



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 02:14 AM GMT

PDB ID : 2O5J
Title : Crystal structure of the T. thermophilus RNAP polymerase elongation complex with the NTP substrate analog
Authors : Vassylyev, D.G.; Vassylyeva, M.N.
Deposited on : 2006-12-06
Resolution : 3.00 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

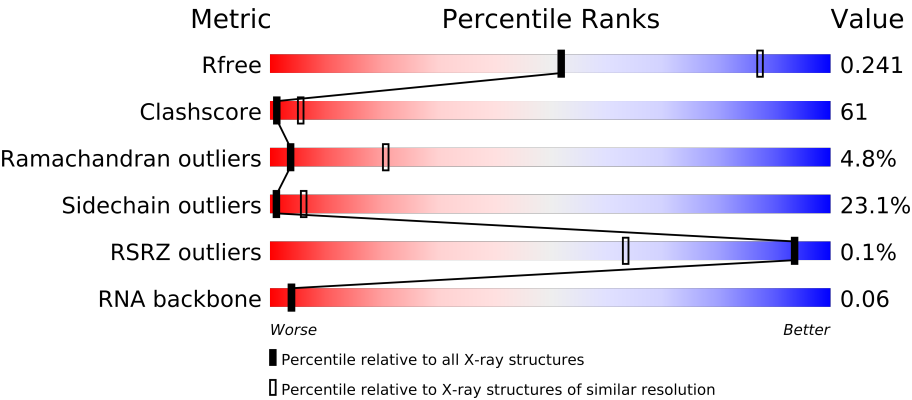
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.00 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.




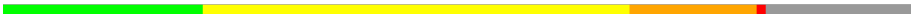
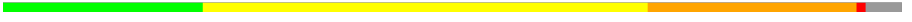

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)
RNA backbone	1838	1070 (3.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	G	23	
1	X	23	
2	H	16	
2	Y	16	
3	I	14	
3	Z	14	
4	A	315	
4	B	315	
4	K	315	
4	L	315	
5	C	1119	
5	M	1119	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	D	1524	
6	N	1524	
7	E	99	
7	O	99	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 51213 atoms, of which 0 are hydrogen and 0 are deuterium.

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 DNA chain called 5'-D(P*CP*CP*CP*TP*GP*TP*CP*TP*GP*GP*CP*GP*TP*TP*CP*GP*CP*GP*CP*GP*CP*GP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	23	Total	C	N	O	P	0	0	0
			467	220	80	144	23			
1	X	23	Total	C	N	O	P	0	0	0
			467	220	80	144	23			

- Molecule 2 is a RNA chain called 5'-R(P*GP*AP*GP*UP*CP*UP*GP*CP*GP*GP*CP*GP*CP*GP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	16	Total	C	N	O	P	0	0	0
			347	153	64	114	16			
2	Y	16	Total	C	N	O	P	0	0	0
			347	153	64	114	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	13	Total	C	N	O	P	0	0	0
			270	126	57	74	13			
3	Z	13	Total	C	N	O	P	0	0	0
			270	126	57	74	13			

- Molecule 4 is a protein called DNA-directed RNA polymerase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
4	B	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
4	L	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			

- Molecule 5 is a protein called DNA-directed RNA polymerase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	1119	Total	C	N	O	S	0	0	0
			8829	5581	1577	1647	24			
5	M	1119	Total	C	N	O	S	0	0	0
			8829	5581	1577	1647	24			

- Molecule 6 is a protein called DNA-directed RNA polymerase beta' chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	1264	Total	C	N	O	S	0	0	0
			9960	6302	1773	1852	33			
6	N	1264	Total	C	N	O	S	0	0	0
			9960	6302	1773	1852	33			

- Molecule 7 is a protein called DNA-directed RNA polymerase omega chain.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	2	Total	Zn	0	0
			2	2		
8	N	2	Total	Zn	0	0
			2	2		

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

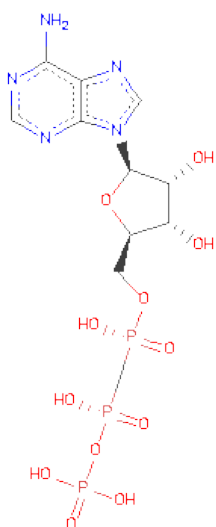
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	2	Total	Mg	0	0
			2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	N	2	Total	Mg	0	0
			2	2		

- Molecule 10 is DIPHOSPHOMETHYLPHOSPHONICACID ADENOSYL ESTER (three-letter code: APC) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	D	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
10	N	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	106	Total	O	0	0
			106	106		
11	B	82	Total	O	0	0
			82	82		
11	C	482	Total	O	0	0
			482	482		
11	D	506	Total	O	0	0
			506	506		
11	E	60	Total	O	0	0
			60	60		
11	G	32	Total	O	0	0
			32	32		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	37	Total 37	O 37	0	0
11	I	22	Total 22	O 22	0	0
11	K	86	Total 86	O 86	0	0
11	L	104	Total 104	O 104	0	0
11	M	483	Total 483	O 483	0	0
11	N	491	Total 491	O 491	0	0
11	O	39	Total 39	O 39	0	0
11	X	43	Total 43	O 43	0	0
11	Y	30	Total 30	O 30	0	0
11	Z	30	Total 30	O 30	0	0

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 errors 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: 5'-D(P*CP*CP*CP*TP*GP*TP*CP*TP*GP*GP*CP*GP*TP*TP*CP*GP*CP*GP*CP*GP*CP*CP*G)-3'

Chain G: 



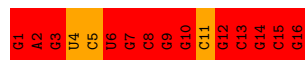
- Molecule 1: 5'-D(P*CP*CP*CP*TP*GP*TP*CP*TP*GP*GP*CP*GP*TP*TP*CP*GP*CP*GP*CP*GP*CP*CP*G)-3'

Chain X: 



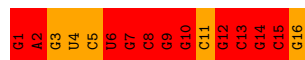
- Molecule 2: 5'-R(P*GP*AP*GP*UP*CP*UP*GP*CP*GP*GP*CP*GP*CP*GP*CP*G)-3',

Chain H: 



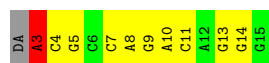
- Molecule 2: 5'-R(P*GP*AP*GP*UP*CP*UP*GP*CP*GP*GP*CP*GP*CP*GP*CP*G)-3',

Chain Y: 



- Molecule 3: 5'-D(*AP*AP*CP*GP*CP*CP*AP*GP*AP*CP*AP*GP*GP*G)-3'

Chain I: 



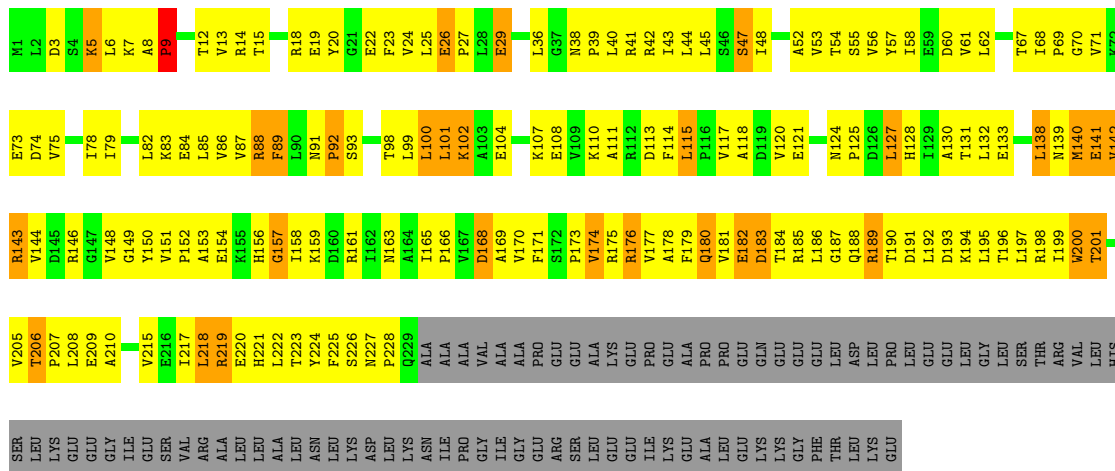
- Molecule 3: 5'-D(*AP*AP*CP*GP*CP*CP*AP*GP*AP*CP*AP*GP*GP*G)-3'

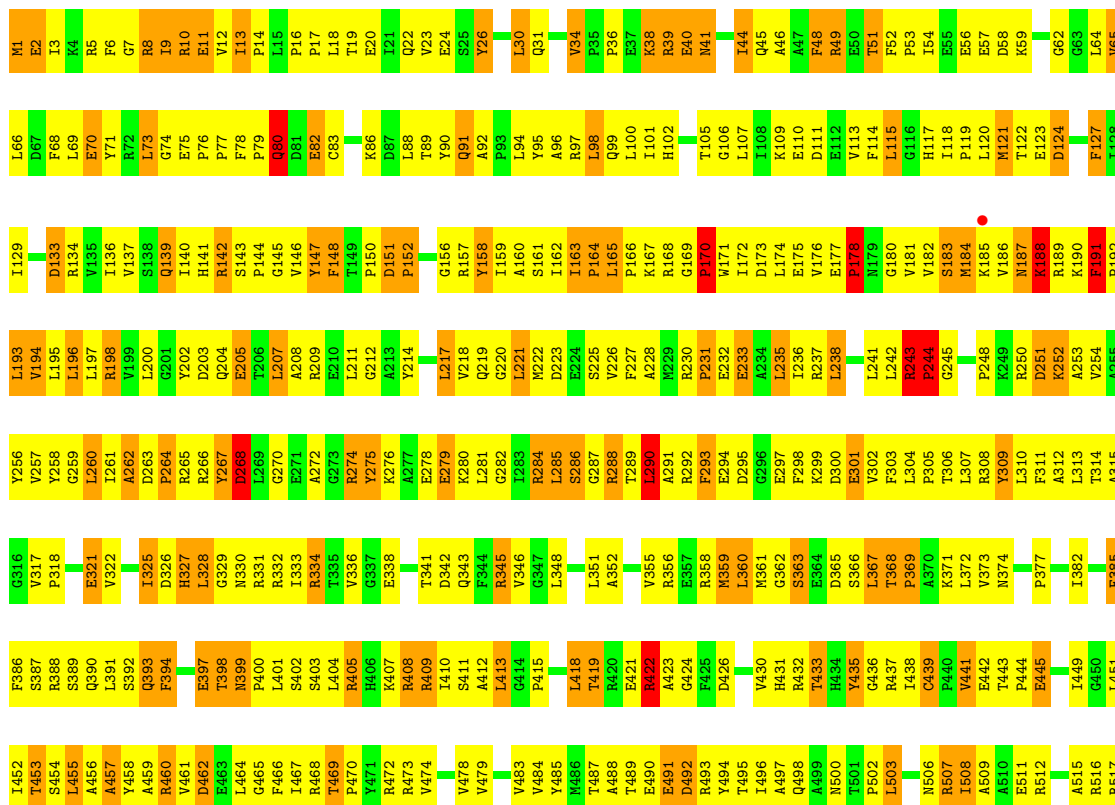
Chain Z: 

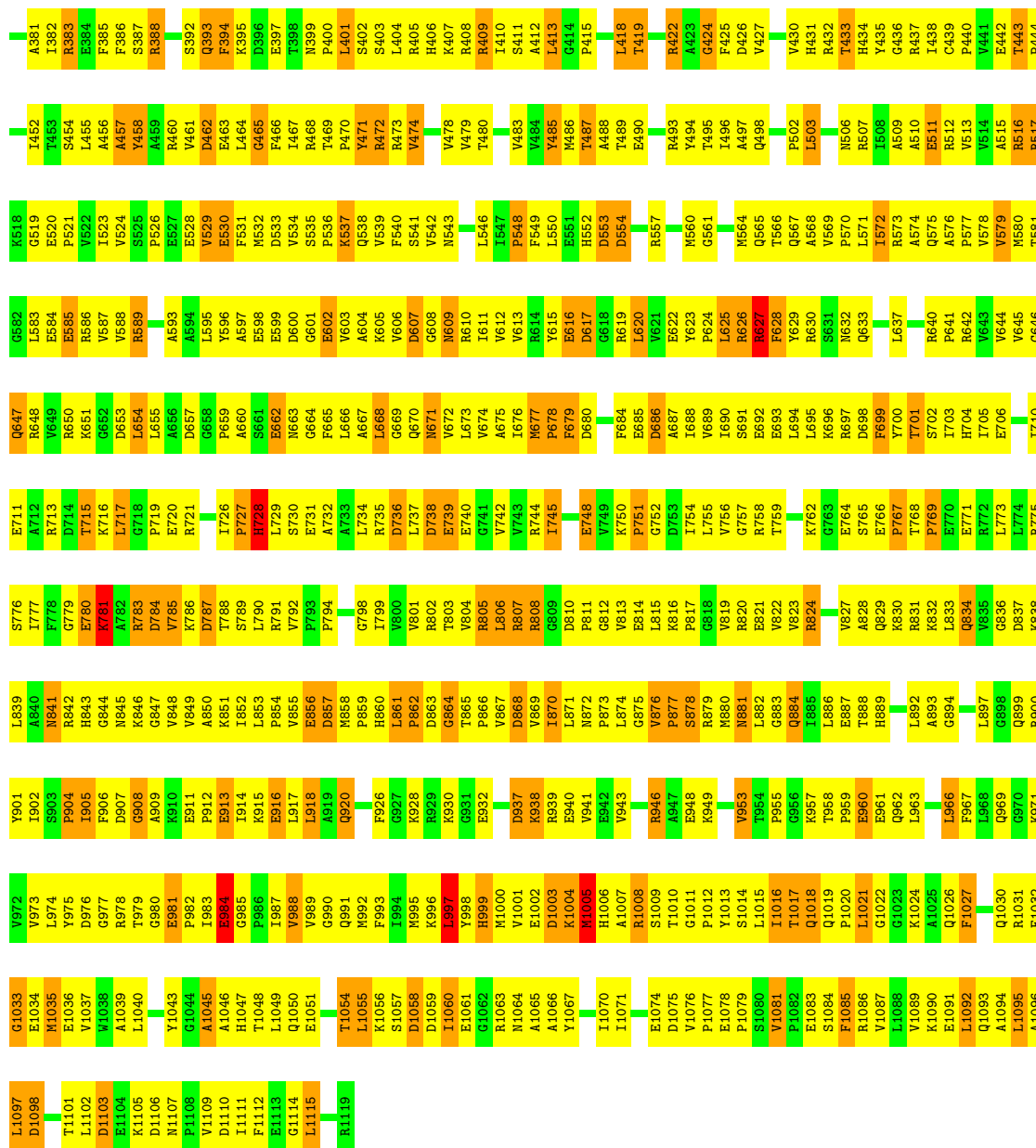


• Molecule 4: DNA-directed RNA polymerase alpha chain

Chain A:

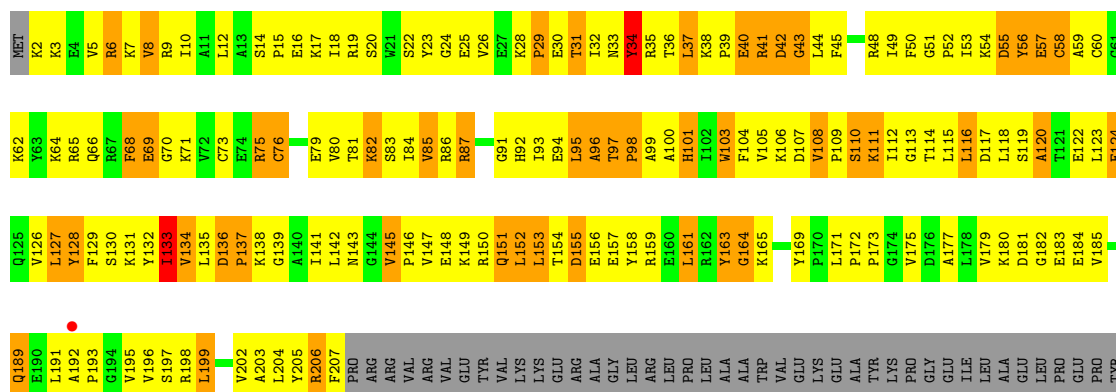






● Molecule 6: DNA-directed RNA polymerase beta' chain

Chain D:



K1271	D1208	D1139	S1073	Q1005	S942	P877	E817	S753	E693	Y625	L558	K434	Y432	ALA	ALA	LEU
ALA	L1209	I1140	S1074	A1006	T943	G878	E818	F754	V694	S626	A559	R494	G433	ILE	ILE	PHE
VAL	M1211	I1140		V1007	I943	R879	R818	F755	I695	S627	Q561	R496	G434	ARG	ARG	LEU
ILE	M1211				I947	I880	G819	G756	H696	G628	Q561	R497	V435	PRO	PRO	ALA
GLY	R1212	G1143	K1079	N1010	T948	L881	E820	A757	G697	S629	A562	V498	E436	GLU	GLU	ARG
ILE	R1214	L1144	G1080	F1011	I949	F882	V821	E758	G697	G630	P563	V499	V437	GLU	GLU	ARG
ASP	V1215	R1147	A1082	M1014	G950	A883	A822	A759	V699	I631	E564	B500	D438	VAL	VAL	GLN
GLY	S1216	V1148	D1083	V1015	I951	R884	L233	A760	V700	V632	I565	A501	D439	GLY	GLY	GLY
VAL	I1217	L1149	T1084	P1016	D952	I885	R824	I761	L701	V633	I566	F502	V440	ARG	ARG	VAL
VAL	G1218	A1150	A1085	F1017	D953	R886	A825	Q762	L702	G634	I567	L503	R441	ALA	ALA	VAL
ARG	E1219	R1151	L1086	F1017	A954	A887	R826	Q763	R703	P635	R568	D504	R442	GLU	GLU	ALA
ILE	A1220	R1152	L1087	L1020	V955		I827	L764	R704	Q636	N569	S505	V443	ALA	ALA	LEU
GLY	V1221	I1153	T1088	Y1021	I956		K828	S765	A705	L637	E570	G506	V444	GLY	GLY	LYS
GLY	G1222	V1154	A1089	Y1022	P957		V829	A766	P706	K638	K571	N507	R445	GLY	GLY	GLY
THR	I1223	V1155	D1090	M1023	E958		A830	H767	T707	L639	R572	R508	V446	VAL	VAL	LEU
GLY	V1224	E1155	K1097	K960	E959		G831	N768	L708	H640	N573	P509	V447	VAL	VAL	LEU
GLY	A1225	L1160	G1092	S1026	K960		R832	L769	H709	Q641	L574	E510	E448	GLY	GLY	GLY
LYS	A1226	E1161	L1093	G1027	Y963		E833	L770	R710	G642	Q575	W511	S449	LEU	LEU	ALA
LEU	Q1227		L1094	G1028	L964		T834	P772	L711	G643	E576	M512	Y450	GLY	GLY	PHE
SER	S1228	R1164	T1095	A1028	E965		S835	G772	G712	L644	A577	I513	D451	THR	THR	GLY
VAL	I1229	Y1165	R1096	G1030	E966		V836	A773	I713	P645	W578	L514	L452	VAL	VAL	LEU
PHE	G1230	L1166	K1097	N1031	A967		G837	S774	Q714	K646	D579	E515	D453	TYR	TYR	VAL
VAL	E1231	S1167	L1098	P1032	D968		R838		A715	R647	A580	A516	A454	LEU	LEU	ARG
GLY	P1232	M1168	V1099	Q1033	R969		E832	L778	R716		L581	P518	R455	THR	THR	ARG
SER	G1233	D1169	D1100	Q1034	K970		T841	A779	Q717		L582	W519	C457	LEU	LEU	GLY
GLY	T1234		V1101	Q1037	L971		H842	K780	P718		D583	B519	G457	PHE	PHE	ASP
GLY	P1235	V1171	T1102	T1037	L972		F843	S781	V719		N584	L520	A458	LEU	LEU	GLY
PHE	T1236	H1172	H1103	L1038	Q973		R839	S782	L720		G585	P521	K397	LEU	LEU	GLY
SER	L1237	L1173	E1104	C1039	I974		A844	T783	W721		R586	D522	A460	TRP	TRP	VAL
LYS	M1238	L1174	I1105	G1040	E975			D784	E722		P580	D524	Q462	THR	THR	ALA
GLY	R1239	L1175	V1106	L1041	Q976		D847	T785	G723		W591	R526	Q463	GLY	GLY	THR
TYR	T1240	K1176	V1107	L1042	Q977		E848	L786	Q724		T592	P526	L464	TYR	TYR	THR
LYS	F1241	A1177	R1108	G1043	Y978		A849	L787	S725		N593	M527	L465	PHE	PHE	LEU
LEU	H1242	E1178	E1109	L1044	E979		L851	Q788	I726		P594	K466	K466	ASP	ASP	LEU
PRO	T1243	E1179	A1110	M1045	M980		L914	L790	Q727		G595	D530	E467	TYR	TYR	PRO
LYS	G1244		D1111	Q1046	G981		V915	L728	H729		L600	W531	D406	ARG	ARG	VAL
GLY			G1112	K1047	F982			T792	P730		G532	D532	D407	VAL	VAL	GLY
ALA	G1248		T1113	G1050	L983		A918	T793	L731		R601	G533	E408	GLN	GLN	MET
ARG			G1114		T984		F919	Q794	V732		S602	R534	V409	PRO	PRO	THR
LEU	D1251	E1185		E1051	D985		L920	C733	C733		L603		S410	HIS	HIS	PRO
LEU	I1252	P1187	Y1117	T1052	R986		R921	V795	E734		T604		T411	MET	MET	LEU
VAL	T1253	V1188	I1118	F1053	E987		L922	R796	E734				L473	VAL	VAL	VAL
LYS	Q1254	R1189	S1119		R988		G923	K797	A735		D605	D538	E474	ASN	ASN	VAL
ASP	G1255	S1190	V1120	V1057	Y989		M924	E798	V736		T606	L540	K475	VAL	VAL	HIS
GLY	L1256	P1191	P1121	R1058	D990		E925	K799	K737		L607		E476	VAL	VAL	GLY
ASP	P1257	L1192	F1122	S1059	Q991		K926	G801	A738		R610	B541	L477	VAL	VAL	GLY
TYR	R1258	L1192	F1123	S1060	I992			R800	D739		D542	L478	P417	PRO	PRO	GLY
VAL	V1259	Q1195	Q1124	F1061	L993		R929	A802	D741		Q611	L543	E479	ILE	ILE	ILE
GLY	E1260	T1196	P1125	R1062	Q994		L930	G803	G741		G612	Y544	E480	VAL	VAL	VAL
ALA	E1261	R1197	D1126	E1063	L995		L931	L804	G742		R613	R545	M481	ALA	ALA	GLY
GLY	F1262	Y1198	E1127	G1064	W996		D932	E805	D743		F614	R546	K482	ARG	ARG	LYS
GLN	F1263	G1199	V1128	L1065	T997		A933	F806	Q744		R615	L547	R483	VAL	VAL	GLY
PRO	E1264	V1200	T1129	T1066	E998		L934	A807	M745		Q616	I548	P484	GLY	GLY	GLN
LEU	A1265	C1201	R1130	V1067	T999		K935	T808	A746		N617	N549	S485	ALA	ALA	PRO
THR	R1266			L1068	T1000		Y936	P809	V747		L618	B550	R486	LEU	LEU	LEU
ARG	K1267	G1204	R1133	E1069	E1001			E810	H748		L619	A487	A487	ASP	ASP	ALA
GLY	P1268	Y1205	L1134	K1002	G938		Y937	E811	V749		G620	L554	R488	LYS	LYS	GLY
	K1269	R1206	L1135	F1070	K1003		F939	A812	P750		R621	K555	R489	ILE	ILE	ALA
		Y1207	K1136	I1072	T1004			L813	S752		R622	L557	R493	VAL	VAL	GLY





M63	AG4	M65	K66	E67	L68	L69	T70	G71	R72	L73	V74	F75		N78	L79	V80	P81	E82	D83	R84	L85	Q86	K87	E88	M89	E90	R91	L92	Y93	P94	V95	E96	ARG	GLU	GLU
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	--	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	152.34Å 152.34Å 524.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.00 38.29 – 3.00	Depositor EDS
% Data completeness (in resolution range)	89.3 (40.00-3.00) 83.5 (38.29-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.257 0.219 , 0.241	Depositor DCC
R_{free} test set	11219 reflections (6.04%)	DCC
Wilson B-factor (Å ²)	64.2	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 143.5	EDS
Estimated twinning fraction	0.146 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 196921 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	51213	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: APC, 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	G	1.04	1/520 (0.2%)	1.12	1/798 (0.1%)
1	X	1.12	2/520 (0.4%)	1.14	1/798 (0.1%)
2	H	1.39	3/387 (0.8%)	2.45	39/601 (6.5%)
2	Y	1.36	3/387 (0.8%)	2.44	33/601 (5.5%)
3	I	0.72	0/304	0.92	1/467 (0.2%)
3	Z	0.73	0/304	0.91	0/467
4	A	0.69	0/1838	0.76	0/2498
4	B	0.76	0/1838	0.76	2/2498 (0.1%)
4	K	0.73	0/1838	0.82	3/2498 (0.1%)
4	L	0.73	0/1838	0.78	4/2498 (0.2%)
5	C	0.79	1/8997 (0.0%)	0.89	17/12164 (0.1%)
5	M	0.78	1/8997 (0.0%)	0.90	17/12164 (0.1%)
6	D	0.79	1/10128 (0.0%)	0.91	18/13681 (0.1%)
6	N	0.79	2/10128 (0.0%)	0.89	22/13681 (0.2%)
7	E	0.83	1/784 (0.1%)	1.07	3/1057 (0.3%)
7	O	0.78	1/784 (0.1%)	1.07	3/1057 (0.3%)
All	All	0.80	16/49592 (0.0%)	0.95	164/67528 (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	G	0	6
1	X	0	5
2	H	0	2
2	Y	0	1
3	I	0	1
All	All	0	15

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	G	OP3-P	10.56	1.73	1.61
1	G	1	DC	OP3-P	-7.74	1.51	1.61
1	X	1	DC	OP3-P	-7.13	1.52	1.61
7	E	94	PRO	N-CA	6.34	1.58	1.47
5	C	439	CYS	CB-SG	-6.08	1.72	1.82

The worst 5 of 164 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	2	A	N9-C1'-C2'	-18.09	90.48	114.00
5	M	409	ARG	NE-CZ-NH1	15.09	127.85	120.30
2	Y	7	G	N9-C1'-C2'	-12.29	98.02	114.00
7	E	94	PRO	CA-N-CD	-11.28	95.71	111.50
2	H	1	G	N9-C1'-C2'	11.20	128.56	114.00

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	13	DT	Sidechain
1	G	15	DC	Sidechain
1	G	16	DG	Sidechain
1	G	17	DC	Sidechain
1	G	18	DG	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	467	0	259	43	0
1	X	467	0	259	43	0
2	H	347	0	174	58	0
2	Y	347	0	174	81	0
3	I	270	0	144	14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Z	270	0	144	12	0
4	A	1806	0	1861	169	0
4	B	1806	0	1861	174	0
4	K	1806	0	1861	182	0
4	L	1806	0	1861	199	0
5	C	8829	0	8933	1208	0
5	M	8829	0	8933	1204	0
6	D	9960	0	10183	1379	0
6	N	9960	0	10183	1351	0
7	E	770	0	784	108	0
7	O	770	0	784	101	0
8	D	2	0	0	0	0
8	N	2	0	0	0	0
9	D	2	0	0	0	0
9	N	2	0	0	0	0
10	D	31	0	14	2	0
10	N	31	0	14	2	0
11	A	106	0	0	16	0
11	B	82	0	0	21	0
11	C	482	0	0	120	0
11	D	506	0	0	138	0
11	E	60	0	0	6	0
11	G	32	0	0	3	0
11	H	37	0	0	3	0
11	I	22	0	0	3	0
11	K	86	0	0	19	0
11	L	104	0	0	23	0
11	M	483	0	0	129	0
11	N	491	0	0	115	0
11	O	39	0	0	6	0
11	X	43	0	0	4	0
11	Y	30	0	0	6	0
11	Z	30	0	0	4	0
All	All	51213	0	48426	5871	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 61.

The worst 5 of 5871 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:Y:7:G:N1	5:M:1014:SER:HA	1.62	1.13
2:Y:16:G:H21	6:N:705:ALA:HB1	1.11	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:N:18:ILE:HG23	6:N:518:PRO:HG3	1.33	1.10
5:C:409:ARG:HA	5:C:454:SER:HA	1.27	1.10
6:N:1189:ARG:HB3	6:N:1204:CYS:HA	1.34	1.09

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	
4	A	227/315 (72%)	206 (91%)	14 (6%)	7 (3%)	7	34
4	B	227/315 (72%)	206 (91%)	15 (7%)	6 (3%)	8	39
4	K	227/315 (72%)	208 (92%)	13 (6%)	6 (3%)	8	39
4	L	227/315 (72%)	206 (91%)	15 (7%)	6 (3%)	8	39
5	C	1117/1119 (100%)	919 (82%)	136 (12%)	62 (6%)	3	16
5	M	1117/1119 (100%)	923 (83%)	133 (12%)	61 (6%)	3	16
6	D	1258/1524 (82%)	1051 (84%)	149 (12%)	58 (5%)	4	22
6	N	1258/1524 (82%)	1058 (84%)	140 (11%)	60 (5%)	4	20
7	E	93/99 (94%)	76 (82%)	11 (12%)	6 (6%)	2	11
7	O	93/99 (94%)	74 (80%)	12 (13%)	7 (8%)	2	8
All	All	5844/6744 (87%)	4927 (84%)	638 (11%)	279 (5%)	4	20

5 of 279 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	29	GLU
4	A	187	GLY
4	B	29	GLU
4	B	187	GLY
5	C	178	PRO

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	
4	A	202/273 (74%)	162 (80%)	40 (20%)	2	11
4	B	202/273 (74%)	159 (79%)	43 (21%)	1	8
4	K	202/273 (74%)	162 (80%)	40 (20%)	2	11
4	L	202/273 (74%)	150 (74%)	52 (26%)	1	4
5	C	941/941 (100%)	704 (75%)	237 (25%)	1	4
5	M	941/941 (100%)	713 (76%)	228 (24%)	1	5
6	D	1063/1279 (83%)	825 (78%)	238 (22%)	1	7
6	N	1063/1279 (83%)	833 (78%)	230 (22%)	1	8
7	E	84/88 (96%)	59 (70%)	25 (30%)	0	2
7	O	84/88 (96%)	68 (81%)	16 (19%)	2	12
All	All	4984/5708 (87%)	3835 (77%)	1149 (23%)	1	6

5 of 1149 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	D	1256	LEU
4	L	67	THR
6	N	1042	ARG
6	D	1365	ASP
4	K	1	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 154 such sidechains are listed below:

Mol	Chain	Res	Type
6	D	1103	HIS
4	K	156	HIS
6	N	906	GLN
6	D	1227	GLN
7	E	29	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	H	16/16 (100%)	10 (62%)	8 (50%)
2	Y	16/16 (100%)	10 (62%)	8 (50%)
All	All	32/32 (100%)	20 (62%)	16 (50%)

5 of 20 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	H	2	A
2	H	3	G
2	H	6	U
2	H	7	G
2	H	8	C

5 of 16 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	H	15	C
2	Y	1	G
2	Y	9	G
2	H	13	C
2	Y	12	G

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 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	APC	D	3999	9	33,33,33	4.47	4 (12%)	52,52,52	2.00	13 (25%)
10	APC	N	4999	9	33,33,33	4.52	4 (12%)	52,52,52	2.05	13 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	APC	D	3999	9	-	0/20/38/38	0/1/3/3
10	APC	N	4999	9	-	0/20/38/38	0/1/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	N	4999	APC	PB-C3A	-18.34	1.64	1.79
10	D	3999	APC	PB-C3A	-17.89	1.64	1.79
10	N	4999	APC	PA-C3A	-17.54	1.64	1.79
10	D	3999	APC	PA-C3A	-17.29	1.64	1.79
10	D	3999	APC	PB-O2B	-3.37	1.48	1.56

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	N	4999	APC	O4'-C1'-N9	6.22	114.23	108.44
10	N	4999	APC	C1'-N9-C4	-6.11	116.08	126.64
10	N	4999	APC	C8-N9-C1'	6.00	138.20	126.38
10	D	3999	APC	C8-N9-C1'	5.90	138.00	126.38
10	D	3999	APC	C1'-N9-C4	-5.74	116.72	126.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	G	23/23 (100%)	-0.57	0 100 100	22, 46, 76, 79	0
1	X	23/23 (100%)	-0.51	0 100 100	21, 38, 71, 90	0
2	H	16/16 (100%)	-0.50	0 100 100	36, 56, 100, 102	0
2	Y	16/16 (100%)	-0.53	0 100 100	21, 73, 101, 103	0
3	I	13/14 (92%)	-0.72	0 100 100	49, 65, 74, 85	0
3	Z	13/14 (92%)	-0.68	0 100 100	54, 67, 80, 81	0
4	A	229/315 (72%)	-0.34	0 100 100	41, 66, 86, 94	0
4	B	229/315 (72%)	-0.31	1 (0%) 90 41	43, 70, 85, 101	0
4	K	229/315 (72%)	-0.34	0 100 100	41, 65, 81, 93	0
4	L	229/315 (72%)	-0.34	0 100 100	38, 68, 80, 90	0
5	C	1119/1119 (100%)	-0.34	1 (0%) 93 63	26, 64, 86, 101	0
5	M	1119/1119 (100%)	-0.33	0 100 100	25, 65, 89, 109	0
6	D	1264/1524 (82%)	-0.37	3 (0%) 93 54	23, 61, 83, 100	0
6	N	1264/1524 (82%)	-0.38	0 100 100	26, 60, 84, 100	0
7	E	95/99 (95%)	-0.38	0 100 100	35, 59, 74, 82	0
7	O	95/99 (95%)	-0.40	0 100 100	45, 66, 80, 84	0
All	All	5976/6850 (87%)	-0.36	5 (0%) 93 63	21, 64, 86, 109	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	D	416	ALA	3.0
4	B	147	GLY	2.5
6	D	391	ALA	2.1
6	D	192	ALA	2.0
5	C	185	LYS	2.0

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 ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
8	ZN	D	6112	1/1	0.15	0.20	59,59,59,59	0
10	APC	N	4999	31/31	0.17	0.18	45,49,51,54	0
10	APC	D	3999	31/31	0.17	0.16	41,49,52,54	0
8	ZN	N	7112	1/1	0.14	-0.80	65,65,65,65	0
8	ZN	N	5058	1/1	0.10	-1.18	66,66,66,66	0
9	MG	N	9001	1/1	0.11	-1.44	21,21,21,21	0
9	MG	N	9002	1/1	0.10	-1.54	23,23,23,23	0
9	MG	D	8001	1/1	0.10	-1.58	23,23,23,23	0
8	ZN	D	4058	1/1	0.10	-1.91	66,66,66,66	0
9	MG	D	8002	1/1	0.09	-2.15	25,25,25,25	0

6.5 Other polymers ⓘ

There are no such residues in this entry.