



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 04:27 AM UTC

PDB ID : 5XJ0 / pdb_00005xj0
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 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

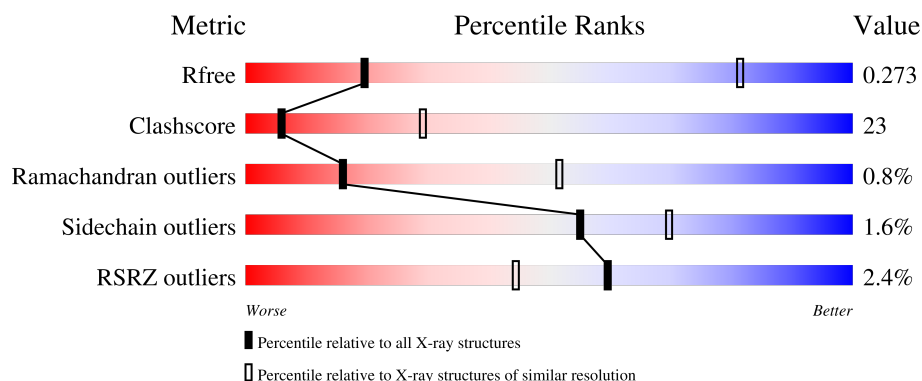
1 Overall quality at a glance

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}	180053	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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 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	44% 25% .. 29%
1	B	315	46% 27% 26%
2	C	1119	% 54% 43% ..
3	D	1524	3% 53% 41% ..
4	E	99	2% 58% 33% ...

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Mol	Chain	Length	Quality of chain
5	F	423	5% 43% 28% 26% ..
6	G	144	% 65% 21% 12% ..
6	H	144	% 40% 22% 37% .
7	Y	54	9% 59% 37% .

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

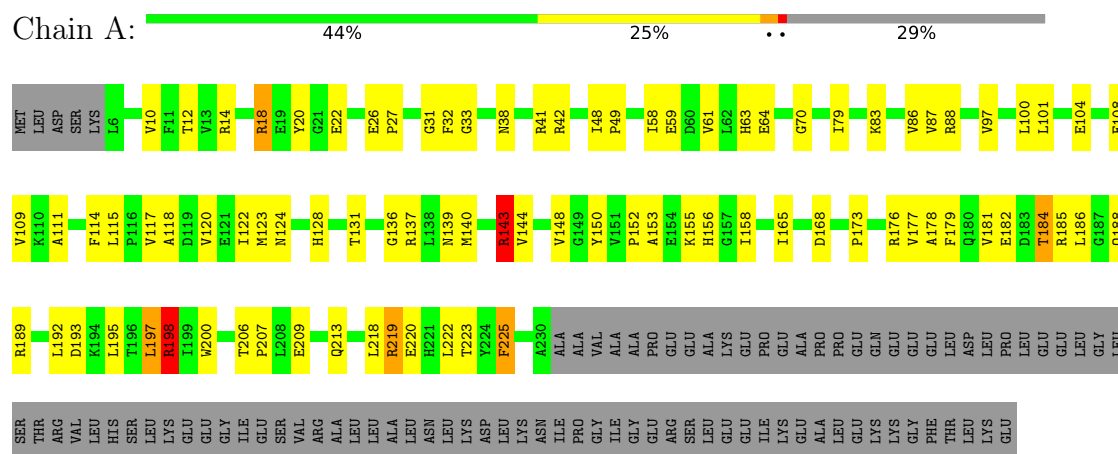
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

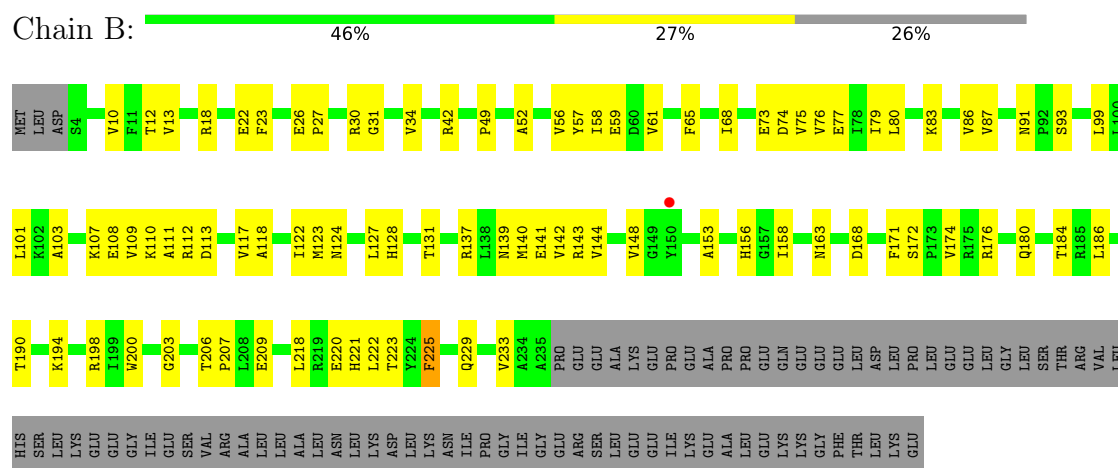
3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

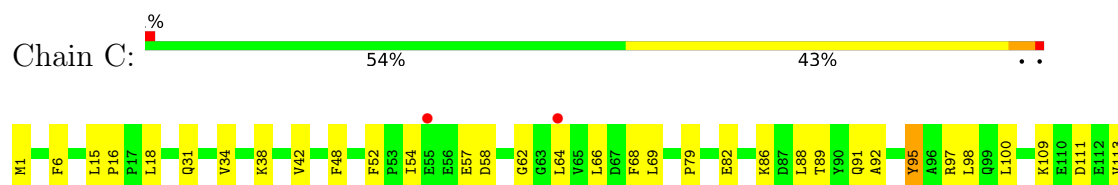
• Molecule 1: DNA-directed RNA polymerase subunit alpha



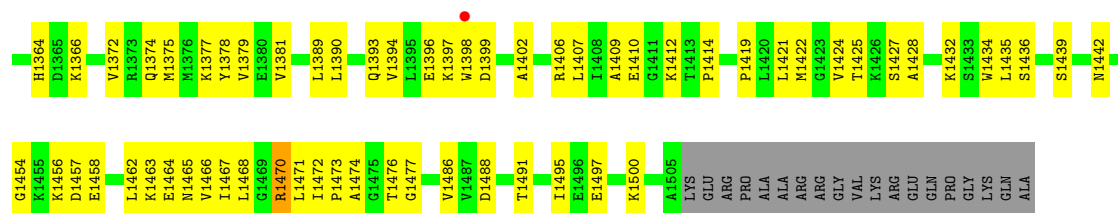
• Molecule 1: DNA-directed RNA polymerase subunit alpha



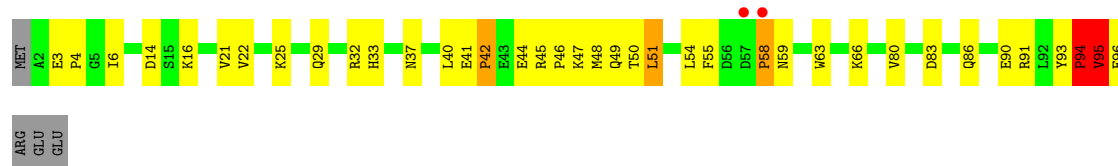
• Molecule 2: DNA-directed RNA polymerase subunit beta



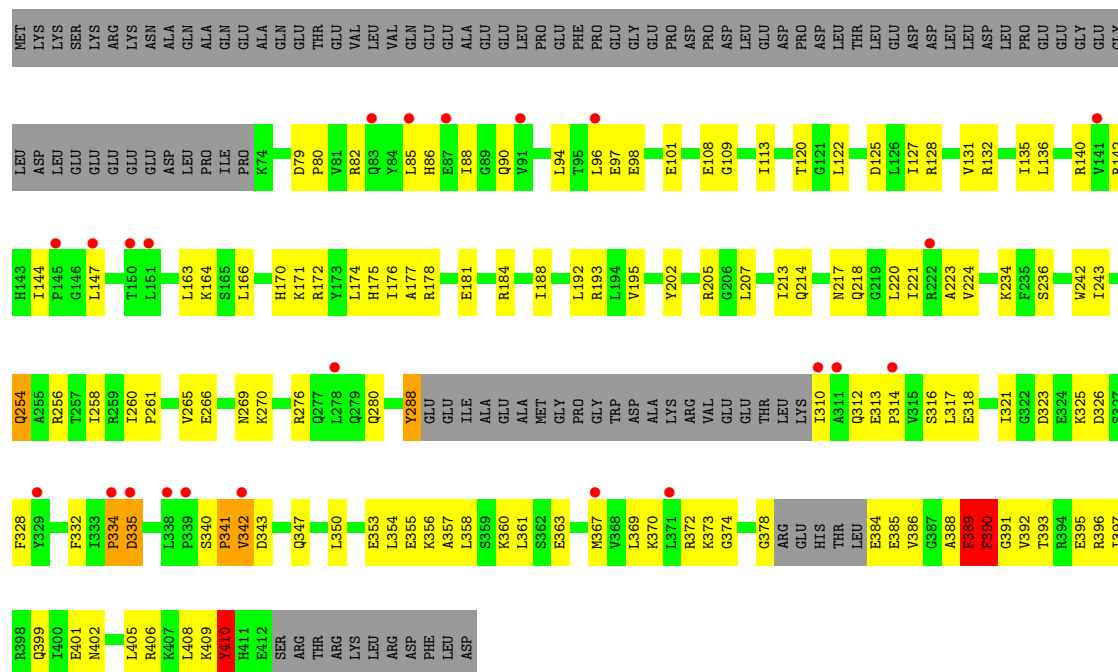
ALA	R1168	K1097	V1003	I880	E810	V732	C642	N549	E459	V377	V298	L223	R150
ASP	D1169	D1100	V1007	L881	E811	C733	G643	R550	A460	G384	E299	R224	Q151
ILE	D1170	F882	F1008	F882	A812	A735	L644	N551	I461	V384	K300	P226	L152
THR	V1101	V1171	A883	A883	L813	A736	P645				Q301	L227	L153
GLN	H1172	H1175	K1009	I885	A814	F736	E651	K555	E474	H388	Q302	L227	T154
G1255	I1175	I1105	R1010	I886	A815	N737	L652	Q560	L477	E389	L304	A228	D155
R1258	K1176	V1106	F1011	V886	R818	A738	F653	K560	L478	P390	A306	A229	E156
A1270	A1177	V1107	E1012	A887	G819	D741	P655	T565	M481	S392	E306	V230	E157
K1269	A1178	R1108	E1013	A888	E820	G742					A307	V231	E160
L1270	E1179	V890	F1017	V890	V821	D743							L161
A1271	A1110	V895	M1023	V895	A822	G744	L658		P484	K397	L310	E234	
K1272	D1111	V895				N745	K659	K571	P484	K397	L311	K237	K165
V1273	C1112	V895				A746	K660	R572	R486	R399	R312	P238	Q186
I1274	G1113	P905	S1026	P905	A825		K660	R573	R487	V400	K313	G239	E187
S1275	G1113	Q906	G1027	Q906	I827	H747	M661	M573	A487	P402	P314	E240	P170
D1278	T1115	T1115	A1028	E907	K828	H748	E662	V578	R489		R315	L242	
D1278	N1116	V829	R1029	K908	V829	V749	E663					L242	
T1196	T1196	A830	G1030	A830	L581	S752	L666		R493	V407	R318	A243	P173
R1197	R1197	G831	M1031	G831	N594				K494	E408	K319	E244	G174
C1201	C1201	F1123	P1032	R832	N594	A755	V670		R495	V408	A320	A244	V175
Q1202	Q1202	Q1124	Q1033	E833	A756	Q756				S410	G321	P246	G176
K1290	K1290	P1125	Q1034	E833	A757					T411	V322	P246	A177
S1291	C1204	I1126	I1035	S835	A758							L250	L178
V1292	Y1292	E1127	Q1037	V836	A759								
F1293	Y1293	V1128	G1038	R838	R760								
E1302	G1206	T1129	C1039	K935	M763								
E1303	D1208	R1130	G1040	Y936	L764								
K1304	S1210	S1131	L1041	Y937									
R1310	V1211	L1132	R1042	F941	H767								
L1311	A1212	R1133	G1043	F941									
D1317	L1134	L1134	L1044	A844									
Y1318	P1214	K1136	M1045	S945									
V1319	V1215	R1137	Q1046	G946									
L1325	S1216	E1141	T1052	T948									
R1327	V1221	L1144	F1053	I949									
G1334	Q1227	Y1145	P1056	V955									
E1231	G1230	G1146	V1057	I956									
P1232	R1147	R1147	R1058	H855									
V1344	E1231	V1148	S1059	G856									
E1345	L1236	L1150	S1060	I857									
R1346	T1237	A1151	E1063	V858									
Y1347	M1238	E1154	L1068	D859									
E1350	ARG	V1155	E1069	L860									
E1351	THR	L1156	Y1070	Q861									
Q1352	PHE	G1157	Y1072	V864									
K1354	HIS	L1158	T1073	R867									
V1355	THR	E1161	D1090	K871									
Y1356	GLY	R1164	Y1093	R988									
A1357	VAL	Y1165	L1094	R872									
A1358	ALA	L1166	T1095	G801									
Q1359	GLY	S1167	R1096	L873									
				E874									
				L593									
				Q994									
				L995									
				W996									
				R879									
				P877									
				G878									
				L804									
				G803									
				R628									
				L543									
				D451									
				N541									
				Y450									
				L540									
				D539									
				S538									
				T537									
				A536									
				F534									
				R525									
				L524									
				D523									
				V431									
				D430									
				S429									
				K339									
				V427									
				L270									
				F269									
				K262									
				L261									
				E260									
				V259									
				E256									
				V186									
				V185									
				E255									
				T330									
				V331									
				V332									
				E326									
				E327									
				E328									
				E329									
				A416									
				P417									
				E414									
				V415									
				S505									
				G506									
				D504									
				E511									
				W510									
				V517									
				P518									
				V519									
				L520									
				P521									
				D522									
				E341									
				P342									
				K343									
				D344									
				V435									
				V436									
				V437									
				D531									
				F534									
				R534									
				F535									
				N442									
				V443									
				V446									
				D365									
				K366									
				I367									
				V368									
				D451									
				I452									
				D453									
				A454									
				R455									
				E296									
				A421									
				E376									



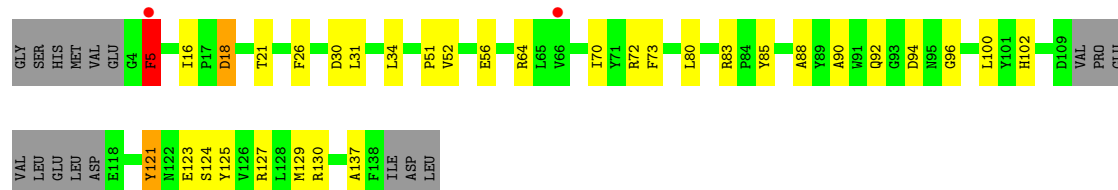
• Molecule 4: DNA-directed RNA polymerase subunit omega



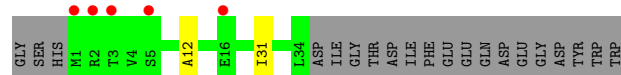
• Molecule 5: RNA polymerase sigma factor SigA



• Molecule 6: gp39



Chain H: %



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) 96.0 (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 0.239 , 0.273	Depositor DCC
R_{free} test set	4644 reflections (3.54%)	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)	0.32 , 157.0	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	0.89	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	0.42	1/1804 (0.1%)	0.81	8/2454 (0.3%)
1	B	0.24	0/1846	0.58	0/2511
2	C	0.41	8/8957 (0.1%)	0.80	23/12113 (0.2%)
3	D	0.42	9/11745 (0.1%)	0.79	31/15882 (0.2%)
4	E	0.49	1/784 (0.1%)	1.00	7/1057 (0.7%)
5	F	0.34	1/2568 (0.0%)	0.73	5/3453 (0.1%)
6	G	0.24	0/1065	0.61	0/1449
6	H	0.27	0/775	0.60	1/1057 (0.1%)
7	Y	0.32	0/171	0.56	0/238
All	All	0.40	20/29715 (0.1%)	0.77	75/40214 (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 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	245	LEU	C-O	-17.29	1.15	1.23
2	C	1081	VAL	C-N	11.07	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	254	GLN	CD-NE2	9.31	1.52	1.33
2	C	276	LYS	CG-CD	-8.35	1.27	1.52
2	C	16	PRO	CA-C	-8.23	1.47	1.51

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1080	SER	N-CA-C	-12.31	84.57	110.80
3	D	879	ARG	CB-CG-CD	-11.24	85.44	111.30
1	A	18	ARG	CB-CG-CD	10.92	136.42	111.30
2	C	16	PRO	O-C-N	-9.36	117.00	121.31
3	D	1164	ARG	NE-CZ-NH2	9.05	127.35	119.20

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

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	71	0
2	C	8789	0	8886	504	0
3	D	11543	0	11785	597	0
4	E	770	0	784	40	0
5	F	2530	0	2611	135	0
6	G	1035	0	1013	33	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	1345	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 23.

The worst 5 of 1345 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%)	9	41
3	D	1456/1524 (96%)	1271 (87%)	179 (12%)	6 (0%)	30	65
4	E	93/99 (94%)	78 (84%)	11 (12%)	4 (4%)	2	20
5	F	307/423 (73%)	271 (88%)	32 (10%)	4 (1%)	9	41
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%)	16	52

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%)	193 (98%)	4 (2%)	48	66
1	B	200/273 (73%)	199 (100%)	1 (0%)	81	82
2	C	937/941 (100%)	919 (98%)	18 (2%)	50	67
3	D	1232/1279 (96%)	1213 (98%)	19 (2%)	57	70
4	E	84/88 (96%)	84 (100%)	0	100	100
5	F	273/371 (74%)	269 (98%)	4 (2%)	57	70
6	G	107/123 (87%)	104 (97%)	3 (3%)	38	60
6	H	79/123 (64%)	79 (100%)	0	100	100
7	Y	1/45 (2%)	1 (100%)	0	100	100
All	All	3110/3516 (88%)	3061 (98%)	49 (2%)	55	70

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	546	ARG
3	D	841	TYR
3	D	549	ASN
3	D	790	TYR

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Mol	Chain	Res	Type
3	D	919	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	767	HIS
3	D	1393	GLN
3	D	1353	GLN
4	E	33	HIS
2	C	728	HIS

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 oligosaccharides 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%)	-0.16	0 100 100	74, 112, 158, 227	0
1	B	232/315 (73%)	-0.04	1 (0%) 88 75	70, 122, 170, 236	0
2	C	1114/1119 (99%)	0.03	13 (1%) 76 59	63, 135, 222, 329	0
3	D	1462/1524 (95%)	0.13	40 (2%) 56 41	69, 160, 249, 295	0
4	E	95/99 (95%)	0.18	2 (2%) 63 47	99, 158, 242, 266	0
5	F	313/423 (73%)	0.42	23 (7%) 21 20	144, 205, 276, 332	0
6	G	127/144 (88%)	0.14	2 (1%) 70 52	108, 172, 219, 238	0
6	H	91/144 (63%)	0.26	2 (2%) 62 46	186, 217, 248, 264	0
7	Y	34/54 (62%)	1.17	5 (14%) 6 9	204, 241, 270, 283	0
All	All	3693/4137 (89%)	0.11	88 (2%) 59 44	63, 153, 245, 332	0

The worst 5 of 88 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	83	SER	5.9
3	D	810	GLU	5.5
4	E	57	ASP	4.4
3	D	420	VAL	4.3
3	D	298	VAL	4.3

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 oligosaccharides in this entry.

6.4 Ligands

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($\text{\AA}^2$)	Q<0.9
8	ZN	D	2001	1/1	0.99	0.04	225,225,225,225	0

6.5 Other polymers

There are no such residues in this entry.