



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:17 PM GMT

PDB ID : 1SMY
Title : Structural basis for transcription regulation by alarmone ppGpp
Authors : Artsimovitch, I.; Patlan, V.; Sekine, S.; Vassylyeva, M.N.; Hosaka, T.; Ochi, K.; Yokoyama, S.; Vassylyev, D.G.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2004-03-10
Resolution : 2.70 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

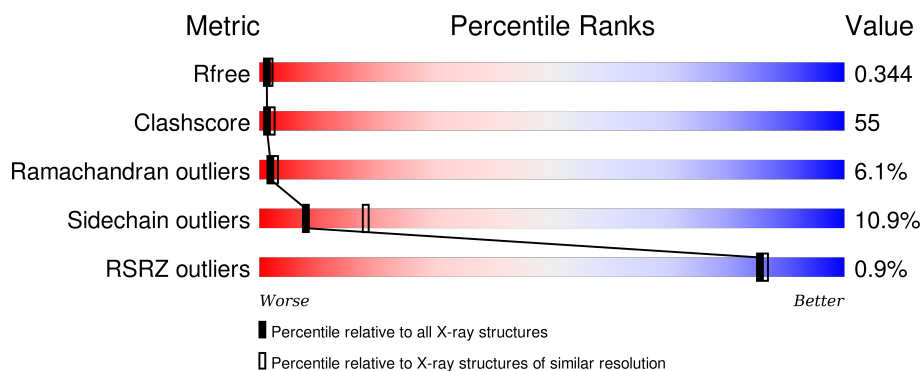
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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></div> <div> <div>21%</div> <div>44%</div> <div>8%</div> <div>27%</div> </div> </div>
1	B	315	<div> <div></div> <div> <div>21%</div> <div>46%</div> <div>5%</div> <div>27%</div> </div> </div>
1	K	315	<div> <div></div> <div> <div>21%</div> <div>46%</div> <div>5%</div> <div>27%</div> </div> </div>
1	L	315	<div> <div></div> <div> <div>23%</div> <div>46%</div> <div>.</div> <div>27%</div> </div> </div>
2	C	1119	<div> <div></div> <div> <div>28%</div> <div>59%</div> <div>12%</div> <div>.</div> </div> </div>

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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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	MG	A	9209	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 63021 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
			8828	5581	1577	1646	24			
2	M	1119	Total	C	N	O	S	0	0	0
			8828	5581	1577	1646	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 SUBUNIT.

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 principal sigma factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	345	Total	C	N	O	S	0	0	0
			2770	1744	504	518	4			
5	P	345	Total	C	N	O	S	0	0	0
			2770	1744	504	518	4			

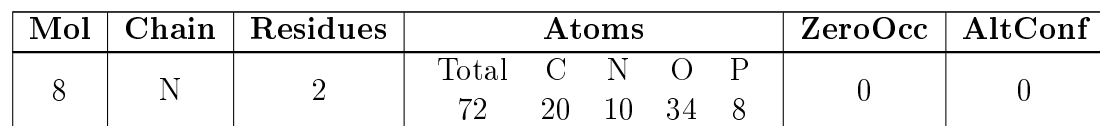
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	150	Total	Mg	0	0
			150	150		
6	E	17	Total	Mg	0	0
			17	17		
6	B	22	Total	Mg	0	0
			22	22		
6	C	92	Total	Mg	0	0
			92	92		
6	A	29	Total	Mg	0	0
			29	29		
6	N	2	Total	Mg	0	0
			2	2		
6	F	49	Total	Mg	0	0
			49	49		
6	M	1	Total	Mg	0	0
			1	1		

- Molecule 7 is ZINC ION (three-letter code: 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 GUANOSINE-5',3'-TETRAPHOSPHATE (three-letter code: G4P) (formula: C₁₀H₁₇N₅O₁₇P₄).



- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|----------------------|---------|---------|
| 9 | A | 296 | Total O
296 296 | 0 | 0 |
| 9 | B | 307 | Total O
307 307 | 0 | 0 |
| 9 | C | 1308 | Total O
1308 1308 | 0 | 0 |
| 9 | D | 1745 | Total O
1745 1745 | 0 | 0 |
| 9 | E | 160 | Total O
160 160 | 0 | 0 |
| 9 | F | 619 | Total O
619 619 | 0 | 0 |
| 9 | K | 316 | Total O
316 316 | 0 | 0 |
| 9 | L | 341 | Total O
341 341 | 0 | 0 |
| 9 | M | 1401 | Total O
1401 1401 | 0 | 0 |
| 9 | N | 1794 | Total O
1794 1794 | 0 | 0 |
| 9 | O | 203 | Total O
203 203 | 0 | 0 |



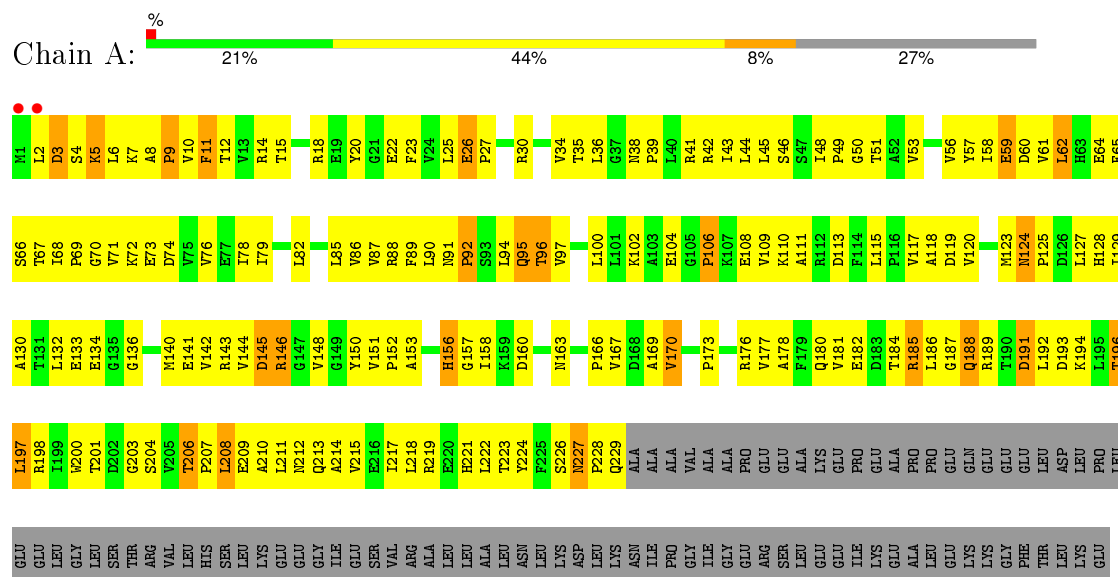
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	P	541	Total	O	0	0
			541	541		

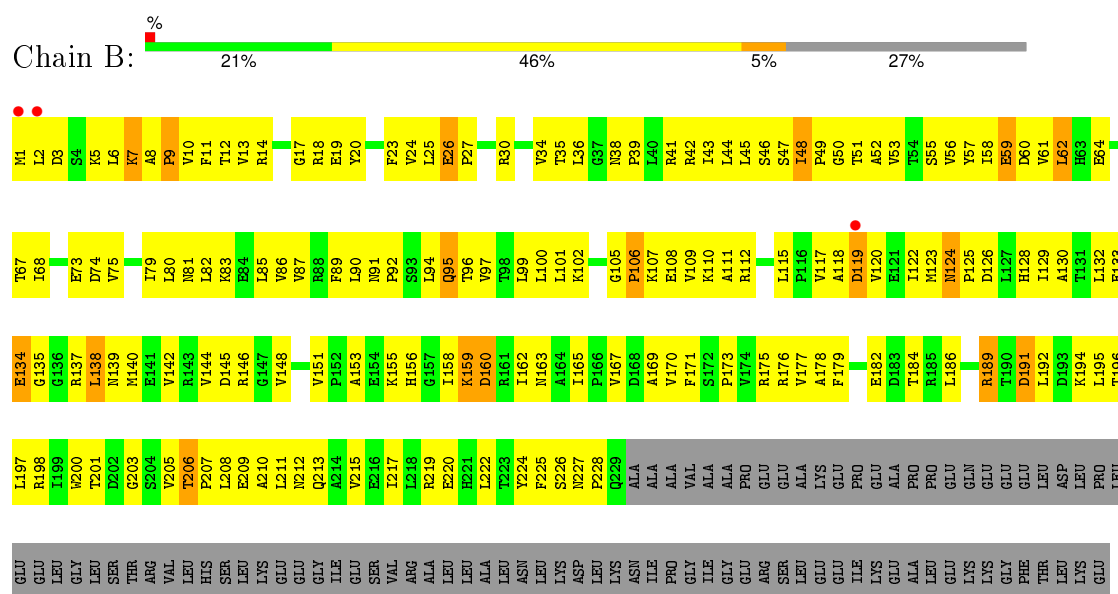
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

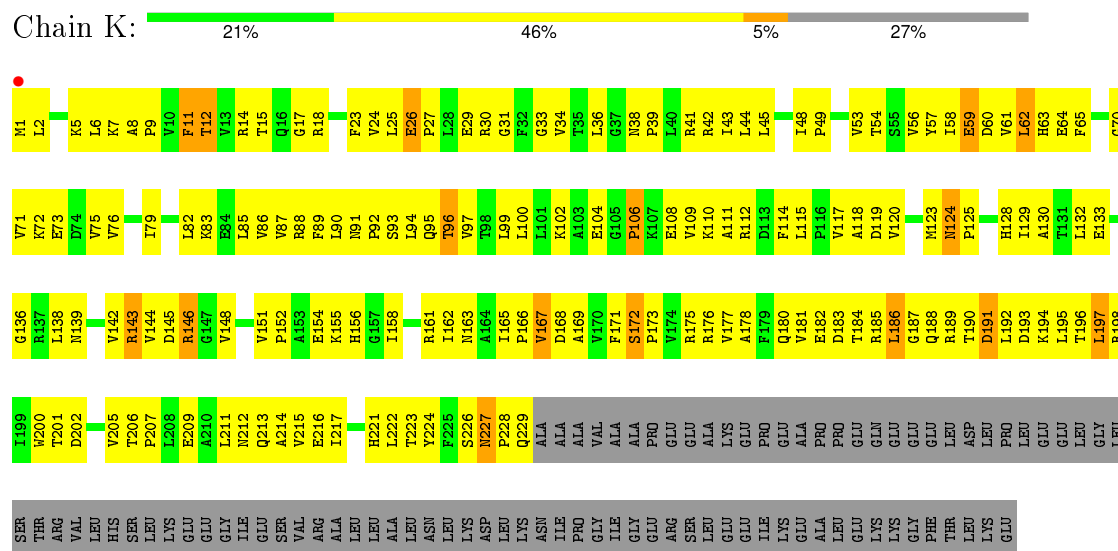
- Molecule 1: DNA-directed RNA polymerase alpha chain



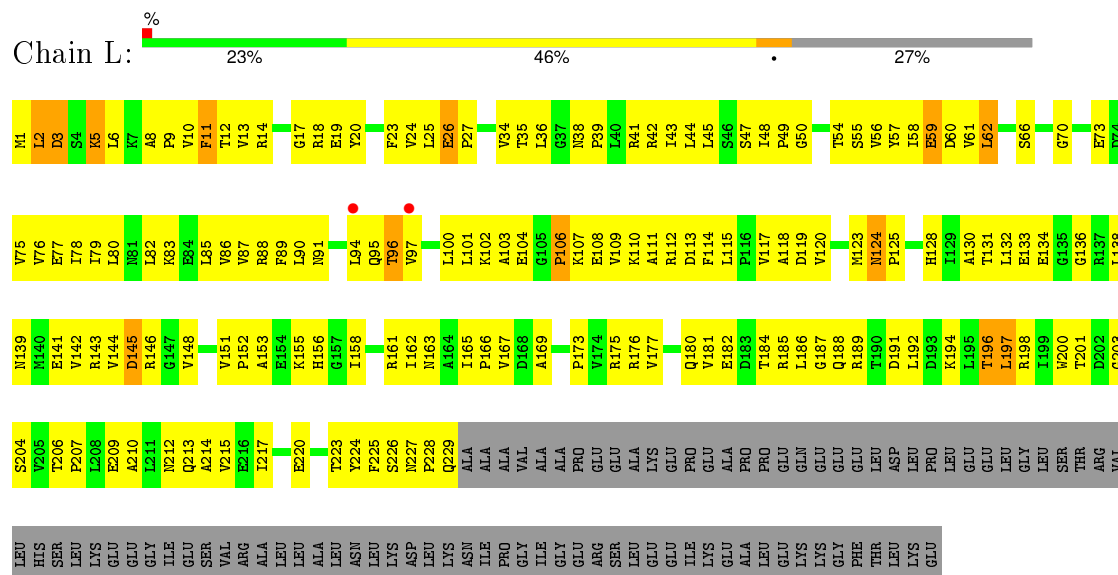
- Molecule 1: DNA-directed RNA polymerase alpha chain



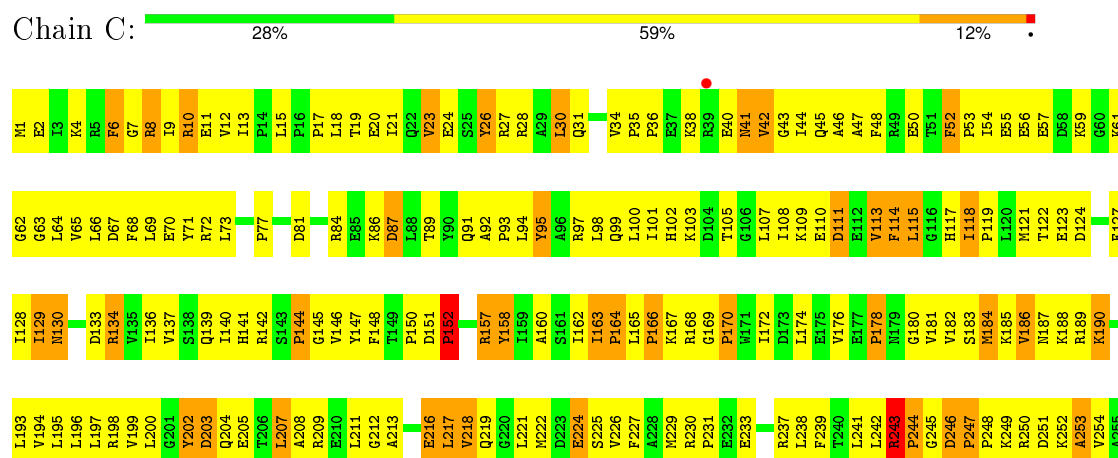
- Molecule 1: DNA-directed RNA polymerase alpha chain



• Molecule 1: DNA-directed RNA polymerase alpha chain



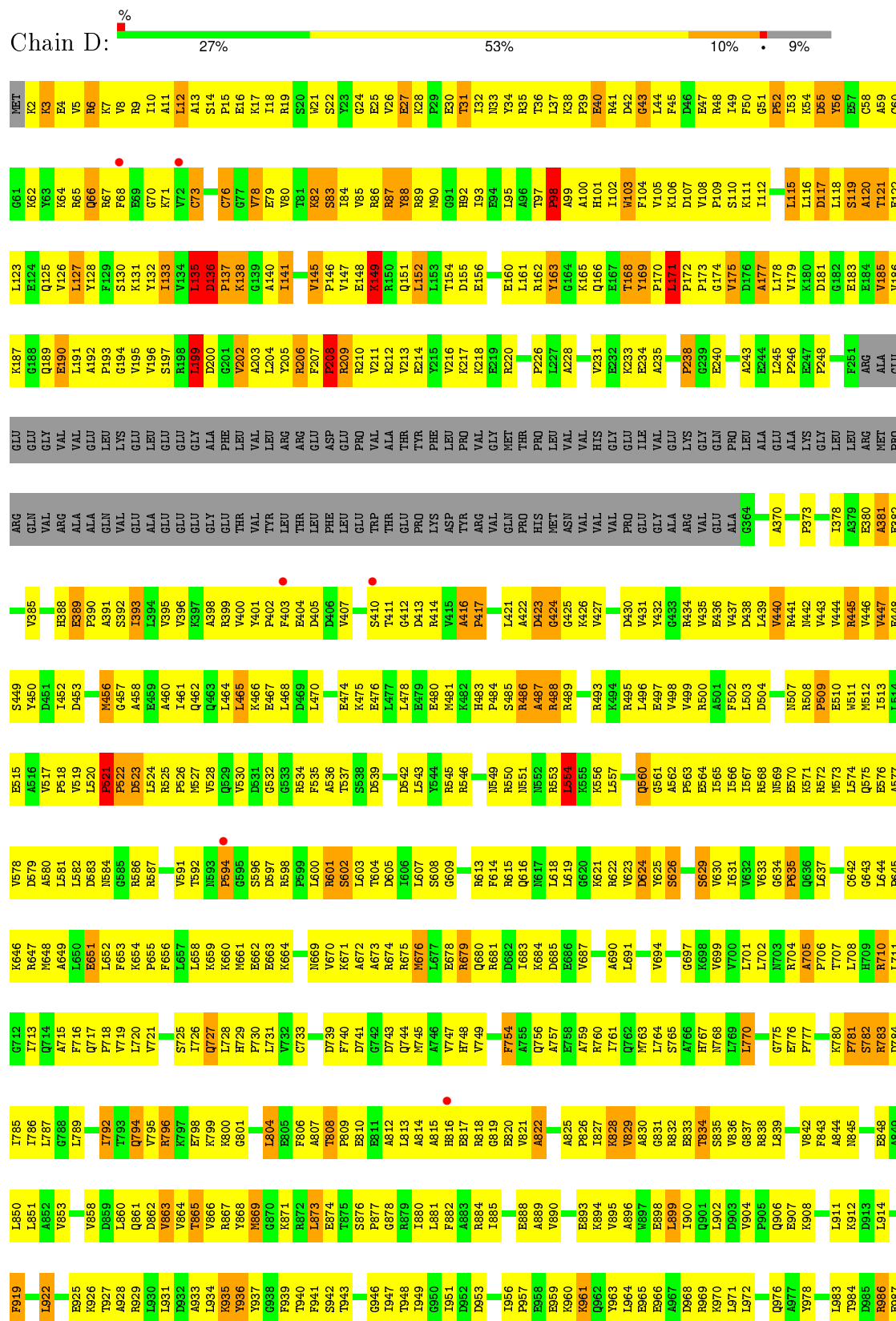
• Molecule 2: DNA-directed RNA polymerase beta chain





F1112	H1047	P982	I910	K846	L773	Y708	P641	P577	A515	I452	F385	H320	G259	L196	D133	G62
L1115	T1048	P983	B911	G847	L774	E709	R642	V578	R516	T463	F386	E321	L260	L197	R134	G63
R1119	L1049	B984	P912	V849	R775	I710	V643	M580	R518	S454		V322	L261	R198	V195	L64
	Q1050	G985	B913	V848	R776	E711	V644	M581	R519	S455	S389	D323	A262	R199	V136	G65
	E1051	P986	I914	A850	I777	A712	V645	T581	G519	A456	Q390	D324	D263	L201	V137	L66
	M1052	P987	K915	K851	F778	R713	G646	G582	B520	A457		I325	P264	G201	S138	D67
	L1053	V988	B916	L852	G779	K716	Q647	L583	P621	Y458	Q393	D826	R265	Y202	Q139	F68
	T1054	V989	I917	L853	E780		R648	E584	V522	A459	F394	H327	R266	D203	I140	L69
	L1055	G990	I918	P854	K781		V649	E585	I523	R460	K395	L328	Y267	Q204	H141	E70
	K1056	Q991	A919	V855	A782		R650	R586	S524	V461	D396		D268	E205	S142	Y71
	S1057	P992	Q920	E856	R783		G651	V587	S525	G462	E397	R331	L269	T206	R144	R72
	D1058	P993	Y925	M857	D784		G652	V588	P526	E463	T398	R332	G270	L207	P144	L73
	L1059		P926	M858	V785		G653	R589	E527	L464	I399	I333	E271	A208	G145	
	I1060	P996	G927	P859	K786		L654	D590	E528	G465		R334	A272	R209	V146	P76
	R1063	P997	G927	B860			L655				S402	T335	A273	E210	F147	
	H1064	P998	K928	G864	L790		D657	A594	F531	R468	S403	T336	G274	E211	F148	E82
	A1065	H999	R929	T865	L791		G658	L595	M532	T469	L404	G337	Y275	G212	T149	R84
	A1066	M1000	K930	P866	R792		P659	Y596	D533	P470	R405	E338	K276	A213	P150	
	Y1067	V1001	G931	V867	V792		A660	A597	V534	Y471	H406	L339	A277		D151	
	D1003	E932	B932	V867			A661	E598	S535	R472	R407	M340	E278	E216	P152	D87
	D1004	D937	K938	D868	G798		S661	E599	P536	R473	R408	T341	E279			L88
	M1005	K938	R939	V869	V799		N663	D600	K537	G476	R409	Q343	L281	Q219	R157	T89
	H1006	R939		L871	V801		G664	E602	V539	G477	S411	F344	G282	G220	I159	Q91
	D1007	R939		M872	R802			V603		V478	A412	R345	L283	L221	A160	A92
	Y1074			P873	T803			A604	S541	V479	L413	V346	R284	V222	S181	P93
	V1076			L874			A667	R605	V542	T480	G414	G347	L285	D223	I162	L94
	E1077			G875	D810		L668	V606	N543	D481	P415	E349	L286	E224	I163	Y95
	P1079			P876	G812		Q670	D607	T544	E482	G416	R350	G287	S225	P164	A96
	S1080			R877	G811		N671	G608	N545	V483	G417	R351	R288	V226	L165	R97
	V1081			S878	V613		V672	N609	L546	V484	L418	R352	T289	P227	P166	L98
	P1082			R879	L613		L673	R610	T547	Y485	T419	A352	L290	A228	K167	Q99
	L1015			R880	K816		V674	L611	P548		R420	R353	A291	L229	R168	L100
	T1017			N881	P817		A675	V612	F549	A488	G424	V355	R292	E230	G169	I101
	D1075			L882	G818		L676	V613	L550	T489	F425			P231	P170	K103
	V1077			G883	V619		N677	R614	E551	E491	D426	M359	D295	E232	W172	
	E1087			Q894	R820		P678	V615	B552	D492	V427	L360	E297	E233	D173	
	L1088			L885	E821		F679	E616	D553	R493	R428		F298	A234	L174	
	V1089			L886	V822		D680	D617	D554	Y494		S363		R237	E175	
	K1090			E887	V823			L620	A555	T495	H431		D300	L238	V176	
	L1092			R889	V825			V621	B557	A497	R432	S366	E301		D111	K109
	Q1093			L892	Y826			E622		Q498	T433	L367	V302	L241	E177	E110
	A1094			A893	V827			L625	N560	Q499	H434	T368	F303	L242	P178	E112
	L1095				A828			R626	G561	M500	V435	P369	L304	L243	R179	V113
	A1096			F896	Q829		L690	R627	S562	T501	G436	A370	F305	R243	V181	F114
	L1097			L897	R830		S691	F628	N564	P502	R437	K371	T306	G245	V182	G116
	D1098			G898	R831		E692	G634	R564	P503	L438	L372	T307	D246	S183	H117
	M1099			Q899	K832		E693	V629	D565	L503	Q439	V373	R308	P247	M184	I118
	Q1100			R900	L833		E694	R630	T566	E504		N374	Y309	P248	K185	P119
	T1101			V901			L694	S631	Q567	G505	B442	S375	L310	R249	V186	L120
	E1104			E764	D837		L695	N632	A568	N506	T443	R376	F311	R250	M187	M121
	K1105			S765	K838		L696	Q633	V569	R507	P444	P377	A312	D251	K188	
	D1106			E766	L839		R697	G634	P570	L508	E445	L378	L313	K252	R189	D124
	N1107			P767	R839		D698	T635	L571	A509	Q446	R379	T314	A253	K190	F127
	P1108			T768	N841		F699	G636	T572	A510	A447	A380	A315	D254	F191	
	Y1109			P769	R842		Y700	L637	R573	E511	M448	A381	G316	A255	P192	
	D1110			E771	T701			D638	A574	R512	L449	L382	V317	A256	L193	
	I1111			R772	R707			R640	A576	V514	L451	E384	G319	V258	P194	
															N130	

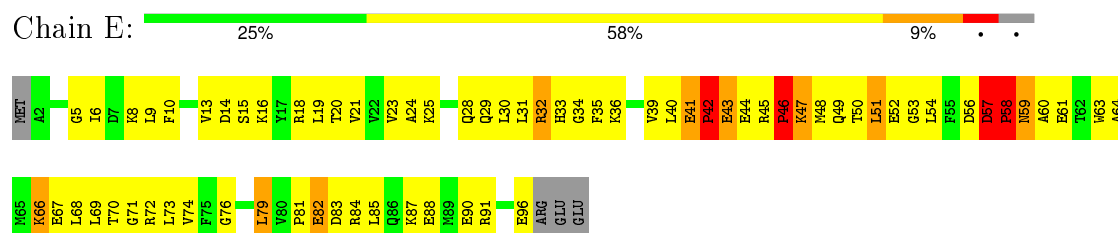
● Molecule 3: DNA-directed RNA polymerase beta' chain



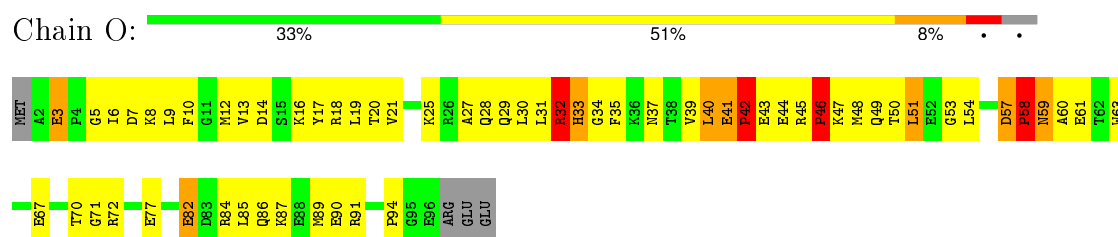


R1388	G1322	T1253	P1191	T1052	1992	A918	L850	G788	V719	L652	G585	A516	D453	I393
L1389	Q1323	L1253	L1192	F1053	L993	F919	L851	L789	L720	F653	R586	V617	A454	L394
E1391	P1324	P1257	T1193	E1054	Q994	L920	A952	L792	W721	K654	R587	P518	R455	V395
G1392	L1325	R1258	C1194	V1055	Q995	R921	V853	T792	E722	P655	G588	V519	R456	V396
G1393	T1326	L1262	Q1195	P1056	W996	L922	A854	T793	G723	F656	R589	P521	K397	K397
V1394	R1327	L1262	P1120	V1057	W997	L922	A854	Q794	Q724	L657	P590	P522	A458	A398
L1395	L1327	L1197	L1122	R1058	E998	E925	V858	T795	L728	L658	P594	P523	E459	R399
L1396	L1328	F1198	F1123	S1059	T999	R926	D859	R796	L729	K660	R595	D523	A460	V400
E1396	D1331	R1266	Q1124	S1060	T1000	T927	L860	K797	H729	K661	G595	L524	L461	P402
H1397	P1332	P1267	P1125	F1061	E1001	A928	Q861	T798	K732	E662	S596	P525	Q462	F403
H1398	H1333	D1268	C1201	R1062	K992	R928	D862	K799	V732	E663	D597	P526	Q463	P403
L1399	Q1334	E1269	E1202	E1063	V1003	L930	V863	K800	G733	K663	R598	V527	L464	E404
V1400	L1335	L1270	K1203	G1064	T1004	L931	V864	G801	E734	K664	P599	V528	L465	D405
E4401	L1336	K1271	C1204	L1065	Q1005	L931	T865	G801	E735	K664	L600	V528	L466	D406
A1402	L1337	A1272	Y1205	T1066	Q1006	R935	V866	L804	F736	N669	R601	F535	E467	V407
L1403	L1338	V1273	G1206	V1067	V1007	R936	R867	R805	N737	V670	S602	A536	L468	E408
N1404	L1339	R1133	L1134	L1068	F1008	R939	V868	F806	A738	K671	L603	T537	D469	V409
L1406	L1340	R1135	R1135	E1069	K1009	F939	G870	A807	D739	A672	T604	D538	L470	S410
L1407	V1344	K1136	K1136	E1070	M1010	S942	K371	T808	D743	R674	D605	D539	E471	T411
I1408	E1345	R1137	R1137	S1073	F1011	T943	R372	R809	D743	R674	L606	L543	A472	G412
A1409	R1346	L1144	L1144	H1075	E1013	T944	L873	E810	Q744	R675	L607	Y544	L473	G413
E1410	Y1347	L1145	L1145	G1076	N1014	S945	E874	A812	M745	M676	S608	Y544	R474	R414
G1411	L1348	Y1145	Y1145	A1077	Y1015	G946	T875	A813	V747	R679	G609	R545	R475	R415
K1412	V1349	G1146	G1146	R1078	P1016	T947	S876	A814	H748	Q680	D611	R546	E476	A416
T1413	E1350	R1147	R1147	K1079	F1017	T948	P877	A815	V749	R881	G612	L547	L477	P417
V1414	E1351	L1148	L1148	G1080	P1018	T948	G878	H816	F750	R882	R613	L548	E479	L478
V1415	L1218	G1218	G1218	D1083	P1019	T951	R879	R818	L751	L683	F614	R549	E480	E479
V1416	E1219	L1149	L1149	D1084	L1020	D952	R879	R818	S752	L683	F614	R549	E480	E479
K1417	G1222	V1155	V1155	L1085	Y1021	D953	E891	G819	S753	D685	L619	N552	N481	N481
K1418	L1223	L1156	L1156	L1086	V1022	A954	R884	E820	F754	E686	G620	R553	D423	D423
L1421	V1224	G1157	G1157	L1087	M1023	V955	A887	E821	Q756	R687	K621	L554	G424	G424
M1422	A1225	V1158	V1158	R1087	A1024	I956	A887	A822	Q756	R687	K621	L554	G424	G424
G1423	Q1227	R1159	R1159	T1088	Q1025	P957	E888	E822	Q756	R687	K621	L554	G424	G424
V1424	S1228	L1160	L1160	A1089	S1026	E958	E888	N824	E758	A690	G623	K556	K426	K426
T1425	L1229	E1161	E1161	D1090	G1027	E959	V890	A825	A759	L691	Y625	L557	K427	K427
L1428	G1230	G1163	G1163	S1091	A1028	E991	E891	P826	R760	E692	G625	L558	R489	R489
L1429	E1231	R1164	R1164	Q1092	R1029	Q962	D892	I827	R763	E693	R628	A559	A490	A490
S1430	P1232	Y1165	Y1165	T1093	G1030	P963	E893	K828	L764	V694	G629	Q560	D430	D430
T1431	L1233	L1166	L1166	L1094	M1031	L964	R894	E829	L764	V694	G629	Q560	D430	D430
K1432	G1234	S1167	S1167	R1096	Q1033	E966	A896	G831	A766	V699	G632	L566	G433	G433
S1433	L1235	M1168	M1168	K1097	Q1034	A967	A897	R832	H767	V700	V633	L566	R434	R434
V1434	L1236	D1169	D1169	L1098	I1035	D968	E897	R833	H768	V700	V633	L566	R434	R434
L1435	T1237	L1175	L1175	V1099	I1036	R969	L899	T834	L769	L701	G634	L567	E437	E437
A1438	M1238	K1176	K1176	D1100	Q1037	R970	L899	R834	L769	L701	G634	L567	E437	E437
F1439	R1239	E1179	E1179	V1101	L1038	L971	Q901	V836	S771	L702	G634	L567	E437	E437
S1439	T1240	A1180	A1180	T1102	C1039	L971	Q901	R837	P772	N703	G636	L567	E437	E437
F1440	F1241	E1179	E1179	H1103	G1040	L971	Q901	R838	P772	N703	G636	L567	E437	E437
N1442	H1242	A1180	A1180	E1104	L1041	E975	V904	I839	S774	T707	G641	L574	D504	D504
L1443	T1243	G1181	G1181	I1105	R1042	L983	P905	K840	P777	L708	G642	Q575	V443	V443
V1446	G1244	E1182	E1182	V1106	G1043	T984	Q906	Y841	P777	L708	G642	Q575	V443	V443
L1447	L1245	L1183	L1183	E1109	M1044	T984	Q906	Y841	P777	L708	G642	Q575	V443	V443
T1448	V1246	Q1184	Q1184	A1110	M1045	D985	K908	F843	P781	L711	P645	V578	V446	V446
D1449	A1247	V1186	V1186	A1110	Q1046	R986	N909	R844	S782	L711	P645	V578	V446	V446
L1450	L1248	F1187	F1187	D1111	K1047	E987	S910	N845	R783	I713	R647	A580	E448	E448
T1451	G1249	P1187	P1187	C1112	F1048	R988	S910	N845	R783	I713	R647	A580	E448	E448
E1450	L1250	V1188	V1188	G1112	F1048	R988	S910	N845	R783	I713	R647	A580	E448	E448
L1451	D1251	L1189	L1189	T1114	S1049	Y989	K912	D847	I785	A715	L649	L582	S449	S449
L1452	I1252	S1190	S1190	T1115	E1051	Q991	Q917	E848	L787	F716	L651	L584	D450	D450

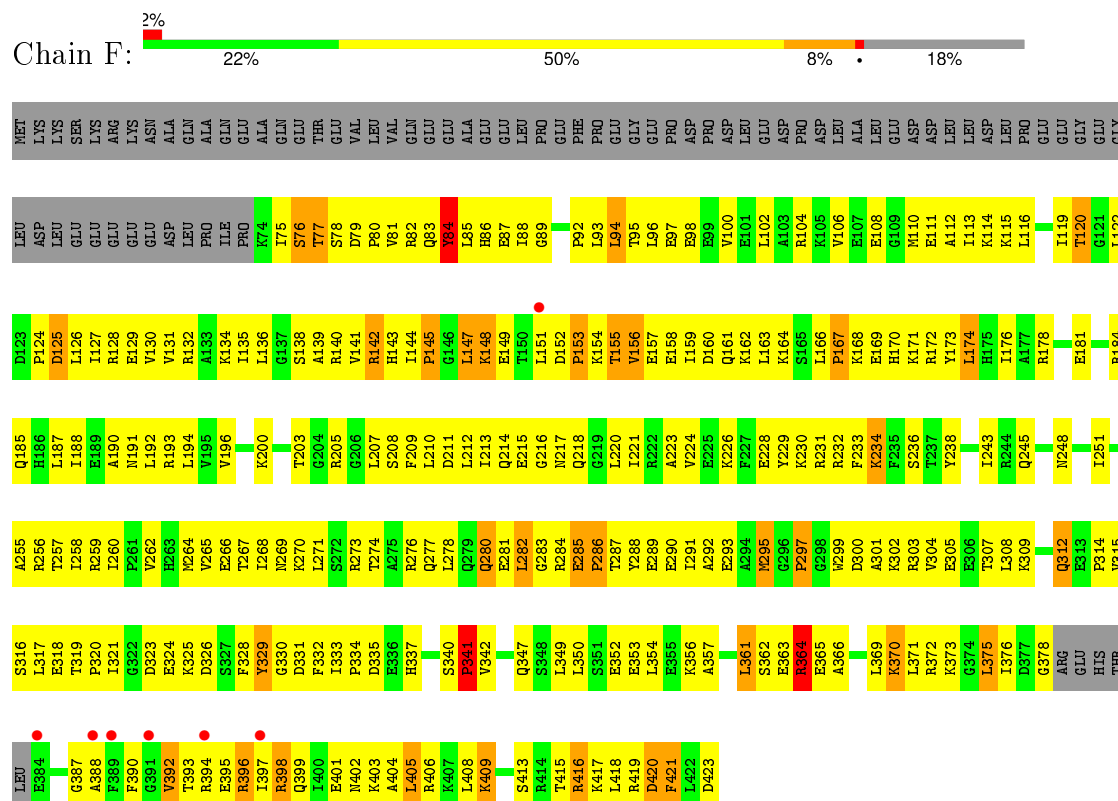
- Molecule 4: RNA POLYMERASE OMEGA SUBUNIT



- Molecule 4: RNA POLYMERASE OMEGA SUBUNIT

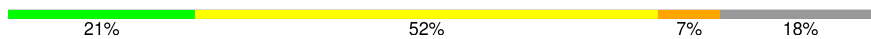


- Molecule 5: principal sigma factor



- Molecule 5: principal sigma factor

Chain P:



WET	LEU	I127	P261	E324	F390
LYS	ASP	R128	V262	K325	G391
LYS	LEU	E129	R263	Y329	T392
SER	GLU	V130	M264		T393
GLY	GLU	V131	V265		R394
ARG	GLU	R132	E266		E395
LYS	GLU	L194	T267		R396
ASN	GLU	A133	I268		I397
ALA	ASP	K134	R269		Q398
ALA	ASP	I135	R270		I400
GLN	LEU	L136	L271		E401
ALA	PRO	G137	L272		M402
GLN	PRO	S138	R273		K403
GLU	PRO	R140	R276		A404
ALA	K74	V141	Q277		L405
GLN	I75	R142	L278		R406
GLU	S76	G204	Q279		K407
THR	T77	H143	Q280		L408
GLU	S78	I144	Q281		K409
VAL	D79	P145	E282		Y410
LEU	P80	G146	R283		E412
VAL	V81	L147	E285		S413
GLN	R82	K148	E286		R416
GLU	Q83	T150	E287		K417
GLU	Y84	L151	Y288		L418
ALA	L85	D152	E289		R419
GLU	H86	P153	E290		D420
GLU	E87	K154	L291		F421
LEU	I88	T155	A292		L422
PRO	V91	V156	E293		D423
GLU	P92	E157	A294		
PHE	L93	E158	R295		
PRO	L94	I159	P297		
GLU	T95	D160	G298		
GLY	L96	Q161	V299		
GLU	E97	K162	K302		
PRO	E98	L163	R303		
ASP	E99	K164	V304		
PRO		S165	E305		
ASP	L102	L166	E306		
LEU	V106	P167	T307		
ASP		K168	L308		
PRO	G109	E169	K309		
ASP	M110	H170	I310		
LEU	I113	K171	A311		
ALA	I114	R172	Q312		
GLU	K115	Y173	E313		
ASP	L116	L174	F314		
ASP	S117	H175	V315		
LEU	E118	I176	S316		
LEU	E119	A177	L317		
ASP	T120	R178	G318		
LEU	G121	I181	E319		
PRO	L122	A182	T319		
GLU	D123	R183	P320		
GLY	P124	R184	I321		
GLU	R125	Q185	G322		
GLY	L126	I188	D323		

4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	236.35Å 236.35Å 249.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.70 50.12 – 2.71	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.70) 97.1 (50.12-2.71)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.73Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.186 , 0.266 0.305 , 0.344	Depositor DCC
R_{free} test set	14873 reflections (3.77%)	DCC
Wilson B-factor (Å ²)	51.1	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.499 for -h,-k,l 0.086 for h,-h-k,-l 0.086 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Outliers	0 of 409145 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	63021	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% 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: G4P, 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	0.68	0/1838	0.70	0/2498
1	B	0.68	0/1838	0.68	0/2498
1	K	0.68	0/1838	0.72	1/2498 (0.0%)
1	L	0.68	0/1838	0.67	1/2498 (0.0%)
2	C	0.75	0/8996	0.79	4/12164 (0.0%)
2	M	0.74	0/8996	0.78	4/12164 (0.0%)
3	D	0.74	0/10975	0.81	10/14836 (0.1%)
3	N	0.73	0/10975	0.81	14/14836 (0.1%)
4	E	0.74	0/783	0.81	0/1054
4	O	0.75	0/783	0.81	0/1054
5	F	0.65	0/2811	0.75	1/3781 (0.0%)
5	P	0.64	0/2811	0.74	1/3781 (0.0%)
All	All	0.72	0/54482	0.78	36/73662 (0.0%)

There are no bond length outliers.

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	243	ARG	C-N-CD	-9.21	100.34	120.60
3	D	199	LEU	CA-CB-CG	-8.95	94.72	115.30
3	N	199	LEU	CA-CB-CG	-8.85	94.94	115.30
1	K	197	LEU	CA-CB-CG	8.22	134.21	115.30
2	C	243	ARG	C-N-CD	-7.23	104.69	120.60

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	211	0
1	B	1806	0	1861	191	0
1	K	1806	0	1861	196	0
1	L	1806	0	1861	183	0
2	C	8828	0	8933	1013	0
2	M	8828	0	8933	1065	0
3	D	10797	0	10873	1260	0
3	N	10797	0	10873	1227	0
4	E	769	0	775	104	0
4	O	769	0	775	96	0
5	F	2770	0	2844	327	0
5	P	2770	0	2844	363	0
6	A	29	0	0	0	0
6	B	22	0	0	0	0
6	C	92	0	0	0	0
6	D	150	0	0	0	0
6	E	17	0	0	0	0
6	F	49	0	0	0	0
6	M	1	0	0	0	0
6	N	2	0	0	0	0
7	D	2	0	0	0	0
7	N	2	0	0	0	0
8	N	72	0	22	9	0
9	A	296	0	0	67	0
9	B	307	0	0	66	0
9	C	1308	0	0	281	0
9	D	1745	0	0	322	0
9	E	160	0	0	37	0
9	F	619	0	0	99	0
9	K	316	0	0	72	0
9	L	341	0	0	64	0
9	M	1401	0	0	325	0
9	N	1794	0	0	330	0
9	O	203	0	0	33	0
9	P	541	0	0	96	0
All	All	63021	0	54316	5952	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 55.

The worst 5 of 5952 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:34:VAL:HB	2:C:38:LYS:HG3	1.28	1.11
2:C:1054:THR:HG21	2:C:1079:PRO:HB3	1.33	1.10
2:M:857:ASP:HB2	2:M:978:ARG:HG2	1.34	1.10
8:N:9100:G4P:H5"	8:N:9100:G4P:H8	1.14	1.09
3:N:148:GLU:HB3	3:N:151:GLN:HB2	1.35	1.08

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%)	187 (82%)	33 (14%)	7 (3%)	5	12
1	B	227/315 (72%)	183 (81%)	38 (17%)	6 (3%)	7	16
1	K	227/315 (72%)	186 (82%)	32 (14%)	9 (4%)	4	8
1	L	227/315 (72%)	185 (82%)	37 (16%)	5 (2%)	8	22
2	C	1117/1119 (100%)	856 (77%)	194 (17%)	67 (6%)	2	3
2	M	1117/1119 (100%)	863 (77%)	187 (17%)	67 (6%)	2	3
3	D	1388/1524 (91%)	1047 (75%)	248 (18%)	93 (7%)	1	2
3	N	1388/1524 (91%)	1042 (75%)	251 (18%)	95 (7%)	1	2
4	E	93/99 (94%)	72 (77%)	11 (12%)	10 (11%)	0	0
4	O	93/99 (94%)	70 (75%)	13 (14%)	10 (11%)	0	0
5	F	341/423 (81%)	264 (77%)	53 (16%)	24 (7%)	1	2
5	P	341/423 (81%)	267 (78%)	53 (16%)	21 (6%)	2	2
All	All	6786/7590 (89%)	5222 (77%)	1150 (17%)	414 (6%)	2	3

5 of 414 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	ALA
1	A	188	GLN
1	B	118	ALA
2	C	10	ARG
2	C	59	LYS

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%)	181 (90%)	21 (10%)	9	20
1	B	202/273 (74%)	186 (92%)	16 (8%)	15	34
1	K	202/273 (74%)	187 (93%)	15 (7%)	17	39
1	L	202/273 (74%)	190 (94%)	12 (6%)	24	51
2	C	941/941 (100%)	827 (88%)	114 (12%)	6	14
2	M	941/941 (100%)	838 (89%)	103 (11%)	8	18
3	D	1123/1279 (88%)	992 (88%)	131 (12%)	7	15
3	N	1123/1279 (88%)	987 (88%)	136 (12%)	6	14
4	E	83/87 (95%)	73 (88%)	10 (12%)	6	14
4	O	83/87 (95%)	73 (88%)	10 (12%)	6	14
5	F	295/370 (80%)	263 (89%)	32 (11%)	8	18
5	P	295/370 (80%)	273 (92%)	22 (8%)	17	38
All	All	5692/6446 (88%)	5070 (89%)	622 (11%)	8	18

5 of 622 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	1487	VAL
1	L	145	ASP
3	N	1287	GLU
4	E	61	GLU

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Mol	Chain	Res	Type
5	F	362	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 162 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	337	HIS
2	M	41	ASN
4	O	33	HIS
1	K	81	ASN
1	L	81	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 368 ligands modelled in this entry, 366 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	$\# Z > 2$
8	G4P	N	9100	6	29,38,38	1.49	4 (13%)	42,61,61	2.32	11 (26%)
8	G4P	N	9101	6	29,38,38	1.66	6 (20%)	42,61,61	2.44	11 (26%)

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
8	G4P	N	9100	6	-	0/23/43/43	0/3/3/3
8	G4P	N	9101	6	-	0/23/43/43	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	N	9101	G4P	C8-N7	-2.53	1.29	1.34
8	N	9100	G4P	C8-N7	-2.50	1.29	1.34
8	N	9101	G4P	C2-N2	2.14	1.38	1.34
8	N	9101	G4P	PD-O3D	2.59	1.64	1.54
8	N	9101	G4P	C2-N1	2.70	1.40	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	N	9100	G4P	C5-C6-N1	-8.54	111.91	123.59
8	N	9101	G4P	C5-C6-N1	-8.45	112.03	123.59
8	N	9101	G4P	C2'-C1'-N9	-5.39	106.05	114.29
8	N	9101	G4P	PC-O3C-PD	-5.37	114.65	132.67
8	N	9100	G4P	PA-O3A-PB	-4.45	117.73	132.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	N	9100	G4P	4	0
8	N	9101	G4P	5	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [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%)	-0.71	2 (0%) 85 86	39, 65, 90, 121	0
1	B	229/315 (72%)	-0.67	3 (1%) 79 79	58, 82, 103, 129	0
1	K	229/315 (72%)	-0.69	1 (0%) 93 94	42, 65, 87, 117	0
1	L	229/315 (72%)	-0.68	2 (0%) 85 86	54, 88, 104, 122	0
2	C	1119/1119 (100%)	-0.77	1 (0%) 95 97	31, 73, 106, 124	0
2	M	1119/1119 (100%)	-0.73	7 (0%) 90 91	30, 75, 110, 122	0
3	D	1392/1524 (91%)	-0.67	17 (1%) 81 81	33, 71, 108, 152	0
3	N	1392/1524 (91%)	-0.69	18 (1%) 79 79	35, 71, 108, 145	0
4	E	95/99 (95%)	-0.87	0 100 100	49, 79, 103, 109	0
4	O	95/99 (95%)	-0.74	0 100 100	42, 81, 111, 119	0
5	F	345/423 (81%)	-0.58	7 (2%) 68 69	53, 84, 111, 126	0
5	P	345/423 (81%)	-0.63	2 (0%) 90 91	41, 83, 110, 117	0
All	All	6818/7590 (89%)	-0.70	60 (0%) 85 86	30, 74, 108, 152	0

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	1246	VAL	7.4
3	D	1245	GLY	7.3
3	D	1246	VAL	6.6
3	N	1247	ALA	6.3
1	K	1	MET	5.5

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	A	9209	1/1	1.00	0.20	2.92	20,20,20,20	0
6	MG	D	9232	1/1	1.00	0.10	0.03	20,20,20,20	0
6	MG	F	9229	1/1	0.99	0.11	-0.14	20,20,20,20	0
6	MG	C	9438	1/1	0.99	0.11	-0.56	20,20,20,20	0
8	G4P	N	9101	36/36	0.99	0.11	-0.60	35,45,50,50	0
6	MG	D	9234	1/1	1.00	0.09	-0.61	20,20,20,20	0
8	G4P	N	9100	36/36	0.98	0.11	-0.66	35,45,54,55	0
7	ZN	N	9105	1/1	0.98	0.10	-0.72	80,80,80,80	0
7	ZN	D	9103	1/1	0.98	0.09	-0.88	87,87,87,87	0
6	MG	C	9346	1/1	1.00	0.10	-1.22	20,20,20,20	0
6	MG	C	9396	1/1	0.99	0.07	-1.39	20,20,20,20	0
6	MG	C	9282	1/1	0.99	0.05	-1.52	20,20,20,20	0
6	MG	D	9220	1/1	0.98	0.07	-1.54	20,20,20,20	0
6	MG	D	9242	1/1	1.00	0.11	-1.56	20,20,20,20	0
6	MG	D	9294	1/1	0.98	0.07	-1.56	20,20,20,20	0
6	MG	B	9235	1/1	0.98	0.06	-1.62	20,20,20,20	0
7	ZN	D	9102	1/1	0.96	0.06	-1.63	115,115,115,115	0
6	MG	C	9238	1/1	0.98	0.07	-1.67	20,20,20,20	0
6	MG	F	9374	1/1	0.99	0.05	-1.67	20,20,20,20	0
7	ZN	N	9104	1/1	0.98	0.05	-1.68	116,116,116,116	0
6	MG	F	9302	1/1	0.99	0.06	-1.70	20,20,20,20	0
6	MG	D	9225	1/1	0.99	0.06	-1.73	20,20,20,20	0
6	MG	F	9303	1/1	0.99	0.06	-1.77	20,20,20,20	0
6	MG	D	9353	1/1	0.99	0.05	-1.77	20,20,20,20	0
6	MG	D	9283	1/1	0.99	0.10	-1.78	20,20,20,20	0
6	MG	E	9432	1/1	0.99	0.06	-1.86	20,20,20,20	0
6	MG	F	9251	1/1	0.99	0.05	-1.92	20,20,20,20	0
6	MG	D	9218	1/1	0.99	0.07	-1.94	20,20,20,20	0
6	MG	E	9366	1/1	1.00	0.05	-1.99	20,20,20,20	0
6	MG	D	9236	1/1	0.99	0.08	-2.11	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	B	9230	1/1	1.00	0.07	-2.14	20,20,20,20	0
6	MG	D	9523	1/1	0.99	0.09	-2.14	20,20,20,20	0
6	MG	F	9244	1/1	0.99	0.05	-2.40	20,20,20,20	0
6	MG	B	9427	1/1	0.99	0.04	-2.45	20,20,20,20	0
6	MG	D	9557	1/1	0.99	0.06	-2.47	20,20,20,20	0
6	MG	C	9507	1/1	0.99	0.03	-2.52	20,20,20,20	0
6	MG	D	9262	1/1	0.99	0.05	-2.55	20,20,20,20	0
6	MG	D	9247	1/1	0.99	0.07	-2.57	20,20,20,20	0
6	MG	D	9211	1/1	0.99	0.06	-2.72	20,20,20,20	0
6	MG	D	9253	1/1	0.99	0.08	-2.83	20,20,20,20	0
6	MG	C	9525	1/1	0.97	0.05	-2.86	20,20,20,20	0
6	MG	D	9312	1/1	1.00	0.05	-2.89	20,20,20,20	0
6	MG	C	9213	1/1	1.00	0.05	-2.90	20,20,20,20	0
6	MG	D	9480	1/1	0.98	0.07	-2.93	20,20,20,20	0
6	MG	C	9264	1/1	0.99	0.07	-3.06	20,20,20,20	0
6	MG	C	9210	1/1	0.98	0.05	-3.12	20,20,20,20	0
6	MG	C	9408	1/1	0.99	0.05	-3.20	20,20,20,20	0
6	MG	C	9221	1/1	0.99	0.07	-3.26	20,20,20,20	0
6	MG	C	9266	1/1	1.00	0.07	-3.36	20,20,20,20	0
6	MG	D	9386	1/1	0.98	0.04	-3.39	20,20,20,20	0
6	MG	A	9473	1/1	0.99	0.05	-3.42	20,20,20,20	0
6	MG	D	9319	1/1	1.00	0.04	-3.45	20,20,20,20	0
6	MG	B	9260	1/1	0.99	0.05	-3.63	20,20,20,20	0
6	MG	D	9419	1/1	0.99	0.05	-3.67	20,20,20,20	0
6	MG	D	9233	1/1	0.99	0.06	-3.78	20,20,20,20	0
6	MG	D	9277	1/1	0.99	0.09	-3.83	20,20,20,20	0
6	MG	C	9300	1/1	0.99	0.03	-3.87	20,20,20,20	0
6	MG	C	9287	1/1	0.99	0.04	-3.91	20,20,20,20	0
6	MG	D	9307	1/1	1.00	0.06	-4.11	20,20,20,20	0
6	MG	C	9263	1/1	0.99	0.08	-4.20	20,20,20,20	0
6	MG	A	9227	1/1	0.99	0.05	-4.21	20,20,20,20	0
6	MG	A	9442	1/1	0.99	0.05	-4.67	20,20,20,20	0
6	MG	C	9316	1/1	0.99	0.05	-4.77	20,20,20,20	0
6	MG	C	9239	1/1	0.99	0.04	-4.82	20,20,20,20	0
6	MG	D	9208	1/1	1.00	0.10	-5.14	20,20,20,20	0
6	MG	C	9243	1/1	0.99	0.06	-5.17	20,20,20,20	0
6	MG	C	9501	1/1	0.99	0.06	-6.49	20,20,20,20	0
6	MG	D	9203	1/1	0.99	0.08	-9.42	25,25,25,25	0
6	MG	A	9437	1/1	1.00	0.07	-	20,20,20,20	0
6	MG	C	9554	1/1	0.98	0.06	-	20,20,20,20	0
6	MG	C	9514	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	C	9383	1/1	0.99	0.04	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	D	9337	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	D	9469	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	D	9421	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	A	9318	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	C	9465	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	A	9368	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	D	9390	1/1	0.98	0.07	-	20,20,20,20	0
6	MG	F	9504	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	A	9329	1/1	1.00	0.08	-	20,20,20,20	0
6	MG	D	9285	1/1	0.99	0.11	-	20,20,20,20	0
6	MG	D	9265	1/1	0.99	0.09	-	20,20,20,20	0
6	MG	A	9423	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	D	9342	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	B	9560	1/1	1.00	0.03	-	20,20,20,20	0
6	MG	F	9463	1/1	0.99	0.08	-	20,20,20,20	0
6	MG	D	9533	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	F	9496	1/1	0.98	0.05	-	20,20,20,20	0
6	MG	F	9398	1/1	0.98	0.07	-	20,20,20,20	0
6	MG	F	9450	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	C	9348	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	D	9393	1/1	0.99	0.08	-	20,20,20,20	0
6	MG	D	9379	1/1	1.00	0.07	-	20,20,20,20	0
6	MG	D	9322	1/1	1.00	0.09	-	20,20,20,20	0
6	MG	C	9359	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	C	9356	1/1	0.98	0.07	-	20,20,20,20	0
6	MG	D	9325	1/1	0.99	0.10	-	20,20,20,20	0
6	MG	C	9444	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	D	9434	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	A	9273	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	A	9295	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	C	9257	1/1	0.97	0.06	-	20,20,20,20	0
6	MG	C	9378	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	C	9347	1/1	1.00	0.04	-	20,20,20,20	0
6	MG	C	9320	1/1	0.98	0.06	-	20,20,20,20	0
6	MG	A	9517	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	E	9373	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	D	9331	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	B	9426	1/1	1.00	0.07	-	20,20,20,20	0
6	MG	D	9301	1/1	0.98	0.05	-	20,20,20,20	0
6	MG	C	9451	1/1	0.99	0.11	-	20,20,20,20	0
6	MG	D	9546	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	C	9429	1/1	1.00	0.04	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	F	9414	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	C	9385	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	C	9459	1/1	1.00	0.06	-	20,20,20,20	0
6	MG	E	9415	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	D	9333	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	D	9492	1/1	1.00	0.08	-	20,20,20,20	0
6	MG	F	9298	1/1	0.99	0.08	-	20,20,20,20	0
6	MG	D	9440	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	D	9304	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	D	9526	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	B	9552	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	D	9332	1/1	0.99	0.09	-	20,20,20,20	0
6	MG	D	9443	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	C	9489	1/1	0.99	0.11	-	20,20,20,20	0
6	MG	E	9494	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	D	9360	1/1	1.00	0.05	-	20,20,20,20	0
6	MG	A	9487	1/1	0.99	0.09	-	20,20,20,20	0
6	MG	C	9222	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	D	9472	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	E	9431	1/1	0.98	0.07	-	20,20,20,20	0
6	MG	D	9518	1/1	0.98	0.06	-	20,20,20,20	0
6	MG	F	9309	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	F	9558	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	B	9491	1/1	0.99	0.08	-	20,20,20,20	0
6	MG	B	9228	1/1	1.00	0.08	-	20,20,20,20	0
6	MG	D	9376	1/1	1.00	0.04	-	20,20,20,20	0
6	MG	C	9430	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	B	9488	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	D	9512	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	D	9271	1/1	0.98	0.06	-	20,20,20,20	0
6	MG	D	9349	1/1	1.00	0.03	-	20,20,20,20	0
6	MG	E	9484	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	F	9290	1/1	0.98	0.06	-	20,20,20,20	0
6	MG	F	9436	1/1	1.00	0.11	-	20,20,20,20	0
6	MG	F	9516	1/1	0.99	0.09	-	20,20,20,20	0
6	MG	M	9206	1/1	0.97	0.10	-	38,38,38,38	0
6	MG	D	9461	1/1	1.00	0.06	-	20,20,20,20	0
6	MG	F	9305	1/1	0.98	0.07	-	20,20,20,20	0
6	MG	D	9456	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	D	9548	1/1	0.99	0.09	-	20,20,20,20	0
6	MG	C	9272	1/1	0.97	0.07	-	20,20,20,20	0
6	MG	D	9406	1/1	0.98	0.06	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	D	9529	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	C	9418	1/1	1.00	0.06	-	20,20,20,20	0
6	MG	F	9340	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	D	9343	1/1	1.00	0.05	-	20,20,20,20	0
6	MG	C	9202	1/1	0.96	0.07	-	43,43,43,43	0
6	MG	B	9541	1/1	1.00	0.07	-	20,20,20,20	0
6	MG	A	9254	1/1	1.00	0.04	-	20,20,20,20	0
6	MG	D	9269	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	F	9483	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	C	9534	1/1	1.00	0.05	-	20,20,20,20	0
6	MG	C	9330	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	A	9327	1/1	0.99	0.09	-	20,20,20,20	0
6	MG	C	9454	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	B	9306	1/1	0.99	0.10	-	20,20,20,20	0
6	MG	B	9311	1/1	0.99	0.11	-	20,20,20,20	0
6	MG	D	9258	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	C	9328	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	F	9530	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	F	9270	1/1	1.00	0.03	-	20,20,20,20	0
6	MG	D	9506	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	A	9334	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	D	9241	1/1	0.98	0.06	-	20,20,20,20	0
6	MG	D	9361	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	F	9323	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	F	9445	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	A	9462	1/1	1.00	0.07	-	20,20,20,20	0
6	MG	F	9513	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	D	9477	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	D	9503	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	F	9471	1/1	1.00	0.08	-	20,20,20,20	0
6	MG	C	9299	1/1	0.98	0.06	-	20,20,20,20	0
6	MG	D	9479	1/1	0.99	0.10	-	20,20,20,20	0
6	MG	D	9428	1/1	1.00	0.03	-	20,20,20,20	0
6	MG	D	9372	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	C	9497	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	F	9297	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	D	9562	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	D	9261	1/1	0.99	0.10	-	20,20,20,20	0
6	MG	D	9400	1/1	0.99	0.08	-	20,20,20,20	0
6	MG	F	9326	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	N	9205	1/1	0.99	0.08	-	16,16,16,16	0
6	MG	D	9214	1/1	0.98	0.07	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	D	9336	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	D	9380	1/1	1.00	0.10	-	20,20,20,20	0
6	MG	B	9420	1/1	1.00	0.07	-	20,20,20,20	0
6	MG	F	9382	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	C	9284	1/1	1.00	0.07	-	20,20,20,20	0
6	MG	F	9425	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	C	9217	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	D	9286	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	D	9403	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	C	9338	1/1	1.00	0.06	-	20,20,20,20	0
6	MG	C	9364	1/1	0.98	0.06	-	20,20,20,20	0
6	MG	A	9464	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	C	9395	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	D	9276	1/1	1.00	0.05	-	20,20,20,20	0
6	MG	D	9490	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	C	9474	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	D	9384	1/1	0.96	0.07	-	20,20,20,20	0
6	MG	F	9388	1/1	1.00	0.09	-	20,20,20,20	0
6	MG	B	9281	1/1	1.00	0.04	-	20,20,20,20	0
6	MG	D	9355	1/1	0.98	0.13	-	20,20,20,20	0
6	MG	A	9521	1/1	1.00	0.06	-	20,20,20,20	0
6	MG	E	9551	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	D	9363	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	D	9350	1/1	1.00	0.05	-	20,20,20,20	0
6	MG	D	9216	1/1	0.98	0.08	-	20,20,20,20	0
6	MG	D	9362	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	C	9371	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	D	9370	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	C	9561	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	D	9291	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	D	9460	1/1	0.98	0.04	-	20,20,20,20	0
6	MG	D	9439	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	F	9278	1/1	1.00	0.07	-	20,20,20,20	0
6	MG	D	9226	1/1	0.98	0.04	-	20,20,20,20	0
6	MG	E	9538	1/1	0.99	0.09	-	20,20,20,20	0
6	MG	D	9470	1/1	0.99	0.09	-	20,20,20,20	0
6	MG	C	9267	1/1	0.99	0.09	-	20,20,20,20	0
6	MG	D	9547	1/1	1.00	0.05	-	20,20,20,20	0
6	MG	E	9275	1/1	1.00	0.11	-	20,20,20,20	0
6	MG	B	9280	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	D	9448	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	D	9455	1/1	1.00	0.10	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	D	9559	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	D	9410	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	B	9412	1/1	1.00	0.06	-	20,20,20,20	0
6	MG	B	9458	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	F	9495	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	D	9391	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	C	9405	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	D	9240	1/1	0.96	0.08	-	20,20,20,20	0
6	MG	D	9416	1/1	0.96	0.08	-	20,20,20,20	0
6	MG	D	9344	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	D	9317	1/1	0.99	0.12	-	20,20,20,20	0
6	MG	A	9365	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	A	9486	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	D	9369	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	C	9553	1/1	1.00	0.05	-	20,20,20,20	0
6	MG	D	9315	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	C	9335	1/1	1.00	0.08	-	20,20,20,20	0
6	MG	D	9377	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	C	9519	1/1	0.98	0.05	-	20,20,20,20	0
6	MG	C	9358	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	D	9467	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	D	9447	1/1	1.00	0.07	-	20,20,20,20	0
6	MG	C	9367	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	F	9407	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	D	9399	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	C	9223	1/1	0.99	0.09	-	20,20,20,20	0
6	MG	D	9536	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	D	9215	1/1	1.00	0.08	-	20,20,20,20	0
6	MG	D	9528	1/1	0.97	0.06	-	20,20,20,20	0
6	MG	D	9296	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	B	9446	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	B	9485	1/1	0.98	0.05	-	20,20,20,20	0
6	MG	F	9537	1/1	1.00	0.05	-	20,20,20,20	0
6	MG	D	9452	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	D	9505	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	C	9354	1/1	0.98	0.07	-	20,20,20,20	0
6	MG	F	9375	1/1	0.99	0.10	-	20,20,20,20	0
6	MG	C	9259	1/1	1.00	0.06	-	20,20,20,20	0
6	MG	D	9475	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	A	9520	1/1	0.99	0.08	-	20,20,20,20	0
6	MG	C	9293	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	F	9250	1/1	0.97	0.06	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	D	9248	1/1	1.00	0.06	-	20,20,20,20	0
6	MG	D	9535	1/1	1.00	0.06	-	20,20,20,20	0
6	MG	C	9255	1/1	0.99	0.10	-	20,20,20,20	0
6	MG	F	9424	1/1	0.99	0.09	-	20,20,20,20	0
6	MG	C	9493	1/1	1.00	0.06	-	20,20,20,20	0
6	MG	D	9478	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	C	9466	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	C	9441	1/1	0.98	0.05	-	20,20,20,20	0
6	MG	D	9417	1/1	0.99	0.08	-	20,20,20,20	0
6	MG	C	9345	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	C	9411	1/1	1.00	0.11	-	20,20,20,20	0
6	MG	D	9308	1/1	0.99	0.09	-	20,20,20,20	0
6	MG	A	9268	1/1	1.00	0.10	-	20,20,20,20	0
6	MG	F	9508	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	D	9515	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	C	9381	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	D	9201	1/1	0.97	0.11	-	30,30,30,30	0
6	MG	D	9498	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	D	9404	1/1	0.99	0.09	-	20,20,20,20	0
6	MG	D	9532	1/1	0.98	0.04	-	20,20,20,20	0
6	MG	C	9524	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	C	9397	1/1	1.00	0.05	-	20,20,20,20	0
6	MG	C	9522	1/1	1.00	0.06	-	20,20,20,20	0
6	MG	F	9468	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	B	9413	1/1	0.98	0.05	-	20,20,20,20	0
6	MG	F	9324	1/1	1.00	0.07	-	20,20,20,20	0
6	MG	C	9339	1/1	0.99	0.11	-	20,20,20,20	0
6	MG	A	9224	1/1	1.00	0.07	-	20,20,20,20	0
6	MG	D	9527	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	D	9392	1/1	1.00	0.07	-	20,20,20,20	0
6	MG	D	9357	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	F	9453	1/1	0.99	0.09	-	20,20,20,20	0
6	MG	C	9549	1/1	1.00	0.05	-	20,20,20,20	0
6	MG	F	9310	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	C	9542	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	D	9556	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	D	9435	1/1	1.00	0.04	-	20,20,20,20	0
6	MG	C	9511	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	A	9394	1/1	0.97	0.09	-	20,20,20,20	0
6	MG	C	9476	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	D	9409	1/1	0.99	0.11	-	20,20,20,20	0
6	MG	D	9246	1/1	0.99	0.07	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	E	9389	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	C	9509	1/1	1.00	0.06	-	20,20,20,20	0
6	MG	D	9279	1/1	1.00	0.06	-	20,20,20,20	0
6	MG	D	9204	1/1	0.96	0.05	-	38,38,38,38	0
6	MG	D	9314	1/1	1.00	0.05	-	20,20,20,20	0
6	MG	D	9502	1/1	0.99	0.10	-	20,20,20,20	0
6	MG	B	9256	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	E	9249	1/1	0.98	0.09	-	20,20,20,20	0
6	MG	D	9499	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	C	9231	1/1	1.00	0.10	-	20,20,20,20	0
6	MG	D	9539	1/1	0.99	0.03	-	20,20,20,20	0
6	MG	C	9422	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	F	9531	1/1	0.99	0.04	-	20,20,20,20	0
6	MG	D	9252	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	D	9433	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	E	9449	1/1	0.99	0.08	-	20,20,20,20	0
6	MG	D	9401	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	N	9207	1/1	1.00	0.08	-	37,37,37,37	0
6	MG	D	9510	1/1	1.00	0.08	-	20,20,20,20	0
6	MG	C	9289	1/1	0.99	0.09	-	20,20,20,20	0
6	MG	E	9288	1/1	1.00	0.08	-	20,20,20,20	0
6	MG	D	9482	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	C	9219	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	E	9341	1/1	0.98	0.06	-	20,20,20,20	0
6	MG	F	9545	1/1	0.98	0.08	-	20,20,20,20	0
6	MG	A	9212	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	F	9540	1/1	0.99	0.05	-	20,20,20,20	0
6	MG	C	9550	1/1	0.99	0.09	-	20,20,20,20	0
6	MG	C	9313	1/1	0.99	0.10	-	20,20,20,20	0
6	MG	F	9500	1/1	0.98	0.08	-	20,20,20,20	0
6	MG	D	9274	1/1	0.99	0.07	-	20,20,20,20	0
6	MG	D	9237	1/1	0.98	0.05	-	20,20,20,20	0
6	MG	A	9544	1/1	1.00	0.07	-	20,20,20,20	0
6	MG	C	9387	1/1	0.99	0.10	-	20,20,20,20	0
6	MG	D	9481	1/1	0.99	0.08	-	20,20,20,20	0
6	MG	C	9292	1/1	1.00	0.05	-	20,20,20,20	0
6	MG	C	9321	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	A	9543	1/1	0.99	0.06	-	20,20,20,20	0
6	MG	E	9457	1/1	1.00	0.04	-	20,20,20,20	0
6	MG	F	9245	1/1	0.99	0.09	-	20,20,20,20	0
6	MG	E	9352	1/1	0.99	0.08	-	20,20,20,20	0
6	MG	D	9402	1/1	1.00	0.05	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	A	9555	1/1	1.00	0.04	-	20,20,20,20	0
6	MG	D	9351	1/1	1.00	0.09	-	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.