



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 03:49 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 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/ValidationPDFNotes.html>

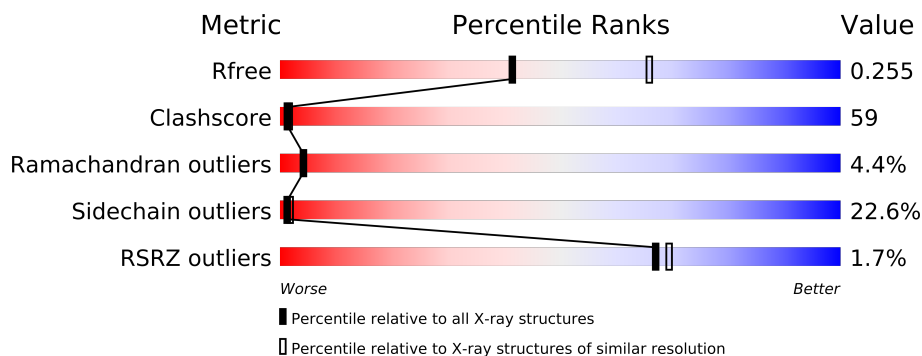
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	315	
1	B	315	
1	K	315	
1	L	315	
2	C	1119	
2	M	1119	
3	D	1524	
3	N	1524	
4	E	99	
4	O	99	
5	F	423	
5	P	423	

The following table lists non-polymeric compounds that are outliers for geometric or electron-

density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
6	MG	B	9419	-	X
6	MG	C	9014	-	X
6	MG	C	9081	-	X
6	MG	C	9106	-	X
6	MG	C	9121	-	X
6	MG	C	9157	-	X
6	MG	C	9185	-	X
6	MG	C	9192	-	X
6	MG	D	9075	-	X
6	MG	D	9112	-	X
6	MG	D	9445	-	X
6	MG	D	9460	-	X
6	MG	E	9187	-	X
6	MG	F	9010	-	X
6	MG	L	9213	-	X
6	MG	L	9378	-	X
6	MG	M	9210	-	X
6	MG	M	9332	-	X
6	MG	N	9246	-	X
6	MG	N	9262	-	X
6	MG	N	9273	-	X
6	MG	N	9292	-	X
6	MG	N	9308	-	X
6	MG	N	9371	-	X
6	MG	N	9482	-	X
6	MG	O	9209	-	X
6	MG	P	9322	-	X
7	RBT	C	8001	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 61089 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

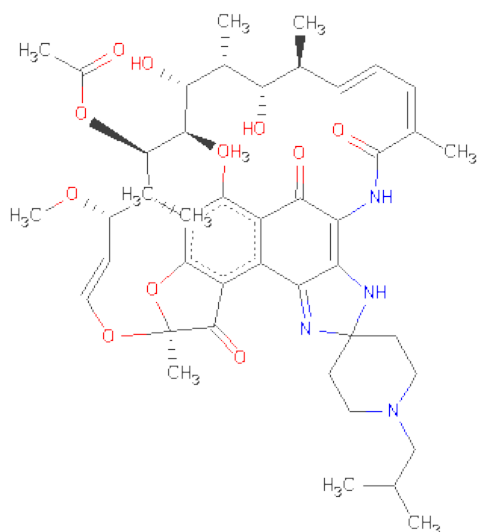
- Molecule 5 is a protein called RNA polymerase sigma factor rpoD.

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: C₄₆H₆₂N₄O₁₁).



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		

Continued on next page...

Continued from previous page...

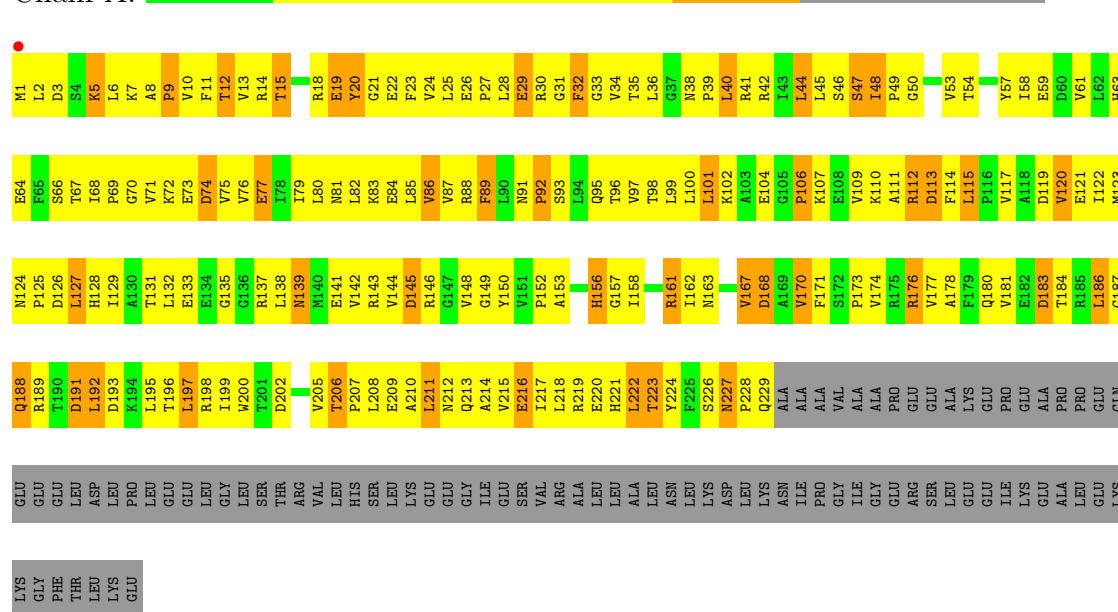
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	F	456	Total 456	O 456	0	0
9	K	213	Total 213	O 213	0	0
9	L	237	Total 237	O 237	0	0
9	M	998	Total 998	O 998	0	0
9	N	1357	Total 1357	O 1357	0	0
9	O	117	Total 117	O 117	0	0
9	P	377	Total 377	O 377	0	0

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 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.

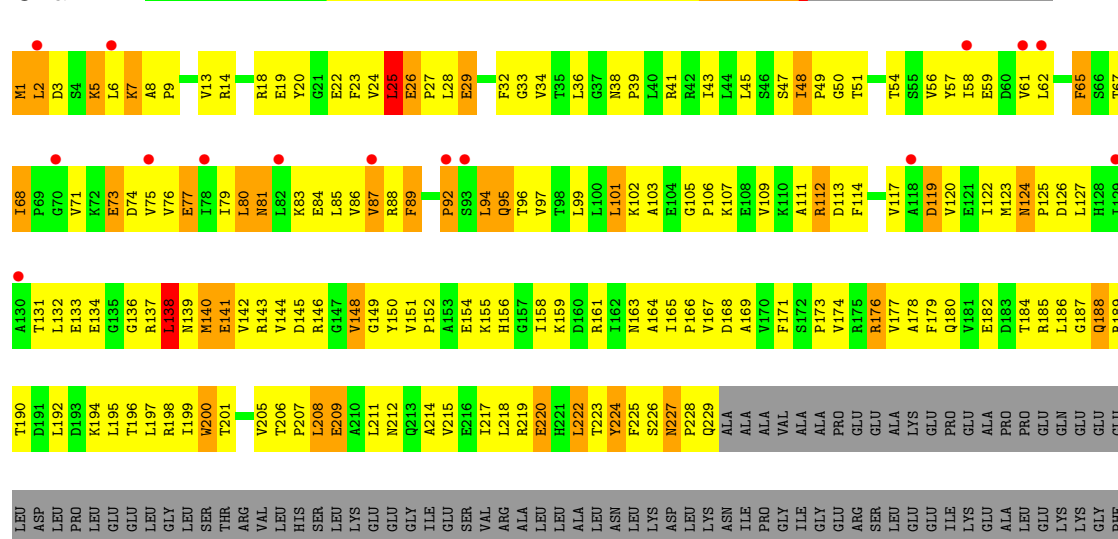
- Molecule 1: DNA-directed RNA polymerase alpha chain

Chain A:



- Molecule 1: DNA-directed RNA polymerase alpha chain

Chain B:



M1	E2	I3	K4	R5	F6	G7	R8	I9	R10	E11	V12	I13	P14	L15	P16	P17	L18	T19	E20	I21	Q22	S25	Y26	A29	L30	Q31	A32	S33	V34	P35	P36	E37	K38	R39	E40	N41	V42	G43	I44	Q45	A46	A47	F48	R49	E50	T51	F52	P53	P54	I54	F55	E56	K59	G60	K61	L62
----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

Q1019	T958	L897	Q829	F761	G634	V569	I508	T443	A381	V254	K190	V65
P1020	P959	G895	K830	F761	T635	P570	A509	P444	I382	A255	F191	L66
L1021	E960	G899	R831	T768	A636	L571	A510	M448	E321	A256	F192	D67
G1022	E961	R900	K832	P769	L637	L572	E511	M449	V322	V256	P193	F68
			L833	T701	D638	R573	R512	I449	D324	Y257	L193	L69
A1025	L963	Y901	K834	T702	G639	A574	V513	G450	F385	Y258	V194	E70
Q1026	G964	S903	R835	T703	R640	Q575	V514	L451	D325	G259	L195	Y71
F1027	E965	P904	G836	T704	P641	A576	A515	L452	I326	L260	L196	R72
G1028	L966	T905	D837	H705	R642	P577	R516		D261	A262	L197	L73
Q1029	P967	F906	K838	T706	V643	V578	R517	A456	L328	A263	P199	G74
G1030	L968	R907	L839	T707	V644	V579	K518	A457	Q329	P264	Q139	E75
	Q969	G908	A840	T708	G645	M580	G519	Y458		R265	L200	P76
G1033	N841	A909	G646	T709	Q647	T581	E520	A459	R332	R266	G201	P77
E1034	R971	K910	Q647	T710	R648	G582	P521	A459	R333	R267	Y202	P78
M1036	V972	E911	R648		V649	L583	V522	R460	T335	D268	Q204	Q80
E1037	V973	G844	V649	R713	L584	E584	I523	V461	V335	D269	Q205	
W1038	L974	E913	R650	T714	R650	R585	V524	D462	G337	G270	T206	C83
A1039	Y975	T914	K651	T715	K651	E586	S525	T469	E338	E271	L207	Y147
	D976	K915	G652	K716	G652	V587	P526	L464	E339	A272	A208	F148
	G977	E916	D653	L717	D653	V588	E527	G465	P400	G273	R209	E85
A1042	R978	L917	L654	D787	L654	R589	E528	F466	T341	R274	E210	K86
	T979	L918	L655	T788	L655	D590	E530	I467	D342	Y275	L211	D87
A1045	E981	Q920	R656	G789	A656		F531	T469	Q343	K276	G212	L88
L1048	P982	L790	K657	T723	D657	L595	M532	P470	F344		A213	T59
L1049	L983	T723	A680	R724	A680	Y596	D583	Y471	R345	E279	Y214	Y90
Q1050	E984	D725				A597	V534	R472	V346	K280	G215	Q91
E1051	G985	T726	G664	D725	G664	E598	S535	R473	G347	L281	E216	A92
M1052	P986	T727	P685	D600	P685	D600	P536	R409	L348	G282	L217	P93
L1053	L987	R728	L666	G601	L666	G601	K537	V474	R408	V218	P157	P93
T1054	V988	H729	A667	E602	A667	E602	Q538	V475	I410	Y158	Y158	L94
L1055	Q928	S730	L668	E603	L668	G603	V539		S411	L285	Q219	Y95
K1056	R929	E731	G669	A604	G669	A604	F540		R405	S286	G220	A96
S1057	Q930	R801	G670	G605	G670	G605	S541	V479	R352	G287	L221	R97
D1058	E931	T732	M671	V606	M671	V606	V542	T480	R353	C287	M222	L98
F993	E932	L734	V672	D607	V672	D607	E482	D481	G354	L290	D223	Q99
L1059	G933	R735	L673	G608	L673	G608			P415	A291	E224	P164
E1060	F934	T736	V674	N609	V674	N609			G416	R356	S225	I101
			A675	R610	A675	R610			G417	R292	V226	H102
G1062	D937	L737	L676	G611	L676	G611			L418	F293	F227	K103
			M677	V612	M677	V612			T419	E294	A228	K104
A1066	R938	E739	P677	G613	P677	G613			R420	T105	M229	D104
Y1067	R939	T740	P678	V613	P678	V613			E421	P170	R230	T105
E1068	E940	G741	F679	R614	F679	R614			R422	G106	P231	G106
A1069	V941	V742	D680	G615	D680	G615			E423	I108	E232	L107
E1070	E942	V743	G681	E616	G681	E616			G424	I172	E233	I108
L1071	L943	T744	V682		V682				F425	K109	E234	K109
K1072	R945	T745	N683	L620	N683	L620			D426	E301	I235	E110
G1073	R946	G746	P684	V621	P684	V621			V427	V302	I236	D111
			G685	E622	G685	E622			T368	L304	R237	E112
E1074	N881	T747	D686	G623	D686	G623			P369	P305	L238	F113
D1075	L882	E748	A687	Y623	A687	Y623			A370	T306	F239	V114
V1076	G883	V749	P688	P624	P688	P624			K371	L307	G180	L115
			V689	L625	V689	L625			L372	R308	H117	G116
P1079	L885	P751	T690	R626	T690	R626			V373	P243	I118	H117
S1080	G951	T752	V691	G627	G951	G627			N500	G245	P119	I118
L1081	L952	L754	S691	F628	L952	F628			K374	S183	S183	P119
S1081	R953	L755	E692	Y629	R953	Y629			S375	D246	M121	L120
L1014	T954	L755	E693	R630	T954	R630			R376	K185	M121	M121
L1015	P955	T756	E694	S631	P955	S631			P377	R250	V186	
F1082	L889	T759	L694	N632	L889	N632			L378	D251	N187	D124
E1083	G956	S760	L695	Q633	G956	Q633			E379	K252	K188	D124
Q1018	K957		K696		K696				A380	P318	R189	F127

R1086
V1087
L1088
L1089
K1090
E1091
L1092
Q1093
A1094
L1095
A1096
L1097
D1098
V1099
Q1100
T1101
L1102
D1103
E1104
K1105
D1106
N1107
P1108
G1114
L1115
A1116
S1117
K1118
R1119

• Molecule 2: DNA-directed RNA polymerase beta chain

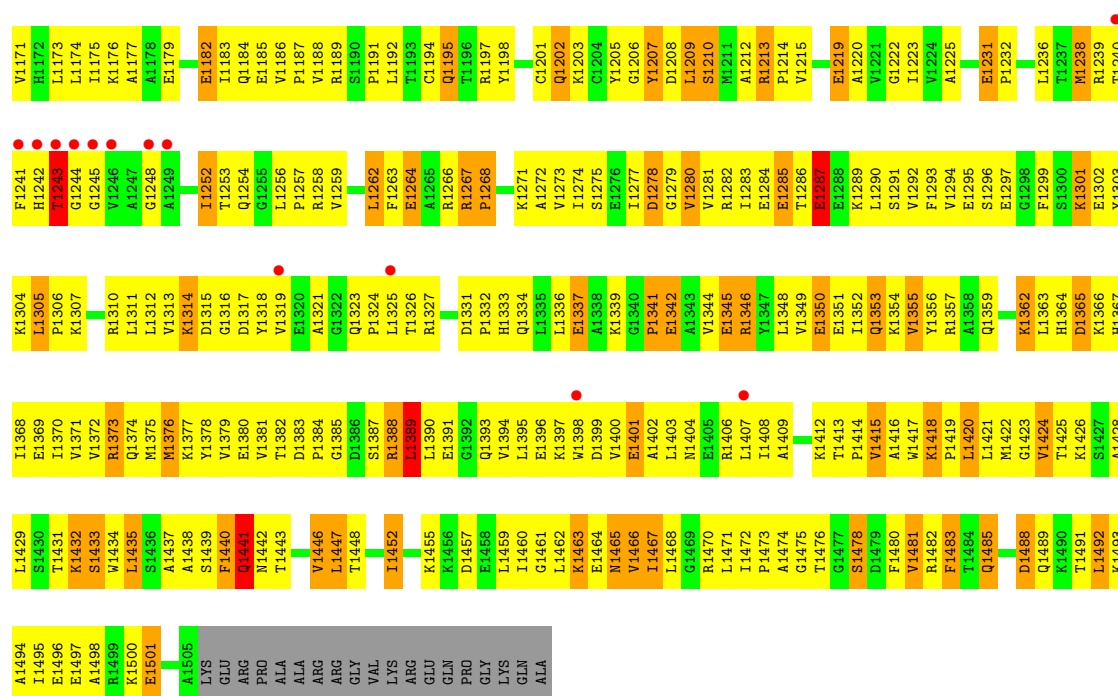
Chain M: 

Y826	Y759	L694	Y629	M564	P502	T433	A370	Y309	K249	R189	I129	G63	M1
Y827	K762	L695	R630	Q565	L503	H434	K371	L310	R250	L130	L310	L64	E2
A828		K696	S631	T566	E504	Y435	L372	F311	D251	F191	G131	V65	I3
		R697	H632		G506	G436	V373	A312	K252	P192	A132	L66	K4
R831	S765	D698	G633	V569	N506	R437	N374	L313	A253	L193	D133	D67	R5
K832		F699	G634	P570	R507	L438	S375	T314	V254	V194	R134	F68	F6
L833	T768	Y700	T635	L571	L508	C439	R376	A315	A255	L195	V135	L69	G7
Q834	P769	T701	A636	L572	A509	E442	P377		E256	L196	G135	E70	R8
R835	E770	S702	L637	R573	A510	E443	L378	P318	Y257	L197	V137	Y71	I9
G836	E771	I703	D638	A574	E511	T443	E379	G319	Y258	R198	S138	R72	R10
R837	R772	H704	Q639	Q575	R512	P444	A380	H320	Y259	V199	Q139	L73	E11
K838	L773	I705	R640	A576	V513	E445		E321	L260	L200	Q139	G74	V12
L839	R774	E706	P641	P577	V514		R383	V322	L261	G201	H141		I13
A840	R775	R707	R642	V578	A515	L451	E384	D323	A262	Y202	R142	F78	P14
N841	S776	Y708	V643	V579	R516	L452	F385	D263	D263	D203	S143	P79	L15
R842	I777	E709	V644	N580	R517	T453	F386	I325	R264	Q204	P144	Q80	P16
H843	F778		V645	T581	K518	S454	S387	D326	R265	E205	G145	D81	P17
G844	G779	R713	G646	G582	G519	L455	R388	H327	R266	T206	V146	E82	L18
N845	E780	D714	R647	L583	E520	A456		L328	Y267	L207	Y147	C83	T19
K846	R781	T715	R648	E584	P521	A457	L391	G329	D268	A208	F148	R84	E20
G847	A782	R716	V649	E585	V522	Y458	S392	N330	L269	R209	T149	E85	I21
H848	R783	L717	R650	R686	I523	A459	Q393	R331	Q270	E210	P150	K86	Q22
Y849	H784	G718	K651	V587	V524	R460	F394	R332	E271	L211	D151	D87	V23
				V588	S525	V461	K395	I333	A272	G212	P152	L88	E24
		R719	L654	V688	S526	D462	D396	R334	G273	A213	A153	T89	S25
I852	K786	E720		R589	P526	D462	D396	R334	G273	A213	A153	T89	S25
L853	H787	R721	A600	D590	E527	E463	E397	T335	R274	Y214	R154	Y90	Y26
P854	T788	I722			E528	L464	T398	V336	Y275	G215	P155	Q91	R27
R855	S789	R723	S661	L595	V529	R465	N399	G337	K276	E216	G156	A92	R28
E856	L790	R724	E662	Y596	E530	E530	P400	E338	A277	L217	R157	P93	A29
D857	R791	D725	N663	A597	F531	L467	L401	L339	E278	V218	Y158	L94	L30
P858	V792	I726	G664	E598	M532	R468	S402	P340	E279	Q219	I159	Y95	L36
N859	P793	R727	L666		D533	T469	S403	T341	K280	G220	A160	A96	V34
H860	P794	L728	A667	G601	V534	P470	R405	D342	L281	L221	S161	R97	P35
		H729		E602	S535		R405	Q343	G282	M222	I162	L98	P36
			L668	V603	P536	R473	H406	F344	T283	D223	I163	Q99	E37
D862	G798		G669	A604	K537	V474	K407	R345	R284	E224	P164	L100	E37
D863	I799	A732	Q670	E605	Q538	V475	R408	V346	L285	S225	P165	K38	K38
G864	A733	R730	R670	F605	Q538	V475	R408	V346	L285	S225	P165	K38	K38
T865	R802	L734	N671	V606	F549	V478	R409	G347	S286	V226	P166	H102	R39
P866	T803	R735	V672	D607	F540	V478	L410	L348	G287	F227	K103	E40	E40
H867	Y804	D736	L673	G608	S541	V479	S411	A349	R288	R168	A168	D104	N41
R868	R805	L737	V674	N609	V542	T480	A412	R350	T289	M229	G169	D104	
H869	L806	D738	A675	R610	M543	D481	L413	L351	L280	R230	P170	L107	G43



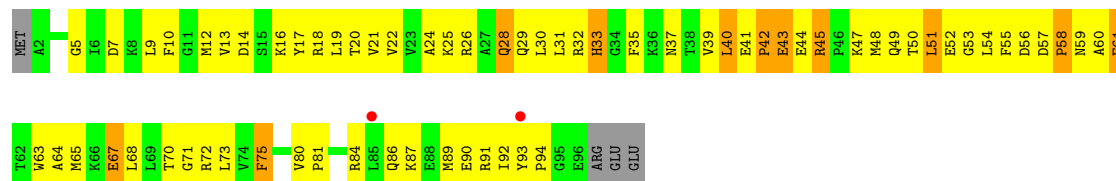


E1109	G1043	F982	E907	R838	E776	L713	R647	V619	E459	I393	GLY	GLY	V126
A1110	L1044	L983	K908	Y841	P777	Q714	M648	L520	A460	L394	ALA	GLY	L127
C1111	M1045	T984	N909	Y842	L778	A715	A649	P521	L461	V395	PHE	THR	L128
G1113	K1046	S910	L911	V841	A779	F716	L850	E822	Q462	K397	LEU	THR	F129
T1114	K1047	D985	K912	F843	K780	Q717	E851	D523	Q463	K398	VAL	VAL	K130
G1115	L1048	R986	K912	A844	P718	Q718	L652	L524	L464	A398	LEU	TYR	K131
T1116	S1049	E987	Y915	N845	S792	W719	F853	R525	L465	R399	ARG	LEU	V132
N1117	K1050	R988	Y916	P846	R783	L720	K654	P526	E467	Y400	ARG	THR	I133
Y1118	E1051	Y989	F916	Y989	D784	G723	P855	G533	E467	Y401	GLU	ARG	I134
S1119	F1052	D990	Q917	L850	T785	Q724	F566	V528	L468	F402	ASP	LEU	V134
P1120	F1053	A918	Q918	L851	T786	W728	F567	Q529	L469	F403	GLU	ASP	L135
P1121	P1056	L992	F919	A852	G725	S725	L658	V630	E470	E404	PRO	PRO	D136
L1122	V1057	R922	L920	V853	Q727	Q727	K660	G534	E471	E408	VAL	VAL	K138
F1123	R1058	G923	L921	T857	L728	W729	M661	R535	L473	G412	ALA	ALA	G139
K1124	S1059	L996	L996	E862	L729	W730	E662	F536	E474	Y205	THR	THR	L140
P1125	S1060	T997	M924	E863	P730	F730	E663	A336	E475	R206	PHE	TYR	I141
L1126	L1061	E998	E925	L860	T732	L731	L666	D539	E476	R414	ASP	LEU	L142
E1127	R1062	T999	K926	Q861	W733	W733	A667	R601	L477	V415	TYR	PRO	N143
V1128	E1063	D962	T927	D862	C734	C734	A668	S602	L478	A416	ARG	VAL	G144
T1129	G1064	E1001	A928	V863	E735	E735	M669	L603	L478	P417	VAL	GLY	V145
R1130	L1065	K1002	L935	V864	F736	D604	E670	T604	E480	G418	GLY	GLY	P146
S1131	T1066	V1003	L937	E874	F737	D605	M676	L643	M481	D419	PRO	THR	V147
L1132	V1067	T1004	G938	T875	W737	T606	K671	Y544	K482	V420	HIS	PRO	E148
R1133	L1068	Q1005	D932	S876	A738	R613	E678	R545	H483	L421	MET	LEU	K149
L1134	E1069	A1006	E933	R877	W745	W745	R679	R607	P484	A422	ASN	VAL	Q151
R1135	V1070	V1007	L936	R872	F740	F740	R674	G609	S495	D423	VAL	VAL	L152
K1136	F1071	F1008	K935	L873	D741	D741	R675	K610	R486	G424	VAL	HIS	L153
L1137	L1072	K1009	L937	E874	Q742	Q742	M676	D611	A487	K425	VAL	GLY	T154
A1138	S1073	N1010	G938	T875	D743	D743	E677	R550	R488	G426	PRO	GLY	E157
D1139	S1074	F1011	F939	S876	Q744	Q744	E678	N551	R489	V427	GLY	TLE	E158
I1140	A1077	E1012	S945	S877	W746	W746	Q680	N552	A490	K428	VAL	VAL	R159
E1141	K1078	N1014	G946	G878	F747	F747	R682	R553	K491	D430	GLY	GLY	E160
G1143	R1079	L1018	T948	R879	W749	W749	I683	L554	A492	V431	ARG	GLY	L161
L1144	D1083	P1019	T949	I880	E811	E811	V687	K556	K494	Y432	GLN	PRO	R162
G1146	T1084	L1020	G950	P882	L813	P750	W687	L557	R495	G433	LEU	LEU	K165
R1147	R1087	Y1021	I951	A883	A814	F754	W688	L558	L496	R434	ALA	ALA	Q166
L1148	D1090	V1022	D952	R884	E817	Q756	D889	Q560	E497	V435	GLY	GLY	E167
A1150	G1091	M1023	D953	I885	E817	Q756	A690	G561	V499	E436	ALA	ALA	T168
R1151	S1091	Q1025	V955	V886	E820	A757	E693	A562	R500	V437	LYS	LYS	Y169
E1152	G1092	S1026	I956	E887	E821	E758	E694	P563	A501	V440	GLY	GLY	P170
V1153	Y1093	G1027	P957	E888	V821	A759	V694	E564	F502	R441	LEU	LEU	L171
L1156	L1094	A1028	E958	A889	A822	R760	I695	I565	L503	N442	ARG	ARG	P172
R1159	T1095	R1029	E959	V890	L823	Q762	H696	I567	D504	V443	MET	ALA	G173
L1160	K1096	G1030	K960	E892	A825	W763	V699	R568	S505	R445	PRO	PRO	V175
E1161	L1098	M1031	K961	E893	P826	L764	W700	N569	N507	V446	ARG	ARG	D176
G1163	V1099	Q1032	L964	K994	I827	S765	L701	E570	S508	V447	GLN	GLY	A177
R1164	T1100	Q1033	E985	V895	K828	A766	L702	K571	P509	E448	VAL	VAL	L178
L1165	V1101	Q1034	E986	A996	V829	R767	N703	R572	E510	S449	ARG	ARG	V179
T1166	L1102	I1035	A830	W897	A830	W768	R704	M573	W511	Y450	ALA	ALA	K180
L1167	R1103	Q1037	D968	E898	G831	L769	A705	L574	M512	H386	ALA	ALA	D181
S1167	E1104	L1038	R969	R833	R832	W770	P706	Q575	W513	I452	GLN	GLN	G182
L1168	L1105	C1039	K970	R834	R833	S771	T707	E576	L514	D453	VAL	VAL	E183
D1169	V1106	L1041	L972	Q901	T834	P772	L708	A577	E515	A454	GLY	GLY	E184
L1170	R1108	R1042	Q976	L902	S835	W773	H709	V578	A516	E455	ALA	ALA	V185
				Q906	V836	S774	R710	D579	W517	M456	GLY	GLY	L186
					G837	G775	K646	A580	P518	S392	GLY	GLY	K187



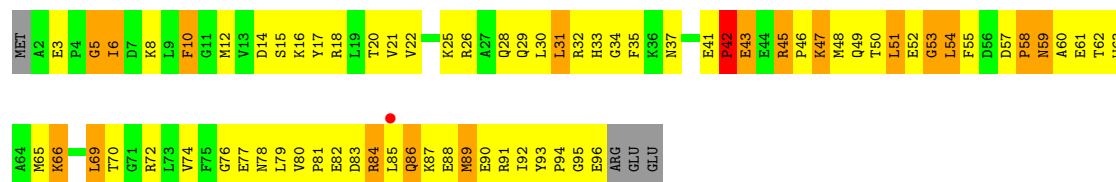
• Molecule 4: RNA polymerase omega chain

Chain E:



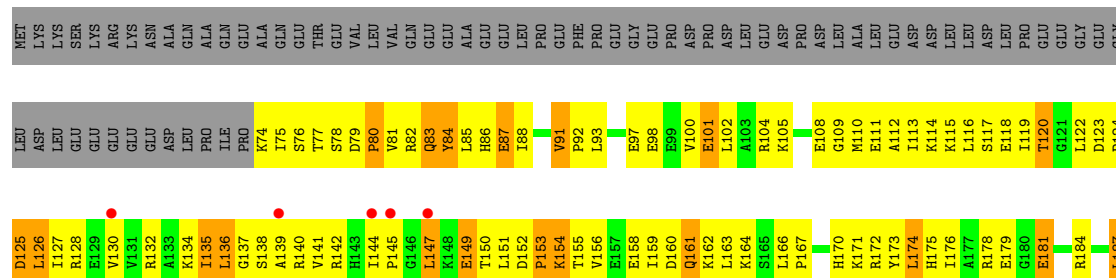
• Molecule 4: RNA polymerase omega chain

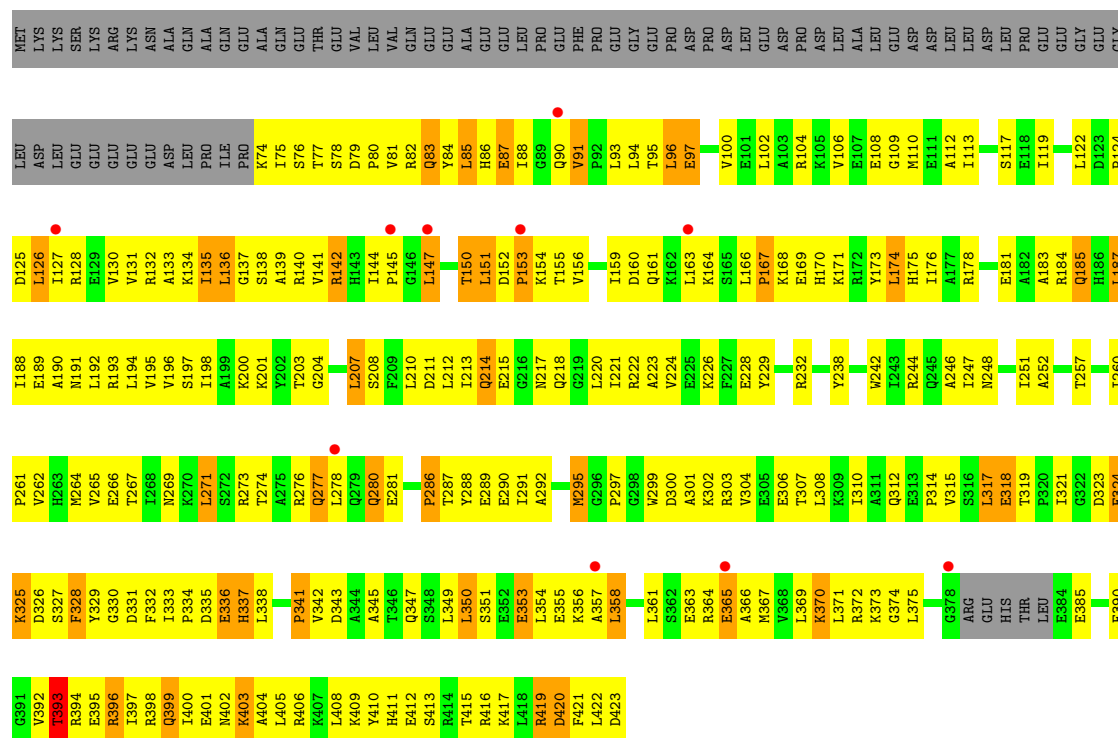
Chain O:



• Molecule 5: RNA polymerase sigma factor rpoD

Chain F:





4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	239.50Å 239.50Å 253.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.50 24.85 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.50) 91.2 (24.85-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.257 0.223 , 0.255	Depositor DCC
R_{free} test set	29386 reflections (6.10%)	DCC
Wilson B-factor (Å ²)	45.1	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 85.5	EDS
Estimated twinning fraction	0.499 for -h,-k,l 0.085 for h,-h-k,-l 0.085 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 511160 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	61089	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	E	112	0	0	22	0
9	F	456	0	0	98	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 59.

The worst 5 of 6365 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	227/315 (72%)	204 (90%)	19 (8%)	4 (2%)	13	20
1	B	227/315 (72%)	201 (88%)	21 (9%)	5 (2%)	10	15
1	K	227/315 (72%)	204 (90%)	19 (8%)	4 (2%)	13	20
1	L	227/315 (72%)	205 (90%)	18 (8%)	4 (2%)	13	20
2	C	1117/1119 (100%)	911 (82%)	153 (14%)	53 (5%)	4	3
2	M	1117/1119 (100%)	904 (81%)	168 (15%)	45 (4%)	5	5

Continued on next page...

Continued from previous page...

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

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%)	1	1
1	B	202/273 (74%)	164 (81%)	38 (19%)	2	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%)	1	1
3	N	1123/1279 (88%)	865 (77%)	258 (23%)	1	2
4	E	83/87 (95%)	67 (81%)	16 (19%)	2	3
4	O	83/87 (95%)	61 (74%)	22 (26%)	1	1
5	F	295/370 (80%)	235 (80%)	60 (20%)	2	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	P	295/370 (80%)	247 (84%)	48 (16%)	3	6
All	All	5692/6446 (88%)	4406 (77%)	1286 (23%)	1	2

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 ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 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	66,66,66	3.27	30 (45%)	101,101,101	1.72	21 (20%)
7	RBT	M	8002	-	66,66,66	3.21	33 (50%)	101,101,101	1.70	17 (16%)

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	0/1/6/6
7	RBT	M	8002	-	-	0/59/116/116	0/1/6/6

The worst 5 of 63 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	8002	RBT	C40-C38	8.13	1.60	1.53
7	C	8001	RBT	C39-C38	8.12	1.60	1.53
7	C	8001	RBT	C9-C8	7.82	1.58	1.41
7	M	8002	RBT	C9-C8	7.55	1.57	1.41
7	C	8001	RBT	C40-C38	7.48	1.60	1.53

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	8002	RBT	C42-C40-C38	5.94	122.58	112.74
7	C	8001	RBT	C42-C40-C38	5.92	122.55	112.74
7	M	8002	RBT	C41-C39-C38	5.78	122.32	112.74
7	C	8001	RBT	C41-C39-C38	5.71	122.20	112.74
7	M	8002	RBT	C20-C21-C22	4.22	121.59	114.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

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, 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%)	-0.21	1 (0%) 90 92	29, 60, 84, 110	0
1	B	229/315 (72%)	0.05	15 (6%) 18 17	44, 89, 114, 118	0
1	K	229/315 (72%)	-0.21	2 (0%) 81 82	33, 58, 89, 120	0
1	L	229/315 (72%)	-0.07	9 (3%) 37 38	49, 89, 109, 119	0
2	C	1119/1119 (100%)	-0.20	14 (1%) 74 76	14, 74, 102, 117	0
2	M	1119/1119 (100%)	-0.21	15 (1%) 74 76	19, 71, 103, 119	0
3	D	1392/1524 (91%)	-0.18	20 (1%) 72 74	19, 62, 107, 125	0
3	N	1392/1524 (91%)	-0.19	29 (2%) 60 63	23, 65, 107, 131	0
4	E	95/99 (95%)	-0.22	2 (2%) 60 63	41, 77, 107, 120	0
4	O	95/99 (95%)	-0.27	1 (1%) 77 79	33, 72, 94, 103	0
5	F	345/423 (81%)	-0.22	8 (2%) 57 60	46, 81, 104, 118	0
5	P	345/423 (81%)	-0.14	10 (2%) 49 51	53, 81, 108, 123	0
All	All	6818/7590 (89%)	-0.18	126 (1%) 67 68	14, 70, 105, 131	0

The worst 5 of 126 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	1243	THR	6.3
5	P	145	PRO	6.0
2	M	269	LEU	5.3
3	D	1244	GLY	4.9
3	D	1240	THR	4.9

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. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	MG	C	9185	1/1	0.20	45.00	60,60,60,60	0
6	MG	N	9292	1/1	0.18	19.25	52,52,52,52	0
6	MG	D	9445	1/1	0.14	13.33	48,48,48,48	0
6	MG	O	9209	1/1	0.13	8.40	37,37,37,37	0
6	MG	L	9213	1/1	0.24	8.14	49,49,49,49	0
6	MG	C	9106	1/1	0.11	8.00	37,37,37,37	0
6	MG	M	9332	1/1	0.16	6.00	54,54,54,54	0
6	MG	E	9187	1/1	0.14	5.20	39,39,39,39	0
6	MG	B	9419	1/1	0.13	4.78	46,46,46,46	0
6	MG	F	9010	1/1	0.20	3.97	57,57,57,57	0
6	MG	N	9308	1/1	0.13	3.50	31,31,31,31	0
6	MG	P	9322	1/1	0.13	3.40	43,43,43,43	0
6	MG	D	9075	1/1	0.13	3.37	39,39,39,39	0
6	MG	C	9081	1/1	0.13	3.33	52,52,52,52	0
6	MG	N	9371	1/1	0.12	3.33	30,30,30,30	0
6	MG	C	9157	1/1	0.18	3.30	44,44,44,44	0
6	MG	C	9014	1/1	0.15	2.83	45,45,45,45	0
6	MG	C	9192	1/1	0.12	2.82	55,55,55,55	0
6	MG	N	9262	1/1	0.15	2.78	49,49,49,49	0
6	MG	D	9460	1/1	0.15	2.67	38,38,38,38	0
6	MG	N	9246	1/1	0.14	2.64	49,49,49,49	0
6	MG	C	9121	1/1	0.16	2.38	43,43,43,43	0
7	RBT	C	8001	61/61	0.19	2.34	25,37,42,48	0
6	MG	L	9378	1/1	0.15	2.20	47,47,47,47	0
6	MG	N	9482	1/1	0.14	2.19	52,52,52,52	0
6	MG	M	9210	1/1	0.14	2.16	35,35,35,35	0
6	MG	N	9273	1/1	0.18	2.10	30,30,30,30	0
6	MG	D	9112	1/1	0.14	2.08	39,39,39,39	0
6	MG	N	9376	1/1	0.14	1.83	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	RBT	M	8002	61/61	0.19	1.78	28,39,48,54	0
6	MG	C	9127	1/1	0.12	1.71	41,41,41,41	0
6	MG	M	9252	1/1	0.14	1.65	37,37,37,37	0
8	ZN	D	7112	1/1	0.14	1.58	72,72,72,72	0
6	MG	M	9255	1/1	0.15	1.50	58,58,58,58	0
6	MG	K	9214	1/1	0.21	1.48	31,31,31,31	0
6	MG	N	9286	1/1	0.13	1.42	46,46,46,46	0
6	MG	C	9130	1/1	0.16	1.40	42,42,42,42	0
6	MG	C	9191	1/1	0.15	1.38	44,44,44,44	0
6	MG	B	9033	1/1	0.11	1.37	44,44,44,44	0
6	MG	D	9060	1/1	0.13	1.34	35,35,35,35	0
6	MG	F	9135	1/1	0.15	1.32	42,42,42,42	0
6	MG	D	9138	1/1	0.13	1.30	38,38,38,38	0
6	MG	A	9001	1/1	0.19	1.18	26,26,26,26	0
6	MG	N	9327	1/1	0.12	1.10	54,54,54,54	0
6	MG	D	9093	1/1	0.12	1.06	34,34,34,34	0
6	MG	M	9309	1/1	0.17	1.00	35,35,35,35	0
6	MG	D	9548	1/1	0.15	0.98	51,51,51,51	0
6	MG	D	9077	1/1	0.11	0.94	32,32,32,32	0
6	MG	D	9002	1/1	0.17	0.91	29,29,29,29	0
6	MG	M	9283	1/1	0.15	0.87	35,35,35,35	0
6	MG	B	9148	1/1	0.17	0.79	54,54,54,54	0
6	MG	N	9358	1/1	0.14	0.78	48,48,48,48	0
6	MG	C	9409	1/1	0.14	0.75	49,49,49,49	0
6	MG	B	9150	1/1	0.11	0.73	43,43,43,43	0
6	MG	N	9320	1/1	0.12	0.67	41,41,41,41	0
8	ZN	N	7113	1/1	0.12	0.66	79,79,79,79	0
6	MG	N	9238	1/1	0.17	0.63	29,29,29,29	0
6	MG	C	9428	1/1	0.14	0.60	42,42,42,42	0
6	MG	C	9141	1/1	0.14	0.59	45,45,45,45	0
6	MG	K	9279	1/1	0.12	0.59	36,36,36,36	0
6	MG	D	9019	1/1	0.16	0.57	35,35,35,35	0
6	MG	D	9096	1/1	0.15	0.57	43,43,43,43	0
6	MG	M	9285	1/1	0.14	0.57	43,43,43,43	0
6	MG	D	9006	1/1	0.16	0.56	30,30,30,30	0
6	MG	D	9082	1/1	0.13	0.56	30,30,30,30	0
6	MG	C	9196	1/1	0.14	0.55	30,30,30,30	0
6	MG	B	9391	1/1	0.13	0.54	27,27,27,27	0
6	MG	C	9068	1/1	0.13	0.51	37,37,37,37	0
6	MG	A	9018	1/1	0.15	0.44	31,31,31,31	0
6	MG	N	9319	1/1	0.13	0.44	41,41,41,41	0
6	MG	C	9074	1/1	0.14	0.42	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	D	9090	1/1	0.12	0.39	48,48,48,48	0
6	MG	N	9218	1/1	0.14	0.31	32,32,32,32	0
6	MG	C	9156	1/1	0.13	0.20	43,43,43,43	0
6	MG	L	9260	1/1	0.10	0.17	41,41,41,41	0
6	MG	D	9061	1/1	0.12	0.16	35,35,35,35	0
8	ZN	N	7059	1/1	0.13	0.14	83,83,83,83	0
6	MG	M	9268	1/1	0.12	0.13	37,37,37,37	0
6	MG	M	9216	1/1	0.13	0.10	44,44,44,44	0
6	MG	N	9314	1/1	0.12	0.07	38,38,38,38	0
6	MG	B	9176	1/1	0.10	0.06	41,41,41,41	0
6	MG	D	9132	1/1	0.11	0.05	33,33,33,33	0
6	MG	N	9303	1/1	0.13	-0.04	35,35,35,35	0
6	MG	L	9258	1/1	0.11	-0.05	47,47,47,47	0
6	MG	B	9040	1/1	0.18	-0.06	29,29,29,29	0
6	MG	D	9049	1/1	0.15	-0.07	31,31,31,31	0
6	MG	C	9029	1/1	0.13	-0.08	36,36,36,36	0
6	MG	A	9097	1/1	0.11	-0.08	41,41,41,41	0
6	MG	D	9009	1/1	0.14	-0.13	53,53,53,53	0
6	MG	D	9059	1/1	0.11	-0.16	40,40,40,40	0
6	MG	M	9384	1/1	0.11	-0.18	35,35,35,35	0
6	MG	D	9015	1/1	0.12	-0.19	37,37,37,37	0
6	MG	M	9488	1/1	0.12	-0.22	42,42,42,42	0
6	MG	D	9154	1/1	0.12	-0.24	31,31,31,31	0
6	MG	M	9220	1/1	0.14	-0.25	45,45,45,45	0
6	MG	N	9306	1/1	0.15	-0.27	30,30,30,30	0
6	MG	N	9504	1/1	0.11	-0.27	32,32,32,32	0
6	MG	D	9189	1/1	0.12	-0.31	34,34,34,34	0
6	MG	E	9115	1/1	0.09	-0.31	39,39,39,39	0
6	MG	C	9198	1/1	0.12	-0.33	36,36,36,36	0
6	MG	N	9242	1/1	0.13	-0.34	36,36,36,36	0
6	MG	M	9233	1/1	0.17	-0.35	38,38,38,38	0
6	MG	M	9259	1/1	0.19	-0.35	57,57,57,57	0
6	MG	M	9340	1/1	0.11	-0.36	43,43,43,43	0
6	MG	D	9042	1/1	0.12	-0.38	47,47,47,47	0
6	MG	F	9421	1/1	0.14	-0.38	30,30,30,30	0
6	MG	M	9336	1/1	0.12	-0.39	31,31,31,31	0
6	MG	M	9347	1/1	0.12	-0.40	37,37,37,37	0
6	MG	D	9021	1/1	0.13	-0.40	34,34,34,34	0
6	MG	K	9265	1/1	0.14	-0.40	37,37,37,37	0
6	MG	N	9245	1/1	0.13	-0.45	28,28,28,28	0
6	MG	D	9038	1/1	0.11	-0.46	35,35,35,35	0
6	MG	K	9484	1/1	0.12	-0.46	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	D	9123	1/1	0.14	-0.47	37,37,37,37	0
6	MG	D	9152	1/1	0.12	-0.48	32,32,32,32	0
6	MG	F	9045	1/1	0.11	-0.48	40,40,40,40	0
6	MG	F	9410	1/1	0.13	-0.49	47,47,47,47	0
6	MG	O	9355	1/1	0.15	-0.49	36,36,36,36	0
6	MG	D	9118	1/1	0.13	-0.51	34,34,34,34	0
6	MG	B	9434	1/1	0.13	-0.52	35,35,35,35	0
6	MG	M	9293	1/1	0.11	-0.53	43,43,43,43	0
6	MG	D	9463	1/1	0.12	-0.54	32,32,32,32	0
6	MG	C	9020	1/1	0.15	-0.56	28,28,28,28	0
6	MG	M	9290	1/1	0.13	-0.58	48,48,48,48	0
6	MG	P	9239	1/1	0.12	-0.60	33,33,33,33	0
6	MG	C	9022	1/1	0.13	-0.61	28,28,28,28	0
6	MG	F	9030	1/1	0.12	-0.62	36,36,36,36	0
6	MG	F	9197	1/1	0.11	-0.63	39,39,39,39	0
6	MG	P	9275	1/1	0.10	-0.66	32,32,32,32	0
6	MG	N	9315	1/1	0.12	-0.67	41,41,41,41	0
6	MG	C	9190	1/1	0.08	-0.68	40,40,40,40	0
6	MG	B	9137	1/1	0.10	-0.69	35,35,35,35	0
6	MG	D	9128	1/1	0.13	-0.70	35,35,35,35	0
6	MG	N	9235	1/1	0.13	-0.70	63,63,63,63	0
6	MG	N	9277	1/1	0.10	-0.71	37,37,37,37	0
6	MG	C	9399	1/1	0.11	-0.71	43,43,43,43	0
6	MG	N	9335	1/1	0.11	-0.72	33,33,33,33	0
6	MG	D	9008	1/1	0.13	-0.74	37,37,37,37	0
6	MG	N	9288	1/1	0.11	-0.74	33,33,33,33	0
6	MG	N	9526	1/1	0.11	-0.75	30,30,30,30	0
6	MG	N	9208	1/1	0.13	-0.77	35,35,35,35	0
6	MG	N	9486	1/1	0.10	-0.77	44,44,44,44	0
6	MG	D	9036	1/1	0.14	-0.77	41,41,41,41	0
6	MG	K	9363	1/1	0.11	-0.78	47,47,47,47	0
6	MG	A	9413	1/1	0.11	-0.78	46,46,46,46	0
6	MG	D	9446	1/1	0.11	-0.79	36,36,36,36	0
6	MG	D	9449	1/1	0.09	-0.79	29,29,29,29	0
6	MG	O	9337	1/1	0.09	-0.81	34,34,34,34	0
6	MG	M	9227	1/1	0.11	-0.81	44,44,44,44	0
6	MG	D	9111	1/1	0.10	-0.83	43,43,43,43	0
6	MG	C	9007	1/1	0.12	-0.83	34,34,34,34	0
6	MG	N	9368	1/1	0.10	-0.84	41,41,41,41	0
6	MG	M	9500	1/1	0.10	-0.84	46,46,46,46	0
6	MG	N	9501	1/1	0.10	-0.84	47,47,47,47	0
6	MG	N	9215	1/1	0.10	-0.86	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	B	9079	1/1	0.12	-0.87	28,28,28,28	0
6	MG	D	9172	1/1	0.11	-0.88	35,35,35,35	0
6	MG	A	9024	1/1	0.10	-0.90	29,29,29,29	0
6	MG	M	9267	1/1	0.13	-0.93	41,41,41,41	0
6	MG	M	9229	1/1	0.10	-0.95	35,35,35,35	0
6	MG	B	9146	1/1	0.10	-0.95	44,44,44,44	0
6	MG	M	9473	1/1	0.11	-0.96	42,42,42,42	0
6	MG	M	9382	1/1	0.10	-0.96	33,33,33,33	0
6	MG	D	9069	1/1	0.13	-0.96	32,32,32,32	0
6	MG	D	9425	1/1	0.11	-0.97	44,44,44,44	0
6	MG	C	9023	1/1	0.10	-0.98	44,44,44,44	0
6	MG	D	9459	1/1	0.12	-0.98	33,33,33,33	0
6	MG	C	9004	1/1	0.10	-0.98	30,30,30,30	0
6	MG	M	9298	1/1	0.13	-0.99	43,43,43,43	0
6	MG	M	9481	1/1	0.10	-1.00	37,37,37,37	0
6	MG	D	9401	1/1	0.13	-1.00	40,40,40,40	0
6	MG	N	9508	1/1	0.13	-1.00	41,41,41,41	0
6	MG	K	9367	1/1	0.09	-1.01	38,38,38,38	0
6	MG	N	9324	1/1	0.09	-1.02	39,39,39,39	0
6	MG	C	9025	1/1	0.11	-1.03	39,39,39,39	0
6	MG	D	9453	1/1	0.12	-1.03	31,31,31,31	0
6	MG	P	9536	1/1	0.09	-1.03	41,41,41,41	0
6	MG	A	9139	1/1	0.10	-1.03	35,35,35,35	0
6	MG	N	9256	1/1	0.11	-1.05	41,41,41,41	0
6	MG	K	9351	1/1	0.10	-1.05	37,37,37,37	0
6	MG	D	9423	1/1	0.10	-1.05	44,44,44,44	0
6	MG	C	9398	1/1	0.11	-1.06	44,44,44,44	0
6	MG	N	9339	1/1	0.12	-1.07	34,34,34,34	0
6	MG	B	9163	1/1	0.07	-1.09	44,44,44,44	0
6	MG	K	9487	1/1	0.12	-1.09	36,36,36,36	0
6	MG	L	9345	1/1	0.14	-1.12	42,42,42,42	0
6	MG	F	9053	1/1	0.10	-1.13	34,34,34,34	0
6	MG	M	9323	1/1	0.11	-1.14	37,37,37,37	0
6	MG	O	9359	1/1	0.09	-1.14	57,57,57,57	0
6	MG	N	9307	1/1	0.10	-1.15	38,38,38,38	0
6	MG	N	9230	1/1	0.11	-1.16	40,40,40,40	0
6	MG	D	9064	1/1	0.12	-1.17	41,41,41,41	0
6	MG	M	9222	1/1	0.10	-1.17	33,33,33,33	0
6	MG	K	9370	1/1	0.06	-1.18	46,46,46,46	0
6	MG	D	9052	1/1	0.09	-1.21	36,36,36,36	0
6	MG	D	9084	1/1	0.11	-1.21	47,47,47,47	0
6	MG	C	9161	1/1	0.08	-1.21	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	M	9328	1/1	0.09	-1.22	48,48,48,48	0
6	MG	C	9011	1/1	0.10	-1.22	39,39,39,39	0
6	MG	C	9005	1/1	0.09	-1.22	31,31,31,31	0
6	MG	P	9274	1/1	0.12	-1.23	45,45,45,45	0
6	MG	C	9044	1/1	0.09	-1.24	37,37,37,37	0
6	MG	N	9365	1/1	0.14	-1.26	43,43,43,43	0
6	MG	M	9383	1/1	0.10	-1.27	46,46,46,46	0
6	MG	N	9498	1/1	0.10	-1.28	45,45,45,45	0
6	MG	D	9441	1/1	0.11	-1.28	46,46,46,46	0
6	MG	M	9312	1/1	0.10	-1.29	37,37,37,37	0
6	MG	F	9035	1/1	0.11	-1.29	40,40,40,40	0
6	MG	N	9354	1/1	0.08	-1.30	42,42,42,42	0
6	MG	D	9169	1/1	0.13	-1.30	45,45,45,45	0
6	MG	P	9284	1/1	0.11	-1.32	51,51,51,51	0
6	MG	D	9057	1/1	0.12	-1.32	33,33,33,33	0
6	MG	P	9329	1/1	0.08	-1.32	46,46,46,46	0
6	MG	D	9055	1/1	0.11	-1.32	51,51,51,51	0
6	MG	M	9287	1/1	0.10	-1.35	36,36,36,36	0
6	MG	A	9200	1/1	0.11	-1.36	49,49,49,49	0
6	MG	N	9221	1/1	0.11	-1.37	30,30,30,30	0
6	MG	C	9193	1/1	0.11	-1.38	37,37,37,37	0
6	MG	N	9289	1/1	0.10	-1.41	35,35,35,35	0
6	MG	B	9199	1/1	0.12	-1.41	52,52,52,52	0
6	MG	N	9357	1/1	0.10	-1.42	41,41,41,41	0
6	MG	L	9236	1/1	0.09	-1.43	41,41,41,41	0
6	MG	A	9117	1/1	0.08	-1.43	32,32,32,32	0
6	MG	D	9026	1/1	0.12	-1.43	37,37,37,37	0
6	MG	C	9031	1/1	0.12	-1.46	43,43,43,43	0
6	MG	A	9109	1/1	0.11	-1.48	33,33,33,33	0
6	MG	C	9144	1/1	0.09	-1.49	39,39,39,39	0
6	MG	B	9180	1/1	0.10	-1.52	36,36,36,36	0
6	MG	D	9110	1/1	0.13	-1.52	38,38,38,38	0
6	MG	N	9263	1/1	0.08	-1.52	37,37,37,37	0
6	MG	A	9165	1/1	0.12	-1.54	65,65,65,65	0
6	MG	M	9369	1/1	0.10	-1.54	35,35,35,35	0
6	MG	C	9124	1/1	0.09	-1.54	33,33,33,33	0
8	ZN	D	7058	1/1	0.08	-1.55	100,100,100,100	0
6	MG	N	9226	1/1	0.07	-1.56	30,30,30,30	0
6	MG	C	9086	1/1	0.12	-1.57	34,34,34,34	0
6	MG	M	9243	1/1	0.12	-1.57	45,45,45,45	0
6	MG	M	9251	1/1	0.14	-1.57	33,33,33,33	0
6	MG	N	9475	1/1	0.07	-1.59	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	D	9070	1/1	0.11	-1.59	46,46,46,46	0
6	MG	D	9136	1/1	0.12	-1.62	41,41,41,41	0
6	MG	P	9296	1/1	0.09	-1.63	42,42,42,42	0
6	MG	N	9301	1/1	0.09	-1.64	50,50,50,50	0
6	MG	C	9028	1/1	0.08	-1.65	41,41,41,41	0
6	MG	L	9278	1/1	0.09	-1.68	46,46,46,46	0
6	MG	K	9264	1/1	0.09	-1.69	36,36,36,36	0
6	MG	D	9179	1/1	0.10	-1.70	30,30,30,30	0
6	MG	N	9313	1/1	0.09	-1.71	39,39,39,39	0
6	MG	C	9027	1/1	0.13	-1.72	28,28,28,28	0
6	MG	A	9050	1/1	0.11	-1.73	41,41,41,41	0
6	MG	B	9101	1/1	0.09	-1.73	40,40,40,40	0
6	MG	C	9415	1/1	0.13	-1.74	38,38,38,38	0
6	MG	A	9194	1/1	0.11	-1.75	40,40,40,40	0
6	MG	F	9465	1/1	0.07	-1.75	36,36,36,36	0
6	MG	N	9280	1/1	0.09	-1.75	34,34,34,34	0
6	MG	C	9046	1/1	0.10	-1.77	31,31,31,31	0
6	MG	P	9502	1/1	0.08	-1.78	43,43,43,43	0
6	MG	E	9186	1/1	0.11	-1.78	35,35,35,35	0
6	MG	O	9231	1/1	0.17	-1.79	41,41,41,41	0
6	MG	D	9181	1/1	0.06	-1.82	36,36,36,36	0
6	MG	M	9350	1/1	0.10	-1.83	37,37,37,37	0
6	MG	M	9372	1/1	0.10	-1.83	47,47,47,47	0
6	MG	L	9272	1/1	0.11	-1.85	29,29,29,29	0
6	MG	M	9219	1/1	0.11	-1.87	39,39,39,39	0
6	MG	K	9212	1/1	0.09	-1.87	33,33,33,33	0
6	MG	D	9125	1/1	0.11	-1.88	35,35,35,35	0
6	MG	N	9244	1/1	0.09	-1.88	37,37,37,37	0
6	MG	D	9561	1/1	0.07	-1.89	38,38,38,38	0
6	MG	C	9546	1/1	0.07	-1.92	49,49,49,49	0
6	MG	N	9550	1/1	0.10	-1.95	34,34,34,34	0
6	MG	N	9225	1/1	0.09	-2.00	40,40,40,40	0
6	MG	L	9234	1/1	0.07	-2.02	41,41,41,41	0
6	MG	D	9105	1/1	0.07	-2.04	48,48,48,48	0
6	MG	P	9269	1/1	0.10	-2.04	41,41,41,41	0
6	MG	D	9134	1/1	0.11	-2.06	40,40,40,40	0
6	MG	P	9240	1/1	0.12	-2.08	38,38,38,38	0
6	MG	N	9247	1/1	0.09	-2.11	29,29,29,29	0
6	MG	N	9207	1/1	0.11	-2.16	30,30,30,30	0
6	MG	D	9037	1/1	0.09	-2.16	31,31,31,31	0
6	MG	M	9380	1/1	0.09	-2.16	32,32,32,32	0
6	MG	N	9387	1/1	0.08	-2.17	28,28,28,28	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	D	9043	1/1	0.13	-2.20	28,28,28,28	0
6	MG	A	9102	1/1	0.10	-2.22	38,38,38,38	0
6	MG	F	9153	1/1	0.08	-2.24	39,39,39,39	0
6	MG	M	9224	1/1	0.07	-2.24	38,38,38,38	0
6	MG	M	9478	1/1	0.06	-2.25	35,35,35,35	0
6	MG	D	9095	1/1	0.07	-2.32	40,40,40,40	0
6	MG	N	9232	1/1	0.11	-2.34	33,33,33,33	0
6	MG	C	9076	1/1	0.11	-2.36	37,37,37,37	0
6	MG	O	9362	1/1	0.05	-2.37	49,49,49,49	0
6	MG	D	9454	1/1	0.09	-2.40	42,42,42,42	0
6	MG	N	9509	1/1	0.11	-2.40	31,31,31,31	0
6	MG	N	9342	1/1	0.07	-2.42	48,48,48,48	0
6	MG	M	9211	1/1	0.10	-2.43	28,28,28,28	0
6	MG	P	9558	1/1	0.10	-2.45	44,44,44,44	0
6	MG	D	9087	1/1	0.10	-2.47	27,27,27,27	0
6	MG	A	9411	1/1	0.11	-2.50	31,31,31,31	0
6	MG	C	9056	1/1	0.06	-2.50	34,34,34,34	0
6	MG	M	9254	1/1	0.09	-2.51	34,34,34,34	0
6	MG	C	9515	1/1	0.09	-2.52	41,41,41,41	0
6	MG	N	9253	1/1	0.09	-2.53	39,39,39,39	0
6	MG	D	9182	1/1	0.08	-2.55	46,46,46,46	0
6	MG	F	9032	1/1	0.10	-2.57	32,32,32,32	0
6	MG	N	9352	1/1	0.06	-2.58	44,44,44,44	0
6	MG	D	9051	1/1	0.08	-2.66	36,36,36,36	0
6	MG	D	9129	1/1	0.10	-2.70	38,38,38,38	0
6	MG	E	9131	1/1	0.09	-2.71	47,47,47,47	0
6	MG	D	9104	1/1	0.10	-2.77	35,35,35,35	0
6	MG	D	9166	1/1	0.10	-2.78	49,49,49,49	0
6	MG	F	9407	1/1	0.07	-2.78	32,32,32,32	0
6	MG	D	9147	1/1	0.10	-2.81	40,40,40,40	0
6	MG	P	9326	1/1	0.09	-2.85	39,39,39,39	0
6	MG	D	9108	1/1	0.12	-2.89	51,51,51,51	0
6	MG	D	9013	1/1	0.09	-2.89	34,34,34,34	0
6	MG	N	9248	1/1	0.06	-2.90	47,47,47,47	0
6	MG	C	9170	1/1	0.11	-2.90	36,36,36,36	0
6	MG	C	9431	1/1	0.06	-2.96	42,42,42,42	0
6	MG	C	9420	1/1	0.08	-3.06	37,37,37,37	0
6	MG	C	9414	1/1	0.07	-3.07	41,41,41,41	0
6	MG	N	9360	1/1	0.06	-3.09	39,39,39,39	0
6	MG	N	9281	1/1	0.11	-3.11	50,50,50,50	0
6	MG	D	9041	1/1	0.11	-3.14	32,32,32,32	0
6	MG	M	9241	1/1	0.10	-3.17	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	C	9171	1/1	0.10	-3.27	33,33,33,33	0
6	MG	M	9485	1/1	0.07	-3.29	42,42,42,42	0
6	MG	P	9333	1/1	0.07	-3.34	28,28,28,28	0
6	MG	A	9126	1/1	0.11	-3.50	39,39,39,39	0
6	MG	M	9373	1/1	0.13	-3.62	38,38,38,38	0
6	MG	C	9047	1/1	0.06	-3.66	47,47,47,47	0
6	MG	N	9531	1/1	0.10	-3.68	38,38,38,38	0
6	MG	D	9017	1/1	0.07	-3.88	37,37,37,37	0
6	MG	N	9349	1/1	0.06	-3.94	37,37,37,37	0
6	MG	D	9100	1/1	0.08	-3.98	31,31,31,31	0
6	MG	C	9444	1/1	0.12	-4.00	40,40,40,40	0
6	MG	A	9178	1/1	0.10	-4.08	28,28,28,28	0
6	MG	D	9397	1/1	0.14	-4.12	31,31,31,31	0
6	MG	D	9168	1/1	0.07	-4.31	38,38,38,38	0
6	MG	A	9107	1/1	0.08	-4.43	40,40,40,40	0
6	MG	D	9003	1/1	0.06	-4.55	43,43,43,43	0
6	MG	D	9120	1/1	0.07	-4.60	34,34,34,34	0
6	MG	D	9122	1/1	0.10	-4.87	31,31,31,31	0
6	MG	N	9381	1/1	0.07	-5.05	35,35,35,35	0
6	MG	D	9012	1/1	0.06	-5.09	39,39,39,39	0
6	MG	E	9151	1/1	0.06	-5.15	48,48,48,48	0
6	MG	N	9310	1/1	0.08	-5.26	36,36,36,36	0
6	MG	D	9099	1/1	0.08	-5.32	38,38,38,38	0
6	MG	M	9364	1/1	0.08	-5.49	37,37,37,37	0
6	MG	K	9217	1/1	0.07	-5.90	36,36,36,36	0
6	MG	F	9054	1/1	0.09	-6.05	37,37,37,37	0
6	MG	D	9451	1/1	0.10	-6.08	37,37,37,37	0
6	MG	N	9476	1/1	0.07	-6.09	44,44,44,44	0
6	MG	D	9162	1/1	0.12	-6.10	44,44,44,44	0
6	MG	N	9266	1/1	0.08	-6.11	36,36,36,36	0
6	MG	C	9458	1/1	0.10	-6.20	38,38,38,38	0
6	MG	N	9228	1/1	0.09	-6.24	49,49,49,49	0
6	MG	D	9195	1/1	0.09	-6.33	32,32,32,32	0
6	MG	F	9437	1/1	0.10	-6.46	47,47,47,47	0
6	MG	C	9462	1/1	0.14	-6.60	50,50,50,50	0
6	MG	C	9177	1/1	0.10	-7.17	40,40,40,40	0
6	MG	N	9282	1/1	0.05	-7.32	38,38,38,38	0
6	MG	D	9523	1/1	0.12	-7.57	41,41,41,41	0
6	MG	D	9203	1/1	0.10	-7.67	46,46,46,46	0
6	MG	C	9456	1/1	0.08	-9.17	37,37,37,37	0
6	MG	C	9426	1/1	0.06	-11.97	47,47,47,47	0
6	MG	K	9495	1/1	0.11	-13.80	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	D	9158	1/1	0.09	-16.64	31,31,31,31	0
6	MG	N	9386	1/1	0.08	-19.67	46,46,46,46	0
6	MG	F	9435	1/1	0.09	-27.22	40,40,40,40	0
6	MG	L	9374	1/1	0.11	-39.00	47,47,47,47	0
6	MG	N	9555	1/1	0.13	-40.25	56,56,56,56	0
6	MG	M	9497	1/1	0.13	-135.00	43,43,43,43	0
6	MG	K	9477	1/1	0.12	-	38,38,38,38	0
6	MG	D	9543	1/1	0.14	-	46,46,46,46	0
6	MG	C	9545	1/1	0.12	-	45,45,45,45	0
6	MG	D	9447	1/1	0.11	-	50,50,50,50	0
6	MG	K	9344	1/1	0.15	-	55,55,55,55	0
6	MG	B	9450	1/1	0.09	-	46,46,46,46	0
6	MG	E	9467	1/1	0.14	-	52,52,52,52	0
6	MG	C	9063	1/1	0.11	-	32,32,32,32	0
6	MG	M	9325	1/1	0.12	-	44,44,44,44	0
6	MG	P	9541	1/1	0.12	-	44,44,44,44	0
6	MG	N	9528	1/1	0.11	-	40,40,40,40	0
6	MG	C	9201	1/1	0.10	-	45,45,45,45	0
6	MG	D	9544	1/1	0.13	-	49,49,49,49	0
6	MG	L	9271	1/1	0.10	-	39,39,39,39	0
6	MG	N	9534	1/1	0.10	-	54,54,54,54	0
6	MG	F	9429	1/1	0.14	-	57,57,57,57	0
6	MG	N	9316	1/1	0.10	-	32,32,32,32	0
6	MG	D	9143	1/1	0.15	-	35,35,35,35	0
6	MG	C	9521	1/1	0.14	-	45,45,45,45	0
6	MG	D	9466	1/1	0.12	-	57,57,57,57	0
6	MG	M	9472	1/1	0.08	-	51,51,51,51	0
6	MG	F	9547	1/1	0.11	-	52,52,52,52	0
6	MG	D	9516	1/1	0.06	-	51,51,51,51	0
6	MG	D	9140	1/1	0.15	-	43,43,43,43	0
6	MG	N	9470	1/1	0.17	-	27,27,27,27	0
6	MG	D	9417	1/1	0.13	-	35,35,35,35	0
6	MG	P	9304	1/1	0.12	-	57,57,57,57	0
6	MG	A	9430	1/1	0.12	-	35,35,35,35	0
6	MG	L	9249	1/1	0.08	-	51,51,51,51	0
6	MG	D	9119	1/1	0.11	-	44,44,44,44	0
6	MG	N	9539	1/1	0.11	-	57,57,57,57	0
6	MG	M	9385	1/1	0.12	-	29,29,29,29	0
6	MG	N	9379	1/1	0.09	-	56,56,56,56	0
6	MG	A	9394	1/1	0.12	-	46,46,46,46	0
6	MG	C	9088	1/1	0.14	-	36,36,36,36	0
6	MG	M	9348	1/1	0.13	-	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	F	9513	1/1	0.16	-	43,43,43,43	0
6	MG	A	9145	1/1	0.13	-	45,45,45,45	0
6	MG	N	9538	1/1	0.11	-	42,42,42,42	0
6	MG	N	9291	1/1	0.16	-	55,55,55,55	0
6	MG	M	9261	1/1	0.11	-	45,45,45,45	0
6	MG	N	9499	1/1	0.10	-	38,38,38,38	0
6	MG	C	9396	1/1	0.17	-	57,57,57,57	0
6	MG	M	9377	1/1	0.14	-	39,39,39,39	0
6	MG	D	9091	1/1	0.15	-	47,47,47,47	0
6	MG	F	9525	1/1	0.10	-	54,54,54,54	0
6	MG	M	9469	1/1	0.16	-	39,39,39,39	0
6	MG	L	9330	1/1	0.10	-	41,41,41,41	0
6	MG	D	9016	1/1	0.09	-	38,38,38,38	0
6	MG	M	9540	1/1	0.18	-	63,63,63,63	0
6	MG	N	9295	1/1	0.06	-	48,48,48,48	0
6	MG	N	9270	1/1	0.15	-	47,47,47,47	0
6	MG	D	9517	1/1	0.11	-	45,45,45,45	0
6	MG	M	9489	1/1	0.10	-	43,43,43,43	0
6	MG	N	9297	1/1	0.15	-	48,48,48,48	0
6	MG	D	9174	1/1	0.11	-	35,35,35,35	0
6	MG	L	9346	1/1	0.16	-	52,52,52,52	0
6	MG	N	9468	1/1	0.13	-	35,35,35,35	0
6	MG	C	9524	1/1	0.10	-	45,45,45,45	0
6	MG	L	9311	1/1	0.08	-	33,33,33,33	0
6	MG	C	9083	1/1	0.12	-	48,48,48,48	0
6	MG	F	9048	1/1	0.17	-	50,50,50,50	0
6	MG	P	9353	1/1	0.14	-	44,44,44,44	0
6	MG	B	9092	1/1	0.12	-	50,50,50,50	0
6	MG	A	9078	1/1	0.15	-	34,34,34,34	0
6	MG	D	9432	1/1	0.11	-	47,47,47,47	0
6	MG	E	9402	1/1	0.14	-	39,39,39,39	0
6	MG	B	9512	1/1	0.22	-	53,53,53,53	0
6	MG	D	9405	1/1	0.12	-	38,38,38,38	0
6	MG	B	9427	1/1	0.14	-	42,42,42,42	0
6	MG	L	9300	1/1	0.10	-	58,58,58,58	0
6	MG	L	9471	1/1	0.11	-	33,33,33,33	0
6	MG	F	9133	1/1	0.12	-	42,42,42,42	0
6	MG	C	9098	1/1	0.10	-	52,52,52,52	0
6	MG	K	9493	1/1	0.11	-	38,38,38,38	0
6	MG	D	9066	1/1	0.12	-	49,49,49,49	0
6	MG	C	9457	1/1	0.11	-	40,40,40,40	0
6	MG	M	9276	1/1	0.14	-	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	D	9403	1/1	0.18	-	30,30,30,30	0
6	MG	L	9530	1/1	0.13	-	58,58,58,58	0
6	MG	A	9440	1/1	0.12	-	53,53,53,53	0
6	MG	D	9418	1/1	0.10	-	47,47,47,47	0
6	MG	L	9505	1/1	0.12	-	58,58,58,58	0
6	MG	D	9510	1/1	0.15	-	51,51,51,51	0
6	MG	C	9422	1/1	0.15	-	41,41,41,41	0
6	MG	C	9408	1/1	0.14	-	38,38,38,38	0
6	MG	K	9492	1/1	0.11	-	40,40,40,40	0
6	MG	A	9173	1/1	0.11	-	41,41,41,41	0
6	MG	N	9343	1/1	0.10	-	45,45,45,45	0
6	MG	N	9237	1/1	0.16	-	40,40,40,40	0
6	MG	L	9483	1/1	0.17	-	44,44,44,44	0
6	MG	B	9442	1/1	0.13	-	47,47,47,47	0
6	MG	D	9155	1/1	0.13	-	56,56,56,56	0
6	MG	N	9527	1/1	0.15	-	42,42,42,42	0
6	MG	A	9522	1/1	0.13	-	57,57,57,57	0
6	MG	D	9424	1/1	0.16	-	50,50,50,50	0
6	MG	B	9103	1/1	0.10	-	37,37,37,37	0
6	MG	C	9455	1/1	0.15	-	61,61,61,61	0
6	MG	C	9439	1/1	0.10	-	35,35,35,35	0
6	MG	D	9452	1/1	0.12	-	32,32,32,32	0
6	MG	N	9506	1/1	0.11	-	56,56,56,56	0
6	MG	M	9557	1/1	0.11	-	54,54,54,54	0
6	MG	M	9321	1/1	0.14	-	40,40,40,40	0
6	MG	L	9479	1/1	0.12	-	48,48,48,48	0
6	MG	D	9519	1/1	0.14	-	55,55,55,55	0
6	MG	A	9560	1/1	0.15	-	49,49,49,49	0
6	MG	N	9474	1/1	0.15	-	56,56,56,56	0
6	MG	N	9305	1/1	0.11	-	42,42,42,42	0
6	MG	N	9554	1/1	0.13	-	45,45,45,45	0
6	MG	D	9142	1/1	0.13	-	40,40,40,40	0
6	MG	A	9514	1/1	0.12	-	42,42,42,42	0
6	MG	C	9205	1/1	0.16	-	53,53,53,53	0
6	MG	D	9433	1/1	0.13	-	46,46,46,46	0
6	MG	F	9072	1/1	0.08	-	40,40,40,40	0
6	MG	M	9331	1/1	0.09	-	49,49,49,49	0
6	MG	L	9532	1/1	0.10	-	51,51,51,51	0
6	MG	K	9553	1/1	0.11	-	50,50,50,50	0
6	MG	D	9436	1/1	0.10	-	46,46,46,46	0
6	MG	K	9507	1/1	0.15	-	45,45,45,45	0
6	MG	N	9341	1/1	0.15	-	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	N	9356	1/1	0.17	-	29,29,29,29	0
6	MG	N	9529	1/1	0.10	-	55,55,55,55	0
6	MG	E	9511	1/1	0.13	-	42,42,42,42	0
6	MG	D	9034	1/1	0.17	-	37,37,37,37	0
6	MG	D	9067	1/1	0.13	-	49,49,49,49	0
6	MG	A	9062	1/1	0.13	-	45,45,45,45	0
6	MG	N	9294	1/1	0.07	-	49,49,49,49	0
6	MG	C	9113	1/1	0.17	-	47,47,47,47	0
6	MG	F	9206	1/1	0.13	-	33,33,33,33	0
6	MG	N	9302	1/1	0.14	-	48,48,48,48	0
6	MG	D	9175	1/1	0.10	-	40,40,40,40	0
6	MG	M	9366	1/1	0.12	-	41,41,41,41	0
6	MG	C	9204	1/1	0.14	-	41,41,41,41	0
6	MG	C	9160	1/1	0.13	-	46,46,46,46	0
6	MG	N	9551	1/1	0.09	-	40,40,40,40	0
6	MG	D	9393	1/1	0.15	-	35,35,35,35	0
6	MG	N	9338	1/1	0.14	-	42,42,42,42	0
6	MG	A	9116	1/1	0.14	-	47,47,47,47	0
6	MG	P	9388	1/1	0.10	-	45,45,45,45	0
6	MG	A	9404	1/1	0.17	-	55,55,55,55	0
6	MG	E	9184	1/1	0.17	-	48,48,48,48	0
6	MG	M	9318	1/1	0.16	-	51,51,51,51	0
6	MG	F	9164	1/1	0.12	-	29,29,29,29	0
6	MG	C	9183	1/1	0.17	-	44,44,44,44	0
6	MG	M	9535	1/1	0.15	-	40,40,40,40	0
6	MG	A	9559	1/1	0.14	-	45,45,45,45	0
6	MG	M	9537	1/1	0.14	-	38,38,38,38	0
6	MG	B	9395	1/1	0.13	-	56,56,56,56	0
6	MG	C	9549	1/1	0.12	-	48,48,48,48	0
6	MG	D	9085	1/1	0.11	-	32,32,32,32	0
6	MG	F	9167	1/1	0.14	-	59,59,59,59	0
6	MG	N	9375	1/1	0.11	-	43,43,43,43	0
6	MG	N	9503	1/1	0.15	-	52,52,52,52	0
6	MG	C	9390	1/1	0.14	-	30,30,30,30	0
6	MG	P	9317	1/1	0.20	-	53,53,53,53	0
6	MG	M	9334	1/1	0.10	-	44,44,44,44	0
6	MG	K	9257	1/1	0.13	-	57,57,57,57	0
6	MG	N	9490	1/1	0.14	-	41,41,41,41	0
6	MG	D	9159	1/1	0.12	-	35,35,35,35	0
6	MG	D	9416	1/1	0.11	-	48,48,48,48	0
6	MG	K	9496	1/1	0.11	-	42,42,42,42	0
6	MG	F	9448	1/1	0.11	-	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	D	9073	1/1	0.17	-	38,38,38,38	0
6	MG	D	9464	1/1	0.13	-	38,38,38,38	0
6	MG	F	9542	1/1	0.21	-	50,50,50,50	0
6	MG	L	9480	1/1	0.15	-	36,36,36,36	0
6	MG	P	9494	1/1	0.12	-	50,50,50,50	0
6	MG	N	9552	1/1	0.13	-	46,46,46,46	0
6	MG	D	9562	1/1	0.19	-	49,49,49,49	0
6	MG	D	9114	1/1	0.11	-	32,32,32,32	0
6	MG	B	9389	1/1	0.12	-	37,37,37,37	0
6	MG	N	9533	1/1	0.14	-	33,33,33,33	0
6	MG	C	9406	1/1	0.13	-	47,47,47,47	0
6	MG	D	9149	1/1	0.15	-	42,42,42,42	0
6	MG	F	9089	1/1	0.11	-	48,48,48,48	0
6	MG	L	9556	1/1	0.11	-	58,58,58,58	0
6	MG	D	9392	1/1	0.10	-	46,46,46,46	0
6	MG	N	9250	1/1	0.17	-	61,61,61,61	0
6	MG	A	9412	1/1	0.14	-	33,33,33,33	0
6	MG	M	9223	1/1	0.13	-	48,48,48,48	0
6	MG	E	9438	1/1	0.12	-	38,38,38,38	0
6	MG	D	9443	1/1	0.08	-	47,47,47,47	0
6	MG	C	9071	1/1	0.16	-	39,39,39,39	0
6	MG	D	9039	1/1	0.14	-	40,40,40,40	0
6	MG	D	9058	1/1	0.12	-	41,41,41,41	0
6	MG	C	9400	1/1	0.14	-	49,49,49,49	0
6	MG	D	9520	1/1	0.15	-	46,46,46,46	0
6	MG	D	9188	1/1	0.10	-	37,37,37,37	0
6	MG	D	9202	1/1	0.19	-	61,61,61,61	0
6	MG	L	9299	1/1	0.08	-	36,36,36,36	0
6	MG	F	9461	1/1	0.13	-	52,52,52,52	0
6	MG	F	9080	1/1	0.14	-	30,30,30,30	0
6	MG	N	9491	1/1	0.13	-	43,43,43,43	0
6	MG	D	9094	1/1	0.11	-	35,35,35,35	0
6	MG	D	9065	1/1	0.15	-	44,44,44,44	0
6	MG	M	9361	1/1	0.11	-	51,51,51,51	0
6	MG	D	9518	1/1	0.13	-	55,55,55,55	0

6.5 Other polymers ⓘ

There are no such residues in this entry.