



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 20, 2017 – 05:33 PM EDT

PDB ID : 1HQM
Title : CRYSTAL STRUCTURE OF THERMUS AQUATICUS CORE RNA POLYMERASE-INCLUDES COMPLETE STRUCTURE WITH SIDE-CHAINS (EXCEPT FOR DISORDERED REGIONS)-FURTHER REFINED FROM ORIGINAL DEPOSITION-CONTAINS ADDITIONAL SEQUENCE INFORMATION
Authors : Minakhin, L.; Bhagat, S.; Brunning, A.; Campbell, E.A.; Darst, S.A.; Ebright, R.H.; Severinov, K.
Deposited on : 2000-12-18
Resolution : 3.30 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
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029077

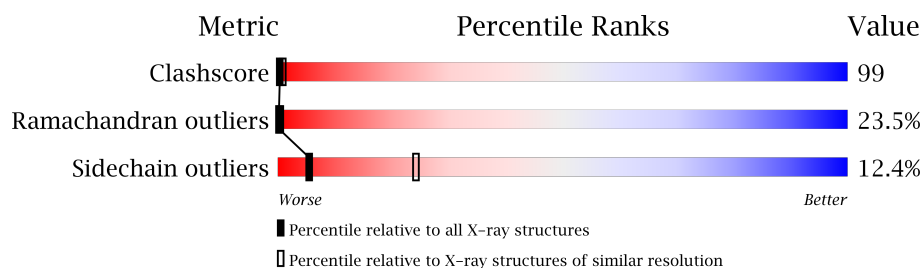
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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))
Clashscore	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	313	
1	B	313	
2	C	1119	
3	D	1265	
4	E	99	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 21254 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	223	Total	C	N	O	S	0	0	0
			1750	1118	302	328	2			
1	B	229	Total	C	N	O	S	0	0	0
			1776	1135	305	334	2			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	deletion	UNP Q9KWU8
A	93	ARG	MET	conflict	UNP Q9KWU8
A	94	TRP	ALA	conflict	UNP Q9KWU8
A	95	ARG	SER	conflict	UNP Q9KWU8
A	111	VAL	GLY	conflict	UNP Q9KWU8
B	?	-	LYS	deletion	UNP Q9KWU8
B	93	ARG	MET	conflict	UNP Q9KWU8
B	94	TRP	ALA	conflict	UNP Q9KWU8
B	95	ARG	SER	conflict	UNP Q9KWU8
B	111	VAL	GLY	conflict	UNP Q9KWU8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1113	Total	C	N	O	S	12	0	0
			8508	5386	1514	1585	23			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2	LYS	GLU	conflict	UNP Q9KWU7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1175	Total	C	N	O	S	17	0	0
			8499	5328	1549	1595	27			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	119	PHE	SER	conflict	UNP Q9KWU6
D	863	THR	VAL	conflict	UNP Q9KWU6
D	866	THR	VAL	conflict	UNP Q9KWU6
D	876	ASN	SER	conflict	UNP Q9KWU6
D	947	ILE	-	insertion	UNP Q9KWU6
D	1010	ASN	LYS	conflict	UNP Q9KWU6
D	1117	LYS	ASN	conflict	UNP Q9KWU6
D	1389	PRO	ARG	conflict	UNP Q9KWU6

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	98	Total	C	N	O	S	0	0	0
			719	453	132	130	4			

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

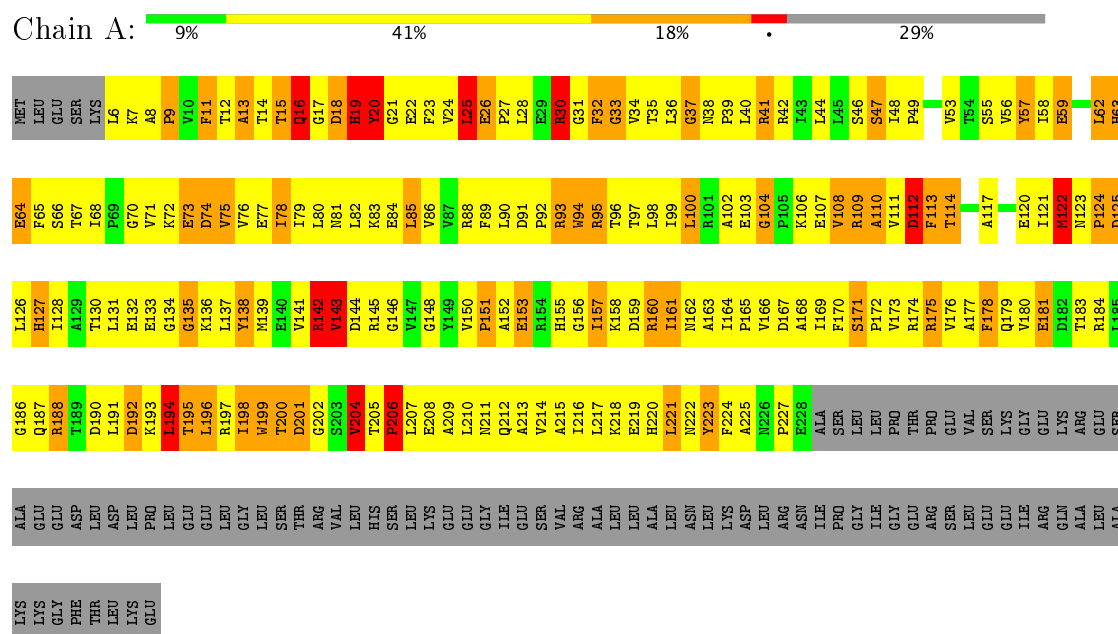
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

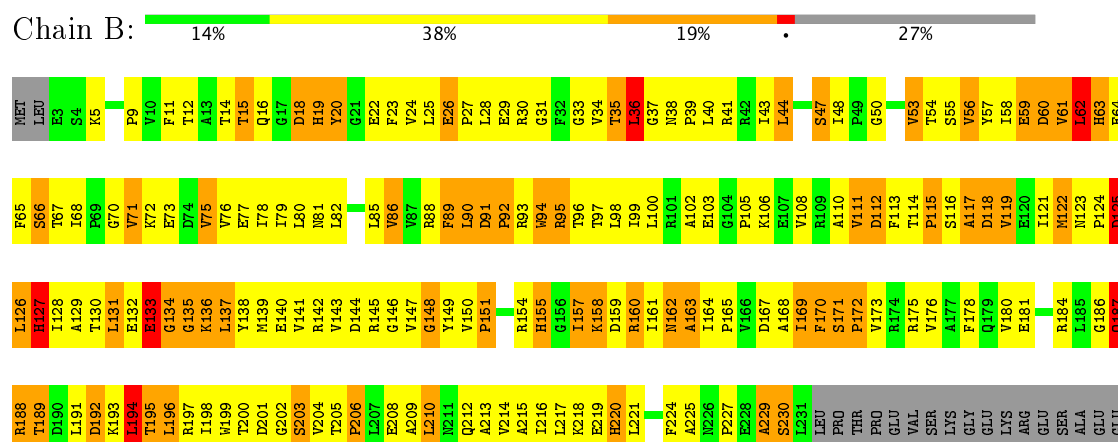
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 1: DNA-directed RNA polymerase subunit alpha



ASP	PHE
LEU	THR
ASP	LEU
LEU	LYS
PRO	GLU
LEU	
GLU	
LEU	
GLY	
LEU	
SER	
THR	
ARG	
VAL	
LEU	
HIS	
SER	
LEU	
LYS	
GLU	
GLY	
GLY	
ILE	
SER	
VAL	
ARG	
ASN	
LEU	
LYS	
ASP	
LEU	
ARG	
ASN	
ILE	
PRO	
GLY	
ILE	
GLY	
GLU	
ILE	
ARG	
GLN	
ALA	
LEU	
ALA	
LYS	
LYS	
GLY	

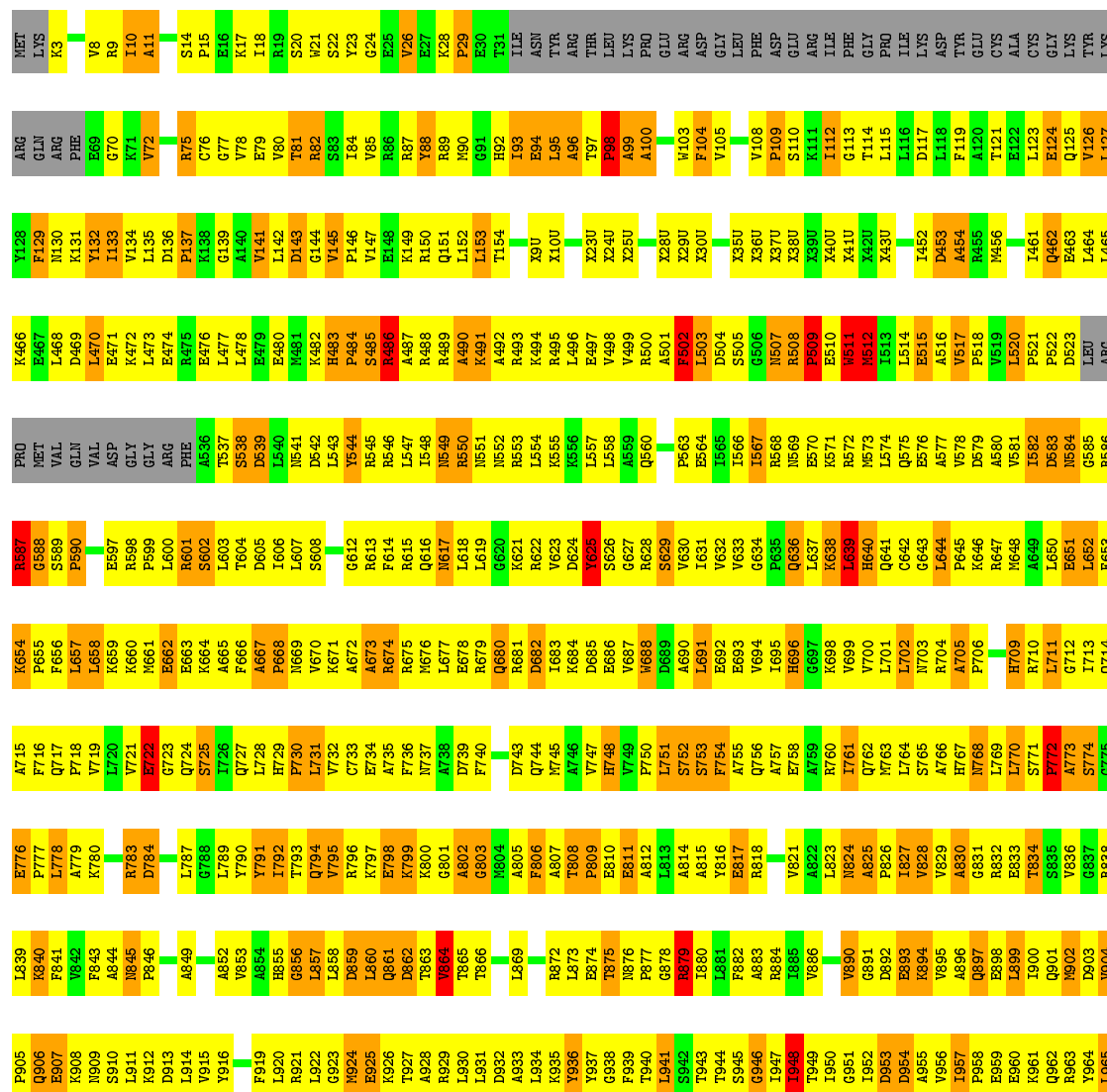
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C: 15% 56% 26% ..

L804	L805	L806	L807	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
I742	I743	I744	I745	I746	I747	I748	I749	I750	I751	I752	I753	I754	I755	I756	I757	I758	I759	I760	I761	I762	I763	I764	I765	I766	I767	I768	I769	I770	I771	I772	I773	I774	I775	I776	I777	I778	I779	I780	I781	I782	I783	I784	I785	I786	I787	I788	I789	I790	I791	I792	I793	I794	I795	I796	I797	I798	I799	I800	I801	I802	I803																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
G681	G682	G683	G684	G685	G686	G687	G688	G689	G690	G691	G692	G693	G694	G695	G696	G697	G698	G699	G700	G701	G702	G703	G704	G705	G706	G707	G708	G709	G710	G711	G712	G713	G714	G715	G716	G717	G718	G719	G720	G721	G722	G723	G724	G725	G726	G727	G728	G729	G730	G731	G732	G733	G734	G735	G736	G737	G738	G739																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
V186	V187	V188	V189	V190	V191	V192	V193	V194	V195	V196	V197	V198	V199	V200	V201	V202	V203	V204	V205	V206	V207	V208	V209	V210	V211	V212	V213	V214	V215	V216	V217	V218	V219	V220	V221	V222	V223	V224	V225	V226	V227	V228	V229	V230	V231	V232	V233	V234	V235	V236	V237	V238	V239	V240	V241	V242	V243	V244	V245	V246	V247	V248	V249	V250																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
T122	T123	T124	T125	T126	T127	T128	T129	T130	T131	T132	T133	T134	T135	T136	T137	T138	T139	T140	T141	T142	T143	T144	T145	T146	T147	T148	T149	T150	T151	T152	T153	T154	T155	T156	T157	T158	T159	T160	T161	T162	T163	T164	T165	T166	T167	T168	T169	T170	T171	T172	T173	T174	T175	T176	T177	T178	T179	T180	T181	T182	T183	T184	T185	T186	T187	T188	T189	T190	T191	T192	T193	T194	T195	T196	T197	T198	T199	T200																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
P247	P248	P249	P250	P251	P252	P253	P254	P255	P256	P257	P258	P259	P260	P261	P262	P263	P264	P265	P266	P267	P268	P269	P270	P271	P272	P273	P274	P275	P276	P277	P278	P279	P280	P281	P282	P283	P284	P285	P286	P287	P288	P289	P290	P291	P292	P293	P294	P295	P296	P297	P298	P299	P300	P301	P302	P303	P304	P305	P306	P307	P308	P309	P310	P311	P312	P313	P314	P315	P316	P317	P318	P319	P320	P321	P322	P323	P324	P325	P326	P327	P328	P329	P330	P331	P332	P333	P334	P335	P336	P337	P338	P339	P340	P341	P342	P343	P344	P345	P346	P347	P348	P349	P350	P351	P352	P353	P354	P355	P356	P357	P358	P359	P360	P361	P362	P363	P364	P365	P366	P367	P368	P369	P370	P371	P372	P373	P374	P375	P376	P377	P378	P379	P380	P381	P382	P383	P384	P385	P386	P387	P388	P389	P390	P391	P392	P393	P394	P395	P396	P397	P398	P399	P400	P401	P402	P403	P404	P405	P406	P407	P408	P409	P410	P411	P412	P413	P414	P415	P416	P417	P418	P419	P420	P421	P422	P423	P424	P425	P426	P427	P428	P429	P430	P431	P432	P433	P434	P435	P436	P437	P438	P439	P440	P441	P442	P443	P444	P445	P446	P447	P448	P449	P450	P451	P452	P453	P454	P455	P456	P457	P458	P459	P460	P461	P462	P463	P464	P465	P466	P467	P468	P469	P470	P471	P472	P473	P474	P475	P476	P477	P478	P479	P480	P481	P482	P483	P484	P485	P486	P487	P488	P489	P490	P491	P492	P493	P494	P495	P496	P497	P498	P499	P500	P501	P502	P503	P504	P505	P506	P507	P508	P509	P510	P511	P512	P513	P514	P515	P516	P517	P518	P519	P520	P521	P522	P523	P524	P525	P526	P527	P528	P529	P530	P531	P532	P533	P534	P535	P536	P537	P538	P539	P540	P541	P542	P543	P544	P545	P546	P547	P548	P549	P550	P551	P552	P553	P554	P555	P556	P557	P558	P559	P560	P561	P562	P563	P564	P565	P566	P567	P568	P569	P570	P571	P572	P573	P574	P575	P576	P577	P578	P579	P580	P581	P582	P583	P584	P585	P586	P587	P588	P589	P590	P591	P592	P593	P594	P595	P596	P597	P598	P599	P600	P601	P602	P603	P604	P605	P606	P607	P608	P609	P610	P611	P612	P613	P614	P615	P616	P617	P618	P619	P620	P621	P622	P623	P624	P625	P626	P627	P628	P629	P630	P631	P632	P633	P634	P635	P636	P637	P638	P639	P640	P641	P642	P643	P644	P645	P646	P647	P648	P649	P650	P651	P652	P653	P654	P655	P656	P657	P658	P659	P660	P661	P662	P663	P664	P665	P666	P667	P668	P669	P670	P671	P672	P673	P674	P675	P676	P677	P678	P679	P680	P681	P682	P683	P684	P685	P686	P687	P688	P689	P690	P691	P692	P693	P694	P695	P696	P697	P698	P699	P700	P701	P702	P703	P704	P705	P706	P707	P708	P709	P710	P711	P712	P713	P714	P715	P716	P717	P718	P719	P720	P721	P722	P723	P724	P725	P726	P727	P728	P729	P730	P731	P732	P733	P734	P735	P736	P737	P738	P739	P740	P741	P742	P743	P744	P745	P746	P747	P748	P749	P750	P751	P752	P753	P754	P755	P756	P757	P758	P759	P760	P761	P762	P763	P764	P765	P766	P767	P768	P769	P770	P771	P772	P773	P774	P775	P776	P777	P778	P779	P780	P781	P782	P783	P784	P785	P786	P787	P788	P789	P790	P791	P792	P793	P794	P795	P796	P797	P798	P799	P800	P801	P802	P803	P804	P805	P806	P807	P808	P809	P810	P811	P812	P813	P814	P815	P816	P817	P818	P819	P820	P821	P822	P823	P824	P825	P826	P827	P828	P829	P830	P831	P832	P833	P834	P835	P836	P837	P838	P839	P840	P841	P842	P843	P844	P845	P846	P847	P848	P849	P850	P851	P852	P853	P854	P855	P856	P857	P858	P859	P860	P861	P862	P863	P864	P865	P866	P867	P868	P869	P870	P871	P872	P873	P874	P875	P876	P877	P878	P879	P880	P881	P882	P883	P884	P885	P886	P887	P888	P889	P890	P891	P892	P893	P894	P895	P896	P897	P898	P899	P900	P901	P902	P903	P904	P905	P906	P907	P908	P909	P910	P911	P912	P913	P914	P915	P916	P917	P918	P919	P920	P921	P922	P923	P924	P925	P926	P927	P928	P929	P930	P931	P932	P933	P934	P935	P936	P937	P938	P939	P940	P941	P942	P943	P944	P945	P946	P947	P948	P949	P950	P951	P952	P953	P954	P955	P956	P957	P958	P959	P960	P961	P962	P963	P964	P965	P966	P967	P968	P969	P970	P971	P972	P973	P974	P975	P976	P977	P978	P979	P980	P981	P982	P983	P984	P985	P986	P987	P988	P989	P990	P991	P992	P993	P994	P995	P996	P997	P998	P999	P1000	P1001	P1002	P1003	P1004	P1005	P1006	P1007	P1008	P1009	P1010	P1011	P1012	P1013	P1014	P1015	P1016	P1017	P1018	P1019	P1020	P1021	P1022	P1023	P1024	P1025	P1026	P1027	P1028	P1029	P1030	P1031	P1032	P1033	P1034	P1035	P1036	P1037	P1038	P1039	P1040	P1041	P1042	P1043	P1044	P1045	P1046	P1047	P1048	P1049	P1050	P1051	P1052	P1053	P1054	P1055	P1056	P1057	P1058	P1059	P1060	P1061	P1062	P1063	P1064	P1065	P1066	P1067	P1068	P1069	P1070	P1071	P1072	P1073	P1074	P1075	P1076	P1077	P1078	P1079	P1080	P1081	P1082	P1083	P1084	P1085	P1086	P1087	P1088	P1089	P1090	P1091	P1092	P1093	P1094	P1095	P1096	P1097	P1098	P1099	P1100	P1101	P1102	P1103	P1104	P1105	P1106	P1107	P1108	P1109	P1110	P1111	P1112	P1113	P1114	P1115	P1116	P1117	P1118	P1119	P1120	P1121	P1122	P1123	P1124	P1125	P1126	P1127	P1128	P1129	P1130	P1131	P1132	P1133	P1134	P1135	P1136	P1137	P1138	P1139	P1140	P1141	P1142	P1143	P1144	P1145	P1146	P1147	P1148	P1149	P1150	P1151	P1152	P1153	P1154	P1155	P1156	P1157	P1158	P1159	P1160	P1161	P1162	P1163	P1164	P1165	P1166	P1167	P1168	P1169	P1170	P1171	P1172	P1173	P1174	P1175	P1176	P1177	P1178	P1179	P1180	P1181	P1182	P1183	P1184	P1185	P1186	P1187	P1188	P1189	P1190	P1191	P1192	P1193	P1194	P1195	P1196	P1197	P1198	P1199	P1200	P1201	P1202	P1203	P1204	P1205	P1206	P1207	P1208	P1209	P1210	P1211	P1212	P1213	P1214	P1215	P1216	P1217	P1218	P1219	P1220	P1221	P1222	P1223	P1224	P1225	P1226	P1227	P1228	P1229	P1230	P1231	P1232	P1233	P1234	P1235	P1236	P1237	P1238	P1239	P1240	P1241	P1242	P1243	P1244	P1245	P1246	P1247	P1248	P1249	P1250	P1251	P1252	P1253	P1254	P1255	P1256	P1257	P1258	P1259	P1260	P1261	P1262	P1263	P1264	P1265	P1266	P1267	P1268	P1269	P1270	P1271	P1272	P1273	P1274	P1275	P1276	P1277	P1278	P1279	P1280	P1281	P1282	P1283	P1284	P1285	P1286	P1287	P1288	P1289	P1290	P1291	P1292	P1293	P1294	P1295	P1296	P1297	P1298	P1299	P1300	P1301	P1302	P1303	P1304	P1305	P1306	P1307	P1308	P1309	P1310	P1311	P1312	P1313	P1314	P1315	P1316	P1317	P1318	P1319	P1320	P1321	P1322	P1323	P1324	P1325	P1326	P1327	P1328	P1329	P1330	P1331	P13



Chain D: 17% 54% 20% 7%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	200.76Å 200.76Å 292.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.30	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.30)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.300 , 0.360	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21254	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.42	0/1786	0.77	0/2434
1	B	0.39	0/1812	0.74	0/2471
2	C	0.42	0/8672	0.78	5/11752 (0.0%)
3	D	0.42	0/8437	0.78	14/11443 (0.1%)
4	E	0.35	0/730	0.65	0/991
All	All	0.41	0/21437	0.77	19/29091 (0.1%)

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	1
2	C	0	1
All	All	0	2

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	834	THR	N-CA-C	-6.40	93.72	111.00
3	D	137	PRO	N-CA-CB	6.22	110.77	103.30
2	C	580	MET	N-CA-C	6.19	127.70	111.00
2	C	836	GLY	N-CA-C	-6.04	97.99	113.10
2	C	329	GLY	N-CA-C	-5.97	98.17	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	138	TYR	Sidechain
2	C	975	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	1750	0	1759	403	0
1	B	1776	0	1776	323	0
2	C	8508	0	8418	1886	0
3	D	8499	0	7993	1651	0
4	E	719	0	685	125	0
5	D	1	0	0	0	0
6	D	1	0	0	0	0
All	All	21254	0	20631	4161	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 99.

The worst 5 of 4161 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:1020:PRO:HB2	3:D:1023:VAL:HB	1.20	1.18
2:C:508:ILE:H	2:C:508:ILE:HD13	1.10	1.15
2:C:438:ILE:HG21	2:C:470:PRO:HB3	1.22	1.15
2:C:605:LYS:HG2	2:C:606:VAL:H	1.05	1.14
2:C:262:ALA:HB1	2:C:266:ARG:HD2	1.23	1.14

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	
1	A	221/313 (71%)	98 (44%)	68 (31%)	55 (25%)	0	0
1	B	227/313 (72%)	109 (48%)	61 (27%)	57 (25%)	0	0
2	C	1111/1119 (99%)	559 (50%)	300 (27%)	252 (23%)	0	0
3	D	1127/1265 (89%)	543 (48%)	319 (28%)	265 (24%)	0	0
4	E	96/99 (97%)	49 (51%)	22 (23%)	25 (26%)	0	0
All	All	2782/3109 (90%)	1358 (49%)	770 (28%)	654 (24%)	0	0

5 of 654 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	59	GLU
1	A	64	GLU
1	A	73	GLU
1	A	75	VAL

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	190/271 (70%)	163 (86%)	27 (14%)	4	19
1	B	191/271 (70%)	171 (90%)	20 (10%)	8	31
2	C	869/936 (93%)	747 (86%)	122 (14%)	4	19
3	D	782/1036 (76%)	693 (89%)	89 (11%)	7	28
4	E	67/88 (76%)	64 (96%)	3 (4%)	32	67
All	All	2099/2602 (81%)	1838 (88%)	261 (12%)	5	24

5 of 261 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	672	VAL

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Continued from previous page...

Mol	Chain	Res	Type
2	C	873	PRO
3	D	1197	THR
2	C	680	ASP
2	C	758	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	845	ASN
2	C	1026	GLN
3	D	1368	HIS
2	C	860	HIS
2	C	889	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 2 ligands modelled in this entry, 2 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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	D	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	155:ASP	C	2(U):UNK	N	55.17
1	D	46(U):UNK	C	452:ILE	N	46.65
1	D	10(U):UNK	C	20(U):UNK	N	14.79

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.