



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 11:49 PM UTC

PDB ID : 1ZYR / pdb_00001zyr
Title : Structure of Thermus thermophilus RNA polymerase holoenzyme in complex with the antibiotic streptolydigin
Authors : Tuske, S.; Sarafianos, S.G.; Wang, X.; Hudson, B.; Sineva, E.; Mukhopadhyay, J.; Birktoft, J.J.; Leroy, O.; Ismail, S.; Clark, A.D.; Dharia, C.; Napoli, A.; Laptenko, O.; Lee, J.; Borukhov, S.; Ebright, R.H.; Arnold, E.
Deposited on : 2005-06-10
Resolution : 3.00 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](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

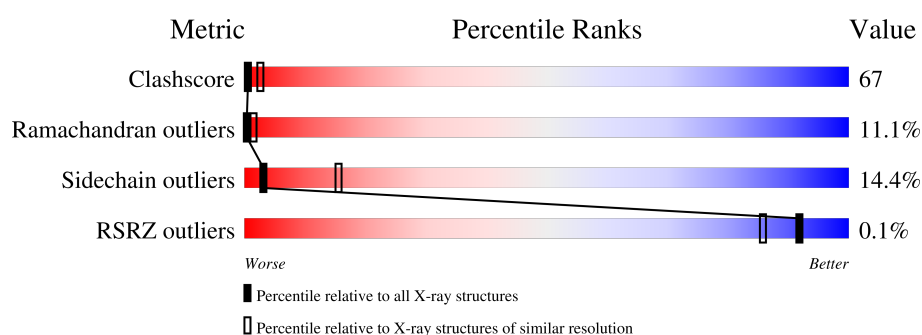
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	
1	B	315	
1	K	315	
1	L	315	
2	C	1119	
2	M	1119	
3	D	1524	

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Mol	Chain	Length	Quality of chain
3	N	1524	19%50%20%•9%
4	E	99	27%51%14%••
4	O	99	21%54%17%••
5	F	423	19%47%14%•18%
5	P	423	21%48%12%•18%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 54048 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 alpha chain.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1392	Total	C	N	O	S	0	0	0
			10975	6953	1941	2048	33			
3	N	1392	Total	C	N	O	S	0	0	0
			10975	6953	1941	2048	33			

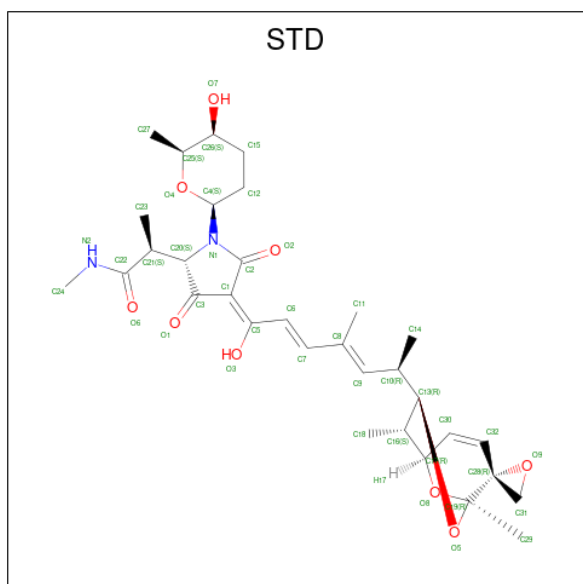
- Molecule 4 is a protein called DNA-directed RNA polymerase omega chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	95	Total	C	N	O	S	0	0	0
			769	488	133	144	4			
4	O	95	Total	C	N	O	S	0	0	0
			769	488	133	144	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	345	Total	C	N	O	S	0	0	0
			2793	1762	504	523	4			
5	P	345	Total	C	N	O	S	0	0	0
			2793	1762	504	523	4			

- Molecule 6 is STREPTOLYDIGIN (CCD ID: STD) (formula: $C_{32}H_{44}N_2O_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	1	Total	C	N	O	0	0
			43	32	2	9		
6	M	1	Total	C	N	O	0	0
			43	32	2	9		

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

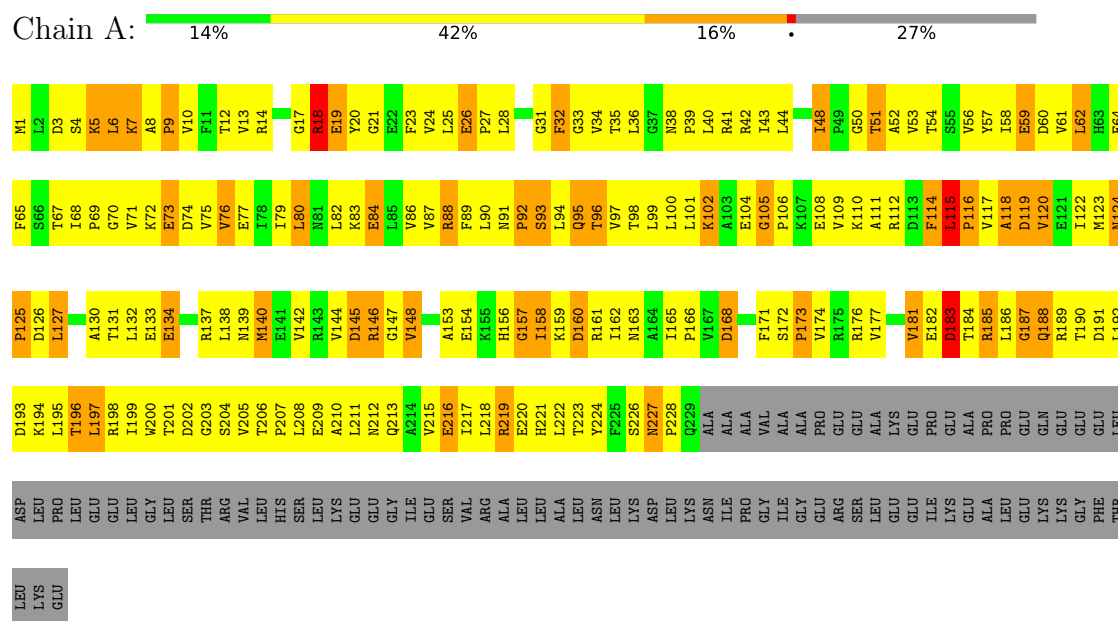
- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	1	Total 1	Mg 1	0	0
8	N	1	Total 1	Mg 1	0	0

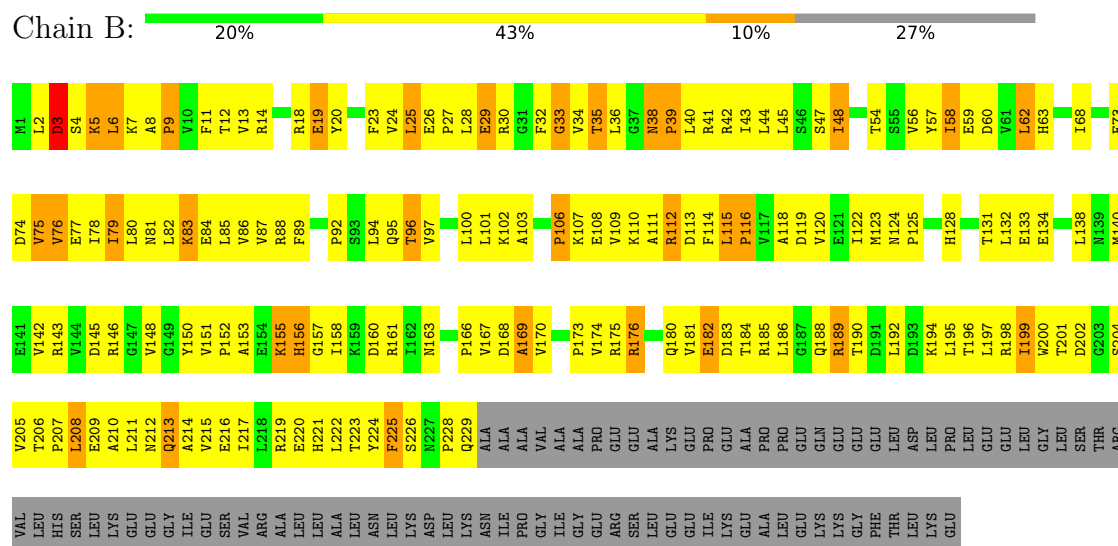
3 Residue-property plots

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 alpha chain



• Molecule 1: DNA-directed RNA polymerase alpha chain



[illegible][illegible]

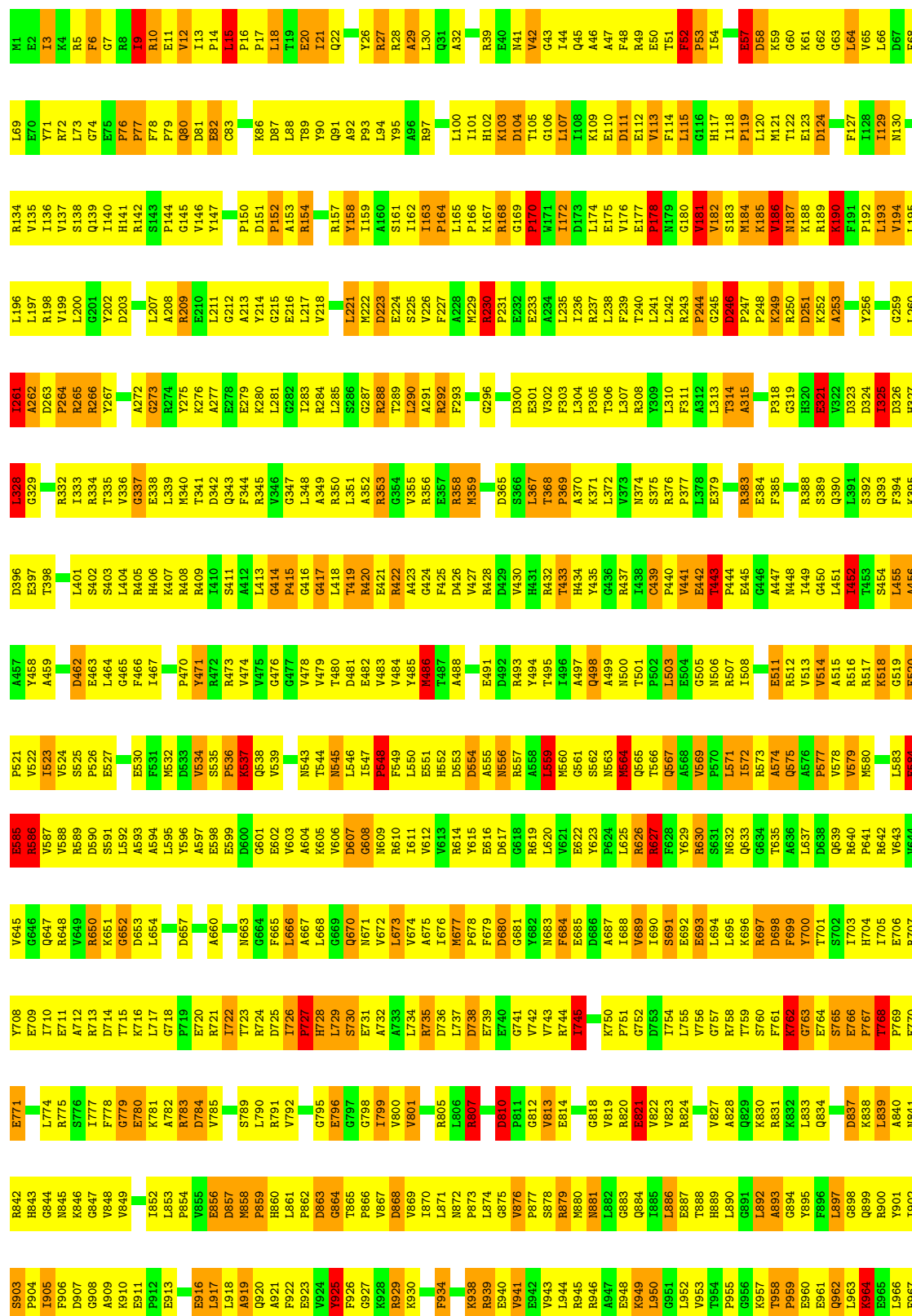
Chain C: 21% 57% 20%

Point	Category
M1	Green
E2	Green
I3	Green
K4	Green
R5	Green
F6	Green
G7	Green
R8	Green
I9	Green
R10	Green
E11	Green
V12	Green
I13	Green
P14	Green
L15	Green
P16	Green
P17	Green
L18	Green
T19	Green
E20	Green
I21	Green
K22	Green
V23	Green
E24	Green
S25	Green
A26	Green
R27	Green
R28	Green
A29	Green
L30	Green
Q31	Green
V32	Green
P33	Green
P36	Green
E37	Green
K38	Green
R39	Green
E40	Green
N41	Green
V42	Green
Q43	Green
I44	Green
Q45	Green
A46	Green
A47	Green
F48	Green
R49	Green
E50	Green
T51	Green
F52	Green
P53	Green
I54	Green
E57	Green
D58	Green
L64	Green
V65	Green
L66	Green
D67	Green
F68	Green
L69	Green
E70	Green
F71	Green
E72	Green
L73	Green
G74	Green
E75	Green
F76	Green
F77	Green
F78	Green
F79	Green
Q80	Green
D81	Green
E82	Green
C83	Green
F84	Green
E85	Green
K86	Green
D87	Green
L88	Green
T89	Green
Y90	Green
Q91	Green
A92	Green
P93	Green
L94	Green
Y95	Green
A96	Green
R97	Green
L100	Green
I101	Green
H102	Green
K103	Green
D104	Green
T105	Green
G106	Green
L107	Green
I108	Green
K109	Green
E110	Green
D111	Green
E112	Green
V113	Green
F114	Green
L115	Green
G116	Green
H117	Green
I118	Green
M121	Green
T122	Green
E123	Green
D124	Green
F127	Green
I128	Green
L129	Green

P1082	E1083	S1084	F1085	L1086	V1087	L1088	V1089	K1090	E1091	L1092	Q1093	A1094	L1095	A1096	L1097	D1098	V1099	Q1100	T1101	L1102	D1103	E1104	K1105	D1106	N1107	V1108	V1109	D1110	I1111	F1112	E1113	G1114	L1115	A1116	S1117	K1118	R1119																									
G891	L892	A893	G894	T895	R896	L897	R900	G901	L902	F903	S904	L905	F906	G907	K971	V972	V973	L974	F911	F912	E913	I914	K915	T979	G980	E981	P982	I983	E984	F922	G985	P986	I987	L988	F989	G927	Q928	Q991	M992	F993	K996	L997	M1000	Y1001	E1002	D1003	K1004	M1005	H1006	A1007	R1008	S1009	T1010	G1011	P1012	Y1013	L1014	S1015	L1016	Y953		
K957	P958	P959	E960	E961	Q962	L963	K964	L965	L966	F967	L968	Q969	G970	K971	V972	V973	L974	F911	F912	E913	I914	K915	T979	G980	E981	P982	I983	E984	F922	G985	P986	I987	L988	F989	G927	Q928	Q991	M992	F993	K996	L997	M1000	Y1001	E1002	D1003	K1004	M1005	H1006	A1007	R1008	S1009	T1010	G1011	P1012	Y1013	L1014	S1015	L1016	Y953			
Q1018	Q1019	P1020	L1021	K1024	F1027	Q1030	R1031	L1032	F1033	E1034	M1035	L1036	V1037	V1038	L1039	L1040	E1041	A1042	Y1043	G1044	A1045	A1046	L1047	T1048	L1049	Q1050	E1051	M1052	L1053	T1054	L1055	L1056	K1057	S1058	D1059	G1062	R1063	A1064	A1065	A1066	Y1067	E1068	A1069	I1070	I1071	K1072	G1073	E1074	D1075	Y1076	P1077	E1078	P1079	S1080	V1081							
R831	K832	L833	Q834	G835	G836	D837	K838	L839	A840	L841	L842	H843	G844	R845	G847	R848	V849	A850	K851	L852	L853	P854	T855	G856	L857	D858	L859	K860	L861	P862	D863	G864	F865	R866	L867	R868	V869	L870	L871	N872	P873	L874	G875	P876	P877	S878	R879	N880	N881	L882	Q883	R884	L885	L886	E887	T888	R889	L890				
E764	S765	E766	P767	T768	P769	E770	E771	R772	L773	L774	S775	S776	L777	E780	R781	A782	R783	S784	V785	K786	D787	T788	L789	R790	R791	V792	P793	F794	G795	E796	L797	V798	G799	R800	V801	R802	R805	L806	R807	D810	P811	G812	R813	E814	L815	K816	V819	G823	R824	V825	R826	V827	F761	K762	R830							
F699	Y700	T701	H704	T705	F706	E707	R708	E709	L710	R713	S714	L715	L716	L717	L718	A719	E720	R721	T722	T723	R724	E725	L726	F727	R728	L729	S730	E731	L734	R735	L736	L737	D738	E739	E740	G741	V742	V743	R744	A747	E748	V749	K750	P751	L754	L755	G756	R757	R758	T759	S760	F761	K762	G763								
D638	Q639	R640	P641	G642	F643	V644	V645	L646	L647	L648	L649	L650	K651	V652	S653	E654	L655	A656	D657	G658	P659	A660	S661	E662	L663	G664	F665	V666	E667	G668	L669	R670	M671	V672	L673	L674	L675	L676	M677	P678	F679	V680	G681	V682	M683	F684	E685	D686	L687	V688	L689	S691	E692	E693	L694	L695	F696	R697	D698			
Q575	V513	V514	A515	R516	V517	K518	G519	E520	V521	V522	V523	V524	S525	P526	E527	L535	E528	D529	E530	F531	M532	D533	V534	S535	P536	K537	Q538	R539	F540	S541	V542	N543	T544	L545	R546	T547	E548	V549	L550	E551	H552	D553	E554	A555	N556	L559	M560	V561	L562	V563	F564	G565	P566	L567	A636	L637						
G446	A447	N448	L449	G450	L451	L452	T453	S454	L455	A456	A457	Y458	A459	R460	V461	D462	E463	L464	G465	F466	L467	R468	T469	P470	Y471	R472	R473	G474	V475	V476	V477	L478	T479	D480	L481	R482	V483	V484	Y485	M486	T487	A488	T489	D490	E491	H492	R493	Y494	T495	L496	A497	Q498	A499	C499	T501	P502	L503	R507	T508			
R383	E384	F385	F386	S389	Q390	L391	S392	F393	L394	L395	R396	E397	T398	L399	P400	S403	L404	R405	H406	K407	R408	R409	A412	L413	L414	G415	R416	R417	L418	T419	V355	D421	P415	G416	A352	R353	G354	R355	R356	E357	R358	R359	G362	D426	V427	R428	D429	V430	H431	R432	T433	H434	Y435	Q436	L438	C439	T440	V441	E442	T443	P444	E445
H320	E321	V322	D323	D324	L325	D326	H327	L328	G329	R330	R331	R332	I333	R334	L335	G336	E337	T341	D342	E279	R344	R345	V346	G347	L348	R349	L351	T289	A352	R353	G354	R355	R356	E357	R358	R359	G362	D426	V427	R428	D429	V430	H431	R432	T433	H434	Y435	Q436	L438	C439	T440	V441	E442	T443	P444	E445						
F191	P192	L193	V194	L195	L196	L197	R198	V199	L200	G201	Y202	D203	Q204	E205	T206	L207	A208	R209	E210	L211	G212	A213	Y214	G220	L221	M222	D223	E224	S225	V226	F227	A228	M229	P166	P231	E232	E233	A234	L235	I236	R237	L238	F239	T240	L241	L242	R243	P244	G245	D246	P247	R248	K249	R250	D251	K252	A253	V254				
A255	Y256	Y257	Y258	G259	L260	L261	A262	D263	R265	G201	Y202	D203	Q204	E205	T206	L207	A208	R209	E210	L211	G212	A213	Y214	G220	L221	M222	D223	E224	S225	V226	F227	A228	M229	P166	P231	E232	E233	A234	L235	I236	R237	L238	F239	T240	L241	L242	R243	P244	G245	D246	P247	R248	K249	R250	D251	K252	A253	V254				

● Molecule 2: DNA-directed RNA polymerase beta chain

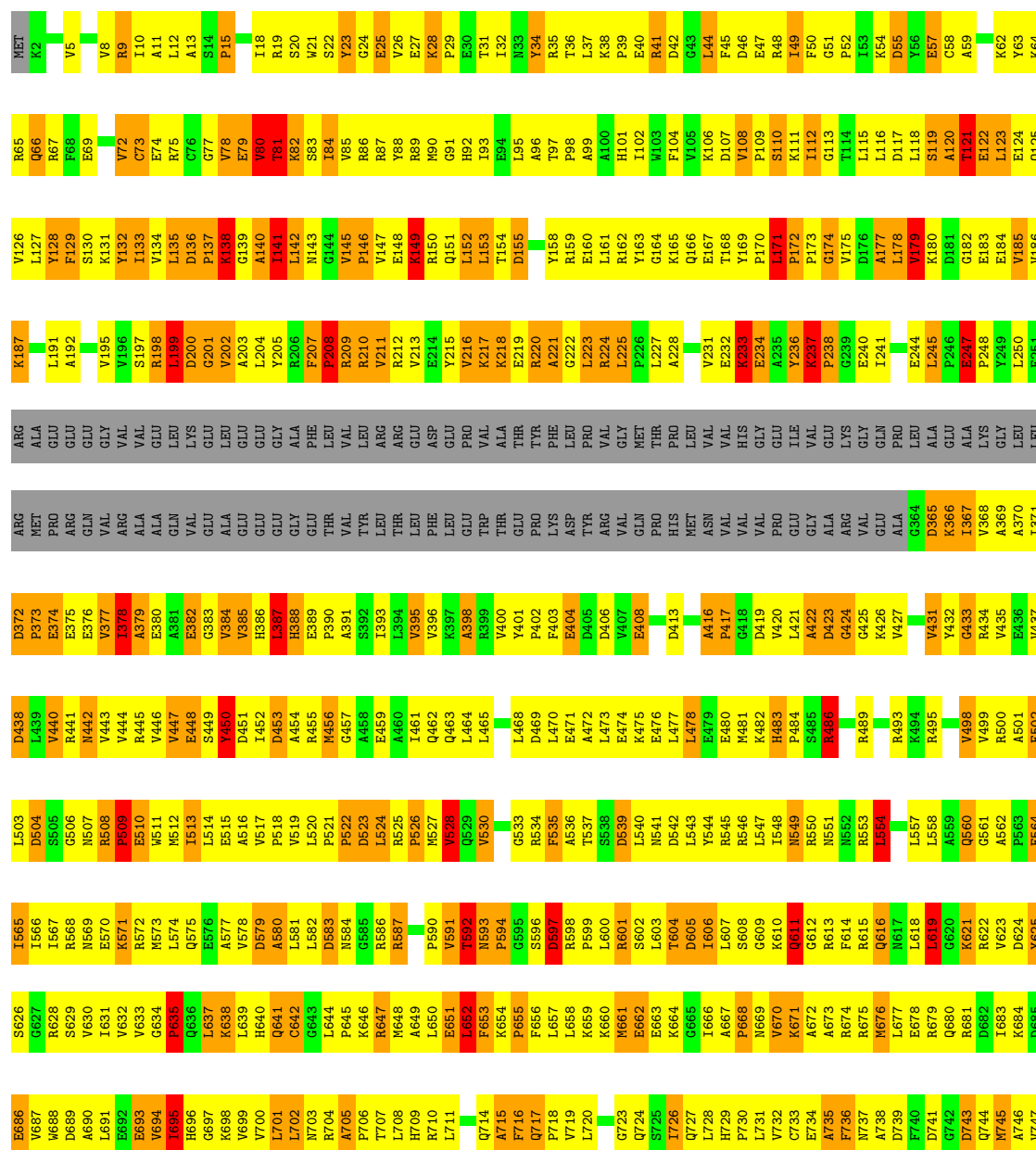
Chain M: 22% 57% 18% .



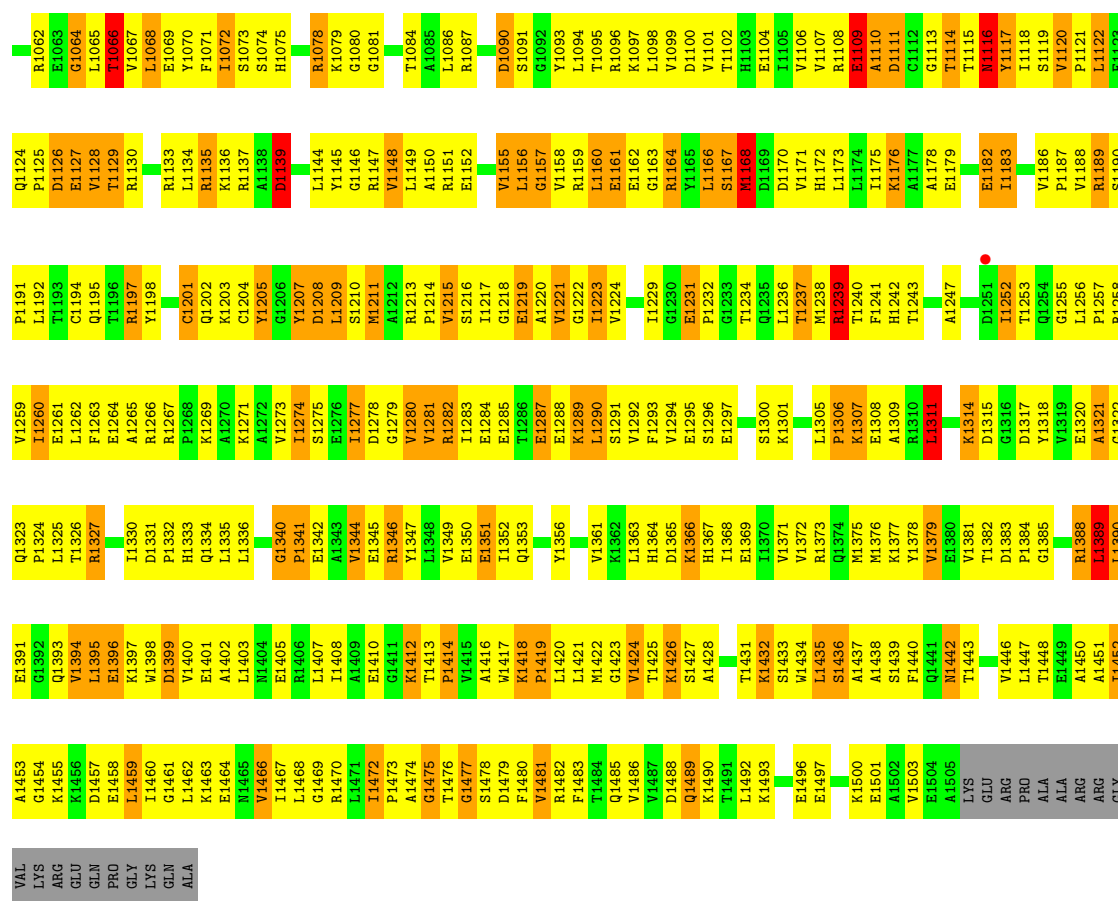


• Molecule 3: DNA-directed RNA polymerase subunit beta' chain

Chain D: 17% 50% 21% 9%

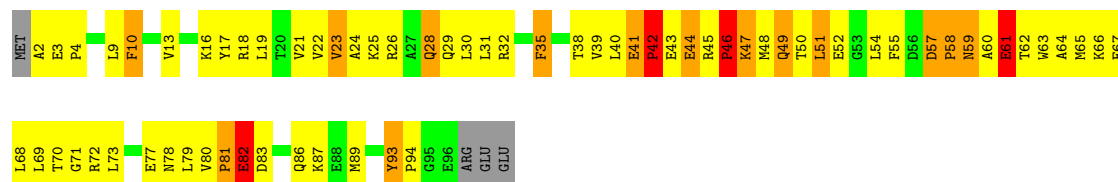






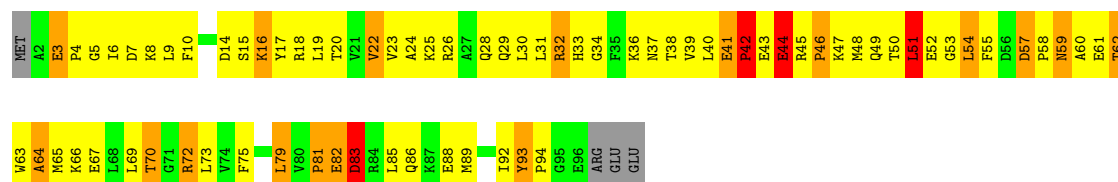
• Molecule 4: DNA-directed RNA polymerase omega chain

Chain E: 27% 51% 14%



• Molecule 4: DNA-directed RNA polymerase omega chain

Chain O: 21% 54% 17%



• Molecule 5: DNA-directed RNA polymerase sigma chain

Chain F: 19% 47% 14% 18%

MET	LEU	I127	I188	I250	V315	G378	ASP	LEU	I127	I188	I250	V315	G378
LYS	ASP	R128	E189	I251	S316	ARG	LYS	LEU	R128	E189	I251	S316	ARG
SER	LEU	I129	E190	A255	S317	HIS	LYS	LEU	I129	E190	A255	S317	HIS
GLY	GLY	V130	M191	A256	E318	THR	GLY	GLY	V130	M191	A256	E318	THR
LYS	GLY	V131	L192	T257	T319	LEU	LYS	GLY	V131	L192	T257	T319	LEU
ARG	GLY	R132	R193	I258	P320	ASP	ARG	GLY	R132	R193	I258	P320	ASP
LYS	GLY	A133	L194	R259	I321	GLY	LYS	GLY	A133	L194	R259	I321	GLY
ASN	GLY	K134	V195	R260	G322	ASP	ASN	GLY	K134	V195	R260	G322	ASP
ALA	GLY	I135	V196	R261	D323	GLY	ALA	GLY	I135	V196	R261	D323	GLY
GLN	LEU	G136	S197	G262	G324	THR	GLN	LEU	G136	S197	G262	G324	THR
ALA	PRO	G137	I198	V263	K325	ALA	ALA	PRO	G137	I198	V263	K325	ALA
GLN	ILE	S138	A199	H264	D326	GLY	GLN	ILE	S138	A199	H264	D326	GLY
GLY	PRO	A139	K200	R265	S327	PRO	GLY	PRO	A139	K200	R265	S327	PRO
ALA	K74	R140	K201	V266	F328	G391	ALA	K74	R140	K201	V266	F328	G391
GLN	I75	V141	Y202	E267	G329	V392	GLN	I75	V141	Y202	E267	G329	V392
THR	T77	G142	T203	T267	G330	THR	THR	T77	G142	T203	T267	G330	THR
VAL	S78	H143	G204	I268	D331	GLY	VAL	S78	H143	G204	I268	D331	GLY
LEU	D79	G145	R205	N269	F332	R395	LEU	D79	G145	R205	N269	F332	R395
VAL	P80	G146	G206	K270	I333	R396	VAL	P80	G146	G206	K270	I333	R396
LEU	V81	L147	L207	L271	F334	R397	LEU	V81	L147	L207	L271	F334	R397
GLN	R82	K148	F209	S272	D335	R398	GLN	R82	K148	F209	S272	D335	R398
GLY	Q83	E149	L210	A275	E336	I400	GLY	Q83	E149	L210	A275	E336	I400
GLY	Y84	L150	D211	R276	S340	N402	GLY	Y84	L150	D211	R276	S340	N402
ALA	L85	L151	L212	Q277	P341	K403	ALA	L85	L151	L212	Q277	P341	K403
GLY	H86	D152	T213	L278	V342	A404	GLY	H86	D152	T213	L278	V342	A404
LEU	E87	P153	Q214	Q279	A345	L405	LEU	E87	P153	Q214	Q279	A345	L405
LEU	G89	K154	E215	Q280	T346	R406	LEU	G89	K154	E215	Q280	T346	R406
PRO	G90	T155	G216	E281	K407	K407	PRO	G90	T155	G216	E281	K407	K407
GLY	V91	V156	Q217	G282	L408	L408	GLY	V91	V156	Q217	G282	L408	L408
PHE	P92	E157	Q218	G283	K409	K409	PHE	P92	E157	Q218	G283	K409	K409
PRO	L93	E158	G219	R284	L349	L349	PRO	L93	E158	G219	R284	L349	L349
GLY	L94	I159	L220	E285	L410	L410	GLY	L94	I159	L220	E285	L410	L410
GLY	T95	Q161	R221	T287	S351	E412	GLY	T95	Q161	R221	T287	S351	E412
PRO	L96	K162	A223	Y288	K353	S413	PRO	L96	K162	A223	Y288	K353	S413
ASP	E87	L163	K226	E289	L354	R414	ASP	E87	L163	K226	E289	L354	R414
PRO	E98	K164	S165	E290	E355	T415	PRO	E98	K164	S165	E290	E355	T415
ASP	L102	L166	Y229	I291	K356	R416	ASP	L102	L166	Y229	I291	K356	R416
LEU	K105	E169	K230	A292	A357	K417	LEU	K105	E169	K230	A292	A357	K417
ASP	V106	H170	R231	E293	L358	L418	ASP	V106	H170	R231	E293	L358	L418
PRO	E107	K171	R232	R295	S359	R419	PRO	E107	K171	R232	R295	S359	R419
ASP	E108	K172	F233	G296	K360	D420	ASP	E108	K172	F233	G296	K360	D420
LEU	G109	Y173	R234	P297	L361	F421	LEU	G109	Y173	R234	P297	L361	F421
ALA	L113	H174	F235	G298	S362	L422	ALA	L113	H174	F235	G298	S362	L422
GLY	L116	I175	S236	W299	E363	D423	GLY	L116	I175	S236	W299	E363	D423
ASP	L117	I176	D300	W299	E365	T415	ASP	L117	I176	D300	W299	E365	T415
ASP	L118	A177	Y238	A301	M367	R416	ASP	L118	A177	Y238	A301	M367	R416
LEU	S117	R178	A239	K302	M368	R417	LEU	S117	R178	A239	K302	M368	R417
LEU	E118	E179	T240	R303	L369	K417	LEU	E118	E179	T240	R303	L369	K417
ASP	T119	G180	W241	E305	L370	L418	ASP	T119	G180	W241	E305	L370	L418
LEU	T120	E181	W242	G306	K370	L419	LEU	T120	E181	W242	G306	K370	L419
PRO	G121	A182	L243	L308	L371	L420	PRO	G121	A182	L243	L308	L371	L420
GLY	D122	K183	Q244	K309	R372	D421	GLY	D122	K183	Q244	K309	R372	D421
GLY	D123	R184	Q245	Q312	G374	L422	GLY	D123	R184	Q245	Q312	G374	L422
GLY	D125	H186	T247	Q313	L375	L423	GLY	D125	H186	T247	Q313	L375	L423
GLY	L126	L187	R249	P314	D377	D423	GLY	L126	L187	R249	P314	D377	D423

• Molecule 5: DNA-directed RNA polymerase sigma chain

Chain P: 21% 48% 12% 18%

MET	LEU	G121	T188	I258	D326	A388
LYS	ASP	L122	E189	R259	Y329	F389
SER	LEU	L126	A190	P261	F332	F390
GLY	GLY	I127	N191	M264	I333	G391
LYS	GLY	R128	L192	T267	P334	T393
ARG	GLY	E129	R193	T267	D335	R394
LYS	GLY	V130	L194	T267	E336	E395
ASN	GLY	I131	V195	L271	H337	R396
ASP	GLY	A132	S197	R272	L338	I397
ALA	LEU	R133	G198	R273	P339	Q399
GLN	PRO	K134	I198	T274	S340	I400
GLN	PRO	L135	A199	A275	T346	R406
ALA	PRO	L136	K200	L275	Q347	K407
K74	K74	G137	K201	E281	S348	L408
I75	I75	I138	Y202	L282	K403	L408
S76	S76	G139	T203	G283	L349	K409
T77	T77	A139	T203	R284	L350	Y410
S78	S78	R140	G204	E285	S351	H411
D79	D79	L141	L207	P286	E352	R414
P80	P80	R142	L207	T287	E353	T415
V81	V81	H143	S208	Y288	L354	R416
R82	R82	I144	F209	E289	E355	L418
Q83	Q83	P145	L210	G298	S362	L369
Y84	Y84	G146	L210	E290	K370	L371
L85	L85	L147	T213	I291	L371	L371
H86	H86	K148	Q214	F227	R372	L371
E87	E87	E149	Q214	E228	G374	L375
G89	G89	T150	N217	E228	L375	I376
Q90	Q90	E158	G218	Y229	D377	G378
V91	V91	D152	Q219	A223	ARG	GLY
P92	P92	T155	G219	V224	GLY	GLY
L93	L93	V156	Q219	E225	THR	THR
R94	R94	E157	G219	E225	E384	E385
G99	G99	E158	Q219	E225	E385	V386
L96	L96	I159	Q219	E225	E386	G387
E97	E97	D160	K226	E225	E387	
E98	E98	Q161	F227	E225		
E99	E99	K162	E228	E225		
V100	V100	L163	E228	E225		
L101	L101	K164	Y229	E225		
L102	L102	S165	R230	E225		
A103	A103	P166	R231	E225		
R104	R104	P167	R232	E225		
K106	K106	K168	R233	E225		
V106	V106	E169	F235	E225		
E107	E107	H170	F235	E225		
E108	E108	K171	S236	E225		
G109	G109	R172	T240	E225		
M110	M110	Y173	W241	E225		
E111	E111	L174	W242	E225		
A112	A112	H175	T243	E225		
T113	T113	I176	R244	E225		
K114	K114	A177	Q245	E225		
L115	L115	R178	Q246	E225		
L116	L116	E181	T247	E225		
S117	S117	E181	A250	E225		
E118	E118	R184	T257	E225		
T120	T120	Q185		E225		

4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	237.00Å 237.00Å 250.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.00 30.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	77.9 (30.00-3.00) 42.8 (30.00-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 3.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.261 , 0.281 0.254 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	71.1	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.499 for -h,-k,l 0.499 for h,-h-k,-l 0.044 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	54048	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.81% 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: STD, 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	0.53	0/1838	1.17	21/2498 (0.8%)
1	B	0.50	0/1838	1.01	9/2498 (0.4%)
1	K	0.57	0/1838	1.10	10/2498 (0.4%)
1	L	0.48	0/1838	1.07	19/2498 (0.8%)
2	C	0.55	1/8997 (0.0%)	1.22	111/12164 (0.9%)
2	M	0.55	1/8997 (0.0%)	1.19	103/12164 (0.8%)
3	D	0.56	0/11165	1.22	127/15088 (0.8%)
3	N	0.56	0/11165	1.20	122/15088 (0.8%)
4	E	0.51	0/783	1.22	14/1054 (1.3%)
4	O	0.51	0/783	1.25	15/1054 (1.4%)
5	F	0.49	0/2836	1.13	31/3812 (0.8%)
5	P	0.49	0/2836	1.12	25/3812 (0.7%)
All	All	0.54	2/54914 (0.0%)	1.19	607/74228 (0.8%)

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
2	C	0	1
3	D	0	1
3	N	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	564	MET	SD-CE	5.72	1.93	1.79
2	C	880	MET	SD-CE	5.46	1.93	1.79

The worst 5 of 607 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	728	HIS	N-CA-C	17.20	131.49	111.71
3	N	207	PHE	CA-C-N	13.63	136.87	119.84
3	N	207	PHE	C-N-CA	13.63	136.87	119.84
3	D	207	PHE	CA-C-N	13.06	136.16	119.84
3	D	207	PHE	C-N-CA	13.06	136.16	119.84

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	258	TYR	Sidechain
3	D	132	TYR	Sidechain
3	N	625	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	1806	0	1861	290	0
1	B	1806	0	1861	221	0
1	K	1806	0	1861	240	0
1	L	1806	0	1861	214	0
2	C	8829	0	8933	1214	0
2	M	8829	0	8933	1239	0
3	D	10975	0	11213	1742	0
3	N	10975	0	11212	1709	0
4	E	769	0	775	109	0
4	O	769	0	775	97	0
5	F	2793	0	2873	341	0
5	P	2793	0	2873	384	0
6	D	43	0	44	10	0
6	M	43	0	44	9	0
7	D	2	0	0	0	0
7	N	2	0	0	0	0
8	D	1	0	0	0	0
8	N	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	54048	0	55119	7278	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 67.

The worst 5 of 7278 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)
2:C:673:LEU:HD23	2:C:867:VAL:HA	1.22	1.20
3:D:141:ILE:H	3:D:141:ILE:HD12	1.11	1.16
3:N:172:PRO:HB3	3:N:178:LEU:HD22	1.22	1.16
2:C:857:ASP:HB2	2:C:978:ARG:HG2	1.29	1.15
3:D:1304:LYS:H	3:D:1304:LYS:HD3	1.03	1.15

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	227/315 (72%)	163 (72%)	48 (21%)	16 (7%)	1	4
1	B	227/315 (72%)	167 (74%)	46 (20%)	14 (6%)	1	6
1	K	227/315 (72%)	154 (68%)	45 (20%)	28 (12%)	0	1
1	L	227/315 (72%)	169 (74%)	41 (18%)	17 (8%)	1	4
2	C	1117/1119 (100%)	768 (69%)	229 (20%)	120 (11%)	0	2
2	M	1117/1119 (100%)	758 (68%)	222 (20%)	137 (12%)	0	1
3	D	1388/1524 (91%)	940 (68%)	286 (21%)	162 (12%)	0	1
3	N	1388/1524 (91%)	916 (66%)	317 (23%)	155 (11%)	0	1
4	E	93/99 (94%)	66 (71%)	17 (18%)	10 (11%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	O	93/99 (94%)	56 (60%)	25 (27%)	12 (13%)	0	1
5	F	341/423 (81%)	239 (70%)	57 (17%)	45 (13%)	0	1
5	P	341/423 (81%)	250 (73%)	54 (16%)	37 (11%)	0	1
All	All	6786/7590 (89%)	4646 (68%)	1387 (20%)	753 (11%)	0	1

5 of 753 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	ALA
1	A	160	ASP
1	A	188	GLN
1	B	3	ASP
1	B	96	THR

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	202/273 (74%)	174 (86%)	28 (14%)	3	17
1	B	202/273 (74%)	180 (89%)	22 (11%)	6	26
1	K	202/273 (74%)	171 (85%)	31 (15%)	3	14
1	L	202/273 (74%)	180 (89%)	22 (11%)	6	26
2	C	941/941 (100%)	807 (86%)	134 (14%)	3	16
2	M	941/941 (100%)	815 (87%)	126 (13%)	4	18
3	D	1170/1279 (92%)	962 (82%)	208 (18%)	2	10
3	N	1170/1279 (92%)	988 (84%)	182 (16%)	2	13
4	E	83/87 (95%)	70 (84%)	13 (16%)	2	13
4	O	83/87 (95%)	74 (89%)	9 (11%)	6	26
5	F	300/370 (81%)	264 (88%)	36 (12%)	5	22
5	P	300/370 (81%)	279 (93%)	21 (7%)	14	44
All	All	5796/6446 (90%)	4964 (86%)	832 (14%)	3	15

5 of 832 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	189	ARG
2	M	698	ASP
3	N	1478	SER
1	L	12	THR
1	K	188	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 183 such sidechains are listed below:

Mol	Chain	Res	Type
2	M	663	ASN
3	N	575	GLN
2	M	829	GLN
2	M	1018	GLN
3	N	724	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 6 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
6	STD	M	1120	-	41,47,47	1.76	10 (24%)	50,73,73	2.25	13 (26%)
6	STD	D	1525	-	41,47,47	2.04	12 (29%)	50,73,73	2.31	10 (20%)

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
6	STD	M	1120	-	-	12/31/101/101	0/6/5/5
6	STD	D	1525	-	-	6/31/101/101	0/6/5/5

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1525	STD	C22-N2	4.97	1.40	1.33
6	D	1525	STD	O5-C19	4.56	1.47	1.43
6	D	1525	STD	O8-C19	4.24	1.46	1.43
6	D	1525	STD	C16-C13	3.87	1.61	1.53
6	M	1120	STD	O4-C4	3.52	1.47	1.42

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1525	STD	C3-C20-N1	-10.56	95.56	103.11
6	M	1120	STD	C3-C20-N1	-6.95	98.14	103.11
6	M	1120	STD	O4-C4-N1	6.74	113.28	105.83
6	D	1525	STD	C29-C19-C28	-5.71	108.73	113.27
6	M	1120	STD	O8-C19-C29	5.27	109.86	105.63

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

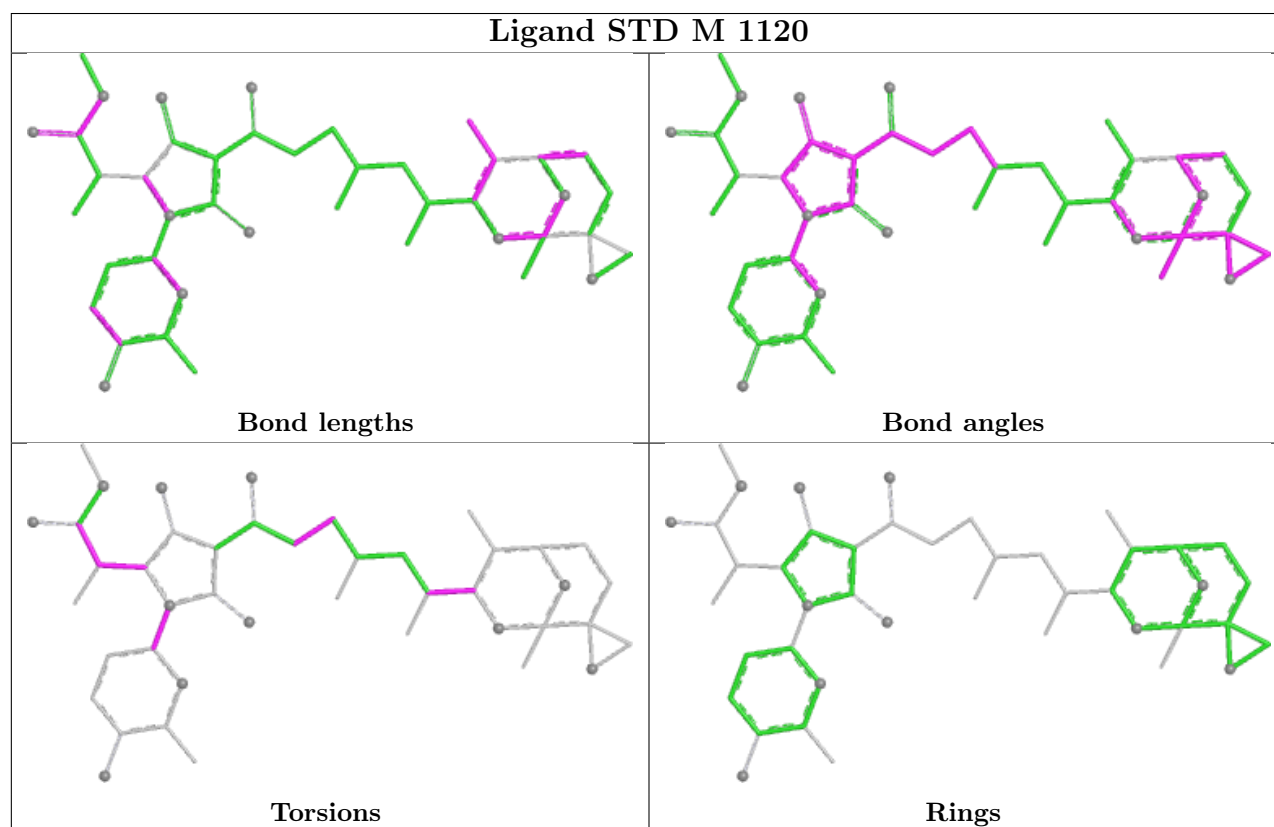
Mol	Chain	Res	Type	Atoms
6	D	1525	STD	N1-C20-C21-C22
6	D	1525	STD	N1-C20-C21-C23
6	D	1525	STD	C3-C20-C21-C22
6	D	1525	STD	C3-C20-C21-C23
6	M	1120	STD	C9-C10-C13-C16

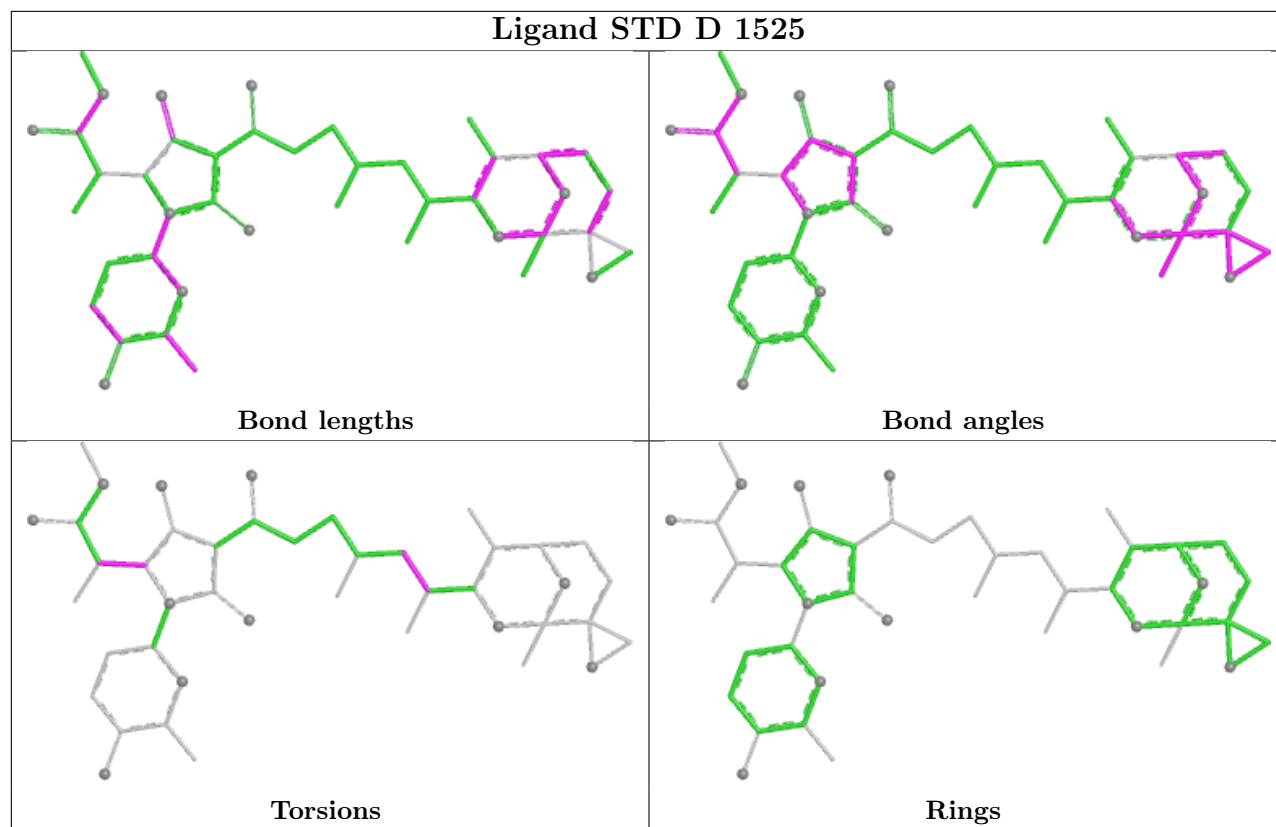
There are no ring outliers.

2 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	1120	STD	9	0
6	D	1525	STD	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	229/315 (72%)	-1.49	0 100 100	32, 58, 89, 110	0
1	B	229/315 (72%)	-1.37	0 100 100	45, 96, 120, 124	0
1	K	229/315 (72%)	-1.51	0 100 100	24, 57, 82, 111	0
1	L	229/315 (72%)	-1.47	0 100 100	43, 78, 96, 117	0
2	C	1119/1119 (100%)	-1.40	0 100 100	21, 67, 123, 137	0
2	M	1119/1119 (100%)	-1.40	0 100 100	21, 69, 120, 130	0
3	D	1392/1524 (91%)	-1.42	2 (0%) 92 86	20, 64, 107, 125	0
3	N	1392/1524 (91%)	-1.39	4 (0%) 90 79	20, 64, 125, 140	0
4	E	95/99 (95%)	-1.40	0 100 100	52, 82, 99, 102	0
4	O	95/99 (95%)	-1.30	0 100 100	46, 86, 114, 119	0
5	F	345/423 (81%)	-1.45	0 100 100	53, 77, 97, 104	0
5	P	345/423 (81%)	-1.41	0 100 100	47, 81, 97, 108	0
All	All	6818/7590 (89%)	-1.41	6 (0%) 92 86	20, 69, 118, 140	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	406	ASP	6.3
3	D	801	GLY	5.3
3	D	802	ALA	3.9
3	N	224	ARG	3.1
3	N	1251	ASP	2.7

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

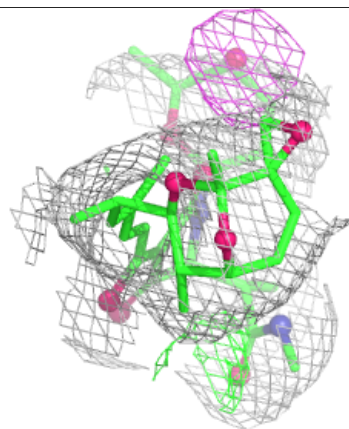
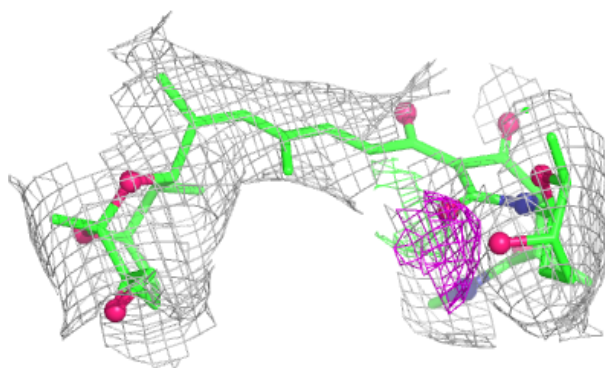
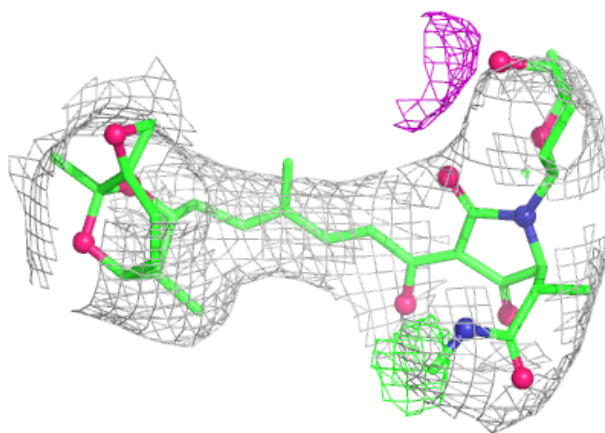
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	STD	D	1525	43/43	0.99	0.04	39,59,62,63	0
6	STD	M	1120	43/43	0.99	0.04	39,51,53,56	0
8	MG	D	9901	1/1	0.99	0.04	20,20,20,20	0
8	MG	N	9902	1/1	0.99	0.02	30,30,30,30	0
7	ZN	N	9003	1/1	1.00	0.01	55,55,55,55	0
7	ZN	N	9004	1/1	1.00	0.02	56,56,56,56	0
7	ZN	D	9001	1/1	1.00	0.01	56,56,56,56	0
7	ZN	D	9002	1/1	1.00	0.01	47,47,47,47	0

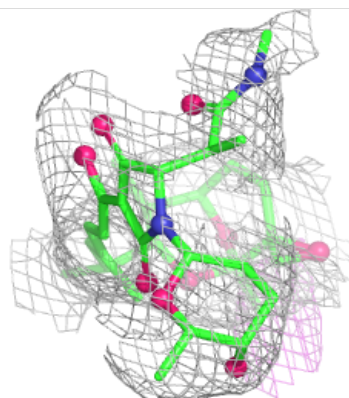
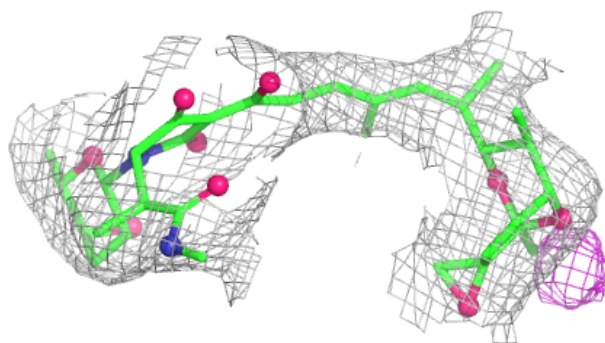
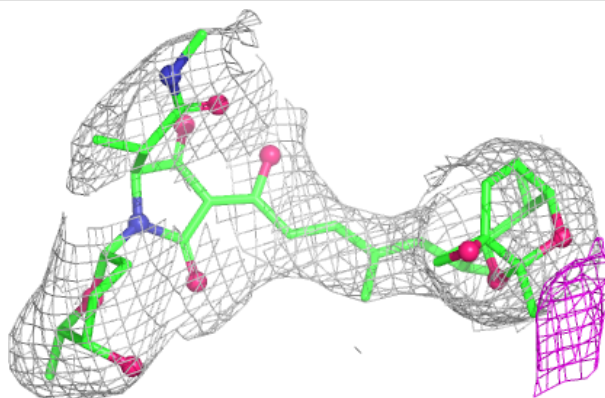
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around STD D 1525:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around STD M 1120:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.