



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 29, 2020 – 09:45 PM BST

PDB ID : 6JCY
Title : Mycobacterium tuberculosis RNA polymerase transcription initiation open complex with a chimeric ECF sigma factor sigH/E
Authors : Li, L.; Zhang, Y.
Deposited on : 2019-01-30
Resolution : 3.11 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
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

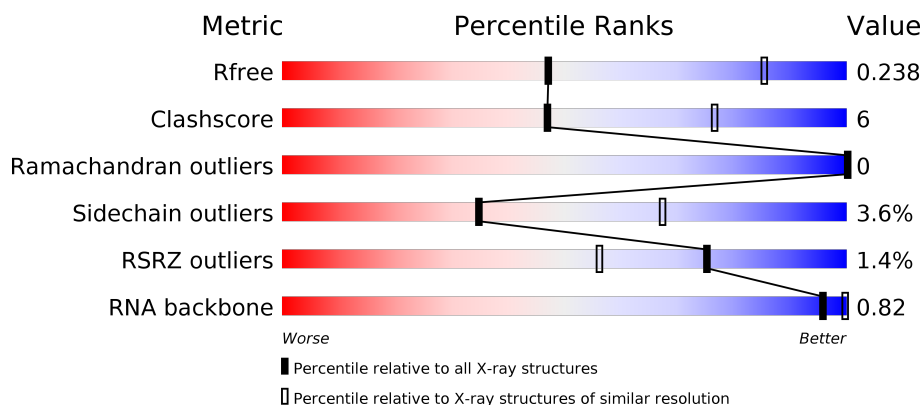
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

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	368	<div> <div>50%</div> <div>10%</div> <div>40%</div> </div>
1	B	368	<div> <div>2%</div> <div>50%</div> <div>13%</div> <div>37%</div> </div>
2	C	1174	<div> <div>81%</div> <div>15%</div> <div>...</div> </div>
3	D	1317	<div> <div>79%</div> <div>16%</div> <div>...</div> </div>

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Mol	Chain	Length	Quality of chain
4	E	110	<div><div><div></div><div></div><div></div><div></div></div><div>3%57%9%31%</div></div>
5	F	209	<div><div><div></div><div></div><div></div><div></div></div><div>3%63%14%22%</div></div>
6	G	23	<div><div><div></div><div></div></div><div>30%70%</div></div>
7	H	20	<div><div><div></div><div></div></div><div>45%55%</div></div>
8	I	6	<div><div><div></div></div><div>100%</div></div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 24729 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	221	Total	C	N	O	S	0	0	0
			1673	1054	288	329	2			
1	B	231	Total	C	N	O	S	0	0	0
			1719	1085	293	338	3			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP P9WGZ1
A	-19	GLY	-	expression tag	UNP P9WGZ1
A	-18	HIS	-	expression tag	UNP P9WGZ1
A	-17	HIS	-	expression tag	UNP P9WGZ1
A	-16	HIS	-	expression tag	UNP P9WGZ1
A	-15	HIS	-	expression tag	UNP P9WGZ1
A	-14	HIS	-	expression tag	UNP P9WGZ1
A	-13	HIS	-	expression tag	UNP P9WGZ1
A	-12	HIS	-	expression tag	UNP P9WGZ1
A	-11	HIS	-	expression tag	UNP P9WGZ1
A	-10	HIS	-	expression tag	UNP P9WGZ1
A	-9	HIS	-	expression tag	UNP P9WGZ1
A	-8	SER	-	expression tag	UNP P9WGZ1
A	-7	SER	-	expression tag	UNP P9WGZ1
A	-6	GLY	-	expression tag	UNP P9WGZ1
A	-5	HIS	-	expression tag	UNP P9WGZ1
A	-4	ILE	-	expression tag	UNP P9WGZ1
A	-3	GLU	-	expression tag	UNP P9WGZ1
A	-2	GLY	-	expression tag	UNP P9WGZ1
A	-1	ARG	-	expression tag	UNP P9WGZ1
A	0	HIS	-	expression tag	UNP P9WGZ1
B	-20	MET	-	initiating methionine	UNP P9WGZ1
B	-19	GLY	-	expression tag	UNP P9WGZ1
B	-18	HIS	-	expression tag	UNP P9WGZ1
B	-17	HIS	-	expression tag	UNP P9WGZ1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	expression tag	UNP P9WGZ1
B	-15	HIS	-	expression tag	UNP P9WGZ1
B	-14	HIS	-	expression tag	UNP P9WGZ1
B	-13	HIS	-	expression tag	UNP P9WGZ1
B	-12	HIS	-	expression tag	UNP P9WGZ1
B	-11	HIS	-	expression tag	UNP P9WGZ1
B	-10	HIS	-	expression tag	UNP P9WGZ1
B	-9	HIS	-	expression tag	UNP P9WGZ1
B	-8	SER	-	expression tag	UNP P9WGZ1
B	-7	SER	-	expression tag	UNP P9WGZ1
B	-6	GLY	-	expression tag	UNP P9WGZ1
B	-5	HIS	-	expression tag	UNP P9WGZ1
B	-4	ILE	-	expression tag	UNP P9WGZ1
B	-3	GLU	-	expression tag	UNP P9WGZ1
B	-2	GLY	-	expression tag	UNP P9WGZ1
B	-1	ARG	-	expression tag	UNP P9WGZ1
B	0	HIS	-	expression tag	UNP P9WGZ1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1139	Total	C	N	O	S	0	0	0
			8572	5364	1504	1665	39			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	5	MET	-	initiating methionine	UNP P9WGY9
C	6	VAL	-	expression tag	UNP P9WGY9

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1260	Total	C	N	O	S	0	0	0
			9802	6141	1774	1847	40			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	MET	-	initiating methionine	UNP P9WGY7
D	1	VAL	-	expression tag	UNP P9WGY7

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	76	Total	C	N	O	0	0	0
			594	379	101	114			

- Molecule 5 is a protein called ECF RNA polymerase sigma factor SigH,ECF RNA polymerase sigma factor SigE,ECF RNA polymerase sigma factor SigH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	164	Total	C	N	O	S	0	0	0
			1238	774	221	238	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	GLY	-	expression tag	UNP P9WGH9
F	0	ALA	-	expression tag	UNP P9WGH9

- Molecule 6 is a DNA chain called DNA (5'-D(*TP*TP*GP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	23	Total	C	N	O	P	0	0	0
			464	221	84	137	22			

- Molecule 7 is a DNA chain called DNA (5'-D(*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*GP*AP*GP*GP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	20	Total	C	N	O	P	0	0	0
			412	196	77	120	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	6	Total	C	N	O	P	0	0	0
			122	56	21	40	5			

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

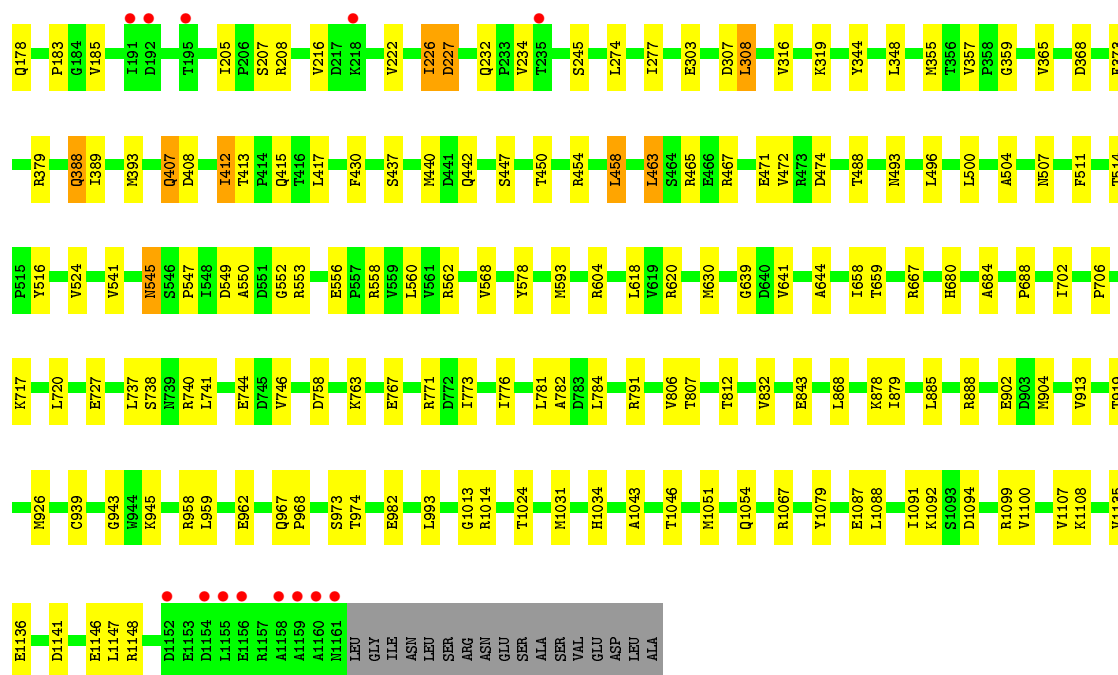
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	2	Total	Zn	0	0
			2	2		

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

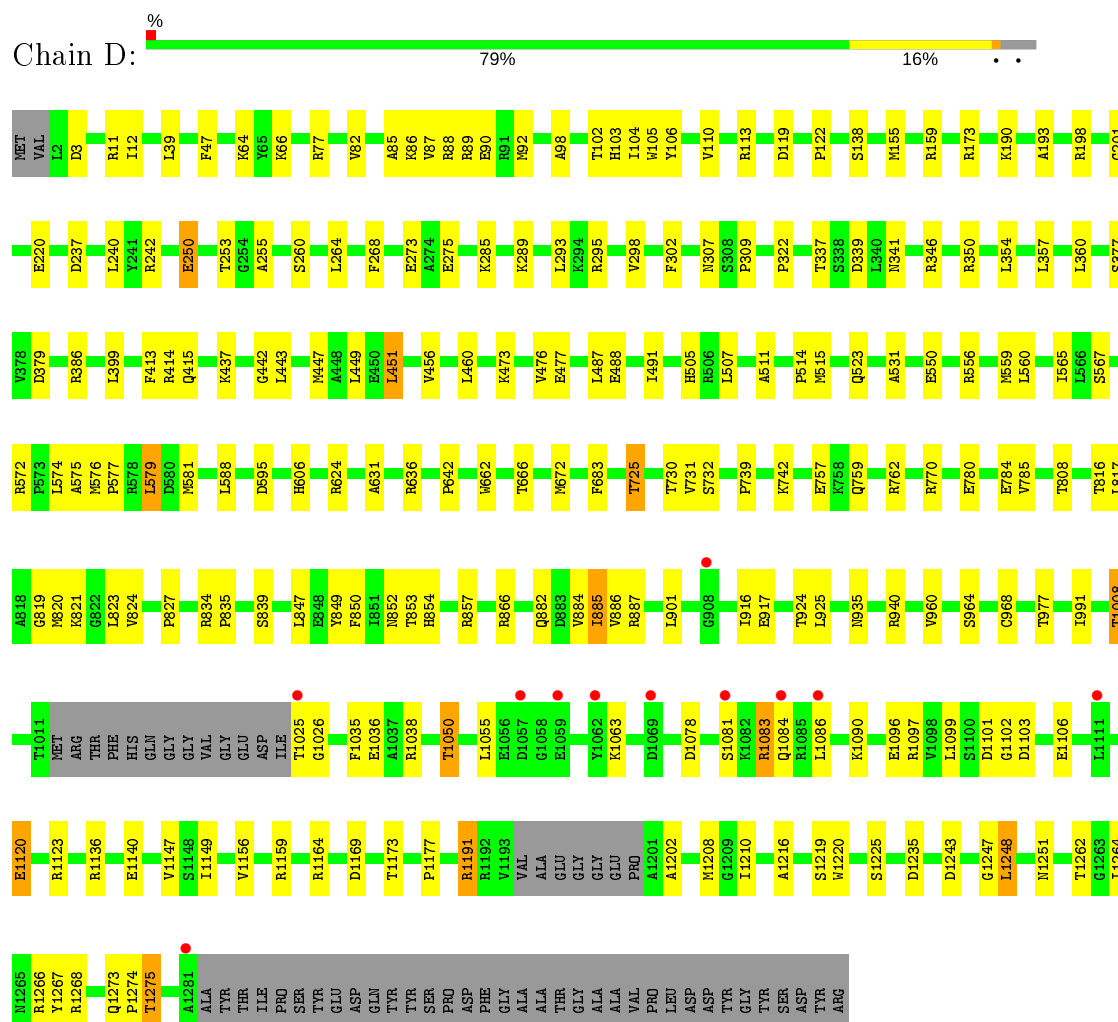
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	1	Total	Mg	0	0
			1	1		

- Molecule 11 is water.

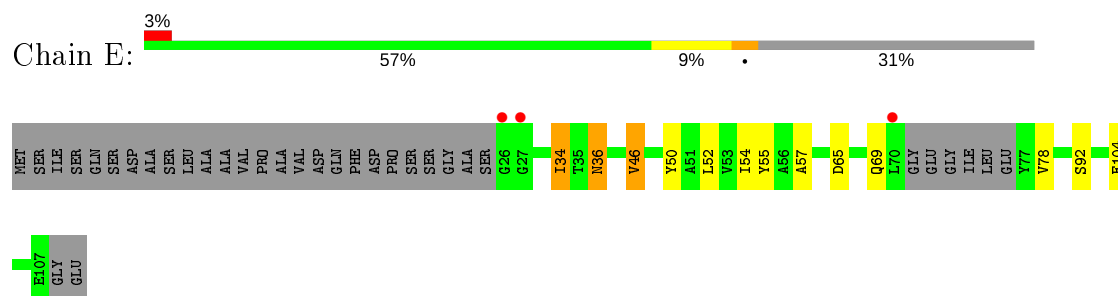
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	11	Total	O	0	0
			11	11		
11	B	9	Total	O	0	0
			9	9		
11	C	37	Total	O	0	0
			37	37		
11	D	58	Total	O	0	0
			58	58		
11	E	2	Total	O	0	0
			2	2		
11	F	5	Total	O	0	0
			5	5		
11	G	1	Total	O	0	0
			1	1		
11	H	6	Total	O	0	0
			6	6		
11	I	1	Total	O	0	0
			1	1		



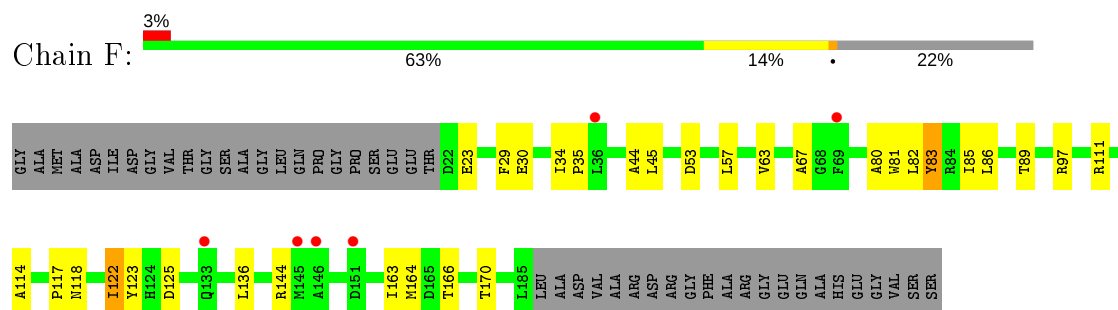
• Molecule 3: DNA-directed RNA polymerase subunit beta'



- Molecule 4: DNA-directed RNA polymerase subunit omega



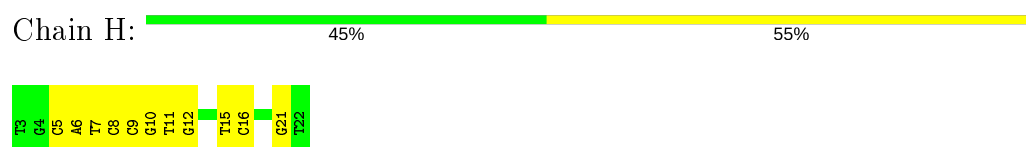
- Molecule 5: ECF RNA polymerase sigma factor SigH, ECF RNA polymerase sigma factor SigE, ECF RNA polymerase sigma factor SigH



- Molecule 6: DNA (5'-D(*TP*TP*GP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*A)-3')



- Molecule 7: DNA (5'-D(*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*GP*AP*GP*GP*GP*T)-3')



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



There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	128.94Å 163.00Å 129.31Å 90.00° 117.81° 90.00°	Depositor
Resolution (Å)	48.77 – 3.11 49.05 – 3.11	Depositor EDS
% Data completeness (in resolution range)	92.5 (48.77-3.11) 92.6 (49.05-3.11)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.195 , 0.238 0.195 , 0.238	Depositor DCC
R_{free} test set	2376 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å ²)	92.6	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.012 for -h-l,k,h 0.012 for l,k,-h-l 0.026 for h,-k,-h-l 0.027 for -h-l,-k,l 0.025 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	24729	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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	0.26	0/1699	0.47	0/2313
1	B	0.25	0/1744	0.46	0/2375
2	C	0.27	0/8730	0.45	0/11869
3	D	0.26	0/9966	0.43	0/13479
4	E	0.25	0/605	0.41	0/823
5	F	0.24	0/1263	0.39	0/1722
6	G	0.62	0/520	0.98	0/802
7	H	0.58	0/462	0.92	0/713
8	I	0.32	0/135	0.88	0/208
All	All	0.28	0/25124	0.48	0/34304

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	1673	0	1707	24	0
1	B	1719	0	1737	28	0
2	C	8572	0	8294	113	0
3	D	9802	0	9817	130	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	594	0	589	9	0
5	F	1238	0	1131	21	0
6	G	464	0	256	16	0
7	H	412	0	227	8	0
8	I	122	0	66	0	0
9	D	2	0	0	0	0
10	D	1	0	0	0	0
11	A	11	0	0	1	0
11	B	9	0	0	0	0
11	C	37	0	0	1	0
11	D	58	0	0	1	0
11	E	2	0	0	0	0
11	F	5	0	0	0	0
11	G	1	0	0	0	0
11	H	6	0	0	0	0
11	I	1	0	0	0	0
All	All	24729	0	23824	298	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 298 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)
1:A:7:PRO:HA	1:A:25:PRO:HG2	1.55	0.89
1:B:62:GLU:HG3	1:B:64:THR:HG22	1.65	0.78
3:D:882:GLN:HB2	3:D:1248:LEU:HD11	1.67	0.75
3:D:1274:PRO:HG3	4:E:78:VAL:HG11	1.70	0.72
1:A:24:GLU:HG2	1:A:191:LYS:HG3	1.70	0.71

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	219/368 (60%)	211 (96%)	8 (4%)	0	100	100
1	B	227/368 (62%)	213 (94%)	14 (6%)	0	100	100
2	C	1137/1174 (97%)	1091 (96%)	46 (4%)	0	100	100
3	D	1254/1317 (95%)	1218 (97%)	36 (3%)	0	100	100
4	E	72/110 (66%)	69 (96%)	3 (4%)	0	100	100
5	F	162/209 (78%)	159 (98%)	3 (2%)	0	100	100
All	All	3071/3546 (87%)	2961 (96%)	110 (4%)	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	188/315 (60%)	177 (94%)	11 (6%)	19	50
1	B	189/315 (60%)	185 (98%)	4 (2%)	53	79
2	C	897/995 (90%)	863 (96%)	34 (4%)	33	66
3	D	1032/1096 (94%)	1003 (97%)	29 (3%)	43	73
4	E	63/90 (70%)	58 (92%)	5 (8%)	12	40
5	F	115/167 (69%)	108 (94%)	7 (6%)	18	49
All	All	2484/2978 (83%)	2394 (96%)	90 (4%)	35	67

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	843	GLU
3	D	102	THR
5	F	23	GLU
2	C	958	ARG
2	C	1046	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	680	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	5/6 (83%)	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 3 ligands modelled in this entry, 3 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	221/368 (60%)	-0.27	4 (1%) 68 47	66, 83, 133, 168	0
1	B	231/368 (62%)	0.03	7 (3%) 50 27	85, 125, 155, 162	0
2	C	1139/1174 (97%)	-0.16	14 (1%) 79 61	54, 88, 147, 170	0
3	D	1260/1317 (95%)	-0.24	11 (0%) 84 69	59, 95, 146, 178	0
4	E	76/110 (69%)	-0.02	3 (3%) 39 20	90, 117, 139, 145	0
5	F	164/209 (78%)	0.21	6 (3%) 41 21	81, 136, 160, 165	0
6	G	23/23 (100%)	-0.19	0 100 100	93, 134, 158, 165	1 (4%)
7	H	20/20 (100%)	-0.54	0 100 100	67, 88, 148, 149	0
8	I	6/6 (100%)	-0.35	0 100 100	60, 62, 72, 87	0
All	All	3140/3595 (87%)	-0.17	45 (1%) 75 56	54, 97, 150, 178	1 (0%)

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	1160	ALA	5.7
3	D	1281	ALA	5.6
4	E	70	LEU	5.5
2	C	1159	ALA	4.7
2	C	1155	LEU	4.4

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 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
10	MG	D	2003	1/1	0.89	0.13	59,59,59,59	0
9	ZN	D	2002	1/1	0.98	0.13	123,123,123,123	0
9	ZN	D	2001	1/1	0.99	0.17	99,99,99,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.