



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 08:57 am BST

PDB ID : 5XJ0
Title : T. thermophilus RNA polymerase holoenzyme bound with gp39 and gp76
Authors : Ooi, W.Y.; Murayama, Y.; Mekler, V.; Minakhin, L.; Severinov, K.;
Yokoyama, S.; Sekine, S.
Deposited on : 2017-04-28
Resolution : 4.00 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	:	2.11
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)	:	2.11

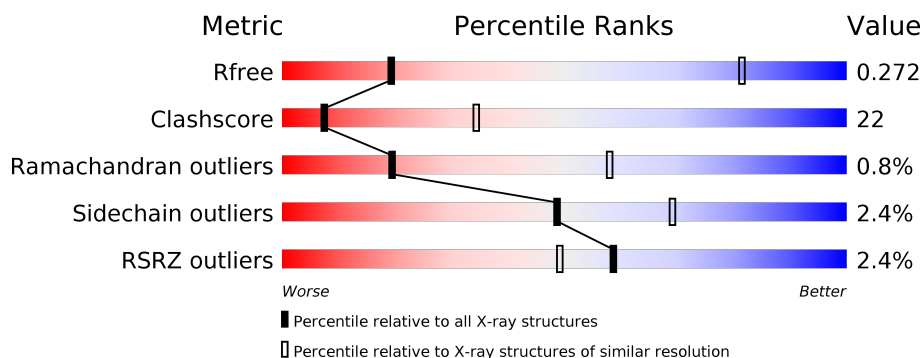
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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	
1	B	315	
2	C	1119	
3	D	1524	
4	E	99	
5	F	423	

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Mol	Chain	Length	Quality of chain
6	G	144	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>3%65%22%••12%</div></div>
6	H	144	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>9%40%22%•37%</div></div>
7	Y	54	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>59%•37%</div></div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 29177 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	225	Total	C	N	O	S	0	0	0
			1772	1132	308	330	2			
1	B	232	Total	C	N	O	S	0	0	0
			1814	1158	316	338	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1114	Total	C	N	O	S	0	0	0
			8789	5557	1568	1640	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1462	Total	C	N	O	S	0	0	0
			11543	7322	2030	2159	32			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	95	Total	C	N	O	S	0	0	0
			770	491	133	142	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	313	Total	C	N	O	S	0	0	0
			2530	1600	456	471	3			

- Molecule 6 is a protein called gp39.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	127	Total	C	N	O	S	0	0	0
			1035	673	175	184	3			
6	H	91	Total	C	N	O	S	0	0	0
			752	495	125	131	1			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-2	GLY	-	expression tag	UNP A7XX65
G	-1	SER	-	expression tag	UNP A7XX65
G	0	HIS	-	expression tag	UNP A7XX65
H	-2	GLY	-	expression tag	UNP A7XX65
H	-1	SER	-	expression tag	UNP A7XX65
H	0	HIS	-	expression tag	UNP A7XX65

- Molecule 7 is a protein called gp76.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	Y	34	Total	C	N	O	0	0	0
			171	103	34	34			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-2	GLY	-	expression tag	UNP A7XXA7
Y	-1	SER	-	expression tag	UNP A7XXA7
Y	0	HIS	-	expression tag	UNP A7XXA7

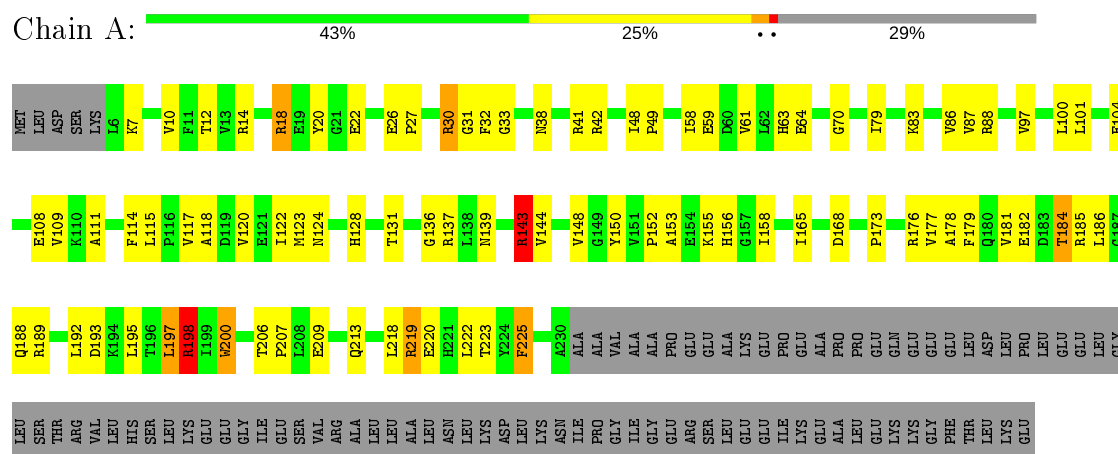
- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	1	Total	Zn	0	0
			1	1		

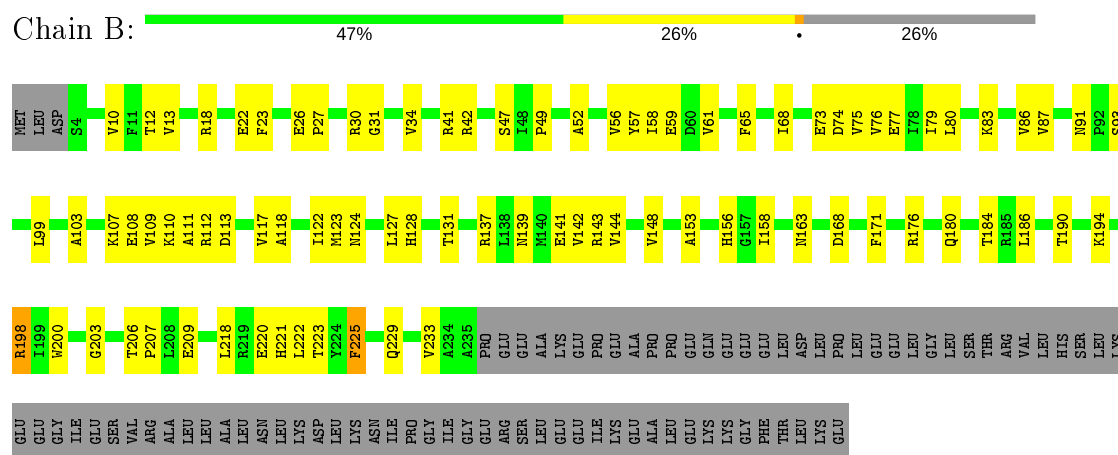
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

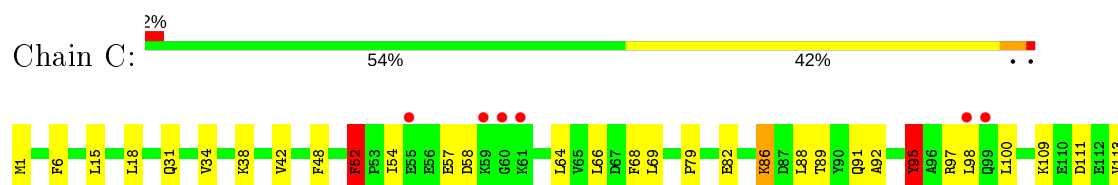
• Molecule 1: DNA-directed RNA polymerase subunit alpha

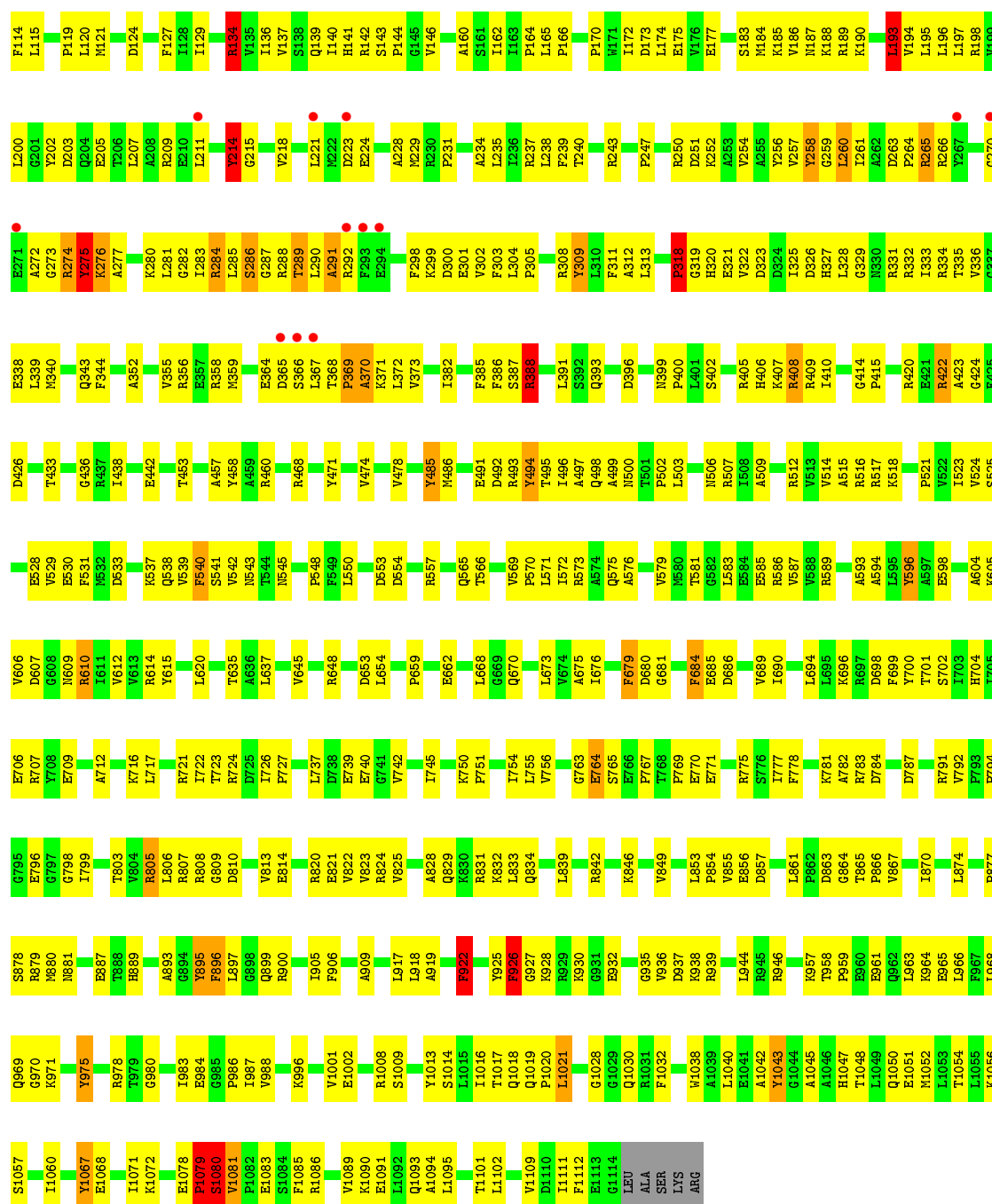


• Molecule 1: DNA-directed RNA polymerase subunit alpha

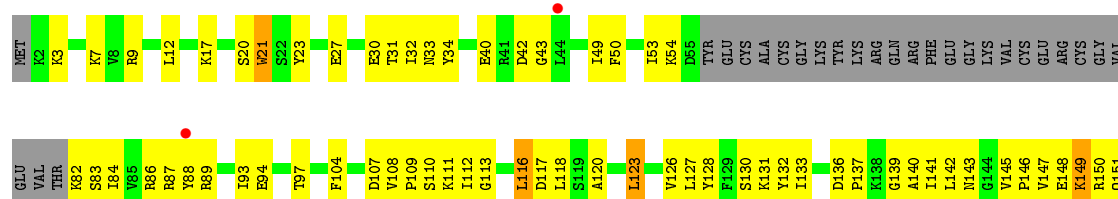


• Molecule 2: DNA-directed RNA polymerase subunit beta

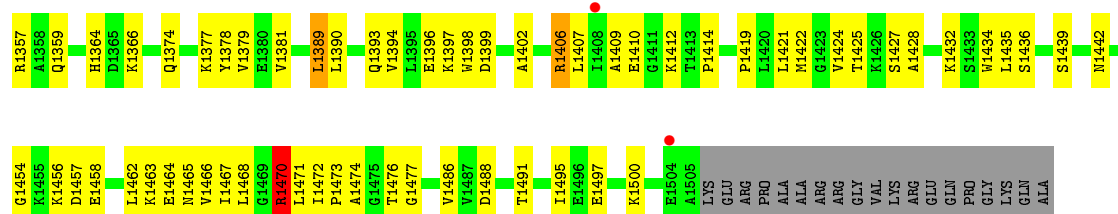




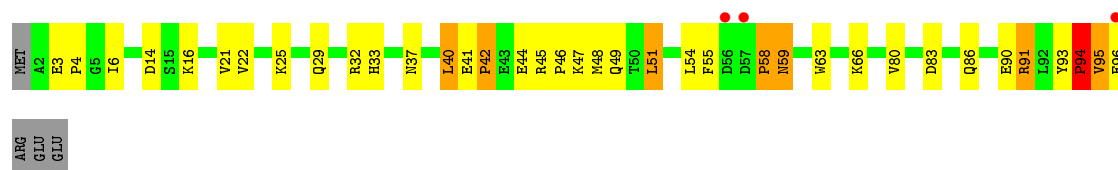
• Molecule 3: DNA-directed RNA polymerase subunit beta'



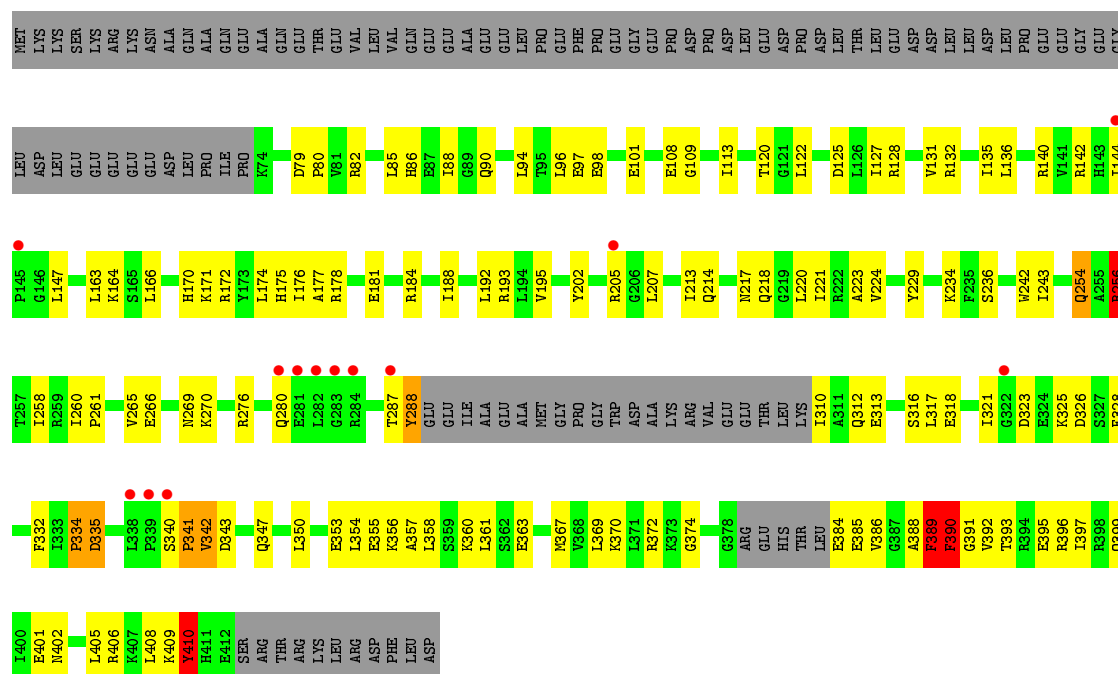
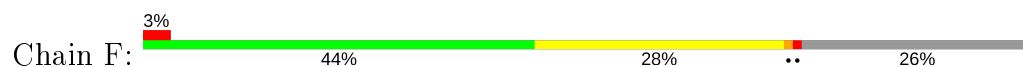




• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 5: RNA polymerase sigma factor SigA

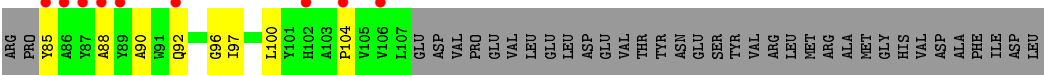


• Molecule 6: gp39





● Molecule 6: gp39



● Molecule 7: gp76



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	294.43Å 294.43Å 222.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.78 – 4.00 49.78 – 4.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.78-4.00) 96.1 (49.78-4.00)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 4.00Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.237 , 0.272 0.237 , 0.272	Depositor DCC
R_{free} test set	4644 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	112.0	Xtriage
Anisotropy	0.548	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 127.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.105 for -h,-k,l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	29177	wwPDB-VP
Average B, all atoms (Å ²)	160.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:
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	0.49	3/1804 (0.2%)	0.89	10/2454 (0.4%)
1	B	0.33	0/1846	0.62	0/2511
2	C	0.43	5/8957 (0.1%)	0.81	28/12113 (0.2%)
3	D	0.44	7/11745 (0.1%)	0.80	40/15882 (0.3%)
4	E	0.52	2/784 (0.3%)	0.81	3/1057 (0.3%)
5	F	0.38	1/2568 (0.0%)	0.71	5/3453 (0.1%)
6	G	0.40	1/1065 (0.1%)	0.66	1/1449 (0.1%)
6	H	0.34	0/775	0.64	1/1057 (0.1%)
7	Y	0.29	0/171	0.48	0/238
All	All	0.43	19/29715 (0.1%)	0.78	88/40214 (0.2%)

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
1	A	0	2
2	C	0	13
3	D	0	11
4	E	0	1
5	F	0	2
6	G	0	1
6	H	0	1
All	All	0	31

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	254	GLN	CD-NE2	7.98	1.52	1.32
2	C	276	LYS	CG-CD	-7.36	1.27	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	879	ARG	CZ-NH2	7.36	1.42	1.33
2	C	134	ARG	CZ-NH2	7.30	1.42	1.33
3	D	1164	ARG	CG-CD	7.04	1.69	1.51

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	388	ARG	NE-CZ-NH2	-17.16	111.72	120.30
3	D	598	ARG	NE-CZ-NH2	-14.88	112.86	120.30
3	D	1164	ARG	NE-CZ-NH2	14.09	127.35	120.30
1	A	185	ARG	NE-CZ-NH2	12.72	126.66	120.30
1	A	185	ARG	NE-CZ-NH1	-11.93	114.34	120.30

There are no chirality outliers.

5 of 31 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	184	THR	Peptide
1	A	197	LEU	Peptide
2	C	214	TYR	Sidechain
2	C	260	LEU	Peptide
2	C	275	TYR	Sidechain

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	1772	0	1821	77	0
1	B	1814	0	1868	69	0
2	C	8789	0	8886	490	0
3	D	11543	0	11785	579	0
4	E	770	0	784	40	0
5	F	2530	0	2611	131	0
6	G	1035	0	1013	30	0
6	H	752	0	748	27	0
7	Y	171	0	91	3	0
8	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	29177	0	29607	1305	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 22.

The worst 5 of 1305 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:198:ARG:HD3	1:A:200:TRP:CH2	1.70	1.24
1:A:143:ARG:NH2	6:H:22:GLU:OE2	1.87	1.07
2:C:277:ALA:HB3	2:C:285:LEU:HD11	1.40	1.02
2:C:274:ARG:HA	2:C:285:LEU:HD12	1.42	1.00
1:A:198:ARG:HD3	1:A:200:TRP:HH2	1.08	0.97

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	223/315 (71%)	207 (93%)	16 (7%)	0	100	100
1	B	230/315 (73%)	216 (94%)	14 (6%)	0	100	100
2	C	1112/1119 (99%)	960 (86%)	138 (12%)	14 (1%)	12	48
3	D	1456/1524 (96%)	1271 (87%)	179 (12%)	6 (0%)	34	71
4	E	93/99 (94%)	78 (84%)	11 (12%)	4 (4%)	2	25
5	F	307/423 (73%)	271 (88%)	32 (10%)	4 (1%)	12	48
6	G	123/144 (85%)	120 (98%)	3 (2%)	0	100	100
6	H	87/144 (60%)	82 (94%)	5 (6%)	0	100	100
7	Y	32/54 (59%)	28 (88%)	4 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3663/4137 (88%)	3233 (88%)	402 (11%)	28 (1%)	19	58

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	284	ARG
2	C	286	SER
2	C	370	ALA
2	C	765	SER
2	C	1080	SER

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	197/273 (72%)	191 (97%)	6 (3%)	41	64
1	B	200/273 (73%)	197 (98%)	3 (2%)	65	80
2	C	937/941 (100%)	911 (97%)	26 (3%)	43	65
3	D	1232/1279 (96%)	1204 (98%)	28 (2%)	50	70
4	E	84/88 (96%)	82 (98%)	2 (2%)	49	69
5	F	273/371 (74%)	267 (98%)	6 (2%)	52	71
6	G	107/123 (87%)	103 (96%)	4 (4%)	34	60
6	H	79/123 (64%)	78 (99%)	1 (1%)	69	82
7	Y	1/45 (2%)	1 (100%)	0	100	100
All	All	3110/3516 (88%)	3034 (98%)	76 (2%)	49	69

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	1067	TYR
3	D	525	ARG
5	F	410	TYR
3	D	3	LYS

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Mol	Chain	Res	Type
3	D	220	ARG

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

Mol	Chain	Res	Type
2	C	899	GLN
3	D	611	GLN
4	E	33	HIS
2	C	704	HIS
3	D	1334	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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 [i](#)

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	225/315 (71%)	-0.34	0	100 100	74, 112, 158, 227	0
1	B	232/315 (73%)	-0.30	0	100 100	70, 122, 170, 236	0
2	C	1114/1119 (99%)	-0.17	18 (1%)	72 62	63, 135, 222, 329	0
3	D	1462/1524 (95%)	0.03	39 (2%)	54 44	69, 160, 249, 295	0
4	E	95/99 (95%)	0.04	3 (3%)	47 37	99, 158, 242, 266	0
5	F	313/423 (73%)	0.08	13 (4%)	36 29	144, 205, 276, 332	0
6	G	127/144 (88%)	0.16	4 (3%)	49 38	108, 172, 219, 238	0
6	H	91/144 (63%)	1.05	13 (14%)	2 3	186, 217, 248, 264	0
7	Y	34/54 (62%)	-0.81	0	100 100	204, 241, 270, 283	0
All	All	3693/4137 (89%)	-0.05	90 (2%)	59 49	63, 153, 245, 332	0

The worst 5 of 90 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	270	GLY	5.4
5	F	282	LEU	5.4
2	C	59	LYS	5.2
3	D	1408	ILE	4.7
5	F	281	GLU	4.6

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. 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
8	ZN	D	2001	1/1	0.97	0.17	225,225,225,225	0

6.5 Other polymers [i](#)

There are no such residues in this entry.