



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 01:26 pm GMT

PDB ID : 2A68  
Title : Crystal structure of the T. thermophilus RNA polymerase holoenzyme in complex with antibiotic rifabutin  
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 : 2005-07-01  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

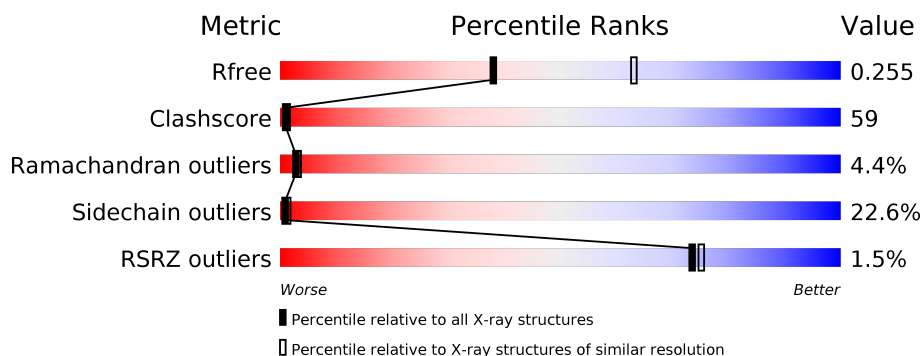
# 1 Overall quality at a glance

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))
$R_{free}$	111664	4155 (2.50-2.50)
Clashscore	122126	4827 (2.50-2.50)
Ramachandran outliers	120053	4735 (2.50-2.50)
Sidechain outliers	120020	4737 (2.50-2.50)
RSRZ outliers	108989	4058 (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  $\geq 3$ , 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	
1	B	315	
1	K	315	
1	L	315	
2	C	1119	
2	M	1119	

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Mol	Chain	Length	Quality of chain
3	D	1524	<div><div><div></div><div></div><div></div><div></div></div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>23%51%16%•9%</div></div>
3	N	1524	<div><div><div></div><div></div><div></div><div></div></div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>25%51%15%•9%</div></div>
4	E	99	<div><div><div></div><div></div><div></div><div></div></div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>27%58%11%•</div></div>
4	O	99	<div><div><div></div><div></div><div></div><div></div></div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>22%56%17%••</div></div>
5	F	423	<div><div><div></div><div></div><div></div><div></div></div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>21%48%11%•18%</div></div>
5	P	423	<div><div><div></div><div></div><div></div><div></div></div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>24%47%10%18%</div></div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 61089 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			

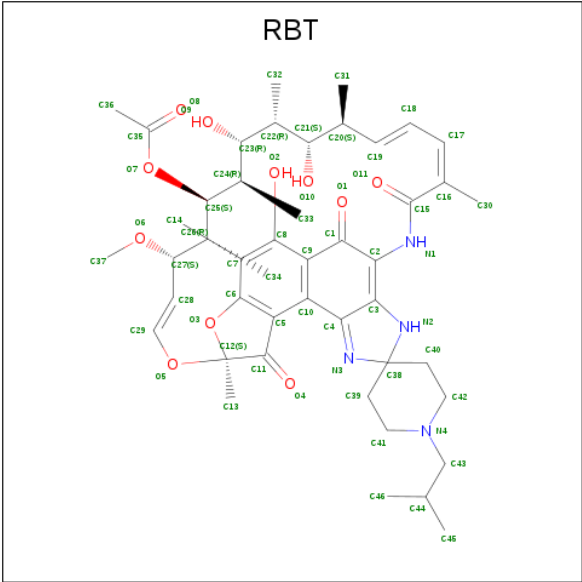
- Molecule 5 is a protein called RNA polymerase sigma factor rpoD.

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	137	Total	Mg	0	0
			137	137		
6	K	21	Total	Mg	0	0
			21	21		
6	E	10	Total	Mg	0	0
			10	10		
6	B	23	Total	Mg	0	0
			23	23		
6	C	81	Total	Mg	0	0
			81	81		
6	A	31	Total	Mg	0	0
			31	31		
6	N	108	Total	Mg	0	0
			108	108		
6	O	6	Total	Mg	0	0
			6	6		
6	L	25	Total	Mg	0	0
			25	25		
6	F	31	Total	Mg	0	0
			31	31		
6	M	69	Total	Mg	0	0
			69	69		

- Molecule 7 is RIFABUTIN (three-letter code: RBT) (formula: C<sub>46</sub>H<sub>62</sub>N<sub>4</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			61	46	4	11		
7	M	1	Total	C	N	O	0	0
			61	46	4	11		

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

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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	253	Total	O	0	0
			253	253		
9	B	307	Total	O	0	0
			307	307		
9	C	1000	Total	O	0	0
			1000	1000		
9	D	1418	Total	O	0	0
			1418	1418		
9	E	112	Total	O	0	0
			112	112		

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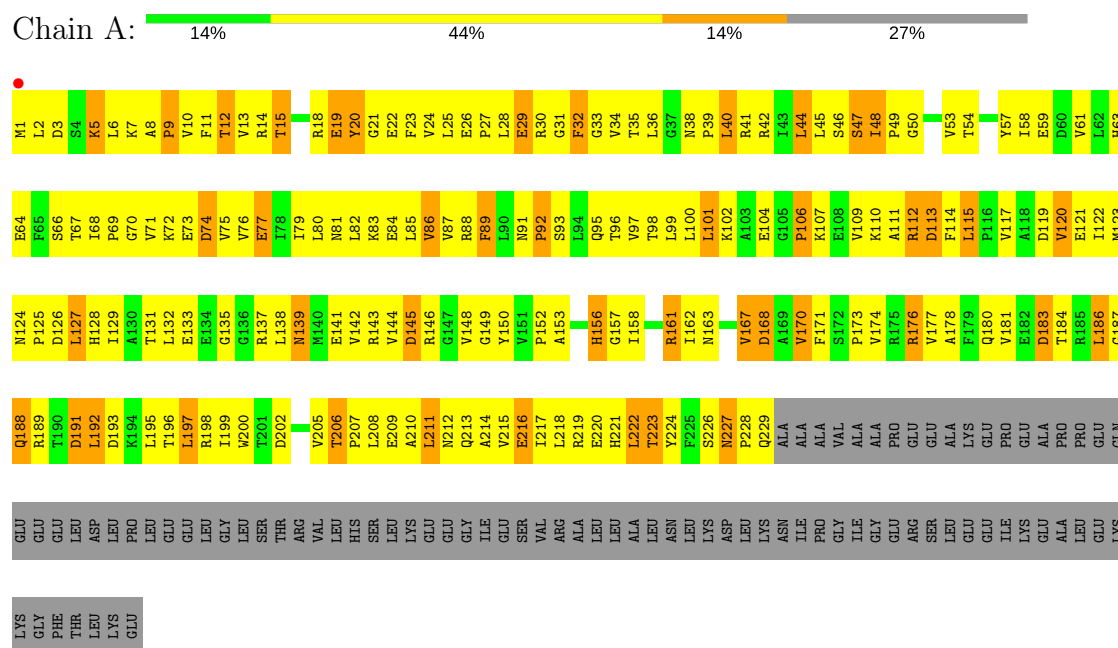
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	F	456	Total 456	O 456	0	0
9	K	213	Total 213	O 213	0	0
9	L	237	Total 237	O 237	0	0
9	M	998	Total 998	O 998	0	0
9	N	1357	Total 1357	O 1357	0	0
9	O	117	Total 117	O 117	0	0
9	P	377	Total 377	O 377	0	0

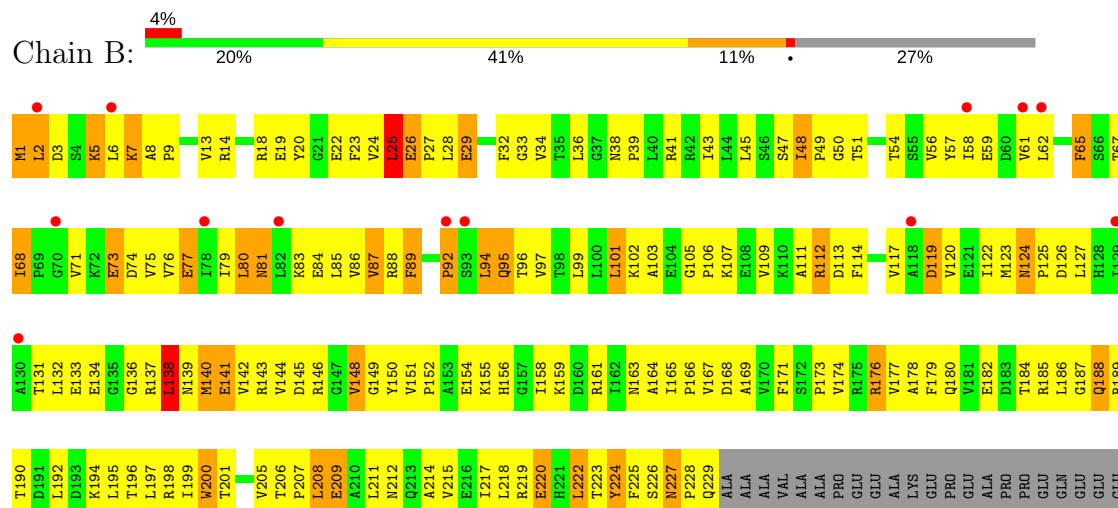
### 3 Residue-property plots

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

#### • Molecule 1: DNA-directed RNA polymerase alpha chain



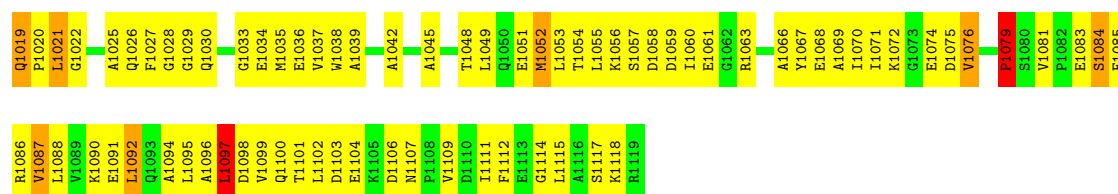
#### • Molecule 1: DNA-directed RNA polymerase alpha chain



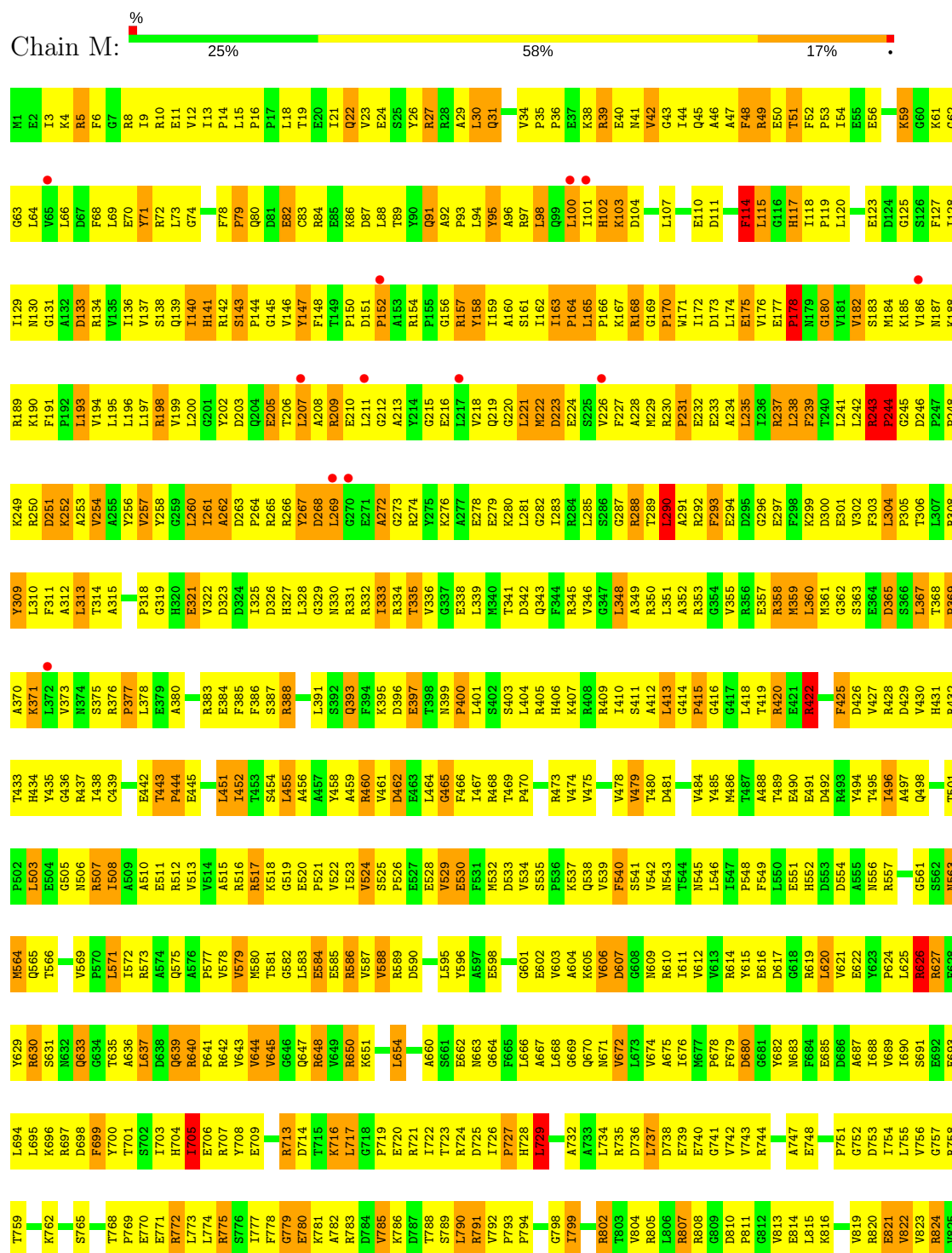


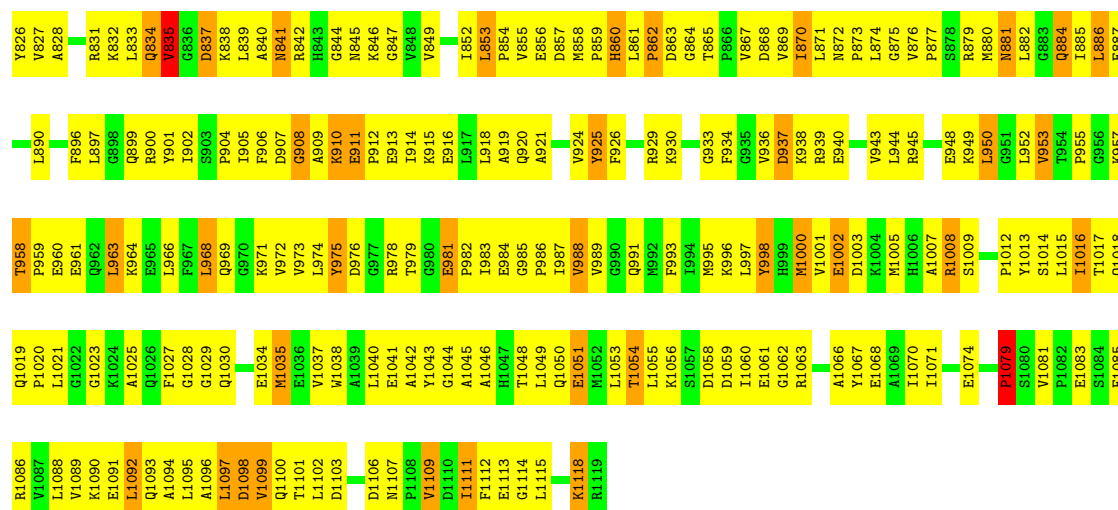


T958	L897	Q829	F761	R697	G634	V569	L508	T443	L381	G321	V254	K190	L128	V65	M1
P959	G996	K830	T761	D698	T635	P570	A509	P444	L382	E321	A255	F191	L129	L66	E2
E960	G999	R831	T768	P699	A636	L571	A510	N448	R383	V322	V256	F192	A132	D67	I3
E961	R900	K832	P769	Y700	L637	L572	E511	I449	E384	D323	V257	L193	L193	F68	K4
Q962	Y901	L833	E770	T701	D638	A574	V513	G450	F386	D325	G259	V194	D133	L69	R5
L963	Q834	Q834	E771	S702	Q639	G575	V514	L451	F387	D326	L260	L195	R134	E70	F6
L964	V835	R835	R772	I703	R640	Q575	A515	I452	R388	H327	L261	L196	V135	Y71	G7
E965	G904	D837	L773	H704	P641	A576	A516	L455	S388	H327	A262	L197	I136	Y72	R8
L966	R837	R642	L774	I705	R642	P577	A517	L456	S389	L328	L262	R198	V137	R73	I9
P967	K838	V643	R775	E706	V643	V578	K518	A456	L391	Q329	G329	L200	S138	G74	R10
L968	L839	V644	R776	R707	V644	V579	K519	A457	L391	Q329	G329	L200	Q139	E75	E11
Q969	G908	V645	I777	Y708	V645	M580	G519	A457	S392	R332	R265	G201	I140	P76	V12
G970	R841	R646	F778	E709	G646	T581	G520	Y458	Q393	R333	R266	Y202	H141	P77	I13
G971	R842	Q647	G779	I710	Q647	G582	P521	A459	F394	R334	Y287	D203	P144	F78	P14
V972	H843	R648	E780	R713	R648	L583	V522	R460	K395	R335	D288	Q204	G145	P79	L15
V973	G844	V649	K781	R714	V649	E584	V523	V461	D396	V336	L269	E205	G146	Q80	P16
L974	R845	R650	A782	T715	R650	E585	V524	D462	E397	G337	G270	L206	V146	P17	P17
Y975	K846	K651	A785	T716	K651	R586	S525	E463	T398	E338	E271	L207	Y147	E84	L18
G976	V849	G652	V785	K716	G652	V587	P526	L464	Q399	L339	A272	A208	F148	T19	E20
G977	V849	D653	K786	L717	D653	V588	E527	G465	P400	M340	G273	R209	T149	E20	I21
R978	L852	L654	D787	R720	L654	R589	E528	F466	L401	T341	R274	E210	P150	D87	L88
L979	L853	L655	T788	R721	L655	D590	V529	I467	S402	Q343	Y275	G212	P152	L88	Q22
Q980	R854	R656	S789	E721	A656	L596	F531	T469	R405	Q343	K276	G212	P152	L88	Q22
E981	P854	A657	L790	R722	A657	L597	N532	P470	L404	R345	E279	A213	R154	T89	S25
P982	V855	D657	L791	T723	D657	A597	N533	Y471	H406	V346	K280	G215	P155	Y90	Y26
L983	E856	A660	V792	R724	A660	E598	D533	R472	R407	G347	E281	G216	P156	Q91	A29
E984	D857	G664	P793	D725	G664	E599	V534	R472	R408	L348	G282	L217	G156	A92	A29
G985	R858	Q670	P794	I726	Q670	D600	S535	V474	R409	L348	G282	L217	R157	P93	L30
P986	G860	L666	G795	H728	L666	G601	P536	V474	R409	A349	G282	L217	Y158	Q99	Q31
L987	R860	L667	G795	L734	L667	D607	K537	V475	L410	R350	L285	Q219	I159	Y95	A32
V988	L861	A677	G798	L729	A677	E602	O538	V475	S411	R351	S286	G220	A160	A96	D33
V989	P862	L668	V799	S730	L668	F603	V539	V478	A412	A352	G287	L221	S161	R97	R34
G990	D863	Q669	V800	E731	Q669	A604	F539	V478	L413	R353	G287	L221	I162	R98	P35
Q991	K864	Q670	R801	A732	Q670	K605	S541	T480	G414	G354	R289	E224	I163	Q99	P36
M992	T865	N671	R802	A733	N671	V606	V542	D481	P415	V355	L290	E224	P164	L100	E37
F993	P866	L672	T803	L734	L672	D607	N543	E482	G416	R356	A291	S225	L165	I101	K38
L994	V867	L673	V804	R735	L673	G608	N543	E482	G417	E357	R292	V226	P166	H102	R39
M995	D868	V674	R805	D736	V674	M609	L546	Y485	L418	R358	F293	F227	K167	E40	E40
K996	V869	A675	R805	L737	A675	M610	L547	M486	L419	R359	E294	A228	R168	K103	E40
L997	I870	L676	R808	D738	L676	L611	P548	T487	R420	L360	E294	A228	G169	D104	M41
Y998	G809	N677	G809	E739	N677	V612	F549	A488	E421	M361	E297	R230	P170	T105	V42
H999	D810	P678	D810	E740	P678	V613	L550	T489	R422	G362	F298	P231	W171	G106	G43
M1000	P811	D680	P811	G741	D680	R614	E551	E490	A423	S363	K299	E232	I172	L107	I44
V1001	G812	D681	G812	V742	D681	V615	H552	E491	G424	E364	D300	E233	I173	I108	Q45
E1002	V813	G881	V813	V743	G881	E616	D553	D492	F425	D865	E301	E233	D173	K109	A46
D1003	E814	N682	E814	R744	N682	L620	D554	R493	D426	S366	V302	L236	E175	D111	F48
K1004	L815	G683	L815	I745	G683	V621	D555	Y494	V427	L367	F303	L236	V176	E112	R49
R946	K816	F684	K816	G746	F684	G621	N556	T495	R428	T368	L304	R237	E177	V113	E50
R946	M880	E685	M880	A747	E685	E622	R557	I496	D429	P369	P305	L238	P178	F114	T51
E947	N881	D686	G818	E748	D686	Y623	A558	A497	V430	A370	T306	F239	M179	L115	F52
E948	L882	A687	V819	V749	A687	F624	L559	Q498	H431	K371	L307	G180	G180	G116	P53
T1010	G983	L688	R820	K750	L688	L625	M560	A499	R432	L372	L307	R243	V181	G117	P53
G1011	Q884	V689	E821	R626	V689	R626	O561	A499	T433	V373	Y309	P244	V182	H117	I54
P1012	L885	L690	E822	G627	L690	R627	S562	T501	H434	N374	L310	G245	P118	P119	E55
L1013	R886	S691	R823	F628	S691	F628	O562	P502	Y435	S375	L310	D246	P118	P119	E56
S1014	E887	E692	R824	L755	E692	F629	N564	L503	C436	R376	A312	D246	M184	L120	K59
L1015	T888	E693	V825	L755	E693	R630	Q665	E504	R437	P377	L313	R250	K185	M121	K59
T1016	H889	L694	Y826	R758	L694	S631	T566	E504	R437	P377	L313	R250	K185	M121	K59
G956	L890	N632	V827	N632	N632	N632	N632	N632	N632	N632	N632	N632	N632	N632	K61
Q1018	K957	G956	V827	N632	N632	N632	N632	N632	N632	N632	N632	N632	N632	N632	K61
															L64

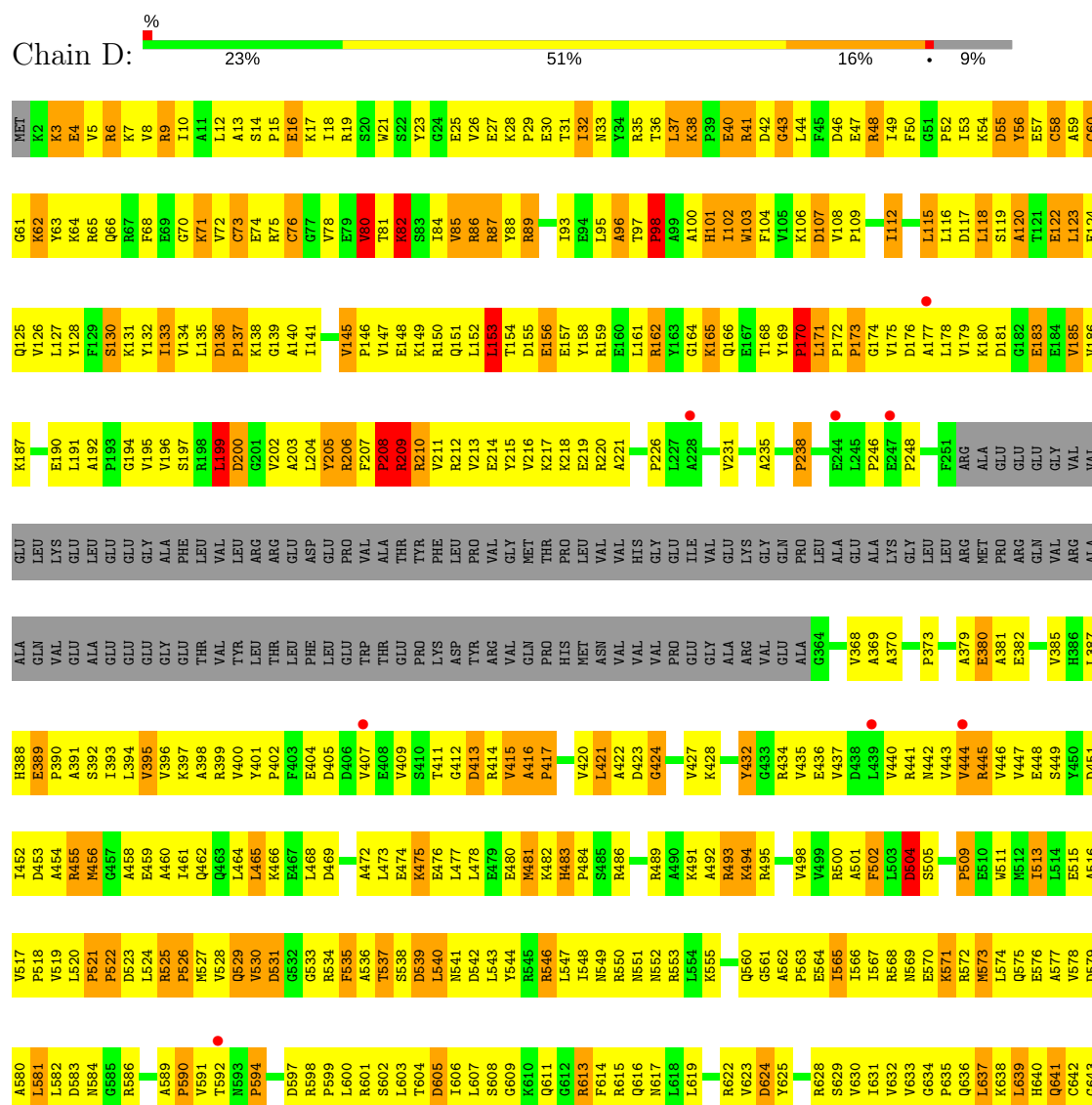


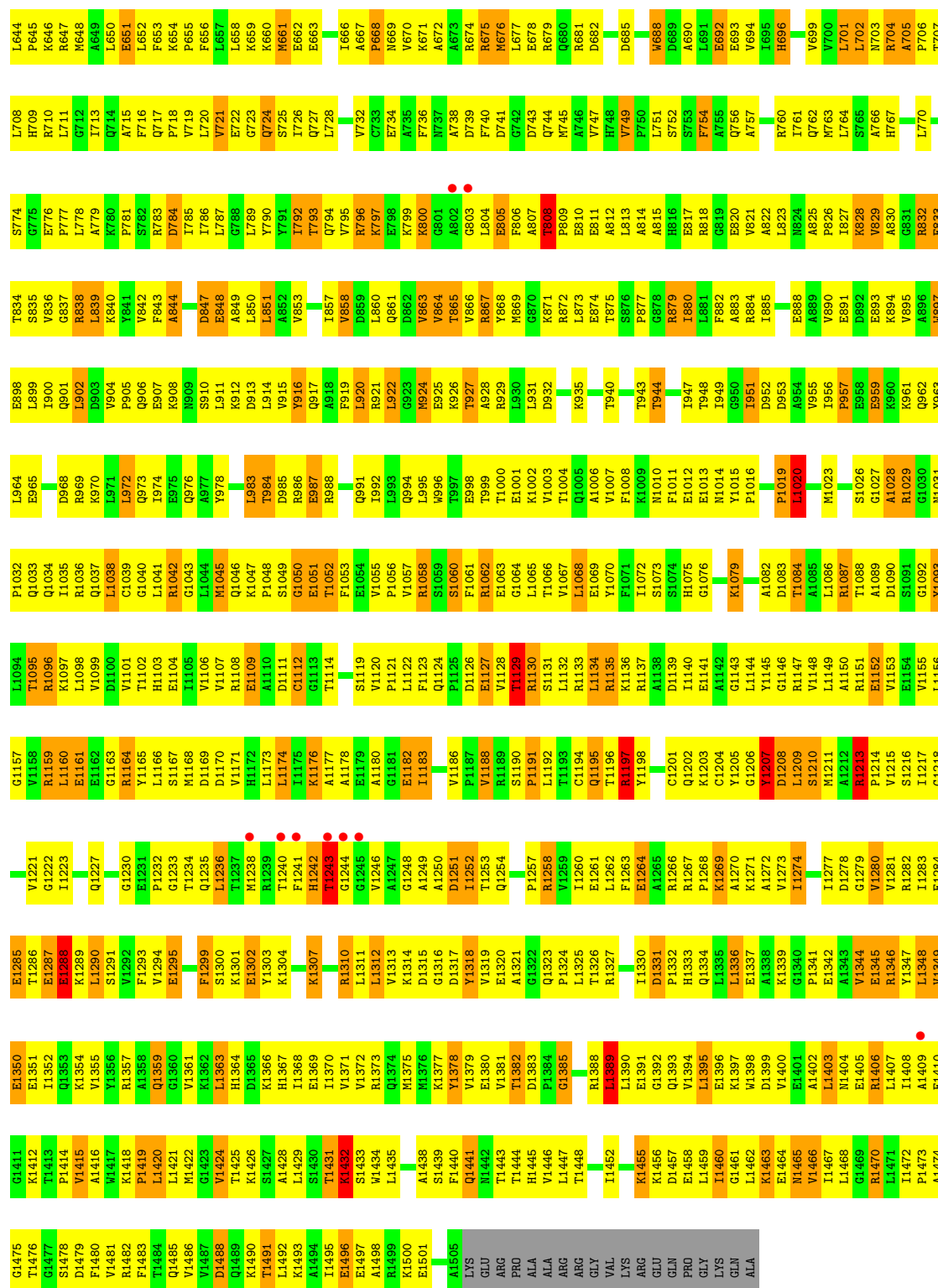
• Molecule 2: DNA-directed RNA polymerase beta chain





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





M1045	L983	N909	Y841	L778	A715	A649	D583	P521	I461	V395	GLU	PHE	V126	Y63
Q1046	T984	S910	V842	A779	F716	L650	M684	P522	Q462	V396	THR	LEU	L127	K64
K1047	D985	L311	F843	K780	Q717	E651	G585	D523	Q463	K397	VAL	VAL	Y128	R65
P1048	R986	K912	A844	P781	P718	L652	R586	L524	L464	A386	LEU	LEU	F129	Q66
S1049	E987		J845	S782	W719	F653	R587	R525	L465	K399	LEU	ARG	S130	R67
G1050	R988	V915	K846	R783	L720	K654	P526	P526	K466	V400	THR	ARG	K131	F68
E1051	Y989	Y916		D784		P655	P590	N527	E467	Y401	LEU	GLU	Y132	
T1052	D990	Q917	L850	I785	Q723	P656	V591	V528	L468	P402	ASP	ASP	I133	K71
F1053	A991	A918	L851	I786	Q724	L657	T592	Q529	D469	F403	LEU	LEU	V134	W72
	I992	F919	A852	I787	S725	L658	N593	V530	L470	E404	PRO	PRO	L135	C73
P1056	L993	L920	V853	Q788	I726	K659	P594		E471		TRP	VAL	D136	E74
V1057	Q994	R921	V857	I789	Q727	K660		G533	A472	E408	ALA	ALA	P137	R75
L1058	L995	L922	I857	W790	I728	M661		P539	L473		GLU	THR	V202	C76
S1059	W996	G923	V858	I791	H729	E662	D597	R534	E474		PRO	THR	K138	G77
T1060	T997	N924	D859	I792	P730	E663	R598	F585	E475		LYS	THR	G139	
F1061	E998	K925	L860	Q793	L731		P599	A536	K476		ASP	LEU	A140	W78
E1062	T999	K926	Q861	Q794	W732		P599		E477		VAL	LEU	E141	E79
E1063	T1000	T927	V862	Q795	C732	A667	S602	L540	L477	V415	PRO	PRO	L142	T80
E1064	E1001	A928	V863	R796	E734	P668	L603	L541	L478	A417	VAL	GLY	N143	T81
L1065	K1002		V864	R797	A735	P669	T804	D542	E479		MET	GLY	G144	K82
T1066	V1003	L931	T865	K798	F736	V670	D805	L543	M481	D419	THR	THR	V145	S83
V1067	T1004	D932	V866	K799	N737	A671	L606	L544	K482	V420	PRO	PRO	P146	L84
L1068	Q1005	A933	R867	K800	Q744	A672	L607	N551	H483	L421	LEU	LEU	V147	V85
E1069	A1006	L934	V867	A807	Q745	A673	S808	R546	P484	A422	ASN	VAL	E148	R86
Y1070	Y1007	K935	R877	T808	F746	K674	G609	L547	S485	D423	VAL	VAL	K149	R87
F1071	F1008	Y936	R872	G803	D741	R675	K610	L548	R486	C424	VAL	HIS	R150	R88
T1072	K1009	Y937	L873	L804	Q742	R676	Q611	R549	A487	G425	VAL	GLY	L152	Q151
S1073	E1010	G938	E874	E805	D743	L677	G612	R550	R488	K432	PRO	GLY	L153	L152
S1074	F1011	F939	T875	F806	Q744	E678	R613	N552	R489	V427	GLY	ILE	K218	T154
	E1012		R876	A807	M745	R679	R614	N552	A490	F414	GLY	VAL	E219	
A1077	E1013	S945	R877	T808	Q746	D680	R615	R553	K491	S429	ALA	GLY	E157	E94
R1078	N1014	Q946	G878	P809	V747	R681	Q616	L584	A492	D430	LYS	LYS	Y158	L95
T1079		I947	R879	E910	H743	D682	L619	K555	R493	V431	GLY	GLY	Y159	A96
D1083	N1018	T948	L880	A812	V749	P683		K556	K494	Y432	GLN	PRO	E160	P98
T1084	Y1020	G950	F882	L813	P750			L557	R495	Q433	ALA	ALA	L161	A99
R1087	Y1021	I951	A883	A814		V687	D624	A559	L496	R434	LEU	LEU	R162	A100
	Y1022	D952	R884		F754	P688	S826	Q560	E497	V435	ALA	ALA	H101	I102
D1090	M1023	D953	T885	E817	Q756	P689	G627	G561	V499	V437	GLU	GLU	K165	I103
S1091	Q1024	A954	V886		A757	A690	R628	A562	R500		ALA	ALA	Q166	T102
G1092	Q1025	V955	A887	E820	E758	E693	S829	P563	A501	V440	LYS	LYS	E167	F104
Y1093	S1026	I956	E888	V821	A759	V694	V630	E564	F502	R441	GLY	GLY	T168	V105
L1094	G1027	P957	A889	A822	R760	T695	I631	I565	L503	N442	LEU	LEU	Y169	K106
T1095	A1028	E958	V890	L823	I761	H696	V632	I566	D504	V443	LEU	LEU	P170	D107
R1096	R1029	E959	E891	N824	Q762		V633	I567	S905	V444	MET	MET	L171	V108
K1097	G1030	K960	D892	A825	M763	P699	G834	R568	G506	R445	PRO	PRO	P172	P109
L1098	P1032	P1031	K894	I827	L764	L700	P635	N569	N507	V446	ARG	ARG	G174	S110
D1100	Q1033	K828	V895	R828	A766	L702	K637	E570	R509	V447	GLN	GLY	V175	K111
V1101	Q1034	A896	A896	V829	H767	W703	L637	K571	P508	E448	VAL	VAL	D176	I112
T1102	T1035	A830	V887	A830	W768	R704	K638	B572	E510	S449	ARG	ARG	A177	L115
H1103	H1036	G831	E898	G831	L769	A705	L839	M573	M511	V450	ALA	ALA	L178	L116
E1104	Q1037	R969	L899	R832	L770	P706	Q841	L574	M512	D451	ALA	ALA	V179	D117
I1105	L1038	K970	L900	E833	S771	T707	C842	Q575	I513	L452	GLN	GLN	K180	L118
V1106	G1039	L971	Q901	T834	W772	L708	G643	E576	L514	D453	VAL	VAL	D181	S119
V1107	G1040	L972	L902	S835	A773	W709	L644	V578	E515	A454	GLU	GLU	G182	A120
R1108	L1041	Q976	Q906	V836	S774	R710	P645	D579	V517	M456	ALA	ALA	E184	T121
E1109	R1042	E907	E837	R837	G775		K646	A580	P518		GLY	GLY	E185	E122
A1110	L1044	F982	K908	R838	E776	I713	R647	L581	P519	E459	GLY	GLY	V186	L123
					P777	Q714	M648	L592	L520	A460	GLY	GLY	K187	Q125







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 91.2 (24.85-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.225 , 0.257 0.223 , 0.255	Depositor DCC
$R_{free}$ test set	29386 reflections (5.75%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.1	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 77.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.499 for -h,-k,l 0.085 for h,-h-k,-l 0.085 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	61089	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, RBT, 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	0.79	1/1838 (0.1%)	0.86	2/2498 (0.1%)
1	B	0.73	0/1838	0.82	3/2498 (0.1%)
1	K	0.75	0/1838	0.84	2/2498 (0.1%)
1	L	0.71	1/1838 (0.1%)	0.78	0/2498
2	C	0.81	0/8997	0.88	6/12164 (0.0%)
2	M	0.79	0/8997	0.88	8/12164 (0.1%)
3	D	0.82	0/10975	0.93	22/14836 (0.1%)
3	N	0.80	0/10975	0.91	14/14836 (0.1%)
4	E	0.82	0/783	0.98	1/1054 (0.1%)
4	O	0.84	0/783	0.96	1/1054 (0.1%)
5	F	0.73	0/2812	0.82	2/3781 (0.1%)
5	P	0.71	0/2812	0.80	1/3781 (0.0%)
All	All	0.79	2/54486 (0.0%)	0.88	62/73662 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	ILE	C-N	5.18	1.44	1.34
1	L	172	SER	N-CA	-5.06	1.36	1.46

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	138	LEU	CA-CB-CG	8.26	134.29	115.30
3	D	199	LEU	CA-CB-CG	-8.08	96.72	115.30
3	N	199	LEU	CA-CB-CG	-7.83	97.28	115.30
3	N	1389	LEU	CA-CB-CG	7.33	132.15	115.30
5	F	361	LEU	CA-CB-CG	7.04	131.49	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	231	0
1	B	1806	0	1861	211	0
1	K	1806	0	1861	199	0
1	L	1806	0	1861	202	0
2	C	8829	0	8933	1201	0
2	M	8829	0	8933	1179	0
3	D	10797	0	10873	1404	0
3	N	10797	0	10873	1285	0
4	E	769	0	775	92	0
4	O	769	0	775	99	0
5	F	2771	0	2844	340	0
5	P	2771	0	2844	315	0
6	A	31	0	0	0	0
6	B	23	0	0	0	0
6	C	81	0	0	0	0
6	D	137	0	0	0	0
6	E	10	0	0	0	0
6	F	31	0	0	0	0
6	K	21	0	0	0	0
6	L	25	0	0	0	0
6	M	69	0	0	0	0
6	N	108	0	0	0	0
6	O	6	0	0	0	0
6	P	20	0	0	0	0
7	C	61	0	61	3	0
7	M	61	0	61	3	0
8	D	2	0	0	0	0
8	N	2	0	0	0	0
9	A	253	0	0	49	0
9	B	307	0	0	49	0
9	C	1000	0	0	202	0
9	D	1418	0	0	282	0
9	E	112	0	0	22	0
9	F	456	0	0	98	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	K	213	0	0	34	0
9	L	237	0	0	58	0
9	M	998	0	0	255	0
9	N	1357	0	0	240	0
9	O	117	0	0	26	0
9	P	377	0	0	75	0
All	All	61089	0	54416	6365	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 59.

The worst 5 of 6365 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:42:ARG:HH12	2:C:857:ASP:HB3	1.08	1.12
2:M:1054:THR:HG21	2:M:1079:PRO:HB3	1.27	1.11
3:N:1045:MET:HG2	3:N:1073:SER:HA	1.35	1.08
2:C:630:ARG:HH21	2:C:705:ILE:HG22	1.18	1.07
3:N:52:PRO:HB2	3:N:80:VAL:HG13	1.34	1.06

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%)	204 (90%)	19 (8%)	4 (2%)	9	16
1	B	227/315 (72%)	201 (88%)	21 (9%)	5 (2%)	7	11
1	K	227/315 (72%)	204 (90%)	19 (8%)	4 (2%)	9	16
1	L	227/315 (72%)	205 (90%)	18 (8%)	4 (2%)	9	16
2	C	1117/1119 (100%)	911 (82%)	153 (14%)	53 (5%)	2	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	M	1117/1119 (100%)	904 (81%)	168 (15%)	45 (4%)	3	4
3	D	1388/1524 (91%)	1112 (80%)	202 (15%)	74 (5%)	2	2
3	N	1388/1524 (91%)	1118 (80%)	195 (14%)	75 (5%)	2	2
4	E	93/99 (94%)	74 (80%)	15 (16%)	4 (4%)	3	3
4	O	93/99 (94%)	76 (82%)	13 (14%)	4 (4%)	3	3
5	F	341/423 (81%)	286 (84%)	40 (12%)	15 (4%)	3	3
5	P	341/423 (81%)	290 (85%)	37 (11%)	14 (4%)	3	4
All	All	6786/7590 (89%)	5585 (82%)	900 (13%)	301 (4%)	3	3

5 of 301 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	156	GLY

### 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%)	148 (73%)	54 (27%)	0	0
1	B	202/273 (74%)	164 (81%)	38 (19%)	1	3
1	K	202/273 (74%)	144 (71%)	58 (29%)	0	0
1	L	202/273 (74%)	159 (79%)	43 (21%)	1	2
2	C	941/941 (100%)	738 (78%)	203 (22%)	1	2
2	M	941/941 (100%)	737 (78%)	204 (22%)	1	2
3	D	1123/1279 (88%)	841 (75%)	282 (25%)	0	1
3	N	1123/1279 (88%)	865 (77%)	258 (23%)	1	1
4	E	83/87 (95%)	67 (81%)	16 (19%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	O	83/87 (95%)	61 (74%)	22 (26%)	0	0
5	F	295/370 (80%)	235 (80%)	60 (20%)	1	2
5	P	295/370 (80%)	247 (84%)	48 (16%)	2	4
All	All	5692/6446 (88%)	4406 (77%)	1286 (23%)	1	1

5 of 1286 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	33	HIS
1	L	29	GLU
3	N	1396	GLU
5	F	87	GLU
1	K	2	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 174 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	277	GLN
1	L	212	ASN
3	N	1374	GLN
1	K	63	HIS
1	K	227	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

Of 568 ligands modelled in this entry, 566 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	RBT	C	8001	6	60,66,66	2.81	21 (35%)	86,101,101	1.80	18 (20%)
7	RBT	M	8002	-	60,66,66	2.77	22 (36%)	86,101,101	1.87	16 (18%)

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	RBT	C	8001	6	-	0/59/116/116	0/5/6/6
7	RBT	M	8002	-	-	0/59/116/116	0/5/6/6

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	8002	RBT	O2-C8	-3.56	1.28	1.37
7	C	8001	RBT	O2-C8	-2.71	1.30	1.37
7	M	8002	RBT	O7-C35	2.02	1.39	1.35
7	C	8001	RBT	C32-C22	2.14	1.58	1.53
7	M	8002	RBT	C9-C1	2.21	1.52	1.46

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	8002	RBT	C39-C38-N3	-4.97	106.87	111.46
7	M	8002	RBT	C40-C38-N3	-3.90	107.86	111.46
7	C	8001	RBT	O3-C6-C5	-3.87	111.08	114.29
7	M	8002	RBT	O3-C6-C5	-3.81	111.13	114.29
7	C	8001	RBT	C39-C38-N3	-3.09	108.61	111.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	8001	RBT	3	0
7	M	8002	RBT	3	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	229/315 (72%)	-0.40	1 (0%) 92 93	29, 60, 84, 110	0
1	B	229/315 (72%)	-0.13	13 (5%) 24 25	44, 89, 114, 118	0
1	K	229/315 (72%)	-0.40	2 (0%) 84 85	33, 58, 89, 120	0
1	L	229/315 (72%)	-0.25	8 (3%) 44 47	49, 89, 109, 119	0
2	C	1119/1119 (100%)	-0.39	10 (0%) 84 85	14, 74, 102, 117	0
2	M	1119/1119 (100%)	-0.39	12 (1%) 80 82	19, 71, 103, 119	0
3	D	1392/1524 (91%)	-0.36	17 (1%) 79 80	19, 62, 107, 125	0
3	N	1392/1524 (91%)	-0.36	24 (1%) 70 72	23, 65, 107, 131	0
4	E	95/99 (95%)	-0.40	2 (2%) 63 66	41, 77, 107, 120	0
4	O	95/99 (95%)	-0.44	1 (1%) 80 82	33, 72, 94, 103	0
5	F	345/423 (81%)	-0.39	7 (2%) 65 67	46, 81, 104, 118	0
5	P	345/423 (81%)	-0.30	8 (2%) 60 63	53, 81, 108, 123	0
All	All	6818/7590 (89%)	-0.36	105 (1%) 73 75	14, 70, 105, 131	0

The worst 5 of 105 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	P	145	PRO	5.8
3	N	1243	THR	5.8
2	M	269	LEU	5.2
3	D	1244	GLY	4.8
3	D	1240	THR	4.8

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	B	9163	1/1	0.92	0.06	44,44,44,44	0
6	MG	N	9538	1/1	0.92	0.10	42,42,42,42	0
6	MG	L	9258	1/1	0.94	0.10	47,47,47,47	0
6	MG	M	9364	1/1	0.94	0.08	37,37,37,37	0
6	MG	F	9410	1/1	0.94	0.12	47,47,47,47	0
6	MG	N	9354	1/1	0.95	0.07	42,42,42,42	0
6	MG	N	9235	1/1	0.95	0.12	63,63,63,63	0
6	MG	C	9068	1/1	0.95	0.12	37,37,37,37	0
8	ZN	D	7058	1/1	0.95	0.07	100,100,100,100	0
6	MG	B	9199	1/1	0.95	0.10	52,52,52,52	0
6	MG	C	9398	1/1	0.95	0.10	44,44,44,44	0
6	MG	N	9250	1/1	0.95	0.16	61,61,61,61	0
6	MG	N	9503	1/1	0.96	0.12	52,52,52,52	0
6	MG	N	9349	1/1	0.96	0.06	37,37,37,37	0
6	MG	M	9261	1/1	0.96	0.10	45,45,45,45	0
6	MG	O	9359	1/1	0.96	0.08	57,57,57,57	0
6	MG	P	9322	1/1	0.96	0.12	43,43,43,43	0
6	MG	A	9062	1/1	0.96	0.11	45,45,45,45	0
6	MG	D	9084	1/1	0.96	0.10	47,47,47,47	0
6	MG	M	9383	1/1	0.96	0.09	46,46,46,46	0
6	MG	K	9257	1/1	0.96	0.12	57,57,57,57	0
6	MG	D	9147	1/1	0.96	0.09	40,40,40,40	0
6	MG	D	9520	1/1	0.96	0.14	46,46,46,46	0
6	MG	D	9155	1/1	0.96	0.12	56,56,56,56	0
6	MG	C	9190	1/1	0.96	0.07	40,40,40,40	0
6	MG	A	9514	1/1	0.96	0.12	42,42,42,42	0
7	RBT	M	8002	61/61	0.96	0.18	28,39,48,54	0
6	MG	F	9048	1/1	0.96	0.16	50,50,50,50	0
6	MG	D	9111	1/1	0.96	0.09	43,43,43,43	0
6	MG	N	9474	1/1	0.96	0.13	56,56,56,56	0
6	MG	M	9255	1/1	0.96	0.13	58,58,58,58	0
6	MG	C	9177	1/1	0.96	0.09	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	N	9253	1/1	0.96	0.08	39,39,39,39	0
6	MG	A	9413	1/1	0.96	0.10	46,46,46,46	0
6	MG	M	9267	1/1	0.96	0.12	41,41,41,41	0
6	MG	M	9220	1/1	0.96	0.13	45,45,45,45	0
6	MG	C	9399	1/1	0.96	0.10	43,43,43,43	0
6	MG	K	9351	1/1	0.97	0.09	37,37,37,37	0
6	MG	M	9334	1/1	0.97	0.09	44,44,44,44	0
6	MG	N	9358	1/1	0.97	0.12	48,48,48,48	0
6	MG	N	9230	1/1	0.97	0.09	40,40,40,40	0
6	MG	E	9467	1/1	0.97	0.12	52,52,52,52	0
6	MG	M	9325	1/1	0.97	0.10	44,44,44,44	0
6	MG	A	9430	1/1	0.97	0.11	35,35,35,35	0
6	MG	N	9539	1/1	0.97	0.10	57,57,57,57	0
6	MG	D	9095	1/1	0.97	0.06	40,40,40,40	0
6	MG	D	9548	1/1	0.97	0.12	51,51,51,51	0
6	MG	D	9543	1/1	0.97	0.12	46,46,46,46	0
6	MG	D	9423	1/1	0.97	0.09	44,44,44,44	0
6	MG	D	9042	1/1	0.97	0.12	47,47,47,47	0
6	MG	P	9304	1/1	0.97	0.10	57,57,57,57	0
6	MG	M	9259	1/1	0.97	0.17	57,57,57,57	0
6	MG	C	9414	1/1	0.97	0.07	41,41,41,41	0
6	MG	N	9486	1/1	0.97	0.09	44,44,44,44	0
6	MG	D	9523	1/1	0.97	0.11	41,41,41,41	0
6	MG	N	9208	1/1	0.97	0.12	35,35,35,35	0
6	MG	C	9455	1/1	0.97	0.12	61,61,61,61	0
6	MG	N	9244	1/1	0.97	0.08	37,37,37,37	0
6	MG	A	9107	1/1	0.97	0.07	40,40,40,40	0
6	MG	A	9145	1/1	0.97	0.11	45,45,45,45	0
6	MG	D	9518	1/1	0.97	0.11	55,55,55,55	0
6	MG	M	9312	1/1	0.97	0.10	37,37,37,37	0
6	MG	K	9363	1/1	0.97	0.09	47,47,47,47	0
6	MG	C	9081	1/1	0.97	0.13	52,52,52,52	0
6	MG	N	9327	1/1	0.97	0.11	54,54,54,54	0
6	MG	L	9249	1/1	0.97	0.07	51,51,51,51	0
7	RBT	C	8001	61/61	0.97	0.19	25,37,42,48	0
6	MG	D	9096	1/1	0.97	0.14	43,43,43,43	0
6	MG	A	9559	1/1	0.97	0.12	45,45,45,45	0
6	MG	O	9209	1/1	0.97	0.11	37,37,37,37	0
6	MG	N	9246	1/1	0.97	0.13	49,49,49,49	0
6	MG	N	9555	1/1	0.97	0.11	56,56,56,56	0
6	MG	N	9247	1/1	0.97	0.08	29,29,29,29	0
6	MG	C	9023	1/1	0.97	0.09	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	A	9050	1/1	0.97	0.10	41,41,41,41	0
6	MG	D	9066	1/1	0.97	0.11	49,49,49,49	0
6	MG	N	9508	1/1	0.97	0.11	41,41,41,41	0
6	MG	L	9346	1/1	0.97	0.14	52,52,52,52	0
6	MG	C	9047	1/1	0.97	0.06	47,47,47,47	0
6	MG	L	9483	1/1	0.97	0.15	44,44,44,44	0
6	MG	P	9284	1/1	0.97	0.10	51,51,51,51	0
6	MG	F	9010	1/1	0.97	0.17	57,57,57,57	0
6	MG	C	9156	1/1	0.97	0.12	43,43,43,43	0
6	MG	D	9152	1/1	0.97	0.11	32,32,32,32	0
6	MG	M	9348	1/1	0.97	0.11	63,63,63,63	0
6	MG	M	9473	1/1	0.97	0.11	42,42,42,42	0
6	MG	D	9026	1/1	0.97	0.12	37,37,37,37	0
6	MG	N	9551	1/1	0.97	0.08	40,40,40,40	0
6	MG	E	9184	1/1	0.97	0.16	48,48,48,48	0
6	MG	M	9332	1/1	0.97	0.13	54,54,54,54	0
6	MG	N	9554	1/1	0.97	0.11	45,45,45,45	0
6	MG	C	9192	1/1	0.97	0.10	55,55,55,55	0
6	MG	D	9067	1/1	0.97	0.12	49,49,49,49	0
6	MG	N	9381	1/1	0.97	0.07	35,35,35,35	0
6	MG	F	9461	1/1	0.97	0.12	52,52,52,52	0
6	MG	C	9549	1/1	0.98	0.11	48,48,48,48	0
6	MG	N	9490	1/1	0.98	0.12	41,41,41,41	0
6	MG	N	9498	1/1	0.98	0.09	45,45,45,45	0
6	MG	N	9207	1/1	0.98	0.10	30,30,30,30	0
6	MG	C	9007	1/1	0.98	0.11	34,34,34,34	0
6	MG	D	9172	1/1	0.98	0.10	35,35,35,35	0
6	MG	D	9401	1/1	0.98	0.12	40,40,40,40	0
6	MG	M	9283	1/1	0.98	0.14	35,35,35,35	0
6	MG	D	9202	1/1	0.98	0.18	61,61,61,61	0
6	MG	N	9342	1/1	0.98	0.07	48,48,48,48	0
6	MG	D	9445	1/1	0.98	0.13	48,48,48,48	0
6	MG	P	9558	1/1	0.98	0.09	44,44,44,44	0
6	MG	A	9097	1/1	0.98	0.09	41,41,41,41	0
6	MG	D	9123	1/1	0.98	0.14	37,37,37,37	0
6	MG	M	9347	1/1	0.98	0.11	37,37,37,37	0
6	MG	P	9541	1/1	0.98	0.10	44,44,44,44	0
6	MG	N	9365	1/1	0.98	0.12	43,43,43,43	0
6	MG	D	9466	1/1	0.98	0.10	57,57,57,57	0
6	MG	D	9168	1/1	0.98	0.06	38,38,38,38	0
6	MG	C	9546	1/1	0.98	0.06	49,49,49,49	0
6	MG	N	9314	1/1	0.98	0.11	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	C	9124	1/1	0.98	0.08	33,33,33,33	0
6	MG	N	9301	1/1	0.98	0.08	50,50,50,50	0
6	MG	D	9003	1/1	0.98	0.06	43,43,43,43	0
6	MG	M	9377	1/1	0.98	0.12	39,39,39,39	0
6	MG	A	9001	1/1	0.98	0.18	26,26,26,26	0
6	MG	N	9295	1/1	0.98	0.05	48,48,48,48	0
6	MG	N	9504	1/1	0.98	0.10	32,32,32,32	0
6	MG	D	9002	1/1	0.98	0.16	29,29,29,29	0
6	MG	E	9131	1/1	0.98	0.08	47,47,47,47	0
6	MG	N	9297	1/1	0.98	0.13	48,48,48,48	0
6	MG	B	9092	1/1	0.98	0.11	50,50,50,50	0
6	MG	L	9505	1/1	0.98	0.10	58,58,58,58	0
6	MG	A	9078	1/1	0.98	0.13	34,34,34,34	0
6	MG	D	9424	1/1	0.98	0.14	50,50,50,50	0
6	MG	N	9313	1/1	0.98	0.09	39,39,39,39	0
6	MG	M	9478	1/1	0.98	0.06	35,35,35,35	0
6	MG	D	9449	1/1	0.98	0.07	29,29,29,29	0
6	MG	M	9219	1/1	0.98	0.10	39,39,39,39	0
6	MG	B	9101	1/1	0.98	0.08	40,40,40,40	0
6	MG	N	9242	1/1	0.98	0.12	36,36,36,36	0
6	MG	C	9515	1/1	0.98	0.08	41,41,41,41	0
6	MG	D	9397	1/1	0.98	0.12	31,31,31,31	0
6	MG	N	9319	1/1	0.98	0.11	41,41,41,41	0
6	MG	C	9457	1/1	0.98	0.10	40,40,40,40	0
6	MG	M	9233	1/1	0.98	0.15	38,38,38,38	0
6	MG	C	9157	1/1	0.98	0.16	44,44,44,44	0
6	MG	B	9395	1/1	0.98	0.11	56,56,56,56	0
6	MG	C	9063	1/1	0.98	0.10	32,32,32,32	0
6	MG	P	9317	1/1	0.98	0.18	53,53,53,53	0
6	MG	D	9012	1/1	0.98	0.06	39,39,39,39	0
6	MG	B	9389	1/1	0.98	0.10	37,37,37,37	0
6	MG	N	9310	1/1	0.98	0.08	36,36,36,36	0
6	MG	D	9015	1/1	0.98	0.12	37,37,37,37	0
6	MG	K	9553	1/1	0.98	0.09	50,50,50,50	0
6	MG	D	9039	1/1	0.98	0.11	40,40,40,40	0
6	MG	E	9151	1/1	0.98	0.05	48,48,48,48	0
6	MG	C	9396	1/1	0.98	0.14	57,57,57,57	0
6	MG	K	9214	1/1	0.98	0.20	31,31,31,31	0
6	MG	N	9228	1/1	0.98	0.08	49,49,49,49	0
6	MG	D	9447	1/1	0.98	0.10	50,50,50,50	0
6	MG	M	9293	1/1	0.98	0.11	43,43,43,43	0
6	MG	N	9526	1/1	0.98	0.10	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	D	9112	1/1	0.98	0.13	39,39,39,39	0
6	MG	F	9153	1/1	0.98	0.07	39,39,39,39	0
6	MG	F	9429	1/1	0.98	0.12	57,57,57,57	0
6	MG	D	9059	1/1	0.98	0.10	40,40,40,40	0
6	MG	D	9099	1/1	0.98	0.07	38,38,38,38	0
6	MG	D	9516	1/1	0.98	0.05	51,51,51,51	0
6	MG	D	9140	1/1	0.98	0.13	43,43,43,43	0
6	MG	C	9014	1/1	0.98	0.14	45,45,45,45	0
6	MG	N	9281	1/1	0.98	0.09	50,50,50,50	0
6	MG	C	9458	1/1	0.98	0.09	38,38,38,38	0
6	MG	A	9102	1/1	0.98	0.09	38,38,38,38	0
6	MG	K	9344	1/1	0.98	0.12	55,55,55,55	0
6	MG	C	9191	1/1	0.98	0.13	44,44,44,44	0
6	MG	N	9534	1/1	0.98	0.09	54,54,54,54	0
6	MG	L	9213	1/1	0.98	0.23	49,49,49,49	0
6	MG	C	9141	1/1	0.98	0.12	45,45,45,45	0
6	MG	N	9499	1/1	0.98	0.08	38,38,38,38	0
6	MG	M	9290	1/1	0.98	0.12	48,48,48,48	0
6	MG	M	9285	1/1	0.98	0.13	43,43,43,43	0
6	MG	N	9262	1/1	0.98	0.14	49,49,49,49	0
6	MG	D	9432	1/1	0.98	0.10	47,47,47,47	0
6	MG	M	9211	1/1	0.98	0.10	28,28,28,28	0
6	MG	D	9019	1/1	0.98	0.15	35,35,35,35	0
6	MG	M	9540	1/1	0.98	0.16	63,63,63,63	0
6	MG	D	9110	1/1	0.98	0.13	38,38,38,38	0
6	MG	N	9315	1/1	0.98	0.11	41,41,41,41	0
6	MG	N	9245	1/1	0.98	0.12	28,28,28,28	0
6	MG	M	9276	1/1	0.98	0.14	54,54,54,54	0
6	MG	L	9311	1/1	0.98	0.07	33,33,33,33	0
6	MG	B	9419	1/1	0.98	0.11	46,46,46,46	0
6	MG	B	9079	1/1	0.98	0.11	28,28,28,28	0
6	MG	M	9485	1/1	0.98	0.06	42,42,42,42	0
6	MG	D	9041	1/1	0.98	0.10	32,32,32,32	0
6	MG	C	9083	1/1	0.98	0.11	48,48,48,48	0
6	MG	L	9378	1/1	0.98	0.14	47,47,47,47	0
6	MG	A	9522	1/1	0.98	0.11	57,57,57,57	0
6	MG	D	9009	1/1	0.98	0.12	53,53,53,53	0
6	MG	D	9057	1/1	0.98	0.11	33,33,33,33	0
6	MG	B	9427	1/1	0.98	0.11	42,42,42,42	0
6	MG	M	9557	1/1	0.98	0.09	54,54,54,54	0
6	MG	D	9036	1/1	0.98	0.13	41,41,41,41	0
6	MG	C	9076	1/1	0.98	0.11	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	N	9266	1/1	0.98	0.08	36,36,36,36	0
6	MG	D	9104	1/1	0.98	0.09	35,35,35,35	0
6	MG	L	9532	1/1	0.98	0.08	51,51,51,51	0
6	MG	D	9451	1/1	0.98	0.09	37,37,37,37	0
6	MG	N	9341	1/1	0.98	0.13	38,38,38,38	0
6	MG	N	9506	1/1	0.98	0.10	56,56,56,56	0
6	MG	D	9034	1/1	0.98	0.16	37,37,37,37	0
6	MG	O	9362	1/1	0.98	0.04	49,49,49,49	0
6	MG	F	9206	1/1	0.98	0.12	33,33,33,33	0
6	MG	B	9148	1/1	0.98	0.15	54,54,54,54	0
6	MG	K	9217	1/1	0.98	0.06	36,36,36,36	0
6	MG	M	9229	1/1	0.98	0.09	35,35,35,35	0
6	MG	N	9338	1/1	0.98	0.12	42,42,42,42	0
6	MG	D	9055	1/1	0.98	0.09	51,51,51,51	0
6	MG	K	9484	1/1	0.98	0.11	30,30,30,30	0
6	MG	C	9183	1/1	0.98	0.16	44,44,44,44	0
6	MG	N	9529	1/1	0.98	0.08	55,55,55,55	0
6	MG	D	9108	1/1	0.98	0.11	51,51,51,51	0
6	MG	F	9167	1/1	0.98	0.12	59,59,59,59	0
6	MG	M	9488	1/1	0.98	0.12	42,42,42,42	0
6	MG	A	9109	1/1	0.98	0.09	33,33,33,33	0
6	MG	M	9350	1/1	0.98	0.09	37,37,37,37	0
6	MG	F	9448	1/1	0.98	0.10	38,38,38,38	0
6	MG	N	9292	1/1	0.98	0.16	52,52,52,52	0
6	MG	F	9437	1/1	0.98	0.09	47,47,47,47	0
6	MG	M	9309	1/1	0.98	0.15	35,35,35,35	0
6	MG	C	9406	1/1	0.98	0.10	47,47,47,47	0
6	MG	M	9227	1/1	0.98	0.10	44,44,44,44	0
6	MG	L	9556	1/1	0.98	0.09	58,58,58,58	0
6	MG	K	9367	1/1	0.98	0.09	38,38,38,38	0
6	MG	D	9441	1/1	0.98	0.10	46,46,46,46	0
6	MG	B	9150	1/1	0.98	0.10	43,43,43,43	0
6	MG	M	9243	1/1	0.98	0.11	45,45,45,45	0
6	MG	M	9298	1/1	0.98	0.12	43,43,43,43	0
6	MG	N	9232	1/1	0.98	0.10	33,33,33,33	0
6	MG	A	9165	1/1	0.98	0.11	65,65,65,65	0
6	MG	N	9288	1/1	0.98	0.10	33,33,33,33	0
6	MG	D	9517	1/1	0.99	0.09	45,45,45,45	0
6	MG	C	9521	1/1	0.99	0.12	45,45,45,45	0
6	MG	F	9072	1/1	0.99	0.07	40,40,40,40	0
6	MG	D	9446	1/1	0.99	0.10	36,36,36,36	0
6	MG	N	9256	1/1	0.99	0.09	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	O	9355	1/1	0.99	0.14	36,36,36,36	0
6	MG	B	9137	1/1	0.99	0.09	35,35,35,35	0
6	MG	F	9135	1/1	0.99	0.14	42,42,42,42	0
6	MG	N	9379	1/1	0.99	0.06	56,56,56,56	0
6	MG	N	9475	1/1	0.99	0.07	43,43,43,43	0
6	MG	C	9088	1/1	0.99	0.12	36,36,36,36	0
6	MG	M	9340	1/1	0.99	0.10	43,43,43,43	0
6	MG	N	9280	1/1	0.99	0.09	34,34,34,34	0
6	MG	N	9218	1/1	0.99	0.12	32,32,32,32	0
6	MG	C	9462	1/1	0.99	0.12	50,50,50,50	0
6	MG	D	9454	1/1	0.99	0.08	42,42,42,42	0
6	MG	E	9438	1/1	0.99	0.10	38,38,38,38	0
6	MG	K	9265	1/1	0.99	0.13	37,37,37,37	0
6	MG	F	9054	1/1	0.99	0.07	37,37,37,37	0
6	MG	F	9197	1/1	0.99	0.10	39,39,39,39	0
6	MG	C	9422	1/1	0.99	0.13	41,41,41,41	0
6	MG	B	9180	1/1	0.99	0.09	36,36,36,36	0
6	MG	C	9029	1/1	0.99	0.12	36,36,36,36	0
6	MG	N	9273	1/1	0.99	0.17	30,30,30,30	0
6	MG	P	9274	1/1	0.99	0.11	45,45,45,45	0
6	MG	F	9435	1/1	0.99	0.08	40,40,40,40	0
6	MG	N	9376	1/1	0.99	0.13	31,31,31,31	0
6	MG	N	9226	1/1	0.99	0.07	30,30,30,30	0
6	MG	C	9011	1/1	0.99	0.10	39,39,39,39	0
6	MG	N	9320	1/1	0.99	0.11	41,41,41,41	0
6	MG	N	9248	1/1	0.99	0.06	47,47,47,47	0
6	MG	E	9186	1/1	0.99	0.10	35,35,35,35	0
6	MG	D	9154	1/1	0.99	0.12	31,31,31,31	0
6	MG	C	9545	1/1	0.99	0.10	45,45,45,45	0
6	MG	D	9169	1/1	0.99	0.12	45,45,45,45	0
6	MG	L	9471	1/1	0.99	0.10	33,33,33,33	0
6	MG	M	9384	1/1	0.99	0.10	35,35,35,35	0
6	MG	P	9333	1/1	0.99	0.07	28,28,28,28	0
6	MG	D	9189	1/1	0.99	0.10	34,34,34,34	0
6	MG	M	9336	1/1	0.99	0.10	31,31,31,31	0
6	MG	M	9287	1/1	0.99	0.08	36,36,36,36	0
6	MG	D	9463	1/1	0.99	0.11	32,32,32,32	0
6	MG	F	9407	1/1	0.99	0.07	32,32,32,32	0
6	MG	D	9122	1/1	0.99	0.10	31,31,31,31	0
6	MG	D	9119	1/1	0.99	0.09	44,44,44,44	0
6	MG	B	9103	1/1	0.99	0.09	37,37,37,37	0
6	MG	D	9077	1/1	0.99	0.10	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	C	9439	1/1	0.99	0.10	35,35,35,35	0
6	MG	N	9356	1/1	0.99	0.14	29,29,29,29	0
6	MG	P	9326	1/1	0.99	0.08	39,39,39,39	0
6	MG	M	9321	1/1	0.99	0.13	40,40,40,40	0
6	MG	P	9502	1/1	0.99	0.07	43,43,43,43	0
6	MG	D	9519	1/1	0.99	0.12	55,55,55,55	0
6	MG	A	9560	1/1	0.99	0.13	49,49,49,49	0
6	MG	C	9044	1/1	0.99	0.08	37,37,37,37	0
6	MG	L	9300	1/1	0.99	0.07	58,58,58,58	0
6	MG	D	9038	1/1	0.99	0.11	35,35,35,35	0
6	MG	C	9196	1/1	0.99	0.13	30,30,30,30	0
6	MG	C	9205	1/1	0.99	0.12	53,53,53,53	0
6	MG	C	9025	1/1	0.99	0.10	39,39,39,39	0
6	MG	D	9393	1/1	0.99	0.13	35,35,35,35	0
6	MG	F	9164	1/1	0.99	0.11	29,29,29,29	0
6	MG	B	9146	1/1	0.99	0.09	44,44,44,44	0
6	MG	N	9335	1/1	0.99	0.10	33,33,33,33	0
6	MG	B	9512	1/1	0.99	0.20	53,53,53,53	0
6	MG	E	9115	1/1	0.99	0.08	39,39,39,39	0
6	MG	C	9121	1/1	0.99	0.15	43,43,43,43	0
6	MG	D	9175	1/1	0.99	0.09	40,40,40,40	0
6	MG	F	9053	1/1	0.99	0.10	34,34,34,34	0
6	MG	D	9159	1/1	0.99	0.11	35,35,35,35	0
6	MG	P	9329	1/1	0.99	0.07	46,46,46,46	0
6	MG	B	9391	1/1	0.99	0.12	27,27,27,27	0
6	MG	D	9100	1/1	0.99	0.07	31,31,31,31	0
6	MG	C	9415	1/1	0.99	0.11	38,38,38,38	0
6	MG	M	9251	1/1	0.99	0.13	33,33,33,33	0
6	MG	D	9021	1/1	0.99	0.12	34,34,34,34	0
6	MG	N	9375	1/1	0.99	0.10	43,43,43,43	0
6	MG	A	9178	1/1	0.99	0.09	28,28,28,28	0
6	MG	N	9307	1/1	0.99	0.09	38,38,38,38	0
6	MG	A	9411	1/1	0.99	0.10	31,31,31,31	0
6	MG	M	9481	1/1	0.99	0.09	37,37,37,37	0
6	MG	D	9561	1/1	0.99	0.06	38,38,38,38	0
8	ZN	N	7113	1/1	0.99	0.11	79,79,79,79	0
6	MG	D	9416	1/1	0.99	0.09	48,48,48,48	0
6	MG	D	9136	1/1	0.99	0.10	41,41,41,41	0
6	MG	D	9073	1/1	0.99	0.15	38,38,38,38	0
6	MG	N	9289	1/1	0.99	0.09	35,35,35,35	0
6	MG	C	9144	1/1	0.99	0.09	39,39,39,39	0
6	MG	D	9166	1/1	0.99	0.08	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	D	9049	1/1	0.99	0.14	31,31,31,31	0
6	MG	D	9203	1/1	0.99	0.09	46,46,46,46	0
6	MG	N	9368	1/1	0.99	0.09	41,41,41,41	0
6	MG	A	9139	1/1	0.99	0.10	35,35,35,35	0
6	MG	C	9074	1/1	0.99	0.13	30,30,30,30	0
6	MG	N	9509	1/1	0.99	0.11	31,31,31,31	0
6	MG	D	9443	1/1	0.99	0.07	47,47,47,47	0
6	MG	C	9071	1/1	0.99	0.13	39,39,39,39	0
6	MG	C	9456	1/1	0.99	0.07	37,37,37,37	0
6	MG	C	9420	1/1	0.99	0.07	37,37,37,37	0
6	MG	M	9366	1/1	0.99	0.10	41,41,41,41	0
6	MG	C	9020	1/1	0.99	0.14	28,28,28,28	0
6	MG	E	9187	1/1	0.99	0.12	39,39,39,39	0
6	MG	A	9018	1/1	0.99	0.14	31,31,31,31	0
6	MG	D	9065	1/1	0.99	0.14	44,44,44,44	0
6	MG	L	9272	1/1	0.99	0.10	29,29,29,29	0
6	MG	D	9562	1/1	0.99	0.17	49,49,49,49	0
6	MG	M	9252	1/1	0.99	0.12	37,37,37,37	0
6	MG	M	9472	1/1	0.99	0.06	51,51,51,51	0
6	MG	D	9417	1/1	0.99	0.11	35,35,35,35	0
6	MG	P	9296	1/1	0.99	0.07	42,42,42,42	0
6	MG	D	9129	1/1	0.99	0.09	38,38,38,38	0
6	MG	F	9032	1/1	0.99	0.09	32,32,32,32	0
6	MG	C	9428	1/1	0.99	0.12	42,42,42,42	0
6	MG	D	9094	1/1	0.99	0.10	35,35,35,35	0
6	MG	D	9090	1/1	0.99	0.11	48,48,48,48	0
6	MG	F	9035	1/1	0.99	0.10	40,40,40,40	0
6	MG	A	9394	1/1	0.99	0.10	46,46,46,46	0
6	MG	D	9544	1/1	0.99	0.11	49,49,49,49	0
6	MG	L	9271	1/1	0.99	0.09	39,39,39,39	0
6	MG	B	9033	1/1	0.99	0.10	44,44,44,44	0
6	MG	K	9496	1/1	0.99	0.09	42,42,42,42	0
6	MG	N	9316	1/1	0.99	0.09	32,32,32,32	0
6	MG	C	9028	1/1	0.99	0.07	41,41,41,41	0
6	MG	N	9476	1/1	0.99	0.06	44,44,44,44	0
6	MG	M	9222	1/1	0.99	0.09	33,33,33,33	0
6	MG	M	9323	1/1	0.99	0.10	37,37,37,37	0
6	MG	L	9236	1/1	0.99	0.08	41,41,41,41	0
6	MG	F	9045	1/1	0.99	0.10	40,40,40,40	0
6	MG	D	9016	1/1	0.99	0.07	38,38,38,38	0
6	MG	P	9536	1/1	0.99	0.07	41,41,41,41	0
6	MG	M	9361	1/1	0.99	0.10	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	N	9282	1/1	0.99	0.06	38,38,38,38	0
6	MG	M	9500	1/1	0.99	0.09	46,46,46,46	0
6	MG	M	9268	1/1	0.99	0.11	37,37,37,37	0
6	MG	M	9385	1/1	0.99	0.10	29,29,29,29	0
6	MG	C	9130	1/1	0.99	0.14	42,42,42,42	0
6	MG	L	9345	1/1	0.99	0.12	42,42,42,42	0
6	MG	D	9460	1/1	0.99	0.14	38,38,38,38	0
6	MG	C	9198	1/1	0.99	0.11	36,36,36,36	0
6	MG	F	9513	1/1	0.99	0.14	43,43,43,43	0
6	MG	A	9194	1/1	0.99	0.09	40,40,40,40	0
6	MG	F	9465	1/1	0.99	0.06	36,36,36,36	0
6	MG	N	9291	1/1	0.99	0.15	55,55,55,55	0
6	MG	D	9093	1/1	0.99	0.11	34,34,34,34	0
6	MG	D	9060	1/1	0.99	0.11	35,35,35,35	0
6	MG	P	9353	1/1	0.99	0.11	44,44,44,44	0
6	MG	D	9091	1/1	0.99	0.14	47,47,47,47	0
6	MG	F	9525	1/1	0.99	0.08	54,54,54,54	0
6	MG	N	9277	1/1	0.99	0.09	37,37,37,37	0
6	MG	D	9425	1/1	0.99	0.09	44,44,44,44	0
6	MG	N	9215	1/1	0.99	0.10	40,40,40,40	0
6	MG	M	9216	1/1	0.99	0.12	44,44,44,44	0
6	MG	C	9431	1/1	0.99	0.06	42,42,42,42	0
6	MG	N	9270	1/1	0.99	0.13	47,47,47,47	0
6	MG	M	9489	1/1	0.99	0.09	43,43,43,43	0
6	MG	P	9275	1/1	0.99	0.09	32,32,32,32	0
6	MG	A	9126	1/1	0.99	0.10	39,39,39,39	0
6	MG	N	9324	1/1	0.99	0.08	39,39,39,39	0
6	MG	C	9524	1/1	0.99	0.08	45,45,45,45	0
6	MG	D	9125	1/1	0.99	0.10	35,35,35,35	0
6	MG	A	9200	1/1	0.99	0.10	49,49,49,49	0
6	MG	C	9056	1/1	0.99	0.06	34,34,34,34	0
6	MG	D	9405	1/1	0.99	0.10	38,38,38,38	0
6	MG	C	9193	1/1	0.99	0.09	37,37,37,37	0
6	MG	M	9373	1/1	0.99	0.12	38,38,38,38	0
6	MG	L	9479	1/1	0.99	0.10	48,48,48,48	0
6	MG	E	9402	1/1	0.99	0.12	39,39,39,39	0
6	MG	M	9497	1/1	0.99	0.12	43,43,43,43	0
6	MG	N	9221	1/1	0.99	0.10	30,30,30,30	0
6	MG	A	9024	1/1	0.99	0.10	29,29,29,29	0
6	MG	C	9098	1/1	0.99	0.09	52,52,52,52	0
6	MG	L	9530	1/1	0.99	0.10	58,58,58,58	0
6	MG	F	9133	1/1	0.99	0.10	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	D	9403	1/1	0.99	0.16	30,30,30,30	0
6	MG	K	9493	1/1	0.99	0.09	38,38,38,38	0
6	MG	P	9240	1/1	0.99	0.11	38,38,38,38	0
6	MG	A	9440	1/1	0.99	0.10	53,53,53,53	0
6	MG	D	9418	1/1	0.99	0.08	47,47,47,47	0
6	MG	M	9224	1/1	0.99	0.06	38,38,38,38	0
6	MG	C	9170	1/1	0.99	0.10	36,36,36,36	0
6	MG	C	9185	1/1	0.99	0.18	60,60,60,60	0
6	MG	D	9452	1/1	0.99	0.10	32,32,32,32	0
6	MG	D	9128	1/1	0.99	0.11	35,35,35,35	0
6	MG	D	9070	1/1	0.99	0.10	46,46,46,46	0
6	MG	D	9052	1/1	0.99	0.09	36,36,36,36	0
6	MG	C	9408	1/1	0.99	0.12	38,38,38,38	0
6	MG	K	9492	1/1	0.99	0.10	40,40,40,40	0
6	MG	A	9173	1/1	0.99	0.10	41,41,41,41	0
6	MG	N	9343	1/1	0.99	0.09	45,45,45,45	0
6	MG	N	9237	1/1	0.99	0.14	40,40,40,40	0
6	MG	N	9305	1/1	0.99	0.09	42,42,42,42	0
6	MG	B	9442	1/1	0.99	0.12	47,47,47,47	0
6	MG	C	9161	1/1	0.99	0.07	40,40,40,40	0
6	MG	N	9386	1/1	0.99	0.08	46,46,46,46	0
6	MG	C	9171	1/1	0.99	0.09	33,33,33,33	0
6	MG	L	9374	1/1	0.99	0.09	47,47,47,47	0
6	MG	D	9459	1/1	0.99	0.10	33,33,33,33	0
6	MG	L	9234	1/1	0.99	0.07	41,41,41,41	0
6	MG	D	9082	1/1	0.99	0.11	30,30,30,30	0
6	MG	N	9550	1/1	0.99	0.09	34,34,34,34	0
6	MG	D	9436	1/1	0.99	0.09	46,46,46,46	0
6	MG	N	9501	1/1	0.99	0.08	47,47,47,47	0
6	MG	D	9120	1/1	0.99	0.07	34,34,34,34	0
6	MG	M	9382	1/1	0.99	0.09	33,33,33,33	0
6	MG	N	9357	1/1	0.99	0.09	41,41,41,41	0
6	MG	D	9158	1/1	0.99	0.08	31,31,31,31	0
6	MG	N	9286	1/1	0.99	0.12	46,46,46,46	0
6	MG	D	9142	1/1	0.99	0.11	40,40,40,40	0
8	ZN	D	7112	1/1	0.99	0.13	72,72,72,72	0
6	MG	D	9174	1/1	0.99	0.10	35,35,35,35	0
6	MG	D	9433	1/1	0.99	0.12	46,46,46,46	0
6	MG	D	9051	1/1	0.99	0.07	36,36,36,36	0
6	MG	D	9181	1/1	0.99	0.06	36,36,36,36	0
6	MG	C	9113	1/1	0.99	0.16	47,47,47,47	0
6	MG	A	9116	1/1	0.99	0.12	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	D	9132	1/1	0.99	0.10	33,33,33,33	0
6	MG	K	9507	1/1	0.99	0.14	45,45,45,45	0
6	MG	C	9031	1/1	0.99	0.12	43,43,43,43	0
6	MG	N	9263	1/1	0.99	0.08	37,37,37,37	0
6	MG	N	9371	1/1	0.99	0.10	30,30,30,30	0
6	MG	M	9318	1/1	0.99	0.14	51,51,51,51	0
6	MG	M	9328	1/1	0.99	0.09	48,48,48,48	0
6	MG	N	9294	1/1	0.99	0.07	49,49,49,49	0
6	MG	M	9210	1/1	0.99	0.13	35,35,35,35	0
6	MG	M	9369	1/1	0.99	0.09	35,35,35,35	0
6	MG	F	9542	1/1	0.99	0.19	50,50,50,50	0
6	MG	C	9005	1/1	0.99	0.08	31,31,31,31	0
6	MG	C	9204	1/1	0.99	0.12	41,41,41,41	0
6	MG	L	9480	1/1	0.99	0.13	36,36,36,36	0
6	MG	D	9138	1/1	0.99	0.12	38,38,38,38	0
6	MG	B	9434	1/1	0.99	0.11	35,35,35,35	0
6	MG	K	9279	1/1	0.99	0.11	36,36,36,36	0
6	MG	P	9388	1/1	0.99	0.08	45,45,45,45	0
6	MG	M	9223	1/1	0.99	0.10	48,48,48,48	0
6	MG	D	9134	1/1	0.99	0.10	40,40,40,40	0
6	MG	N	9238	1/1	0.99	0.16	29,29,29,29	0
6	MG	L	9260	1/1	0.99	0.09	41,41,41,41	0
6	MG	M	9535	1/1	0.99	0.12	40,40,40,40	0
6	MG	A	9117	1/1	0.99	0.07	32,32,32,32	0
6	MG	M	9537	1/1	0.99	0.13	38,38,38,38	0
6	MG	K	9370	1/1	0.99	0.06	46,46,46,46	0
6	MG	D	9118	1/1	0.99	0.12	34,34,34,34	0
6	MG	D	9085	1/1	0.99	0.10	32,32,32,32	0
6	MG	N	9533	1/1	0.99	0.12	33,33,33,33	0
6	MG	F	9089	1/1	0.99	0.10	48,48,48,48	0
6	MG	C	9004	1/1	0.99	0.09	30,30,30,30	0
6	MG	D	9061	1/1	0.99	0.11	35,35,35,35	0
6	MG	M	9372	1/1	0.99	0.09	47,47,47,47	0
6	MG	D	9017	1/1	0.99	0.07	37,37,37,37	0
6	MG	P	9269	1/1	0.99	0.09	41,41,41,41	0
6	MG	D	9008	1/1	0.99	0.13	37,37,37,37	0
6	MG	D	9058	1/1	0.99	0.11	41,41,41,41	0
6	MG	N	9482	1/1	0.99	0.14	52,52,52,52	0
6	MG	D	9464	1/1	0.99	0.12	38,38,38,38	0
6	MG	C	9426	1/1	0.99	0.06	47,47,47,47	0
6	MG	K	9487	1/1	0.99	0.12	36,36,36,36	0
6	MG	P	9494	1/1	0.99	0.10	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	N	9552	1/1	0.99	0.11	46,46,46,46	0
6	MG	N	9303	1/1	0.99	0.12	35,35,35,35	0
6	MG	D	9114	1/1	0.99	0.10	32,32,32,32	0
6	MG	D	9162	1/1	0.99	0.11	44,44,44,44	0
6	MG	L	9330	1/1	0.99	0.09	41,41,41,41	0
6	MG	N	9387	1/1	0.99	0.07	28,28,28,28	0
6	MG	D	9105	1/1	0.99	0.07	48,48,48,48	0
6	MG	M	9254	1/1	0.99	0.08	34,34,34,34	0
6	MG	C	9046	1/1	0.99	0.09	31,31,31,31	0
6	MG	D	9392	1/1	0.99	0.09	46,46,46,46	0
6	MG	C	9444	1/1	0.99	0.09	40,40,40,40	0
6	MG	A	9412	1/1	0.99	0.12	33,33,33,33	0
6	MG	B	9040	1/1	0.99	0.16	29,29,29,29	0
6	MG	B	9450	1/1	0.99	0.08	46,46,46,46	0
6	MG	N	9225	1/1	0.99	0.08	40,40,40,40	0
6	MG	N	9306	1/1	0.99	0.13	30,30,30,30	0
6	MG	N	9339	1/1	0.99	0.11	34,34,34,34	0
6	MG	C	9400	1/1	0.99	0.12	49,49,49,49	0
6	MG	D	9064	1/1	0.99	0.11	41,41,41,41	0
6	MG	D	9188	1/1	0.99	0.09	37,37,37,37	0
6	MG	K	9495	1/1	0.99	0.10	35,35,35,35	0
6	MG	D	9075	1/1	0.99	0.11	39,39,39,39	0
6	MG	N	9352	1/1	0.99	0.05	44,44,44,44	0
6	MG	F	9080	1/1	0.99	0.12	30,30,30,30	0
6	MG	C	9086	1/1	0.99	0.10	34,34,34,34	0
6	MG	C	9022	1/1	0.99	0.12	28,28,28,28	0
6	MG	N	9528	1/1	0.99	0.10	40,40,40,40	0
6	MG	C	9409	1/1	0.99	0.12	49,49,49,49	0
6	MG	C	9201	1/1	0.99	0.08	45,45,45,45	0
6	MG	D	9037	1/1	1.00	0.08	31,31,31,31	0
6	MG	C	9390	1/1	1.00	0.12	30,30,30,30	0
6	MG	B	9176	1/1	1.00	0.09	41,41,41,41	0
8	ZN	N	7059	1/1	1.00	0.12	83,83,83,83	0
6	MG	D	9195	1/1	1.00	0.08	32,32,32,32	0
6	MG	E	9511	1/1	1.00	0.12	42,42,42,42	0
6	MG	L	9299	1/1	1.00	0.07	36,36,36,36	0
6	MG	D	9510	1/1	1.00	0.12	51,51,51,51	0
6	MG	D	9043	1/1	1.00	0.11	28,28,28,28	0
6	MG	F	9547	1/1	1.00	0.09	52,52,52,52	0
6	MG	N	9527	1/1	1.00	0.14	42,42,42,42	0
6	MG	N	9531	1/1	1.00	0.10	38,38,38,38	0
6	MG	F	9030	1/1	1.00	0.11	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	D	9006	1/1	1.00	0.14	30,30,30,30	0
6	MG	P	9239	1/1	1.00	0.11	33,33,33,33	0
6	MG	K	9264	1/1	1.00	0.09	36,36,36,36	0
6	MG	N	9308	1/1	1.00	0.12	31,31,31,31	0
6	MG	D	9453	1/1	1.00	0.12	31,31,31,31	0
6	MG	O	9337	1/1	1.00	0.08	34,34,34,34	0
6	MG	D	9182	1/1	1.00	0.07	46,46,46,46	0
6	MG	D	9087	1/1	1.00	0.09	27,27,27,27	0
6	MG	N	9302	1/1	1.00	0.14	48,48,48,48	0
6	MG	N	9468	1/1	1.00	0.11	35,35,35,35	0
6	MG	N	9470	1/1	1.00	0.15	27,27,27,27	0
6	MG	N	9360	1/1	1.00	0.05	39,39,39,39	0
6	MG	C	9160	1/1	1.00	0.12	46,46,46,46	0
6	MG	N	9491	1/1	1.00	0.11	43,43,43,43	0
6	MG	M	9380	1/1	1.00	0.08	32,32,32,32	0
6	MG	M	9241	1/1	1.00	0.09	35,35,35,35	0
6	MG	K	9212	1/1	1.00	0.08	33,33,33,33	0
6	MG	F	9421	1/1	1.00	0.13	30,30,30,30	0
6	MG	L	9278	1/1	1.00	0.08	46,46,46,46	0
6	MG	A	9404	1/1	1.00	0.16	55,55,55,55	0
6	MG	D	9149	1/1	1.00	0.13	42,42,42,42	0
6	MG	C	9027	1/1	1.00	0.12	28,28,28,28	0
6	MG	C	9106	1/1	1.00	0.09	37,37,37,37	0
6	MG	O	9231	1/1	1.00	0.15	41,41,41,41	0
6	MG	D	9179	1/1	1.00	0.09	30,30,30,30	0
6	MG	M	9469	1/1	1.00	0.14	39,39,39,39	0
6	MG	D	9069	1/1	1.00	0.12	32,32,32,32	0
6	MG	K	9477	1/1	1.00	0.11	38,38,38,38	0
6	MG	M	9331	1/1	1.00	0.08	49,49,49,49	0
6	MG	C	9127	1/1	1.00	0.10	41,41,41,41	0
6	MG	D	9143	1/1	1.00	0.14	35,35,35,35	0
6	MG	D	9013	1/1	1.00	0.09	34,34,34,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.