5.57	95.97	111.00
3	D	919	PHE	N-CA-CB	5.19	119.95	110.60
3	D	1041	LEU	CA-CB-CG	5.14	127.12	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	922	LEU	Peptide

5.2 Too-close contacts

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	1814	0	1869	38	0
1	B	1750	0	1802	44	0
2	C	8792	0	8902	160	0
3	D	11759	0	12002	231	0
4	E	758	0	770	10	0
5	F	2737	0	2819	41	0
6	G	372	0	203	10	0
7	H	495	0	272	13	0
8	I	142	0	78	2	0
9	B	1	0	0	0	0
9	D	2	0	0	0	0
9	F	1	0	0	0	0
10	D	2	0	0	0	0
11	A	12	0	0	1	0
11	B	12	0	0	6	0
11	C	49	0	0	0	0
11	D	62	0	0	5	0
11	E	5	0	0	1	0
11	F	8	0	0	0	0
11	G	5	0	0	0	0
11	H	4	0	0	2	0
11	I	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	28784	0	28717	488	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 9.

The worst 5 of 488 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)
3:D:918:ALA:O	3:D:923:GLY:N	1.80	1.12
3:D:919:PHE:O	3:D:923:GLY:HA2	1.51	1.09
3:D:919:PHE:C	3:D:923:GLY:HA2	1.98	0.84
3:D:921:ARG:O	3:D:923:GLY:HA3	1.80	0.82
6:G:20:DG:H1	8:I:2:C:H42	1.32	0.77

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	230/315 (73%)	228 (99%)	2 (1%)	0	100	100
1	B	218/315 (69%)	210 (96%)	7 (3%)	1 (0%)	34	78
2	C	1111/1119 (99%)	1081 (97%)	29 (3%)	1 (0%)	56	91
3	D	1485/1524 (97%)	1445 (97%)	40 (3%)	0	100	100
4	E	92/99 (93%)	90 (98%)	2 (2%)	0	100	100
5	F	333/443 (75%)	329 (99%)	4 (1%)	0	100	100
All	All	3469/3815 (91%)	3383 (98%)	84 (2%)	2 (0%)	56	91

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	925	TYR
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	201/273 (74%)	199 (99%)	2 (1%)	82	95
1	B	195/273 (71%)	192 (98%)	3 (2%)	72	91
2	C	939/941 (100%)	922 (98%)	17 (2%)	66	89
3	D	1256/1279 (98%)	1234 (98%)	22 (2%)	66	89
4	E	82/88 (93%)	81 (99%)	1 (1%)	78	93
5	F	293/388 (76%)	290 (99%)	3 (1%)	82	95
All	All	2966/3242 (92%)	2918 (98%)	48 (2%)	70	91

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	807[B]	ARG
3	D	288	MET
4	E	50	THR
3	D	35	ARG
3	D	270	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	538	GLN
2	C	962	GLN
3	D	669	ASN
2	C	506	ASN
3	D	143	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	6/7 (85%)	1 (16%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	I	2	C

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 carbohydrates 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 ⓘ

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, 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%)	-0.37	4 (1%) 73 60	40, 54, 82, 135	0
1	B	222/315 (70%)	-0.30	0 100 100	38, 61, 96, 118	0
2	C	1112/1119 (99%)	-0.35	7 (0%) 90 84	20, 49, 113, 153	0
3	D	1486/1524 (97%)	-0.19	18 (1%) 81 69	18, 53, 118, 151	1 (0%)
4	E	94/99 (94%)	-0.41	0 100 100	24, 49, 86, 107	0
5	F	337/443 (76%)	-0.04	15 (4%) 37 23	42, 73, 124, 149	0
6	G	18/21 (85%)	-0.18	0 100 100	36, 64, 143, 151	0
7	H	24/27 (88%)	-0.02	0 100 100	59, 83, 139, 168	0
8	I	7/7 (100%)	-0.08	1 (14%) 4 2	33, 35, 85, 108	0
All	All	3531/3870 (91%)	-0.25	45 (1%) 79 67	18, 55, 116, 168	1 (0%)

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	63	GLY	5.0
5	F	146	GLY	4.9
1	A	232	ALA	4.6
5	F	149	GLU	4.5
5	F	377	ASP	3.8

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 ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
9	MG	D	1601	1/1	0.97	0.17	-0.44	37,37,37,37	0
10	ZN	D	1603	1/1	0.90	0.07	-1.44	45,45,45,45	0
9	MG	F	2001	1/1	0.95	0.14	-1.58	62,62,62,62	0
10	ZN	D	1602	1/1	0.98	0.03	-3.83	6,6,6,6	0
9	MG	D	1604	1/1	0.98	0.12	-	19,19,19,19	0
9	MG	B	2001	1/1	0.70	0.27	-	64,64,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.