



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:26 AM GMT

PDB ID : 2A69
Title : Crystal structure of the T. Thermophilus RNA polymerase holoenzyme in complex with antibiotic rifapentin
Authors : Artsimovitch, I.; Vassilyeva, M.N.; Svetlov, D.; Svetlov, V.; Perederina, A.; Igarashi, N.; Matsugaki, N.; Wakatsuki, S.; Tahirov, T.H.; Vassilyev, D.G.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2005-07-02
Resolution : 2.50 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

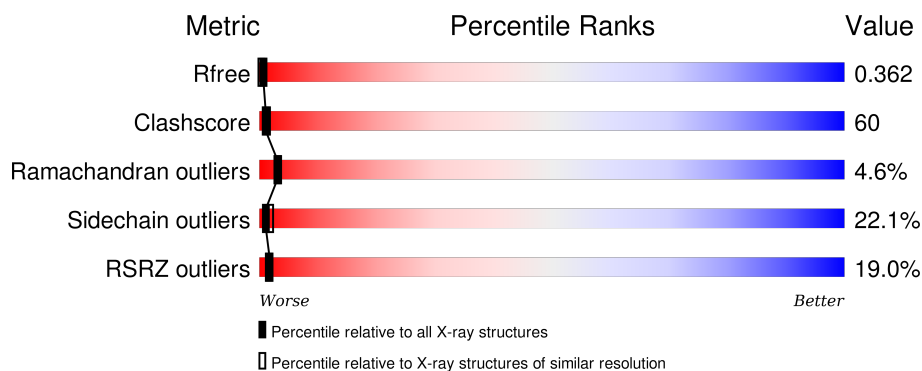
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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. 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	<div> <div>8%</div> <div>17% 44% 10% 27%</div> </div>
1	B	315	<div> <div>22%</div> <div>18% 43% 11% 27%</div> </div>
1	K	315	<div> <div>7%</div> <div>23% 40% 9% 27%</div> </div>
1	L	315	<div> <div>15%</div> <div>19% 43% 10% 27%</div> </div>
2	C	1119	<div> <div>17%</div> <div>22% 59% 18%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	M	1119	
3	D	1524	
3	N	1524	
4	E	99	
4	O	99	
5	F	423	
5	P	423	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 60572 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 beta' chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1392	Total	C	N	O	S	0	0	0
			10797	6819	1925	2020	33			
3	N	1392	Total	C	N	O	S	0	0	0
			10797	6819	1925	2020	33			

- Molecule 4 is a protein called 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			

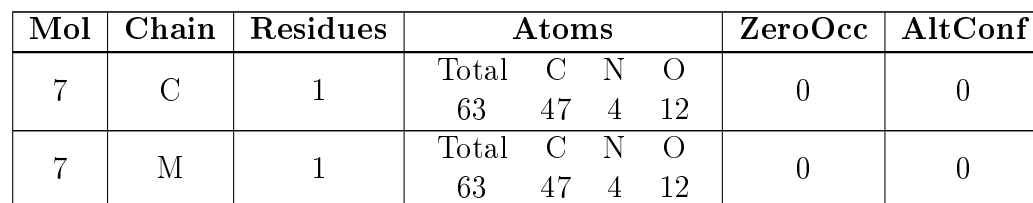
- Molecule 5 is a protein called RNA polymerase sigma factor rpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	345	Total	C	N	O	S	0	0	0
			2771	1744	504	519	4			
5	P	345	Total	C	N	O	S	0	0	0
			2771	1744	504	519	4			

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	P	20	Total	Mg	0	0
			20	20		
6	D	106	Total	Mg	0	0
			106	106		
6	K	19	Total	Mg	0	0
			19	19		
6	E	5	Total	Mg	0	0
			5	5		
6	B	21	Total	Mg	0	0
			21	21		
6	C	73	Total	Mg	0	0
			73	73		
6	A	33	Total	Mg	0	0
			33	33		
6	N	92	Total	Mg	0	0
			92	92		
6	O	8	Total	Mg	0	0
			8	8		
6	L	17	Total	Mg	0	0
			17	17		
6	F	28	Total	Mg	0	0
			28	28		
6	M	65	Total	Mg	0	0
			65	65		

- Molecule 7 is RIFAPENTINE (three-letter code: RPT) (formula: C₄₇H₆₄N₄O₁₂).



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

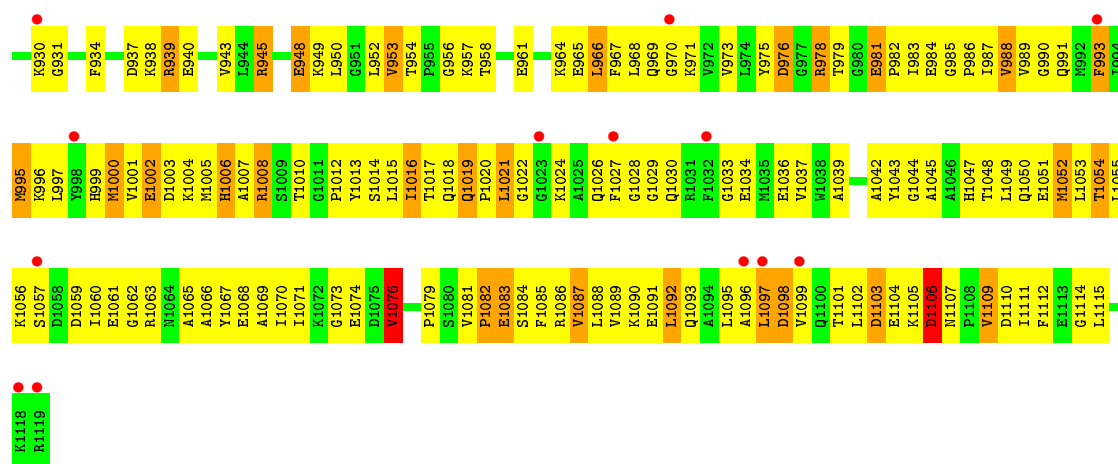
- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|----------------------|---------|---------|
| 9 | A | 239 | Total O
239 239 | 0 | 0 |
| 9 | B | 258 | Total O
258 258 | 0 | 0 |
| 9 | C | 979 | Total O
979 979 | 0 | 0 |
| 9 | D | 1252 | Total O
1252 1252 | 0 | 0 |
| 9 | E | 117 | Total O
117 117 | 0 | 0 |



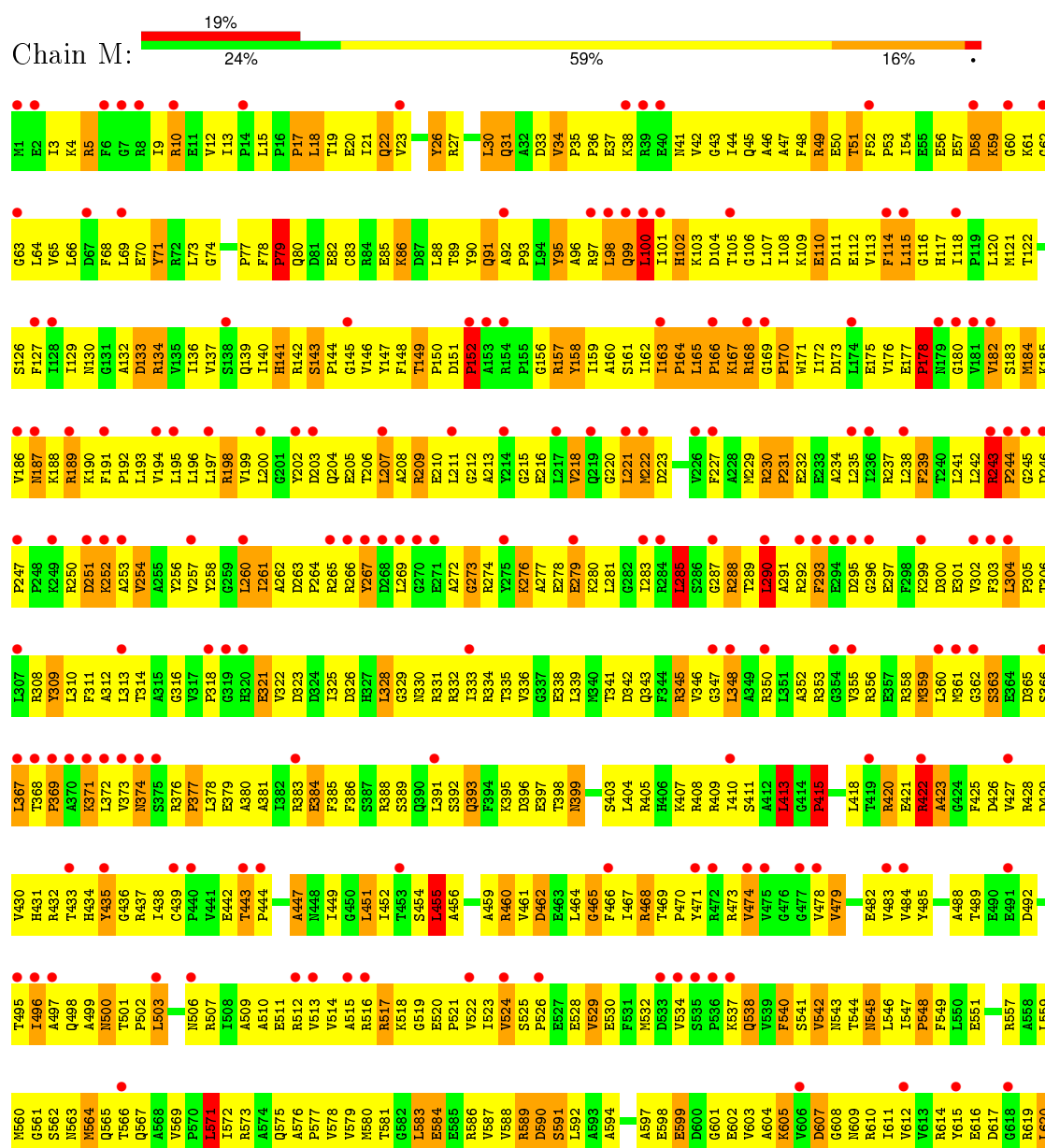
Continued from previous page...

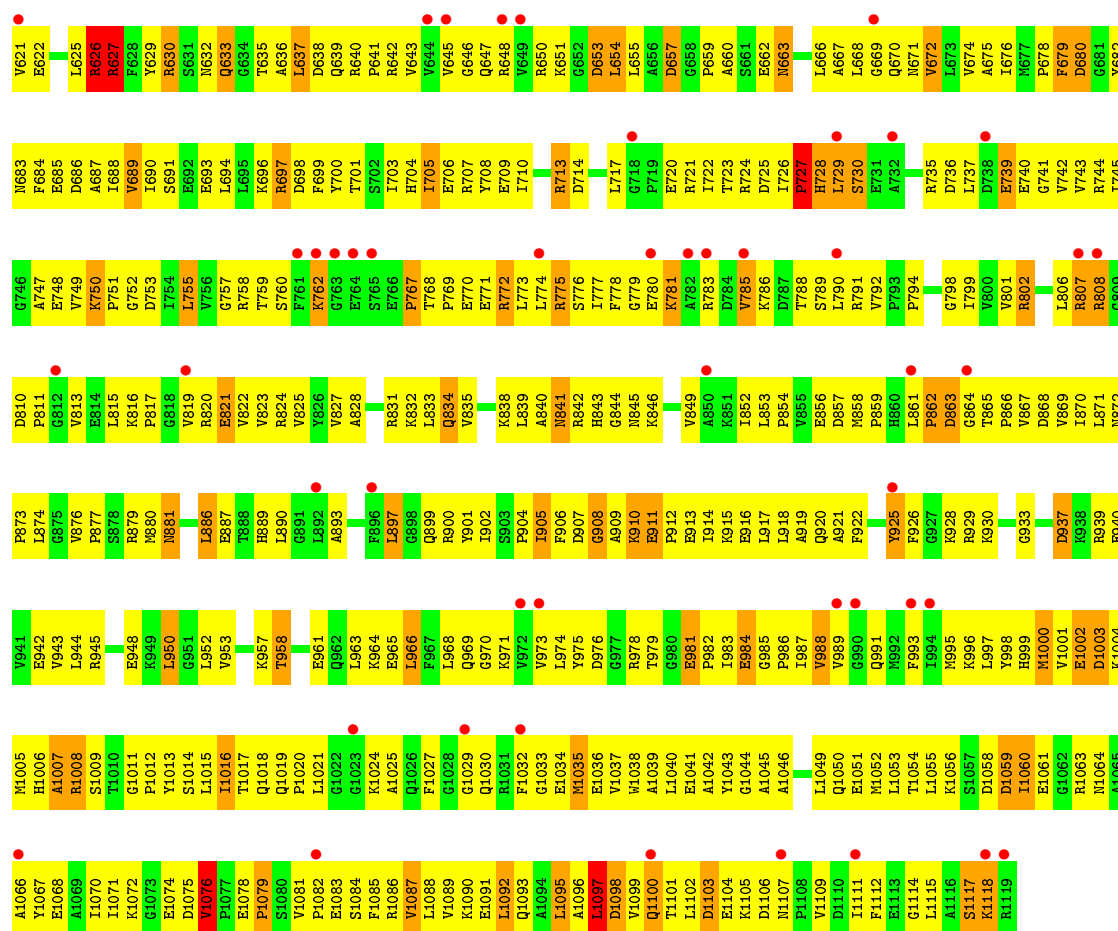
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	F	420	Total 420	O 420	0	0
9	K	183	Total 183	O 183	0	0
9	L	219	Total 219	O 219	0	0
9	M	998	Total 998	O 998	0	0
9	N	1265	Total 1265	O 1265	0	0
9	O	108	Total 108	O 108	0	0
9	P	361	Total 361	O 361	0	0

G884	R802	E740	F679	G618	N556	Y494	R432	P369	R308	F247	K185	D124	M1
T865	T803	G741	D680	R619	R557	T495	T433	A370	Y309	P248	V186	G125	E2
P866	V804	V742	G681	L620	A558	I496	H434	K371	L310	K249	S126	V65	I3
V867	R805	V743	V682	W621	N559	A497	Y435	L372	F311	R250	K188	I127	K4
D868	B808	R744	N683	E622	M560	Q498	G436	V373	A312	D251	R189	I128	R5
V669	G809	T745	N684	E622	G561	A499	R437	N374	L313	K282	K190	I129	F6
L870	D810	G746	E685	L625	N562	N500	L438	S375	A315	A253	F191	G7	
P873	P811	A747	D686	R626	N563	T501	C439	R376	A315	V284	F192	R8	
L874	G812	E748	A687	R627	N564	P502	P440	P377	P318	A295	L193	I9	
G875	V813	V749	V688	F628	N565	L503	V441	R378	G319	Y256	V194	R10	
V876	E814	K750	V689	W629	T566	E504	A442	E379	G319	Y257	R195	L73	
P877	L815	G752	S691	R630	Q567	G505	T443	A380	H320	Y258	L196	L73	
S878	L816	L755	E692	R631	A568	N506	P444	L381	E321	G259	L197	G74	
R879	P817	L756	B693	Q633	F570	R507	E445	I382	F322	L260	R198	P76	
R880	G818	V756	L694	G634	L571	A509	A447	D324	D323	I261	V199	P77	
L881	V819	V757	L695	R635	L572	A510	M448	F385	D324	A262	L200	F78	
L882	R820	R758	L449	A636	E511	E510	I449	F386	D326	D263	Y202	P79	
G883	E821	T759	R697	L637	Q575	R512	G450	S387	H327	R265	I203	Q80	
Q884	V822	S760	D698	W645	A576	V513	L451	R388	L328	I266	Q204	D81	
L885	V823	F761	F699	G646	P577	V514	L452	S389	G329	Y267	T206	E82	
L886	R824	K762	T700	R640	W578	A515	T453	Q390	N330	D268	G145	C83	
E887	V825	E763	T701	P641	W579	R516	S454	L391	R331	L269	Y147	R84	
T888	Y826	E764	S702	R642	W580	R517	L455	S392	R332	G270	A208		
R889	R827	S765	T703	W643		K518	A456	Q393	I333	E271	F148	D87	
L890	A828	E766	H704	W645	L583	G519	A457	F394	R334	A272	K209	L88	
G891	Q829	P767	I705	V645	E584	E520	Y458	K395	T335	G273	E210	T89	
L892	R830	T768	E706	G646	E585	P621	R459	D396	V336	R274	L211	Y90	
A893	R831	P769	R707	Q647	E586	V522	R460	E397	G337	Y275	G212	Q91	
	K832	E770	T708	R648	W587	L523	V461	T398	E338	K276	A213	A92	
	L833	E771	V693	W649	E588	V524	D462	R399	L339		Y214	P93	
	Q834	R772	I710	R650	W589	S525	E463	P400	M340		G215	L94	
G898	V835	L773	E711	K651	D590	P526	L464	F384	T341	K280	V218	Y95	
R899	A774	R774	A712	G652	E591	E527	G465	S403	D342	L281	R97	P35	
Y900	K837	S775	R713	D653	L592	E528	F466	R405	Q343	G282	Y158	R37	
I901	L838	I777	D714	L654	A593	V529	I467	H406	F344	I283	A160	L98	
I902	L839	I777	T715	L655	A594	E530	R468	K407	R345	R284	S161	Q99	
S903	N841	G779	K716	W596	E595	F531	T469	K407	V346	L285	I162	L100	
P904	H841	E780	P859	D657	L656	M532	P470	R408	G347	S286	I101	I101	
L905	R842	E781	G658	R658	A597	D533	Y471	R409	L348	G287	K103	H102	
F906	H843	K781	S659	W659	E598	V534	R472	I410	A349	T227	L165	K103	
G907	G844	A782	R721	A660	E599	S535	R473	S411	R350	T289	P166	D104	
A908	N845	D784	T722	S661	D600	P536	V474	A412	L351	L290	K167	T105	
K910	V849	V785	E602	W663	B602	K537	L413	R421	A352	A291	R168	G106	
E911	A850	T788	V603	G664	V603	Q538	G414	P415	R353	R292	G169	L107	
P912	R851	V789	A604	F665	A604	S541	W479	G416	F354	R293	K109	I108	
E913	K852	P727	K605	L666	K605	V542	T480	G417	V355	E294	E110	E110	
L914	I853	L790	V606	A667	V606	N543	D481	L418	R356	D295	D234	D111	
E915	P854	R791	D607	L668	D607	T544	V483	T419	R358	G296	L235	E112	
L916	R855	V792	G669	L688	G608	W483	Y484	R420	M359	E297	L236	V113	
L918	E856	P793	R731	Q670	N609	T547	Y485	E421	L360	K299	L238	F114	
A919	D857	G795	I611	W672	R610	P548	W486	R422	M361	D300	F239	L115	
	M858	E796	V612	L673	L611	F549	T487	A423	G362	E301	T246	G116	
T923	P859	G797	V613	W674	W612	L590	A488	G424	S363	V302	L241	H117	
V924	H860	G798	R614	A675	L614	F425	T489	F425	E364	P303	L242	V102	
F925	R862	V799	E615	W676	W615	H552	T489	D426	D365	L304	R243	E175	
G927	D863	W800	D617	D677	W616	D554	D492	V427	S366	P305	P244	F176	

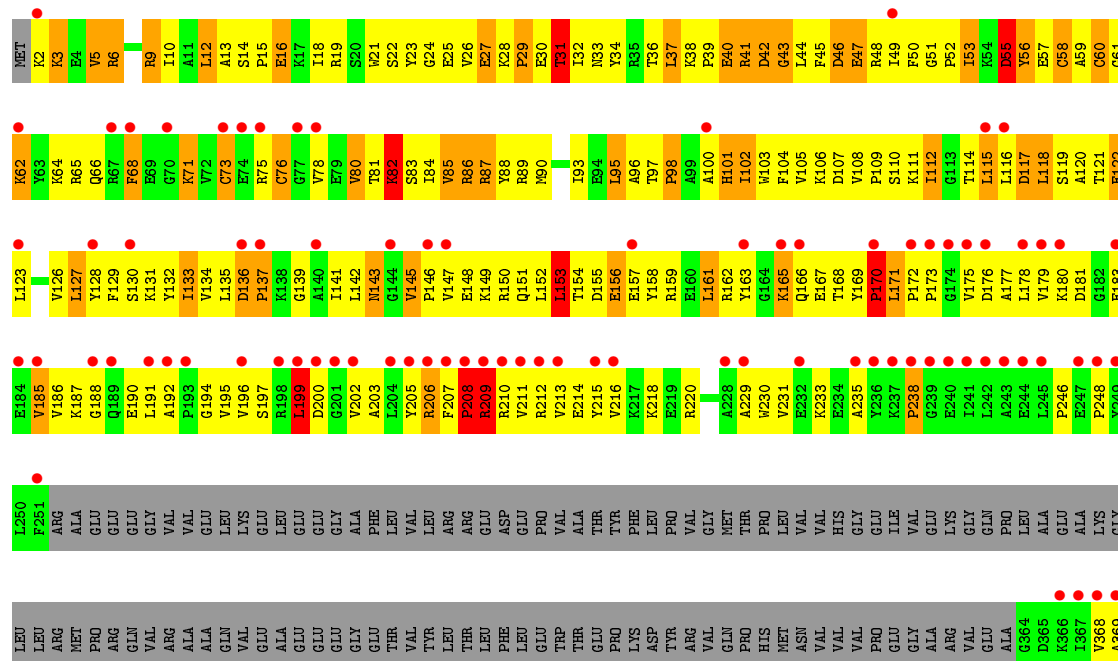


• Molecule 2: DNA-directed RNA polymerase beta chain

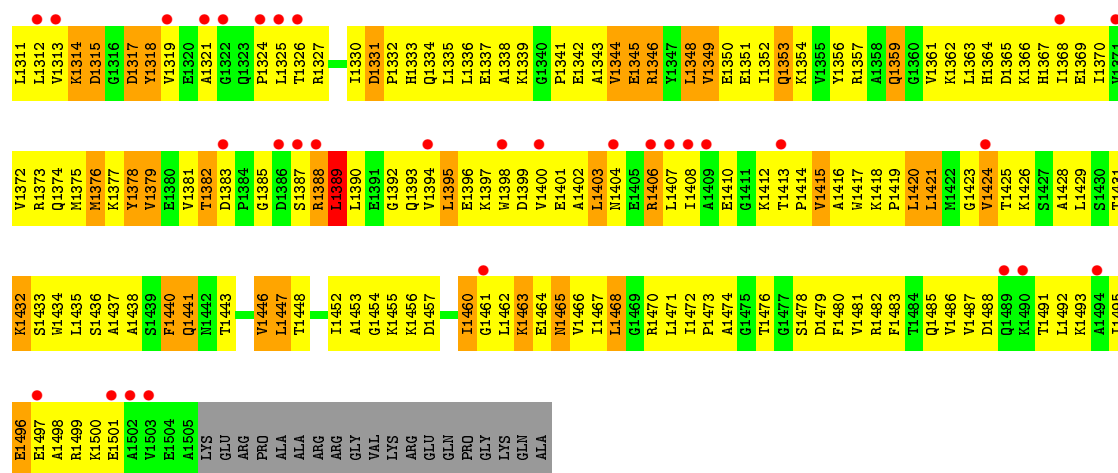




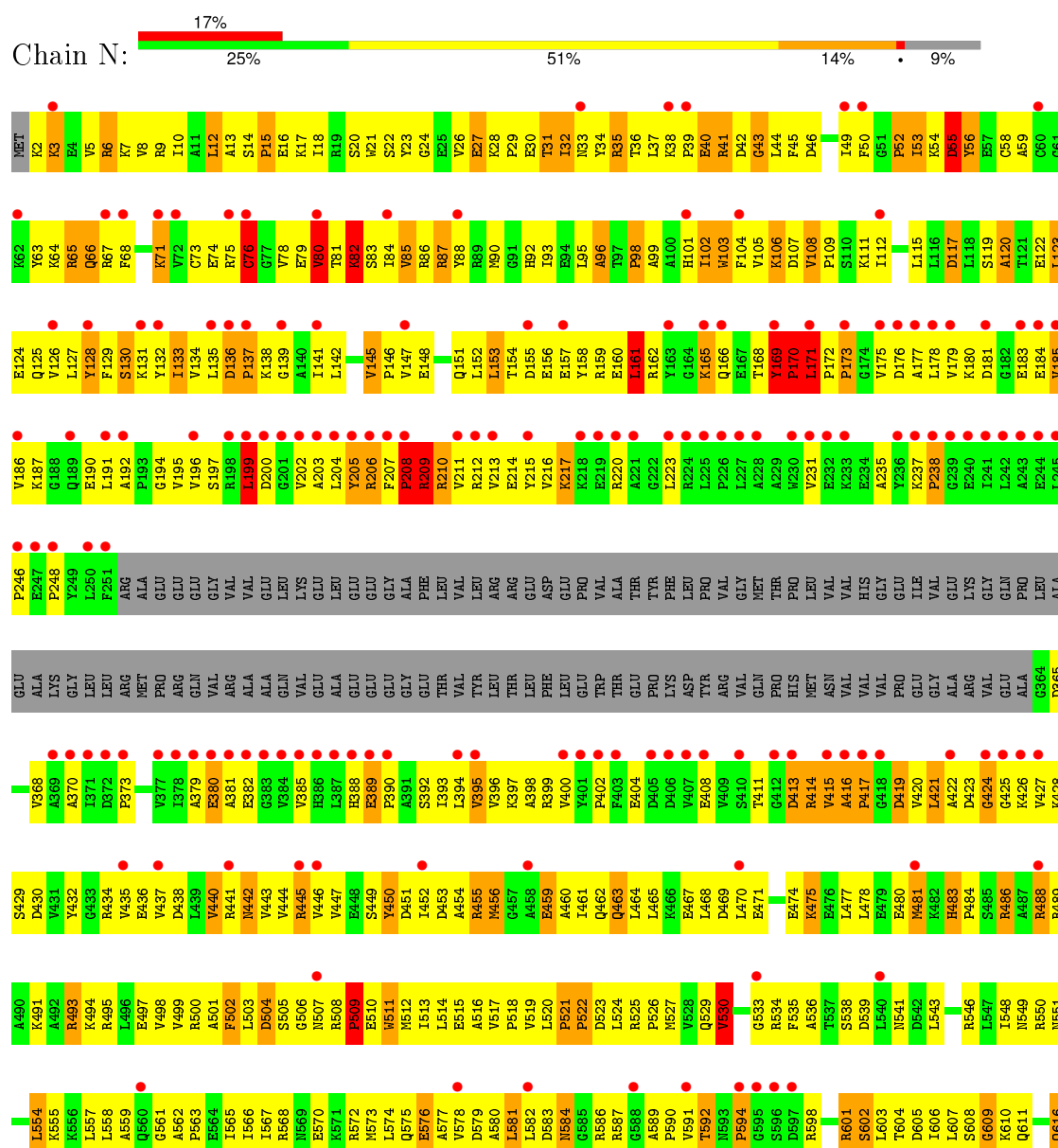
• Molecule 3: DNA-directed RNA polymerase beta' chain



D1251	P1191	E1063	E998	K926	V854	G803	D741	M676	R615	R553	A493	Y431	A370
I1252	L1192	G1064	T999	I927	T855	L804	G742	L677	Q616	L554	R493	Y432	I371
L1253	T1193	L1065	T1000	A928	V856	E805	D743	E678	Q617	R494	K494	G433	P372
Q1254	C1194	T1066	E1001	R929	R867	F806	Q744	R679	L618	K555	R495	R434	D373
G1255	G1195	V1067	K1002	L930	V868	A807	M745	Q680	L619	L558	V498	V435	E374
L1256	R1197	L1068	V1003	L931	R869	T808	A746	R681	Q620	A559	V499	V436	E375
P1257	R1198	E1069	T1004	T940	G870	P809	V747	D682	V621	Q560	R500	V437	E376
R1258	K1136	E1070	Q1005	T941	K871	E810	H748	L683	V622	G561	R501	V438	V377
V1259	R1137	F1071	A1006	T943	R872	E811	V749	E684	V623	A562	F502	V439	I378
L1260	V1200	S1072	F1007	T944	L873	A812	P750	D685	V624	P563	F503	R440	E380
E1261	D1139	S1073	F1008	T945	E874	R813	L751	E686	V625	E564	L502	R441	A381
Q1262	I1140	S1074	K1009	I947	T875	A814	S752	V687	R628	I565	D504	M442	A382
K1263	L1203	H1075	M1010	I948	R876	A815	S753	V688	S629	I566	S505	V443	A383
F1264	A1142	G1076	F1011	T949	P877	H616	F754	V689	S630	I567	G506	V444	G382
G1265	G1143	A1077	E1012	I950	G878	E817	A755	V694	V630	R568	G507	V445	G383
L1266	L1144	K1078	R1007	G950	R879	R818	A756	E696	V631	N569	R508	V446	R445
P1267	Y1145	K1079	D1008	I951	L880	E819	A757	E697	V632	E570	P509	V447	E448
D1268	G1146	G1080	Y1015	D952	T880	E820	E758	K698	V633	K571	E510	E449	E448
K1269	R1147	G1081	P1016	D953	A883	V821	A759	V699	Q634	R572	H511	S449	E389
S1270	V1148	A1082	P1019	A954	R884	A822	R760	K699	Q635	H573	H512	V450	P390
M1271	L1149	D1083	L1020	V955	E887	L823	I761	V700	P636	L574	I513	D451	A391
A1272	A1150	T1084	Y1021	I956	E888	R824	Q762	L701	L637	Q575	L514	L452	S392
R1273	R1151	A1085	V1022	P957	E889	A825	M763	L702	V638	E576	E515	D453	I393
I1274	E1152	L1086	M1023	E958	A899	P826	L764	N703	L639	A577	A516	A454	L394
V1275	V1214	L1087	L1086	E959	V890	T827	S765	R704	H640	V577	V517	R455	L395
S1276	V1215	D1087	L1087	K960	E891	K828	A766	A705	Q641	D579	P518	K456	V396
E1276	E1154	D1090	S1026	Y963	E892	V829	H767	P706	C642	A580	V519	G457	K397
L1277	V1155	S1091	G1027	L964	E893	A830	M768	T707	Q643	L581	L520	E458	E397
D1278	L1156	G1092	A1028	L965	R894	E831	L769	R708	L644	L582	P521	E459	R399
G1279	R1159	Y1093	G1030	E965	V895	R832	P645	H709	P645	D833	P522	A460	V400
A1280	A1210	L1094	N1031	E966	A896	E833	L770	R710	V646	N584	D523	I461	Y401
V1281	V1221	T1095	P1032	A967	V897	T834	A773	L711	R647	G855	L524	Q482	Y402
R1282	G1222	R1096	Q1033	E968	E898	S835	S774	G712	R648	R587	R525	Q463	F403
E1283	L1223	K1097	Q1034	R969	L899	E837	E776	I713	L649	G888	P526	L464	E404
L1284	R1164	L1098	I1035	K970	Q901	R838	P777	A715	E651	A539	M527	L465	D405
E1285	Y1165	V1099	R1036	L971	L902	L839	K780	F716	L652	P590	V528	L468	D406
T1286	L1166	D1100	Q1037	L972	D903	K840	P781	Q717	R653	V591	Q529	V407	V407
E1287	S1167	V1101	L1038	Q973	P904	T841	S782	F718	R654	T592	R530	E408	E408
E1288	M1168	T1102	G1039	I974	P905	V842	R783	V719	P655	N593	D531	L470	V409
K1289	D1169	H1103	G1040	E975	G1041	R843	R784	L720	F656	P594	G532	E471	S410
L1290	E1291	E1104	L1041	Q976	Q906	F844	D784	V721	L657	G595	G533	A472	T411
V1291	P1232	I1105	R1042	Y977	E907	N845	I785	E722	L658	S596	R534	L473	G412
F1292	V1171	V1106	G1043	Y978	K908	D846	I786	Q723	L659	D597	F535	E474	D413
P1293	L1173	V1107	L1044	E979	S940	P847	L787	Q724	R660	R598	A536	K475	R414
Q1235	L1174	R1108	M1045	M980	S941	D848	R788	Q725	R661	P599	T537	E476	V415
E1295	L1175	E1109	Q1046	F982	L911	E849	G789	S725	R661	S538	D539	E477	A416
S1296	K1176	A1110	K1047	G981	K912	A849	L789	T726	E562	L600	E478	L478	P417
E1297	A1177	D1112	P1048	T984	D913	L850	Y790	Q727	E563	R601	L540	E479	G418
G1298	E1178	G1113	E1051	D985	L914	A851	Y791	L728	V663	S602	N541	E480	D419
F1299	E1179	G1113	T1052	D985	V915	A852	I792	H729	V665	L603	D542	V420	V420
S1300	T1240	T1114	F1053	R986	Q917	V853	Q794	F730	L666	I606	L543	K482	L421
K1301	F1241	T1115	P1056	E987	A918	G856	V795	C733	A667	L607	Y544	R483	A422
E1302	E1181	M1116	Q1056	R988	F919	R857	R796	E734	P668	L607	R545	P484	D423
K1304	G1244	Y1117	V1057	Y989	L920	V858	K797	E735	N669	S608	R546	S485	G424
L1305	V1245	I1183	V1057	I992	R921	D859	E798	V736	V670	G609	L547	R486	G425
P1306	V1246	S1118	K1058	I992	R921	D859	E798	V736	V670	K610	I548	A487	K426
K1307	P1187	S1119	S1059	I992	R921	D859	E798	V736	V670	Q611	I548	A487	V427
E1308	V1188	V1120	S1060	L995	R921	D859	E798	V736	V670	G612	N549	R488	V427
A1309	R1189	P1121	F1061	W996	G923	R861	K900	I737	A672	R613	R550	R489	K428
K1310	S1190	Q1124	R1062	T997	E925	V863	A802	F740	R675	A490	N551	A490	E429

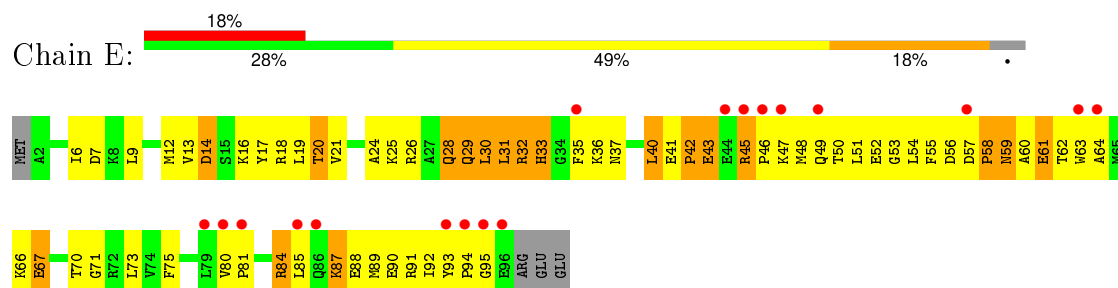


● Molecule 3: DNA-directed RNA polymerase beta' chain

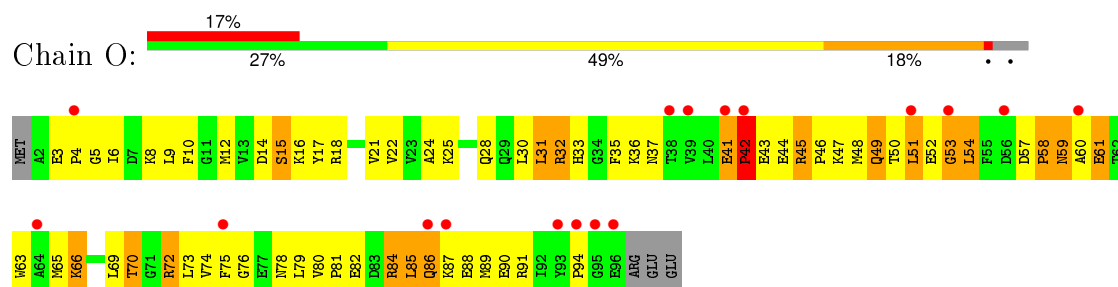


VAL	K1455	K1456	K1457	D1458	E1459	I1460	G1461	L1462	K1463	N1464	M1465	V1466	T1467	L1468	G1469	R1470	L1471	I1472	P1473	A1474	G1475	T1476	G1477	S1478	D1479	F1480	V1481	F1482	F1483	P1484	Q1485	V1486	V1487	D1488	Q1489	K1490	T1491	L1492	K1493	A1494	I1495	E1496	E1497	A1498	R1499	K1500	E1501	V1502	S1503	F1504	A1505	LYS	GLU	ARG	PRO	ALA	ALA	ARG	ARG	GLY												
	R1388	L1325	F1263	T1193	L1065	E998	A933	Y868	F806	D743	E678	N617	L618	L619	K620	G621	V622	D623	D624	Y625	S626	G627	R628	G629	V630	L631	E632	V633	G634	P635	Q636	L637	K638	V639	L640	N641	G642	G643	P644	P645	T646	G647	N648	H649	R650	L651	F652	K653	A654	P655	F656	L657	L658	K659	V660	G661	E662	K663	G664	I665	L666	V667	N668	P669	K670	C671	A672	A673	R674	G675	A676	L677
	L1326	F1264	T1194	C1194	T1066	T999	A937	Y869	F807	D744	E679	L618	L619	K620	G621	V622	D623	D624	Y625	S626	G627	R628	G629	V630	L631	E632	V633	G634	P635	Q636	L637	K638	V639	L640	N641	G642	G643	P644	P645	T646	G647	N648	H649	R650	L651	F652	K653	A654	P655	F656	L657	L658	K659	V660	G661	E662	K663	G664	I665	L666	V667	N668	P669	K670	C671	A672	A673	R674	G675	A676	L677	
	L1327	E1265	T1195	Q1195	V1067	T1000	Y937	Y870	T808	M745	E680	L619	L620	K621	G622	V623	D624	Y625	S626	G627	R628	G629	V630	L631	E632	V633	G634	P635	Q636	L637	K638	V639	L640	N641	G642	G643	P644	P645	T646	G647	N648	H649	R650	L651	F652	K653	A654	P655	F656	L657	L658	K659	V660	G661	E662	K663	G664	I665	L666	V667	N668	P669	K670	C671	A672	A673	R674	G675	A676	L677		
	L1328	E1266	T1196	R1196	E1068	E1001	Y937	Y871	T809	M746	E681	L620	L621	K622	G623	D624	Y626	S627	G628	R629	G630	V631	L632	E633	V634	G635	P636	Q637	L638	K639	V640	L641	N642	G643	G644	P645	T647	G648	N649	H650	R651	L652	F653	K654	A655	F656	L657	L658	K659	V660	G661	E662	K663	G664	I665	L666	V667	N668	P669	K670	C671	A672	A673	R674	G675	A676	L677					
	L1329	E1267	T1197	R1197	E1069	E1002	Y937	Y872	T810	M747	E682	L621	L622	K623	G624	D625	Y627	S628	G629	R630	G631	V632	L633	E634	V635	G636	P637	Q638	L639	K640	V641	L642	N643	G644	G645	P646	T648	G649	N650	H651	R652	L653	F654	K655	A656	F657	L658	L659	K660	E661	E662	K663	G664	I665	L666	V667	N668	P669	K670	C671	A672	A673	R674	G675	A676	L677						
	L1330	E1268	T1198	R1198	E1070	E1003	Y937	Y873	T811	M748	E683	L622	L623	K624	G625	D626	Y628	S629	G630	R631	G632	V633	L634	E635	V636	G637	P638	Q639	L640	K641	V642	L643	N644	G645	G646	P647	T649	G650	N651	H652	R653	L654	F655	K656	A657	F658	L659	L660	K661	E662	K663	G664	I665	L666	V667	N668	P669	K670	C671	A672	A673	R674	G675	A676	L677							
	L1331	E1269	T1199	R1199	S1073	E1004	Y937	Y874	T812	M749	E684	L623	L624	K625	G626	D627	Y629	S630	G631	R632	G633	V634	L635	E636	V637	G638	P639	Q640	L641	K642	V643	L644	N645	G646	G647	P648	T650	G651	N652	H653	R654	L655	F656	K657	A658	F659	L660	L661	K662	E663	K664	G665	L666	V667	N668	P669	K670	C671	A672	A673	R674	G675	A676	L677								
	L1332	E1270	T1200	R1200	S1074	E1005	Y937	Y875	T813	M750	E685	L624	L625	K626	G627	D628	Y630	S631	G632	R633	G634	V635	L636	E637	V638	G639	P640	Q641	L642	K643	V644	L645	N646	G647	G648	P649	T651	G652	N653	H654	R655	L656	F657	K658	A659	F660	L661	L662	K663	E664	K665	L666	V667	N668	P669	K670	C671	A672	A673	R674	G675	A676	L677									
	L1333	E1271	T1201	R1201	S1075	E1006	Y937	Y876	T814	M751	E686	L625	L626	K627	G628	D629	Y631	S632	G633	R634	G635	V636	L637	E638	V639	G640	P641	Q642	L643	K644	V645	L646	N647	G648	G649	P650	T652	G653	N654	H655	R656	L657	F658	K659	A660	F661	L662	L663	K664	E665	K666	L667	V668	N669	P670	K671	C672	A673	A674	R675	G676	A677	L678									
	L1334	E1272	T1202	R1202	H1076	E1007	Y937	Y877	T815	M752	E687	L626	L627	K628	G629	D630	Y632	S633	G634	R635	G636	V637	L638	E639	V640	G641	P642	Q643	L644	K645	V646	L647	N648	G649	G650	P651	T653	G654	N655	H656	R657	L658	F659	K660	A661	F662	L663	L664	K665	E666	K667	L668	V669	N670	P671	K672	C673	A674	A675	R676	G677	A678	L679									
	L1335	E1273	T1203	R1203	H1077	E1008	Y937	Y878	T816	M753	E688	L627	L628	K629	G630	D631	Y633	S634	G635	R636	G637	V638	L639	E640	V641	G642	P643	Q644	L645	K646	V647	L648	N649	G650	G651	P652	T654	G655	N656	H657	R658	L659	F660	K661	A662	F663	L664	L665	K666	E667	K668	L669	V670	N671	P672	K673	C674	A675	A676	R677	G678	A679	L680									
	L1336	E1274	T1204	R1204	A1078	E1009	Y937	Y879	T817	M754	E689	L628	L629	K630	G631	D632	Y634	S635	G636	R637	G638	V639	L640	E641	V642	G643	P644	Q645	L646	K647	V648	L649	N650	G651	G652	P653	T655	G656	N657	H658	R659	L660	F661	K662	A663	F664	L665	L666	K667	E668	K669	L670	V671	N672	P673	K674	C675	A676	A677	R678	G679	A680	L681									
	L1337	E1275	T1205	R1205	A1079	E1010	Y937	Y880	T818	M755	E690	L629	L630	K631	G632	D633	Y635	S636	G637	R638	G639	V640	L641	E642	V643	G644	P645	Q646	L647	K648	V649	L650	N651	G652	G653	P654	T656	G657	N658	H659	R660	L661	F662	K663	A664	F665	L666	L667	K668	E669	K670	L671	V672	N673	P674	K675	C676	A677	A678	R679	G680	A681	L682									
	L1338	E1276	T1206	R1206	D1083	E1011	Y937	Y881	T819	M756	E691	L630	L631	K632	G633	D634	Y636	S637	G638	R639	G640	V641	L642	E643	V644	G645	P646	Q647	L648	K649	V650	L651	N652	G653	G654	P655	T657	G658	N659	H660	R661	L662	F663	K664	A665	F666	L667	L668	K669	E670	K671	L672	V673	N674	P675	K676	C677	A678	A679	R680	G681	A682	L683									
	L1339	E1277	T1207	R1207	D1084	E1012	Y937	Y882	T820	M757	E692	L631	L632	K633	G634	D635	Y637	S638	G639	R640	G641	V642	L643	E644	V645	G646	P647	Q648	L649	K650	V651	L652	N653	G654	G655	P656	T658	G659	N660	H661	R662	L663	F664	K665	A666	F667	L668	L669	K670	E671	K671	L672	V673	N674	P675	K676	C677	A678	A679	R680	G681	A682	L683									
	L1340	E1278	T1208	R1208	A1085	E1013	Y937	Y883	T821	M758	E693	L632	L633	K634	G635	D636	Y638	S639	G640	R641	G642	V643	L644	E645	V646	G647	P648	Q649	L650	K651	V652	L653	N654	G655	G656	P657	T659	G660	N661	H662	R663	L664	F665	K666	A667	F668	L669	L670	K671	E672	K672	L673	V674	N675	P676	K677	C678	A679	A680	R681	G682	A683	L684									
	L1341	E1279	T1209	R1209	A1086	E1014	Y937	Y884	T822	M759	E694	L633	L634	K635	G636	D637	Y639	S640	G641	R642	G643	V644	L645	E646	V647	G648	P649	Q650	L651	K652	V653	L654	N655	G656	G657	P658	T660	G661	N662	H663	R664	L665	F666	K667	A668	F669	L670	L671	K672	E673	K673	L674	V675	N676	P677	K678	C679	A680	A681	R682	G683	A684	L685									
	L1342	E1280	T1210	R1210	A1087	E1015	Y937	Y885	T823	M760	E695	L634	L635	K636	G637	D638	Y640	S641	G642	R643	G644	V645	L646	E647	V648	G649	P650	Q651	L652	K653	V654	L655	N656	G657	G658	P659	T661	G662	N663	H664	R665	L666	F667	K668	A669	F670	L671	L672	K673	E674	K674	L675	V676	N677	P678	K679	C680	A681	A682	R683	G684	A685	L686									
	L1343	E1281	T1211	R1211	A1088	E1016	Y937	Y886	T824	M761	E696	L635	L636	K637	G638	D639	Y641	S642	G643	R644	G645	V646	L647	E648	V649	G650	P651	Q652	L653	K654	V655	L656	N657	G658	G659	P660	T662	G663	N664	H665	R666	L667	F668	K669	A670	F671	L672	L673	K674	E675	K675	L676	V677	N678	P679	K680	C681	A682	A683	R684	G685	A686	L687									
	L1344	E1282	T1212	R1212	A1089	E1017	Y937	Y887	T825	M762	E697	L636	L637	K638	G639	D640	Y642	S643	G644	R645	G646	V647	L648	E649	V650	G651	P652	Q653	L654	K655	V656	L657	N658	G659	G660	P661	T663	G664	N665	H666	R667	L668	F669	K670	A671	F672	L673	L674	K675	E676	K676	L677	V678	N679	P680	K681	C682	A683	A684	R685	G686	A687	L688									
	L1345	E1283	T1213	R1213	A1090	E1018	Y937	Y888	T826	M763	E698	L637	L638	K639	G640	D641	Y643	S644	G645	R646	G647	V648	L649	E650	V651	G652	P653	Q654	L655	K656	V657	L658	N659	G660	G661	P662	T664	G665	N666	H667	R668	L669	F670	K671	A672	F673	L674	L675	K676	E677	K677	L678	V679	N680	P681	K682	C683	A684	A685	R686	G687	A688	L689									
	L1346	E1284	T1214	R1214	A1091	E1019	Y937	Y889	T827	M764	E699	L638	L639	K640	G641	D642	Y644	S645	G646	R647	G648	V649	L650	E651	V652	G653	P654	Q655	L656	K657	V658	L659	N660	G661	G662	P663	T665	G666	N667	H668	R669	L670	F671	K672	A673	F674	L675	L676	K677	E678	K678	L679	V680	N681																		

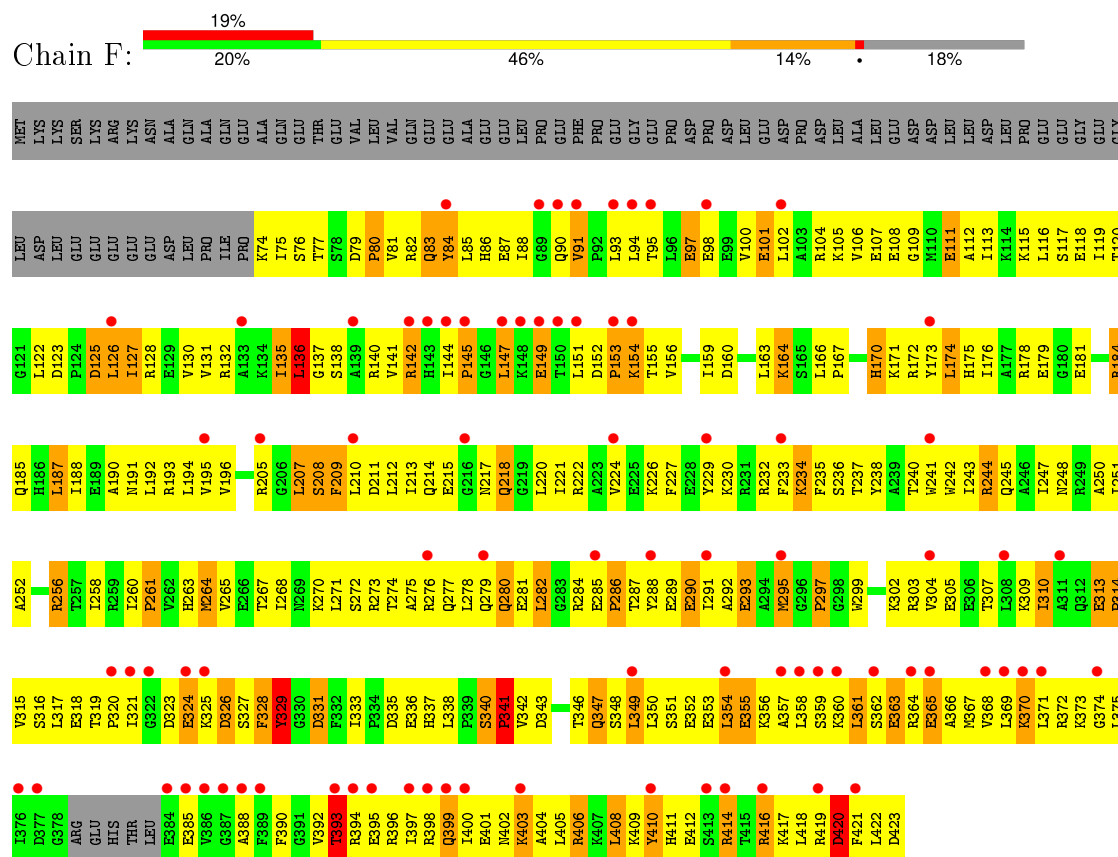
Chain E:



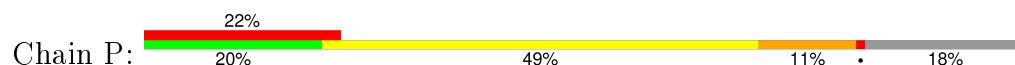
Chain O:



Chain F:



Chain P:



K373	E313	I251	L187	L126	LEU	MET
G374	F314	Q254	I188	I127	ASP	LYS
L376	V315	Q255	E189	R128	LEU	LYS
I377	S316	A255	A190	E129	GLU	SER
D377	L317	R256	N191	V130	GLU	LYS
G378	E318	T257	L192	R132	GLU	ARG
ARG	T319	I258	R193	R133	GLU	LYS
GLU	F320	R259	L194	A134	GLU	ASN
HIS	I321	I260	V195	K135	ASP	ALA
THR	G322	P261	V196	I135	LEU	GLN
LEU	D323	V262	S197	L136	PRO	ALA
E384	E324	H263	G137	I137	ILE	GLN
E385	K325	M264	K200	S138	PRO	GLU
V386	D326	V265	K201	A139	K74	ALA
G387	S327	E266	Y202	R140	I75	GLN
A388	F328	T267	G204	T203	S76	GLU
F389	Y329	I268	G204	R142	T77	THR
F390	G330	N269	S208	R143		GLU
G391	D331	K270	F209	H144		VAL
V392	F332	L271	L210	P145		LEU
T393	I333	S272	D211	G146		VAL
R394	F334	R273	L212	L147		GLN
E395	D335	T274	L213	T150		GLU
R396	E336	A275	I214	L85		ALA
I397	R337	R276	E215	H86		GLU
R398	L338	Q277	G216	E87		GLU
Q399	F339	L278	N217	I88		GLU
I400	S340	Q279	K154	G89		LEU
E401	P341	Q280	T155	Q90		PRO
H402	V342	E281	G219	V91		GLU
K403	D343	L282	I220	P32		PHE
A404	A344	G283	I221	L93		PRO
L405	A345	R284	R222	L94		GLU
R406	T346	E285	A223	T95		GLY
K407	Q347	P286	V224	L96		GLU
L408	S348	T287	E225	E97		PRO
K409	L349	Y288	K226	E98		ASP
Y410	L350	E289	F227	E99		PRO
H411	S351	E290	E228	V100		ASP
E412	E352	I291	Y229	E101		LEU
S413	E353	A292	K230	L102		GLU
R414	L354	E293	R231	A103		ASP
T415	E355	A294	R232	R104		PRO
R416	K356	M295	F233	K105		ASP
K417	A357	G296	K234	V106		ASP
L418	L358	G297	F235	E107		ALA
R419	S359	G298	S236	E108		LEU
D420	K360	W299	T237			GLU
L422	L361		Y238	A112		ASP
D423	S362		A239	I113		ASP
	E363		T240			LEU
	R364		W241	S117		LEU
	E365		W242	E118		ASP
	A366		I243	I119		LEU
	N367		R244	T120		PRO
	V368		Q245	G121		GLU
	L369		A246	L122		GLU
	R370		I247	D123		GLY
	L371		N248	P124		GLU
	R372			D125		GLY

4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	239.50Å 239.50Å 253.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.50 24.85 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.50) 92.6 (24.85-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.267 0.336 , 0.362	Depositor DCC
R_{free} test set	29710 reflections (6.10%)	DCC
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 80.8	EDS
Estimated twinning fraction	0.499 for -h,-k,l 0.076 for h,-h-k,-l 0.076 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 517107 reflections	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	60572	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 2.14% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, ZN, RPT

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	0.81	1/1838 (0.1%)	0.88	4/2498 (0.2%)
1	B	0.74	0/1838	0.81	2/2498 (0.1%)
1	K	0.75	0/1838	0.86	3/2498 (0.1%)
1	L	0.73	1/1838 (0.1%)	0.80	2/2498 (0.1%)
2	C	0.83	2/8997 (0.0%)	0.89	7/12164 (0.1%)
2	M	0.81	0/8997	0.88	8/12164 (0.1%)
3	D	0.84	0/10975	0.94	20/14836 (0.1%)
3	N	0.82	0/10975	0.92	17/14836 (0.1%)
4	E	0.84	0/783	0.94	0/1054
4	O	0.82	0/783	0.96	2/1054 (0.2%)
5	F	0.74	0/2812	0.82	4/3781 (0.1%)
5	P	0.71	0/2812	0.80	1/3781 (0.0%)
All	All	0.81	4/54486 (0.0%)	0.89	70/73662 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	ILE	C-N	6.06	1.45	1.34
1	L	172	SER	N-CA	-5.43	1.35	1.46
2	C	792	VAL	CB-CG1	-5.28	1.41	1.52
2	C	393	GLN	CD-OE1	5.25	1.35	1.24

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1389	LEU	CA-CB-CG	8.13	133.99	115.30
1	K	211	LEU	CA-CB-CG	8.11	133.95	115.30
1	B	138	LEU	CA-CB-CG	7.70	133.00	115.30
1	A	192	LEU	CA-CB-CG	7.60	132.79	115.30
3	D	199	LEU	CA-CB-CG	-7.59	97.84	115.30

There are no chirality outliers.

There are no planarity outliers.

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	232	0
1	B	1806	0	1861	216	0
1	K	1806	0	1861	173	0
1	L	1806	0	1861	186	0
2	C	8829	0	8933	1215	0
2	M	8829	0	8933	1174	0
3	D	10797	0	10873	1490	0
3	N	10797	0	10873	1288	0
4	E	769	0	775	89	0
4	O	769	0	775	95	0
5	F	2771	0	2844	346	0
5	P	2771	0	2844	352	0
6	A	33	0	0	0	0
6	B	21	0	0	0	0
6	C	73	0	0	0	0
6	D	106	0	0	0	0
6	E	5	0	0	0	0
6	F	28	0	0	0	0
6	K	19	0	0	0	0
6	L	17	0	0	0	0
6	M	65	0	0	0	0
6	N	92	0	0	0	0
6	O	8	0	0	0	0
6	P	20	0	0	0	0
7	C	63	0	62	6	0
7	M	63	0	62	7	0
8	D	2	0	0	0	0
8	N	2	0	0	0	0
9	A	239	0	0	50	0
9	B	258	0	0	46	0
9	C	979	0	0	224	0
9	D	1252	0	0	277	0
9	E	117	0	0	28	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	F	420	0	0	94	0
9	K	183	0	0	39	0
9	L	219	0	0	46	0
9	M	998	0	0	249	0
9	N	1265	0	0	250	0
9	O	108	0	0	26	0
9	P	361	0	0	78	0
All	All	60572	0	54418	6470	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 60.

The worst 5 of 6470 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:95:GLN:HA	1:A:146:ARG:HH12	1.07	1.11
2:M:952:LEU:HD12	2:M:969:GLN:HE22	1.13	1.11
3:D:1087:ARG:HG2	3:D:1234:THR:HA	1.27	1.07
1:B:152:PRO:HD2	1:B:155:LYS:HD3	1.36	1.05
2:M:605:LYS:HB2	2:M:610:ARG:HH12	1.16	1.05

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%)	201 (88%)	21 (9%)	5 (2%)	8	13
1	B	227/315 (72%)	198 (87%)	23 (10%)	6 (3%)	7	10
1	K	227/315 (72%)	200 (88%)	23 (10%)	4 (2%)	11	18
1	L	227/315 (72%)	203 (89%)	20 (9%)	4 (2%)	11	18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	1117/1119 (100%)	907 (81%)	157 (14%)	53 (5%)	3	3
2	M	1117/1119 (100%)	906 (81%)	158 (14%)	53 (5%)	3	3
3	D	1388/1524 (91%)	1108 (80%)	207 (15%)	73 (5%)	2	2
3	N	1388/1524 (91%)	1105 (80%)	208 (15%)	75 (5%)	2	2
4	E	93/99 (94%)	75 (81%)	15 (16%)	3 (3%)	5	6
4	O	93/99 (94%)	75 (81%)	15 (16%)	3 (3%)	5	6
5	F	341/423 (81%)	285 (84%)	38 (11%)	18 (5%)	2	2
5	P	341/423 (81%)	287 (84%)	38 (11%)	16 (5%)	3	3
All	All	6786/7590 (89%)	5550 (82%)	923 (14%)	313 (5%)	3	3

5 of 313 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	B	29	GLU
1	B	48	ILE
2	C	152	PRO
2	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	
1	A	202/273 (74%)	159 (79%)	43 (21%)	1	2
1	B	202/273 (74%)	161 (80%)	41 (20%)	1	2
1	K	202/273 (74%)	158 (78%)	44 (22%)	1	2
1	L	202/273 (74%)	160 (79%)	42 (21%)	1	2
2	C	941/941 (100%)	714 (76%)	227 (24%)	1	1
2	M	941/941 (100%)	738 (78%)	203 (22%)	1	2
3	D	1123/1279 (88%)	868 (77%)	255 (23%)	1	1
3	N	1123/1279 (88%)	871 (78%)	252 (22%)	1	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	83/87 (95%)	62 (75%)	21 (25%)	1	1
4	O	83/87 (95%)	65 (78%)	18 (22%)	1	2
5	F	295/370 (80%)	233 (79%)	62 (21%)	1	2
5	P	295/370 (80%)	246 (83%)	49 (17%)	3	5
All	All	5692/6446 (88%)	4435 (78%)	1257 (22%)	1	2

5 of 1257 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	28	GLN
1	L	55	SER
3	N	1363	LEU
4	E	84	ARG
5	F	365	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 169 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	218	GLN
2	M	117	HIS
4	O	86	GLN
5	F	337	HIS
1	K	229	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 493 ligands modelled in this entry, 491 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	$\# Z > 2$
7	RPT	C	8001	-	68,68,68	2.25	22 (32%)	87,101,101	1.40	12 (13%)
7	RPT	M	8002	-	68,68,68	2.29	22 (32%)	87,101,101	1.40	10 (11%)

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
7	RPT	C	8001	-	-	0/64/96/96	0/2/6/6
7	RPT	M	8002	-	-	0/64/96/96	0/2/6/6

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	8002	RPT	O2-C8	-2.07	1.28	1.35
7	M	8002	RPT	C32-C22	2.02	1.58	1.53
7	C	8001	RPT	C27-C28	2.27	1.59	1.50
7	M	8002	RPT	C27-C28	2.35	1.59	1.50
7	C	8001	RPT	C45-C38	2.38	1.59	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	8002	RPT	C34-C26-C25	-2.89	105.97	111.38
7	M	8002	RPT	C31-C20-C19	-2.88	103.02	110.07
7	C	8001	RPT	C31-C20-C19	-2.71	103.44	110.07
7	M	8002	RPT	C4-C3-C43	-2.48	115.16	119.67
7	C	8001	RPT	C34-C26-C25	-2.25	107.18	111.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	8001	RPT	6	0
7	M	8002	RPT	7	0

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%)	0.84	26 (11%)	7 6	27, 63, 91, 115	0
1	B	229/315 (72%)	1.69	70 (30%)	1 0	48, 93, 115, 119	0
1	K	229/315 (72%)	0.81	23 (10%)	9 10	34, 65, 94, 134	0
1	L	229/315 (72%)	1.22	48 (20%)	1 1	52, 92, 110, 131	0
2	C	1119/1119 (100%)	1.04	191 (17%)	2 2	21, 75, 106, 118	0
2	M	1119/1119 (100%)	1.15	215 (19%)	2 1	25, 79, 109, 122	0
3	D	1392/1524 (91%)	1.13	252 (18%)	2 2	24, 65, 112, 132	0
3	N	1392/1524 (91%)	1.15	264 (18%)	2 1	25, 69, 117, 138	0
4	E	95/99 (95%)	1.34	18 (18%)	2 1	42, 83, 108, 126	0
4	O	95/99 (95%)	1.13	17 (17%)	2 2	46, 80, 107, 114	0
5	F	345/423 (81%)	1.21	82 (23%)	1 1	49, 84, 110, 127	0
5	P	345/423 (81%)	1.41	92 (26%)	1 1	63, 89, 114, 124	0
All	All	6818/7590 (89%)	1.15	1298 (19%)	2 1	21, 75, 112, 138	0

The worst 5 of 1298 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	177	ALA	14.7
1	B	130	ALA	13.8
1	L	6	LEU	13.7
4	E	85	LEU	13.3
3	D	229	ALA	12.2

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 ⓘ

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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	MG	D	9029	1/1	0.93	0.20	1.86	33,33,33,33	0
6	MG	K	9410	1/1	0.90	0.33	1.80	36,36,36,36	0
6	MG	D	9095	1/1	0.93	0.25	1.24	30,30,30,30	0
7	RPT	M	8002	63/63	0.89	0.28	1.19	33,45,55,57	0
6	MG	N	9402	1/1	0.99	0.30	1.09	45,45,45,45	0
6	MG	N	9200	1/1	0.90	0.20	0.65	38,38,38,38	0
7	RPT	C	8001	63/63	0.89	0.26	0.46	26,40,66,82	0
6	MG	M	9400	1/1	0.99	0.19	0.38	40,40,40,40	0
6	MG	D	9038	1/1	0.96	0.20	0.13	39,39,39,39	0
6	MG	O	9197	1/1	0.88	0.32	0.03	57,57,57,57	0
6	MG	D	9001	1/1	0.78	0.18	-0.05	36,36,36,36	0
6	MG	B	9033	1/1	0.96	0.22	-0.14	33,33,33,33	0
6	MG	D	9017	1/1	0.95	0.17	-0.33	42,42,42,42	0
6	MG	M	9219	1/1	0.94	0.20	-0.47	47,47,47,47	0
6	MG	L	9183	1/1	0.91	0.17	-0.52	37,37,37,37	0
6	MG	N	9398	1/1	0.98	0.20	-0.58	48,48,48,48	0
6	MG	P	9189	1/1	0.87	0.13	-0.59	49,49,49,49	0
6	MG	L	9182	1/1	0.83	0.17	-0.60	47,47,47,47	0
8	ZN	D	7058	1/1	0.63	0.18	-0.62	106,106,106,106	0
6	MG	M	9247	1/1	0.84	0.17	-0.65	51,51,51,51	0
6	MG	N	9211	1/1	0.79	0.11	-0.67	44,44,44,44	0
6	MG	M	9407	1/1	0.92	0.17	-0.83	35,35,35,35	0
6	MG	D	9073	1/1	0.98	0.14	-0.83	34,34,34,34	0
6	MG	A	9354	1/1	0.93	0.12	-0.93	37,37,37,37	0
6	MG	K	9213	1/1	0.88	0.16	-0.95	43,43,43,43	0
6	MG	E	9007	1/1	0.88	0.14	-1.01	40,40,40,40	0
6	MG	F	9057	1/1	0.98	0.14	-1.04	30,30,30,30	0
6	MG	M	9242	1/1	0.94	0.20	-1.05	35,35,35,35	0
6	MG	C	9031	1/1	0.93	0.10	-1.22	40,40,40,40	0
6	MG	M	9208	1/1	0.92	0.10	-1.23	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	D	9009	1/1	0.97	0.11	-1.29	43,43,43,43	0
6	MG	D	9054	1/1	0.75	0.11	-1.32	44,44,44,44	0
6	MG	M	9299	1/1	0.90	0.14	-1.34	43,43,43,43	0
6	MG	M	9300	1/1	0.91	0.11	-1.37	39,39,39,39	0
6	MG	A	9081	1/1	0.88	0.10	-1.39	40,40,40,40	0
6	MG	A	9002	1/1	0.98	0.16	-1.39	31,31,31,31	0
6	MG	D	9028	1/1	0.91	0.12	-1.44	34,34,34,34	0
6	MG	N	9467	1/1	0.92	0.18	-1.48	35,35,35,35	0
6	MG	C	9004	1/1	0.77	0.15	-1.51	39,39,39,39	0
6	MG	M	9196	1/1	0.97	0.10	-1.53	42,42,42,42	0
6	MG	M	9434	1/1	0.98	0.09	-1.55	34,34,34,34	0
6	MG	D	9087	1/1	0.92	0.12	-1.58	43,43,43,43	0
6	MG	B	9059	1/1	0.89	0.14	-1.60	48,48,48,48	0
6	MG	N	9207	1/1	0.94	0.09	-1.63	41,41,41,41	0
6	MG	N	9199	1/1	0.98	0.07	-1.67	35,35,35,35	0
6	MG	K	9188	1/1	0.92	0.14	-1.68	40,40,40,40	0
6	MG	B	9032	1/1	0.87	0.08	-1.70	34,34,34,34	0
6	MG	N	9271	1/1	0.97	0.08	-1.73	43,43,43,43	0
6	MG	E	9074	1/1	0.96	0.04	-1.82	59,59,59,59	0
6	MG	D	9036	1/1	0.83	0.09	-1.84	44,44,44,44	0
6	MG	F	9035	1/1	0.96	0.10	-1.86	40,40,40,40	0
6	MG	D	9024	1/1	0.91	0.08	-1.87	36,36,36,36	0
8	ZN	N	7059	1/1	0.84	0.06	-1.89	93,93,93,93	0
6	MG	N	9238	1/1	0.96	0.13	-1.94	43,43,43,43	0
6	MG	D	9113	1/1	0.97	0.09	-1.99	34,34,34,34	0
6	MG	P	9228	1/1	0.97	0.08	-2.02	43,43,43,43	0
6	MG	A	9013	1/1	0.94	0.07	-2.02	44,44,44,44	0
6	MG	D	9365	1/1	0.93	0.25	-2.04	41,41,41,41	0
6	MG	C	9003	1/1	0.95	0.11	-2.06	38,38,38,38	0
6	MG	D	9367	1/1	0.89	0.12	-2.13	31,31,31,31	0
6	MG	D	9330	1/1	0.86	0.15	-2.22	39,39,39,39	0
6	MG	D	9011	1/1	0.98	0.07	-2.23	33,33,33,33	0
6	MG	M	9239	1/1	0.92	0.11	-2.28	34,34,34,34	0
6	MG	M	9260	1/1	0.90	0.10	-2.32	36,36,36,36	0
6	MG	C	9092	1/1	0.95	0.06	-2.35	44,44,44,44	0
6	MG	N	9298	1/1	0.98	0.04	-2.40	55,55,55,55	0
6	MG	C	9046	1/1	0.99	0.04	-2.40	38,38,38,38	0
8	ZN	N	7113	1/1	0.87	0.07	-2.41	84,84,84,84	0
6	MG	A	9156	1/1	0.91	0.07	-2.45	43,43,43,43	0
6	MG	C	9015	1/1	0.98	0.11	-2.47	38,38,38,38	0
6	MG	N	9243	1/1	0.91	0.12	-2.50	35,35,35,35	0
6	MG	N	9214	1/1	0.99	0.06	-2.50	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	A	9010	1/1	0.93	0.08	-2.53	30,30,30,30	0
6	MG	D	9089	1/1	0.97	0.06	-2.59	36,36,36,36	0
6	MG	N	9431	1/1	0.96	0.09	-2.63	39,39,39,39	0
6	MG	D	9329	1/1	0.90	0.09	-2.74	33,33,33,33	0
8	ZN	D	7112	1/1	0.94	0.05	-2.90	80,80,80,80	0
6	MG	N	9316	1/1	0.99	0.06	-3.06	37,37,37,37	0
6	MG	A	9088	1/1	0.99	0.05	-3.22	36,36,36,36	0
6	MG	A	9027	1/1	0.88	0.07	-3.26	37,37,37,37	0
6	MG	D	9333	1/1	0.98	0.05	-3.37	33,33,33,33	0
6	MG	M	9268	1/1	0.96	0.11	-3.43	32,32,32,32	0
6	MG	D	9062	1/1	0.85	0.07	-3.54	47,47,47,47	0
6	MG	N	9184	1/1	0.95	0.07	-3.61	29,29,29,29	0
6	MG	C	9051	1/1	0.98	0.08	-3.66	37,37,37,37	0
6	MG	K	9180	1/1	0.99	0.11	-3.81	42,42,42,42	0
6	MG	M	9195	1/1	0.97	0.04	-4.07	34,34,34,34	0
6	MG	C	9061	1/1	0.96	0.06	-4.47	34,34,34,34	0
6	MG	M	9205	1/1	0.97	0.06	-4.65	38,38,38,38	0
6	MG	C	9053	1/1	0.99	0.07	-5.19	30,30,30,30	0
6	MG	N	9293	1/1	0.82	0.07	-	42,42,42,42	0
6	MG	L	9421	1/1	0.92	0.07	-	53,53,53,53	0
6	MG	B	9110	1/1	0.96	0.13	-	49,49,49,49	0
6	MG	M	9486	1/1	0.86	0.13	-	48,48,48,48	0
6	MG	A	9124	1/1	0.96	0.10	-	39,39,39,39	0
6	MG	M	9248	1/1	0.97	0.23	-	48,48,48,48	0
6	MG	D	9364	1/1	0.97	0.06	-	47,47,47,47	0
6	MG	L	9252	1/1	0.96	0.15	-	45,45,45,45	0
6	MG	D	9039	1/1	0.95	0.09	-	44,44,44,44	0
6	MG	K	9290	1/1	0.92	0.12	-	51,51,51,51	0
6	MG	M	9295	1/1	0.96	0.23	-	42,42,42,42	0
6	MG	A	9345	1/1	0.96	0.07	-	41,41,41,41	0
6	MG	K	9264	1/1	0.95	0.05	-	42,42,42,42	0
6	MG	F	9008	1/1	0.93	0.07	-	40,40,40,40	0
6	MG	M	9220	1/1	0.86	0.10	-	51,51,51,51	0
6	MG	M	9440	1/1	0.97	0.08	-	50,50,50,50	0
6	MG	F	9356	1/1	0.93	0.10	-	37,37,37,37	0
6	MG	M	9256	1/1	0.94	0.05	-	56,56,56,56	0
6	MG	D	9351	1/1	0.96	0.14	-	43,43,43,43	0
6	MG	D	9058	1/1	0.95	0.11	-	38,38,38,38	0
6	MG	B	9358	1/1	0.99	0.13	-	39,39,39,39	0
6	MG	D	9084	1/1	0.97	0.06	-	37,37,37,37	0
6	MG	N	9292	1/1	0.90	0.07	-	56,56,56,56	0
6	MG	B	9359	1/1	0.97	0.04	-	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	C	9067	1/1	0.92	0.08	-	57,57,57,57	0
6	MG	C	9020	1/1	0.97	0.09	-	34,34,34,34	0
6	MG	K	9433	1/1	0.94	0.09	-	50,50,50,50	0
6	MG	F	9389	1/1	0.96	0.18	-	53,53,53,53	0
6	MG	C	9176	1/1	0.87	0.18	-	28,28,28,28	0
6	MG	C	9138	1/1	0.92	0.18	-	43,43,43,43	0
6	MG	M	9319	1/1	0.96	0.18	-	41,41,41,41	0
6	MG	D	9135	1/1	0.95	0.13	-	50,50,50,50	0
6	MG	A	9043	1/1	0.97	0.05	-	37,37,37,37	0
6	MG	C	9361	1/1	0.93	0.10	-	41,41,41,41	0
6	MG	K	9405	1/1	0.92	0.07	-	56,56,56,56	0
6	MG	D	9102	1/1	0.92	0.10	-	44,44,44,44	0
6	MG	B	9093	1/1	0.95	0.10	-	40,40,40,40	0
6	MG	B	9457	1/1	0.97	0.18	-	43,43,43,43	0
6	MG	D	9163	1/1	0.94	0.15	-	52,52,52,52	0
6	MG	N	9221	1/1	0.97	0.06	-	44,44,44,44	0
6	MG	D	9121	1/1	0.93	0.06	-	35,35,35,35	0
6	MG	A	9125	1/1	0.93	0.09	-	36,36,36,36	0
6	MG	C	9362	1/1	0.94	0.09	-	55,55,55,55	0
6	MG	C	9126	1/1	0.97	0.13	-	46,46,46,46	0
6	MG	C	9168	1/1	0.91	0.13	-	45,45,45,45	0
6	MG	F	9481	1/1	0.96	0.23	-	57,57,57,57	0
6	MG	D	9144	1/1	0.98	0.13	-	39,39,39,39	0
6	MG	C	9128	1/1	0.99	0.16	-	52,52,52,52	0
6	MG	D	9373	1/1	0.97	0.07	-	51,51,51,51	0
6	MG	C	9340	1/1	0.90	0.29	-	60,60,60,60	0
6	MG	P	9315	1/1	0.97	0.12	-	35,35,35,35	0
6	MG	L	9289	1/1	0.68	0.19	-	62,62,62,62	0
6	MG	D	9374	1/1	0.99	0.17	-	41,41,41,41	0
6	MG	C	9461	1/1	0.94	0.17	-	50,50,50,50	0
6	MG	D	9152	1/1	0.94	0.12	-	67,67,67,67	0
6	MG	D	9339	1/1	0.95	0.08	-	37,37,37,37	0
6	MG	D	9166	1/1	0.92	0.11	-	40,40,40,40	0
6	MG	C	9455	1/1	0.93	0.09	-	40,40,40,40	0
6	MG	D	9118	1/1	0.92	0.12	-	44,44,44,44	0
6	MG	A	9016	1/1	0.97	0.09	-	36,36,36,36	0
6	MG	M	9452	1/1	0.95	0.16	-	42,42,42,42	0
6	MG	C	9107	1/1	0.76	0.12	-	42,42,42,42	0
6	MG	D	9379	1/1	0.96	0.07	-	47,47,47,47	0
6	MG	C	9122	1/1	0.97	0.06	-	56,56,56,56	0
6	MG	N	9215	1/1	0.92	0.08	-	32,32,32,32	0
6	MG	N	9415	1/1	0.95	0.05	-	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	D	9348	1/1	0.82	0.16	-	57,57,57,57	0
6	MG	D	9023	1/1	0.90	0.08	-	34,34,34,34	0
6	MG	M	9412	1/1	0.84	0.21	-	43,43,43,43	0
6	MG	C	9044	1/1	0.95	0.11	-	34,34,34,34	0
6	MG	M	9320	1/1	0.99	0.26	-	34,34,34,34	0
6	MG	N	9419	1/1	0.92	0.27	-	51,51,51,51	0
6	MG	P	9235	1/1	0.92	0.13	-	40,40,40,40	0
6	MG	K	9432	1/1	0.89	0.08	-	49,49,49,49	0
6	MG	M	9409	1/1	0.97	0.10	-	36,36,36,36	0
6	MG	M	9284	1/1	0.97	0.06	-	54,54,54,54	0
6	MG	C	9154	1/1	0.98	0.12	-	43,43,43,43	0
6	MG	C	9055	1/1	0.97	0.10	-	38,38,38,38	0
6	MG	D	9120	1/1	0.98	0.14	-	31,31,31,31	0
6	MG	D	9331	1/1	0.86	0.13	-	43,43,43,43	0
6	MG	D	9069	1/1	0.95	0.10	-	48,48,48,48	0
6	MG	N	9303	1/1	0.98	0.08	-	54,54,54,54	0
6	MG	C	9464	1/1	0.98	0.26	-	48,48,48,48	0
6	MG	C	9021	1/1	0.97	0.13	-	37,37,37,37	0
6	MG	D	9158	1/1	0.83	0.22	-	60,60,60,60	0
6	MG	K	9438	1/1	0.86	0.10	-	52,52,52,52	0
6	MG	M	9305	1/1	0.98	0.14	-	46,46,46,46	0
6	MG	L	9314	1/1	0.94	0.18	-	56,56,56,56	0
6	MG	N	9435	1/1	0.90	0.08	-	53,53,53,53	0
6	MG	B	9080	1/1	0.91	0.26	-	56,56,56,56	0
6	MG	N	9472	1/1	0.98	0.07	-	56,56,56,56	0
6	MG	N	9404	1/1	0.89	0.17	-	55,55,55,55	0
6	MG	M	9442	1/1	0.98	0.24	-	59,59,59,59	0
6	MG	P	9216	1/1	0.85	0.10	-	48,48,48,48	0
6	MG	N	9313	1/1	0.93	0.05	-	43,43,43,43	0
6	MG	L	9414	1/1	0.88	0.10	-	51,51,51,51	0
6	MG	F	9159	1/1	0.90	0.06	-	57,57,57,57	0
6	MG	D	9336	1/1	0.95	0.06	-	53,53,53,53	0
6	MG	D	9386	1/1	0.99	0.07	-	40,40,40,40	0
6	MG	C	9022	1/1	0.94	0.07	-	37,37,37,37	0
6	MG	N	9181	1/1	0.92	0.07	-	47,47,47,47	0
6	MG	D	9091	1/1	0.99	0.04	-	27,27,27,27	0
6	MG	C	9360	1/1	0.91	0.16	-	53,53,53,53	0
6	MG	C	9119	1/1	0.91	0.11	-	43,43,43,43	0
6	MG	C	9042	1/1	0.97	0.08	-	47,47,47,47	0
6	MG	D	9174	1/1	0.94	0.16	-	47,47,47,47	0
6	MG	N	9276	1/1	0.95	0.20	-	61,61,61,61	0
6	MG	P	9285	1/1	0.95	0.10	-	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	F	9148	1/1	0.97	0.13	-	54,54,54,54	0
6	MG	M	9230	1/1	0.90	0.15	-	50,50,50,50	0
6	MG	D	9041	1/1	0.94	0.07	-	47,47,47,47	0
6	MG	C	9350	1/1	0.74	0.14	-	60,60,60,60	0
6	MG	C	9366	1/1	0.99	0.04	-	41,41,41,41	0
6	MG	M	9324	1/1	0.84	0.18	-	41,41,41,41	0
6	MG	N	9267	1/1	0.91	0.12	-	42,42,42,42	0
6	MG	D	9146	1/1	0.99	0.07	-	31,31,31,31	0
6	MG	D	9167	1/1	0.95	0.09	-	49,49,49,49	0
6	MG	D	9137	1/1	0.97	0.04	-	47,47,47,47	0
6	MG	D	9369	1/1	0.97	0.20	-	49,49,49,49	0
6	MG	F	9048	1/1	0.97	0.16	-	41,41,41,41	0
6	MG	D	9177	1/1	0.93	0.18	-	64,64,64,64	0
6	MG	B	9378	1/1	0.97	0.17	-	47,47,47,47	0
6	MG	D	9133	1/1	0.98	0.14	-	42,42,42,42	0
6	MG	F	9387	1/1	0.96	0.12	-	53,53,53,53	0
6	MG	N	9186	1/1	0.92	0.07	-	49,49,49,49	0
6	MG	D	9063	1/1	0.94	0.10	-	33,33,33,33	0
6	MG	F	9109	1/1	0.79	0.09	-	60,60,60,60	0
6	MG	L	9306	1/1	0.97	0.05	-	57,57,57,57	0
6	MG	N	9288	1/1	0.96	0.09	-	49,49,49,49	0
6	MG	M	9294	1/1	0.92	0.10	-	52,52,52,52	0
6	MG	D	9480	1/1	0.97	0.23	-	55,55,55,55	0
6	MG	F	9363	1/1	0.95	0.11	-	53,53,53,53	0
6	MG	N	9449	1/1	0.84	0.15	-	51,51,51,51	0
6	MG	A	9384	1/1	0.96	0.09	-	39,39,39,39	0
6	MG	M	9263	1/1	0.95	0.15	-	56,56,56,56	0
6	MG	D	9346	1/1	0.90	0.16	-	47,47,47,47	0
6	MG	D	9396	1/1	0.96	0.26	-	62,62,62,62	0
6	MG	N	9249	1/1	0.94	0.13	-	45,45,45,45	0
6	MG	D	9328	1/1	0.98	0.05	-	30,30,30,30	0
6	MG	M	9272	1/1	0.94	0.24	-	45,45,45,45	0
6	MG	A	9368	1/1	0.95	0.05	-	43,43,43,43	0
6	MG	N	9270	1/1	0.94	0.07	-	39,39,39,39	0
6	MG	C	9071	1/1	0.91	0.11	-	42,42,42,42	0
6	MG	B	9116	1/1	0.91	0.07	-	38,38,38,38	0
6	MG	D	9132	1/1	0.97	0.13	-	43,43,43,43	0
6	MG	M	9321	1/1	0.99	0.04	-	41,41,41,41	0
6	MG	D	9453	1/1	0.90	0.10	-	38,38,38,38	0
6	MG	N	9323	1/1	0.97	0.17	-	38,38,38,38	0
6	MG	K	9223	1/1	0.96	0.16	-	32,32,32,32	0
6	MG	D	9072	1/1	0.99	0.06	-	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	M	9222	1/1	0.97	0.12	-	35,35,35,35	0
6	MG	A	9357	1/1	0.92	0.08	-	54,54,54,54	0
6	MG	C	9065	1/1	0.94	0.13	-	37,37,37,37	0
6	MG	D	9385	1/1	0.92	0.17	-	35,35,35,35	0
6	MG	D	9129	1/1	0.90	0.13	-	42,42,42,42	0
6	MG	D	9005	1/1	0.96	0.11	-	40,40,40,40	0
6	MG	N	9187	1/1	0.98	0.05	-	33,33,33,33	0
6	MG	N	9465	1/1	0.91	0.06	-	49,49,49,49	0
6	MG	O	9296	1/1	0.96	0.05	-	42,42,42,42	0
6	MG	L	9307	1/1	0.96	0.08	-	35,35,35,35	0
6	MG	M	9424	1/1	0.93	0.08	-	34,34,34,34	0
6	MG	P	9280	1/1	0.93	0.11	-	51,51,51,51	0
6	MG	P	9325	1/1	0.74	0.34	-	49,49,49,49	0
6	MG	N	9444	1/1	0.97	0.13	-	49,49,49,49	0
6	MG	A	9342	1/1	0.97	0.06	-	39,39,39,39	0
6	MG	M	9310	1/1	0.80	0.13	-	46,46,46,46	0
6	MG	A	9078	1/1	0.90	0.18	-	66,66,66,66	0
6	MG	D	9151	1/1	0.93	0.07	-	57,57,57,57	0
6	MG	M	9401	1/1	0.98	0.08	-	37,37,37,37	0
6	MG	D	9165	1/1	0.98	0.20	-	32,32,32,32	0
6	MG	D	9070	1/1	0.97	0.05	-	33,33,33,33	0
6	MG	C	9047	1/1	0.95	0.18	-	53,53,53,53	0
6	MG	N	9317	1/1	0.97	0.31	-	43,43,43,43	0
6	MG	C	9143	1/1	0.97	0.16	-	35,35,35,35	0
6	MG	M	9471	1/1	0.89	0.16	-	47,47,47,47	0
6	MG	A	9460	1/1	0.94	0.22	-	55,55,55,55	0
6	MG	D	9127	1/1	0.98	0.04	-	48,48,48,48	0
6	MG	C	9086	1/1	0.97	0.08	-	39,39,39,39	0
6	MG	M	9224	1/1	0.93	0.13	-	40,40,40,40	0
6	MG	N	9287	1/1	0.91	0.16	-	53,53,53,53	0
6	MG	F	9123	1/1	0.94	0.15	-	37,37,37,37	0
6	MG	D	9014	1/1	0.94	0.10	-	41,41,41,41	0
6	MG	K	9413	1/1	0.90	0.17	-	54,54,54,54	0
6	MG	M	9411	1/1	0.97	0.14	-	47,47,47,47	0
6	MG	O	9198	1/1	0.98	0.06	-	36,36,36,36	0
6	MG	M	9474	1/1	0.96	0.23	-	49,49,49,49	0
6	MG	D	9392	1/1	0.97	0.10	-	52,52,52,52	0
6	MG	M	9406	1/1	0.91	0.13	-	67,67,67,67	0
6	MG	A	9352	1/1	0.79	0.28	-	46,46,46,46	0
6	MG	P	9258	1/1	0.98	0.06	-	51,51,51,51	0
6	MG	N	9448	1/1	0.95	0.06	-	51,51,51,51	0
6	MG	F	9393	1/1	0.97	0.19	-	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	K	9469	1/1	0.99	0.13	-	50,50,50,50	0
6	MG	O	9420	1/1	0.95	0.16	-	51,51,51,51	0
6	MG	N	9426	1/1	0.93	0.29	-	41,41,41,41	0
6	MG	D	9130	1/1	0.98	0.06	-	51,51,51,51	0
6	MG	D	9341	1/1	0.91	0.07	-	41,41,41,41	0
6	MG	K	9244	1/1	0.97	0.14	-	44,44,44,44	0
6	MG	C	9149	1/1	0.94	0.17	-	48,48,48,48	0
6	MG	C	9050	1/1	0.98	0.07	-	37,37,37,37	0
6	MG	N	9445	1/1	0.93	0.06	-	51,51,51,51	0
6	MG	O	9439	1/1	0.96	0.09	-	56,56,56,56	0
6	MG	M	9225	1/1	0.94	0.13	-	56,56,56,56	0
6	MG	C	9162	1/1	0.84	0.23	-	50,50,50,50	0
6	MG	M	9441	1/1	0.87	0.17	-	45,45,45,45	0
6	MG	D	9343	1/1	0.91	0.13	-	59,59,59,59	0
6	MG	M	9210	1/1	0.91	0.11	-	41,41,41,41	0
6	MG	D	9397	1/1	0.96	0.12	-	51,51,51,51	0
6	MG	D	9082	1/1	0.76	0.17	-	60,60,60,60	0
6	MG	M	9201	1/1	0.95	0.09	-	45,45,45,45	0
6	MG	N	9232	1/1	0.96	0.07	-	47,47,47,47	0
6	MG	L	9309	1/1	0.87	0.13	-	49,49,49,49	0
6	MG	A	9097	1/1	0.97	0.07	-	34,34,34,34	0
6	MG	A	9111	1/1	0.92	0.10	-	35,35,35,35	0
6	MG	C	9353	1/1	0.93	0.16	-	48,48,48,48	0
6	MG	C	9371	1/1	0.93	0.08	-	54,54,54,54	0
6	MG	F	9376	1/1	0.93	0.06	-	62,62,62,62	0
6	MG	M	9261	1/1	0.98	0.04	-	47,47,47,47	0
6	MG	C	9175	1/1	0.81	0.15	-	68,68,68,68	0
6	MG	B	9094	1/1	0.95	0.06	-	38,38,38,38	0
6	MG	P	9399	1/1	0.97	0.11	-	34,34,34,34	0
6	MG	P	9202	1/1	0.89	0.08	-	49,49,49,49	0
6	MG	B	9458	1/1	0.90	0.13	-	44,44,44,44	0
6	MG	N	9326	1/1	0.98	0.09	-	62,62,62,62	0
6	MG	A	9332	1/1	0.94	0.18	-	35,35,35,35	0
6	MG	A	9395	1/1	0.93	0.10	-	50,50,50,50	0
6	MG	D	9100	1/1	0.95	0.09	-	43,43,43,43	0
6	MG	N	9322	1/1	0.96	0.09	-	54,54,54,54	0
6	MG	N	9192	1/1	0.89	0.10	-	62,62,62,62	0
6	MG	N	9318	1/1	0.98	0.17	-	34,34,34,34	0
6	MG	N	9443	1/1	0.95	0.13	-	54,54,54,54	0
6	MG	F	9382	1/1	0.92	0.13	-	40,40,40,40	0
6	MG	C	9178	1/1	0.96	0.07	-	39,39,39,39	0
6	MG	N	9179	1/1	0.97	0.16	-	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	D	9349	1/1	0.89	0.09	-	33,33,33,33	0
6	MG	N	9217	1/1	0.96	0.04	-	48,48,48,48	0
6	MG	D	9338	1/1	0.95	0.07	-	42,42,42,42	0
6	MG	N	9253	1/1	0.97	0.04	-	42,42,42,42	0
6	MG	N	9262	1/1	0.99	0.07	-	51,51,51,51	0
6	MG	L	9437	1/1	0.94	0.14	-	40,40,40,40	0
6	MG	F	9139	1/1	1.00	0.12	-	38,38,38,38	0
6	MG	C	9355	1/1	0.91	0.23	-	58,58,58,58	0
6	MG	M	9234	1/1	0.94	0.08	-	53,53,53,53	0
6	MG	D	9335	1/1	0.98	0.11	-	52,52,52,52	0
6	MG	D	9006	1/1	0.89	0.06	-	40,40,40,40	0
6	MG	D	9052	1/1	0.96	0.11	-	65,65,65,65	0
6	MG	N	9231	1/1	0.98	0.15	-	52,52,52,52	0
6	MG	N	9429	1/1	0.95	0.13	-	45,45,45,45	0
6	MG	F	9390	1/1	0.97	0.24	-	46,46,46,46	0
6	MG	M	9275	1/1	0.95	0.06	-	55,55,55,55	0
6	MG	D	9173	1/1	0.98	0.17	-	48,48,48,48	0
6	MG	C	9372	1/1	0.76	0.15	-	61,61,61,61	0
6	MG	B	9083	1/1	0.99	0.16	-	40,40,40,40	0
6	MG	D	9134	1/1	0.99	0.06	-	47,47,47,47	0
6	MG	N	9417	1/1	0.98	0.14	-	39,39,39,39	0
6	MG	N	9302	1/1	0.98	0.14	-	31,31,31,31	0
6	MG	F	9172	1/1	0.87	0.24	-	51,51,51,51	0
6	MG	C	9142	1/1	0.97	0.23	-	48,48,48,48	0
6	MG	D	9108	1/1	0.92	0.07	-	51,51,51,51	0
6	MG	P	9436	1/1	0.96	0.12	-	49,49,49,49	0
6	MG	M	9227	1/1	0.92	0.10	-	35,35,35,35	0
6	MG	C	9145	1/1	0.94	0.13	-	66,66,66,66	0
6	MG	F	9101	1/1	0.96	0.11	-	44,44,44,44	0
6	MG	L	9246	1/1	0.82	0.15	-	52,52,52,52	0
6	MG	D	9030	1/1	0.89	0.12	-	48,48,48,48	0
6	MG	M	9190	1/1	0.97	0.05	-	29,29,29,29	0
6	MG	C	9115	1/1	0.95	0.16	-	36,36,36,36	0
6	MG	N	9204	1/1	0.99	0.03	-	44,44,44,44	0
6	MG	D	9334	1/1	0.94	0.06	-	54,54,54,54	0
6	MG	P	9277	1/1	0.91	0.07	-	41,41,41,41	0
6	MG	M	9212	1/1	0.95	0.10	-	32,32,32,32	0
6	MG	N	9468	1/1	0.97	0.20	-	55,55,55,55	0
6	MG	A	9106	1/1	0.95	0.10	-	38,38,38,38	0
6	MG	N	9185	1/1	0.98	0.06	-	56,56,56,56	0
6	MG	L	9278	1/1	0.88	0.17	-	44,44,44,44	0
6	MG	C	9026	1/1	0.97	0.07	-	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	D	9456	1/1	0.96	0.14	-	55,55,55,55	0
6	MG	N	9274	1/1	0.97	0.10	-	40,40,40,40	0
6	MG	C	9160	1/1	0.86	0.14	-	44,44,44,44	0
6	MG	F	9370	1/1	0.89	0.38	-	46,46,46,46	0
6	MG	C	9112	1/1	0.97	0.07	-	39,39,39,39	0
6	MG	C	9090	1/1	0.91	0.22	-	47,47,47,47	0
6	MG	D	9161	1/1	0.89	0.09	-	57,57,57,57	0
6	MG	B	9104	1/1	0.96	0.05	-	45,45,45,45	0
6	MG	N	9430	1/1	0.92	0.32	-	57,57,57,57	0
6	MG	L	9245	1/1	0.96	0.28	-	62,62,62,62	0
6	MG	B	9136	1/1	0.98	0.07	-	47,47,47,47	0
6	MG	A	9012	1/1	0.97	0.14	-	47,47,47,47	0
6	MG	P	9255	1/1	0.95	0.05	-	34,34,34,34	0
6	MG	F	9383	1/1	0.92	0.26	-	48,48,48,48	0
6	MG	C	9394	1/1	0.96	0.13	-	33,33,33,33	0
6	MG	N	9269	1/1	0.97	0.10	-	42,42,42,42	0
6	MG	P	9482	1/1	0.97	0.07	-	48,48,48,48	0
6	MG	E	9045	1/1	0.91	0.08	-	61,61,61,61	0
6	MG	K	9257	1/1	0.91	0.22	-	58,58,58,58	0
6	MG	O	9254	1/1	0.93	0.10	-	39,39,39,39	0
6	MG	L	9283	1/1	0.97	0.07	-	59,59,59,59	0
6	MG	N	9408	1/1	0.99	0.15	-	45,45,45,45	0
6	MG	N	9233	1/1	0.83	0.09	-	62,62,62,62	0
6	MG	M	9281	1/1	0.94	0.25	-	49,49,49,49	0
6	MG	O	9266	1/1	0.94	0.14	-	47,47,47,47	0
6	MG	N	9427	1/1	0.74	0.21	-	58,58,58,58	0
6	MG	N	9229	1/1	0.93	0.08	-	41,41,41,41	0
6	MG	C	9487	1/1	0.98	0.14	-	32,32,32,32	0
6	MG	A	9380	1/1	0.89	0.09	-	44,44,44,44	0
6	MG	M	9416	1/1	0.96	0.20	-	45,45,45,45	0
6	MG	F	9157	1/1	0.97	0.06	-	42,42,42,42	0
6	MG	N	9428	1/1	0.97	0.12	-	42,42,42,42	0
6	MG	L	9466	1/1	0.96	0.14	-	49,49,49,49	0
6	MG	L	9218	1/1	0.96	0.14	-	33,33,33,33	0
6	MG	N	9291	1/1	0.84	0.12	-	64,64,64,64	0
6	MG	K	9470	1/1	0.89	0.06	-	55,55,55,55	0
6	MG	N	9418	1/1	0.87	0.11	-	49,49,49,49	0
6	MG	N	9265	1/1	0.96	0.07	-	61,61,61,61	0
6	MG	F	9105	1/1	0.97	0.03	-	36,36,36,36	0
6	MG	B	9478	1/1	0.94	0.15	-	61,61,61,61	0
6	MG	C	9377	1/1	0.96	0.06	-	44,44,44,44	0
6	MG	D	9085	1/1	0.99	0.15	-	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	D	9459	1/1	0.94	0.17	-	54,54,54,54	0
6	MG	D	9117	1/1	0.99	0.13	-	48,48,48,48	0
6	MG	O	9483	1/1	0.79	0.26	-	63,63,63,63	0
6	MG	C	9037	1/1	0.96	0.04	-	51,51,51,51	0
6	MG	B	9056	1/1	0.97	0.08	-	43,43,43,43	0
6	MG	M	9447	1/1	0.85	0.19	-	64,64,64,64	0
6	MG	D	9347	1/1	0.88	0.28	-	49,49,49,49	0
6	MG	A	9477	1/1	0.96	0.12	-	52,52,52,52	0
6	MG	D	9337	1/1	0.95	0.10	-	53,53,53,53	0
6	MG	C	9025	1/1	0.96	0.08	-	39,39,39,39	0
6	MG	P	9297	1/1	0.91	0.12	-	45,45,45,45	0
6	MG	N	9484	1/1	0.92	0.20	-	37,37,37,37	0
6	MG	D	9388	1/1	0.94	0.16	-	37,37,37,37	0
6	MG	D	9096	1/1	0.97	0.11	-	60,60,60,60	0
6	MG	D	9064	1/1	0.88	0.07	-	44,44,44,44	0
6	MG	N	9206	1/1	0.99	0.02	-	31,31,31,31	0
6	MG	A	9153	1/1	0.91	0.06	-	66,66,66,66	0
6	MG	E	9155	1/1	0.97	0.04	-	44,44,44,44	0
6	MG	N	9451	1/1	0.97	0.11	-	41,41,41,41	0
6	MG	D	9077	1/1	0.94	0.11	-	35,35,35,35	0
6	MG	M	9203	1/1	0.98	0.04	-	32,32,32,32	0
6	MG	C	9049	1/1	0.97	0.04	-	46,46,46,46	0
6	MG	K	9191	1/1	0.94	0.07	-	32,32,32,32	0
6	MG	N	9311	1/1	1.00	0.11	-	39,39,39,39	0
6	MG	B	9103	1/1	0.94	0.11	-	43,43,43,43	0
6	MG	F	9098	1/1	0.93	0.17	-	54,54,54,54	0
6	MG	C	9463	1/1	0.95	0.23	-	55,55,55,55	0
6	MG	C	9114	1/1	0.95	0.10	-	30,30,30,30	0
6	MG	M	9273	1/1	0.84	0.12	-	44,44,44,44	0
6	MG	D	9018	1/1	0.91	0.10	-	39,39,39,39	0
6	MG	D	9140	1/1	0.99	0.12	-	40,40,40,40	0
6	MG	D	9344	1/1	0.96	0.07	-	55,55,55,55	0
6	MG	F	9060	1/1	0.94	0.10	-	41,41,41,41	0
6	MG	F	9375	1/1	0.94	0.07	-	36,36,36,36	0
6	MG	N	9240	1/1	0.97	0.16	-	46,46,46,46	0
6	MG	N	9423	1/1	0.83	0.12	-	58,58,58,58	0
6	MG	N	9476	1/1	0.97	0.09	-	54,54,54,54	0
6	MG	B	9131	1/1	0.94	0.10	-	33,33,33,33	0
6	MG	C	9381	1/1	0.80	0.15	-	53,53,53,53	0
6	MG	D	9150	1/1	0.98	0.05	-	31,31,31,31	0
6	MG	C	9391	1/1	0.79	0.24	-	60,60,60,60	0
6	MG	P	9209	1/1	0.95	0.19	-	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	N	9308	1/1	0.96	0.19	-	55,55,55,55	0
6	MG	N	9259	1/1	0.94	0.08	-	34,34,34,34	0
6	MG	N	9473	1/1	0.94	0.23	-	51,51,51,51	0
6	MG	M	9485	1/1	0.88	0.11	-	54,54,54,54	0
6	MG	A	9068	1/1	0.97	0.09	-	39,39,39,39	0
6	MG	N	9193	1/1	0.98	0.08	-	34,34,34,34	0
6	MG	N	9304	1/1	0.93	0.17	-	47,47,47,47	0
6	MG	C	9019	1/1	0.90	0.08	-	57,57,57,57	0
6	MG	M	9250	1/1	0.97	0.06	-	38,38,38,38	0
6	MG	N	9327	1/1	0.89	0.08	-	40,40,40,40	0
6	MG	N	9279	1/1	0.97	0.20	-	54,54,54,54	0
6	MG	M	9312	1/1	0.90	0.09	-	37,37,37,37	0
6	MG	C	9454	1/1	0.93	0.22	-	55,55,55,55	0
6	MG	D	9147	1/1	0.91	0.14	-	41,41,41,41	0
6	MG	N	9286	1/1	0.98	0.13	-	31,31,31,31	0
6	MG	C	9076	1/1	1.00	0.09	-	33,33,33,33	0
6	MG	P	9226	1/1	0.71	0.17	-	43,43,43,43	0
6	MG	F	9099	1/1	0.94	0.18	-	56,56,56,56	0
6	MG	D	9141	1/1	0.91	0.11	-	50,50,50,50	0
6	MG	C	9169	1/1	0.91	0.06	-	42,42,42,42	0
6	MG	K	9251	1/1	0.96	0.06	-	43,43,43,43	0
6	MG	K	9301	1/1	0.93	0.19	-	43,43,43,43	0
6	MG	D	9034	1/1	0.94	0.15	-	41,41,41,41	0
6	MG	N	9422	1/1	0.94	0.11	-	56,56,56,56	0
6	MG	N	9194	1/1	0.79	0.13	-	51,51,51,51	0
6	MG	N	9236	1/1	0.97	0.12	-	39,39,39,39	0
6	MG	C	9170	1/1	0.98	0.10	-	41,41,41,41	0
6	MG	P	9446	1/1	0.97	0.05	-	34,34,34,34	0
6	MG	N	9450	1/1	0.93	0.07	-	48,48,48,48	0
6	MG	C	9079	1/1	0.96	0.20	-	38,38,38,38	0
6	MG	N	9425	1/1	0.93	0.11	-	46,46,46,46	0
6	MG	E	9479	1/1	0.93	0.17	-	62,62,62,62	0
6	MG	M	9475	1/1	0.97	0.23	-	62,62,62,62	0
6	MG	N	9403	1/1	0.96	0.10	-	34,34,34,34	0
6	MG	M	9241	1/1	0.98	0.14	-	36,36,36,36	0
6	MG	A	9171	1/1	0.95	0.15	-	58,58,58,58	0
6	MG	C	9164	1/1	0.97	0.10	-	49,49,49,49	0
6	MG	B	9040	1/1	0.98	0.04	-	36,36,36,36	0
6	MG	M	9237	1/1	0.93	0.16	-	52,52,52,52	0
6	MG	P	9282	1/1	0.95	0.06	-	56,56,56,56	0
6	MG	A	9066	1/1	0.95	0.06	-	47,47,47,47	0
6	MG	A	9075	1/1	0.95	0.07	-	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	C	9462	1/1	0.97	0.13	-	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.