



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 08:42 am GMT

PDB ID : 2A69
Title : Crystal structure of the T. Thermophilus RNA polymerase holoenzyme in complex with antibiotic rifapentin
Authors : Artsimovitch, I.; Vassilyeva, M.N.; Svetlov, D.; Svetlov, V.; Perederina, A.; Igarashi, N.; Matsugaki, N.; Wakatsuki, S.; Tahirov, T.H.; Vassilyev, D.G.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2005-07-02
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

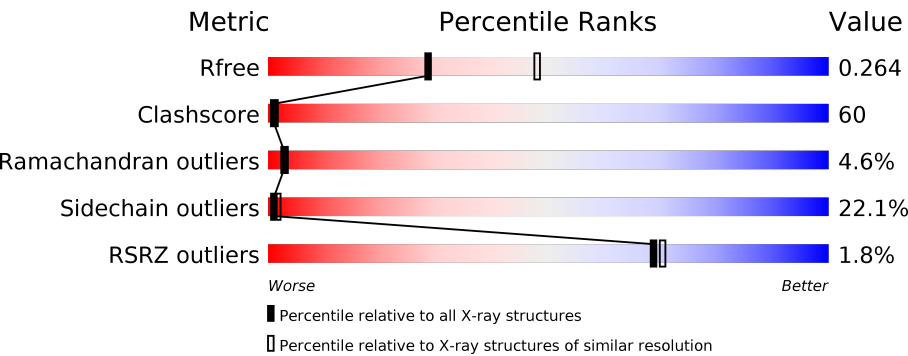
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

1 Overall quality at a glance i

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}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	315	<div><div></div><div><div>17%</div><div>44%</div><div>10%</div><div>•</div><div>27%</div></div></div>
1	B	315	<div><div>4%</div><div><div>18%</div><div>43%</div><div>11%</div><div>27%</div></div></div>
1	K	315	<div><div>%</div><div><div>23%</div><div>40%</div><div>9%</div><div>•</div><div>27%</div></div></div>
1	L	315	<div><div>2%</div><div><div>19%</div><div>43%</div><div>10%</div><div>27%</div></div></div>
2	C	1119	<div><div>%</div><div><div>22%</div><div>59%</div><div>18%</div><div>•</div></div></div>
2	M	1119	<div><div>%</div><div><div>24%</div><div>59%</div><div>16%</div><div>•</div></div></div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	RPT	C	8001	-	-	-	X
7	RPT	M	8002	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 60572 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase alpha chain.

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

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

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

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

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

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

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

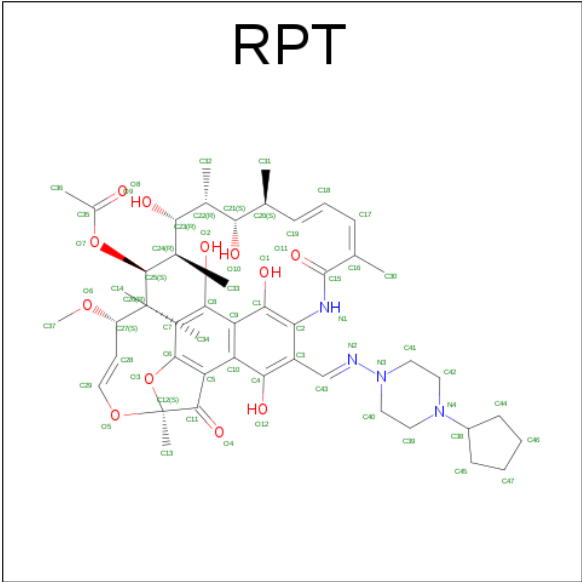
- Molecule 5 is a protein called RNA polymerase sigma factor rpoD.

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

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

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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			63	47	4	12		
7	M	1	Total	C	N	O	0	0
			63	47	4	12		

- 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	239	Total	O	0	0
			239	239		
9	B	258	Total	O	0	0
			258	258		
9	C	979	Total	O	0	0
			979	979		
9	D	1252	Total	O	0	0
			1252	1252		
9	E	117	Total	O	0	0
			117	117		

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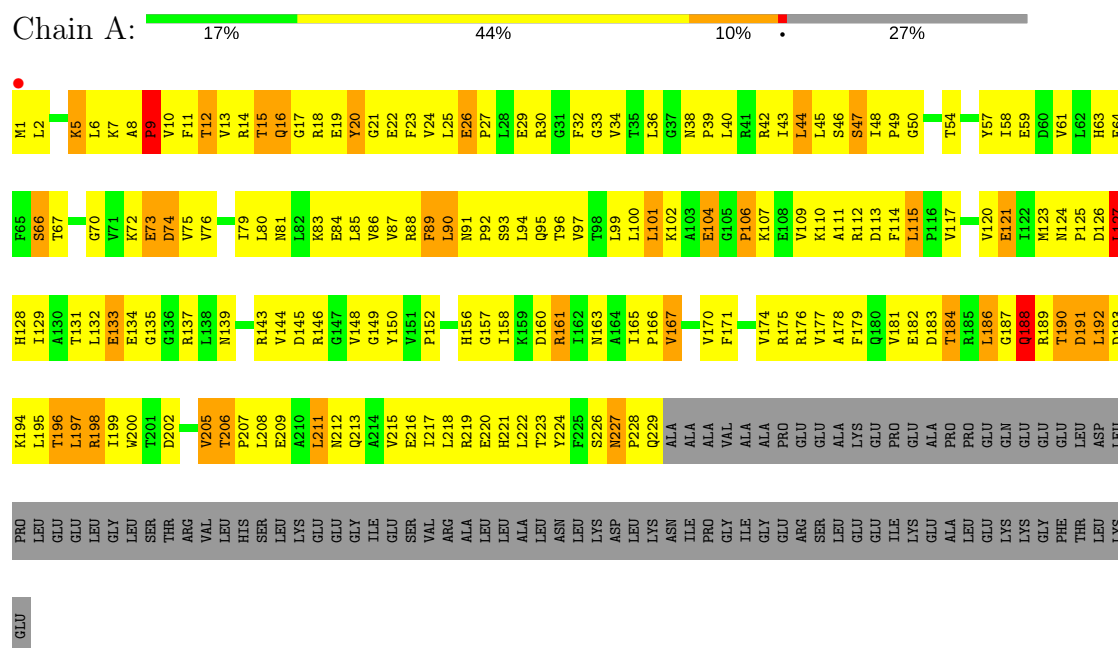
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	F	420	Total 420	O 420	0	0
9	K	183	Total 183	O 183	0	0
9	L	219	Total 219	O 219	0	0
9	M	998	Total 998	O 998	0	0
9	N	1265	Total 1265	O 1265	0	0
9	O	108	Total 108	O 108	0	0
9	P	361	Total 361	O 361	0	0

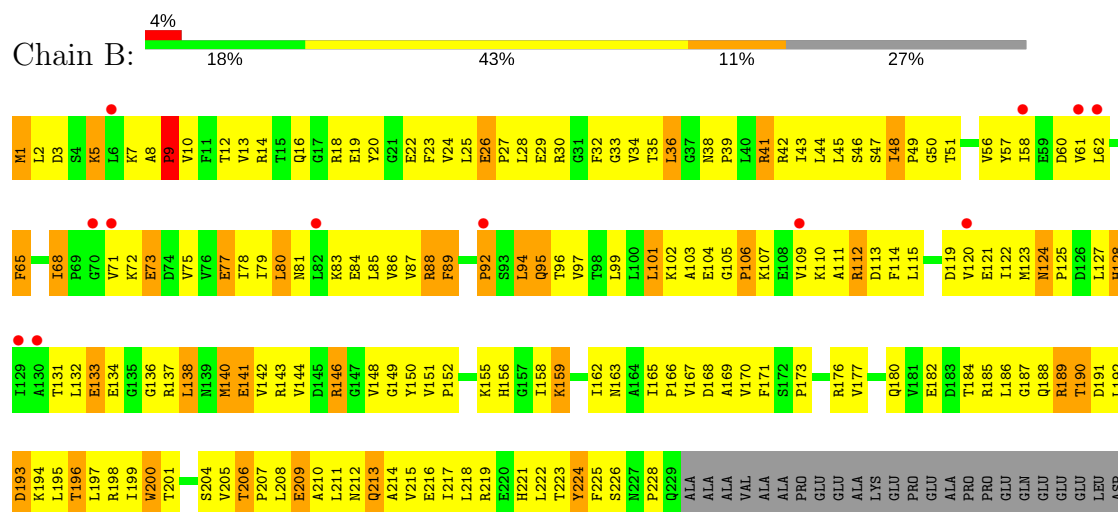
3 Residue-property plots

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

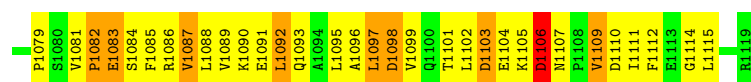


• Molecule 1: DNA-directed RNA polymerase alpha chain

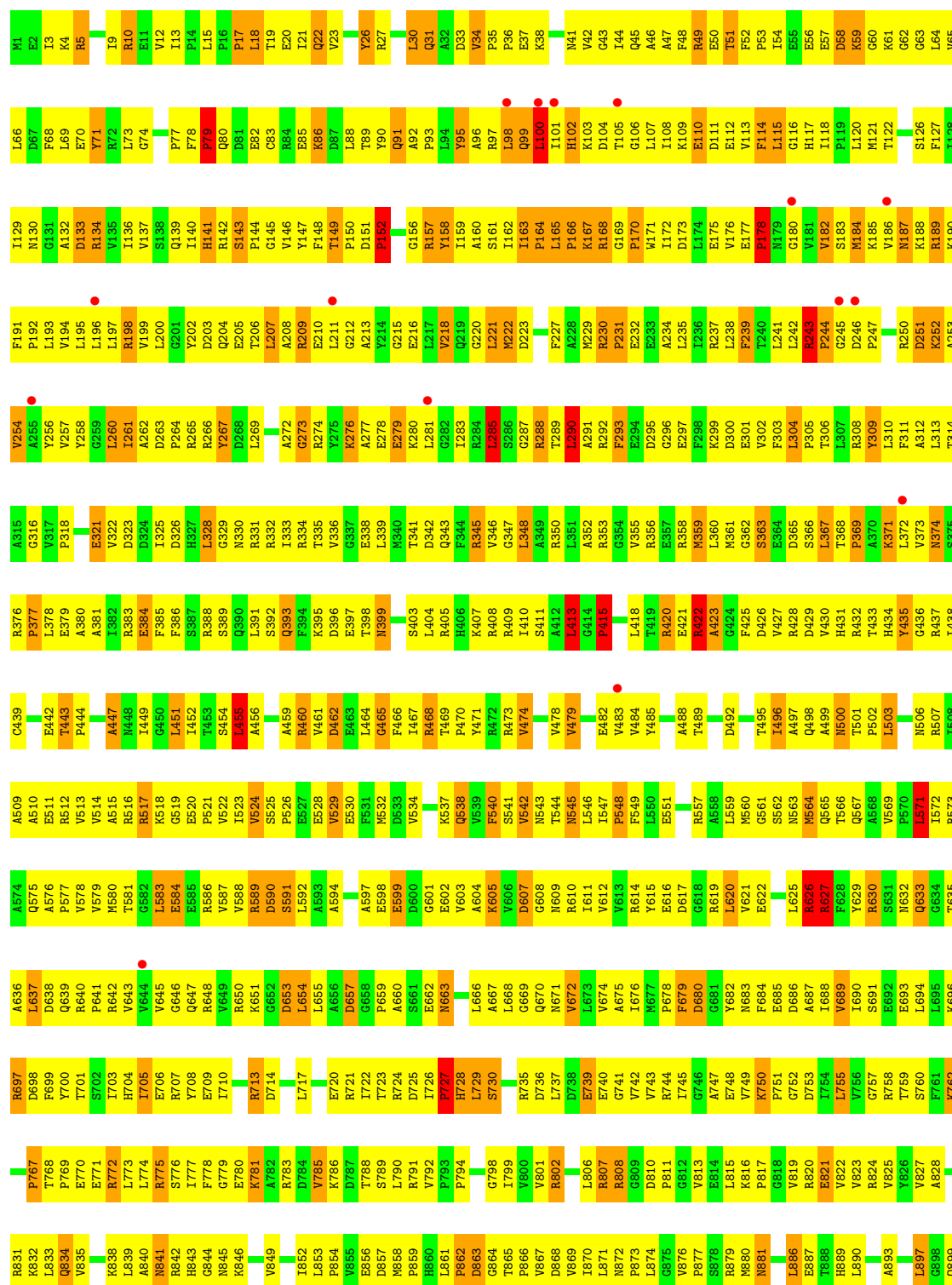
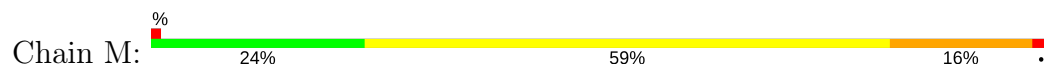


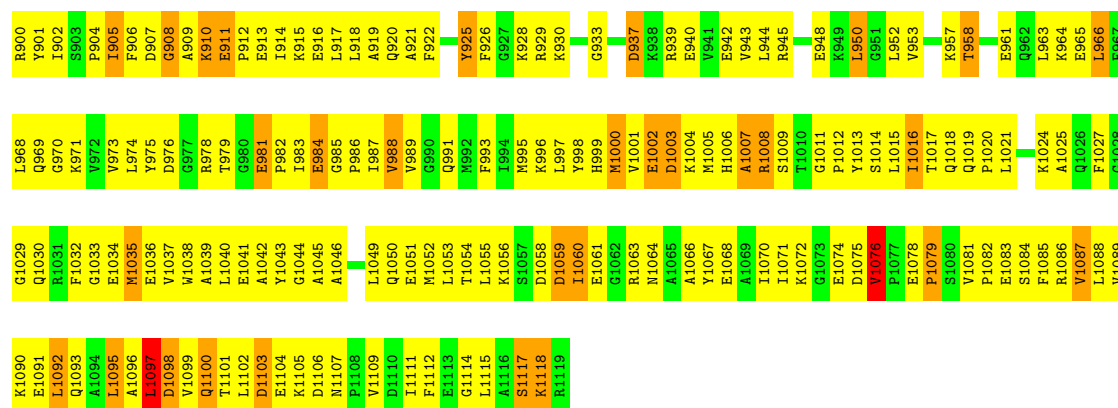


L1015	V953	Q884	V819	E692	N632	Q567	Q505	T443	L378	P318	V254	N187	S126	V65
I1016	T954	I885	R820	E693	Q633	A588	N506	P444	E379	G319	A255	K188	F127	L66
T1017	P955	L886	E521	L694	G634	V569	I508	E445	A380	H320	V256	R189	I128	F68
Q1018	G956	T635	L695	T635	T635	P570	I508	G446	A381	E321	V257	K190	I129	L69
Q1019	K957	H889	V825	K696	A636	R758	A510	A447	I382	V322	G258	L193	A132	E70
P1020	T958	L890	V826	K697	L637	T759	A511	N448	I383	D323	G259	V194	D133	V71
L1021	E961	G891	V827	D698	D638	S760	E511	I449	E384	D324	L260	L196	D134	R72
G1022	E961	L892	A828	F699	Q639	F761	R512	G450	F386	I325	L261	L196	V135	L73
G1023	E961	A893	Q829	T700	R640	A576	V513	L451	F386	D326	A262	L196	R135	L73
K1024	E965	T701	R830	T701	Q641	A577	V514	L452	F387	I327	D263	L197	V136	G74
A1025	E965	R831	K831	S702	R642	V578	A515	L453	S388	H327	P264	R198	V137	E75
Q1026	L966	L897	K832	T703	V643	V579	R516	S454	S389	G329	R265	V199	S138	P76
F1027	F967	G898	L833	H704	V644	M580	R517	G455	Q390	N330	Q266	L200	Q139	P77
G1028	L968	Q899	Q834	T705	V645	E583	K518	A456	L391	R331	Y267	G201	I140	P77
Q1029	Q969	A900	V835	E706	Q646	L584	G519	A457	S392	R332	D268	Y202	H141	F78
Q1030	Q970	Y901	G836	R707	Q647	E583	E520	Y458	Q393	I333	L269	D203	R142	Q80
G1033	K971	I902	D837	E708	R648	E585	P521	A459	F394	R334	G270	Q204	S143	D81
I1034	V973	P904	K838	T710	V649	V587	I523	R460	K395	T335	E271	Q205	S144	E82
A1035	L974	I905	A840	E711	K651	V588	V524	V461	D396	V336	A272	T206	G145	C83
E1036	Y975	R941	R841	A712	A712	R589	S525	D462	E397	G337	G273	L207	V146	R84
V1037	D976	D907	R842	R713	D653	S526	P526	L464	N399	E338	R274	A208	F148	E82
W1038	G977	G908	H843	D714	L654	S591	E527	G465	P400	M340	Y275	E209	F149	C83
A1039	T978	A909	G844	T715	L655	L592	E528	F466	T341	T341	K276	E210	T149	R84
I1040	T979	K910	N845	K716	A556	A593	V529	L467	S403	D342	E279	L211	P150	T89
G1043	G980	E911	K846	L717	D657	A594	E530	R468	L404	Q343	K280	G212	D151	Y90
E1044	E981	P912	A782	E720	G658	L595	F531	T469	L404	Q343	L281	A213	P152	Q91
P982	E982	E913	V849	R721	P659	Y596	M532	P470	H406	F344	L281	Y214	A153	A92
A1045	E983	I914	T784	R722	A660	A597	E534	Y471	R405	R345	G282	G215	R154	P93
I1046	E984	K915	I852	T723	S661	E598	D533	R472	R408	G346	L283	G215	P155	L94
H1047	E985	E916	L853	R724	E662	E599	S535	R473	R409	L348	L285	V218	G156	Y95
T1048	P986	L917	P854	R725	N663	D600	P336	V474	I410	L348	S286	L221	R157	A96
L1049	I987	L918	V855	D725	G664	G601	K337	V478	S411	R350	G287	M222	Y158	E97
Q1050	V988	A919	E856	F726	F665	E602	Q538	V479	A412	L351	R288	D223	I159	L98
I1051	V989	E923	D857	P727	L666	V603	S541	T480	G414	R353	L290	F227	I162	I101
M1052	G990	P924	K858	H728	A667	A604	V542	D481	P415	G354	A291	A228	I163	H102
L1053	Q991	L861	P859	L729	L668	K605	N542	D481	P415	G354	A291	M229	I164	K103
T1054	K992	R925	H860	S730	G669	V606	N543	E482	T419	V355	R292	P230	L165	L104
L1055	F993	F926	L861	E731	Q670	D607	T544	E483	T419	R356	F293	R231	P166	T105
K1056	T994	G927	P862	A732	N671	G608	I547	V484	R420	E357	G296	E232	K167	G106
S1057	M995	K930	D863	A733	V672	N609	P548	Y485	E421	R358	E297	E232	G168	L107
D1058	K996	L734	L673	L734	L673	R610	F549	M486	R422	M359	F298	E233	G169	I108
I1059	L997	T735	T675	R735	V674	Y487	F549	T487	A423	L360	K299	A234	V170	K109
T1060	Y998	D736	A675	D736	A675	A488	L550	A488	G424	M361	D300	L235	R170	E110
E1061	H999	L737	L676	L737	V613	E551	E551	T489	F425	G362	D300	I236	W171	E110
G1062	M1000	R802	R614	H738	R614	H552	H552	E490	D426	S363	E301	R237	I172	D111
R1063	V1001	T803	Y615	E739	Y615	D553	D553	E491	V427	E364	V302	L238	D173	E112
H1064	E1002	R804	E616	E740	E616	E616	E616	D492	L304	D365	F303	F239	L174	F114
A1065	D1003	R939	G741	G741	D680	A555	A555	R493	H431	S366	L304	T240	E175	V113
I1066	K1004	E940	V742	V742	G681	N556	N556	Y494	R432	L367	P305	L241	V176	L115
Y1067	M1005	L874	V743	V743	Y682	R557	R557	T495	T433	T368	T306	L242	E177	G116
E1068	H1006	G875	R744	R744	N683	B622	A559	T496	H434	P369	L307	R243	R178	H117
A1069	A1007	V876	T745	T745	F684	L625	M560	A497	Y435	A370	R308	P244	M179	I118
I1070	R1008	P811	G746	G746	E685	L625	M560	Q498	G436	K371	Y309	G245	G180	P119
H1071	S1009	G812	A747	A747	D686	R626	S562	A499	R437	L372	F311	D246	V181	L120
K1072	T1010	V813	E748	E748	A687	R627	S562	N500	L438	V373	L310	G246	V182	M121
G1073	G1011	K816	V749	V749	L888	F628	N563	T501	C439	N374	A312	R250	S183	T122
E1074	P1012	H889	K750	K750	R689	F629	M564	P502	V441	S375	R251	D251	M184	E123
D1075	Y1013	R817	F751	F751	I690	R630	Q565	L503	T314	R376	K252	D124	K185	D124
Y1076	S1014	G818	G752	G752	S691	S631	T566	E504	E442	P377	A253	G125	V186	G125

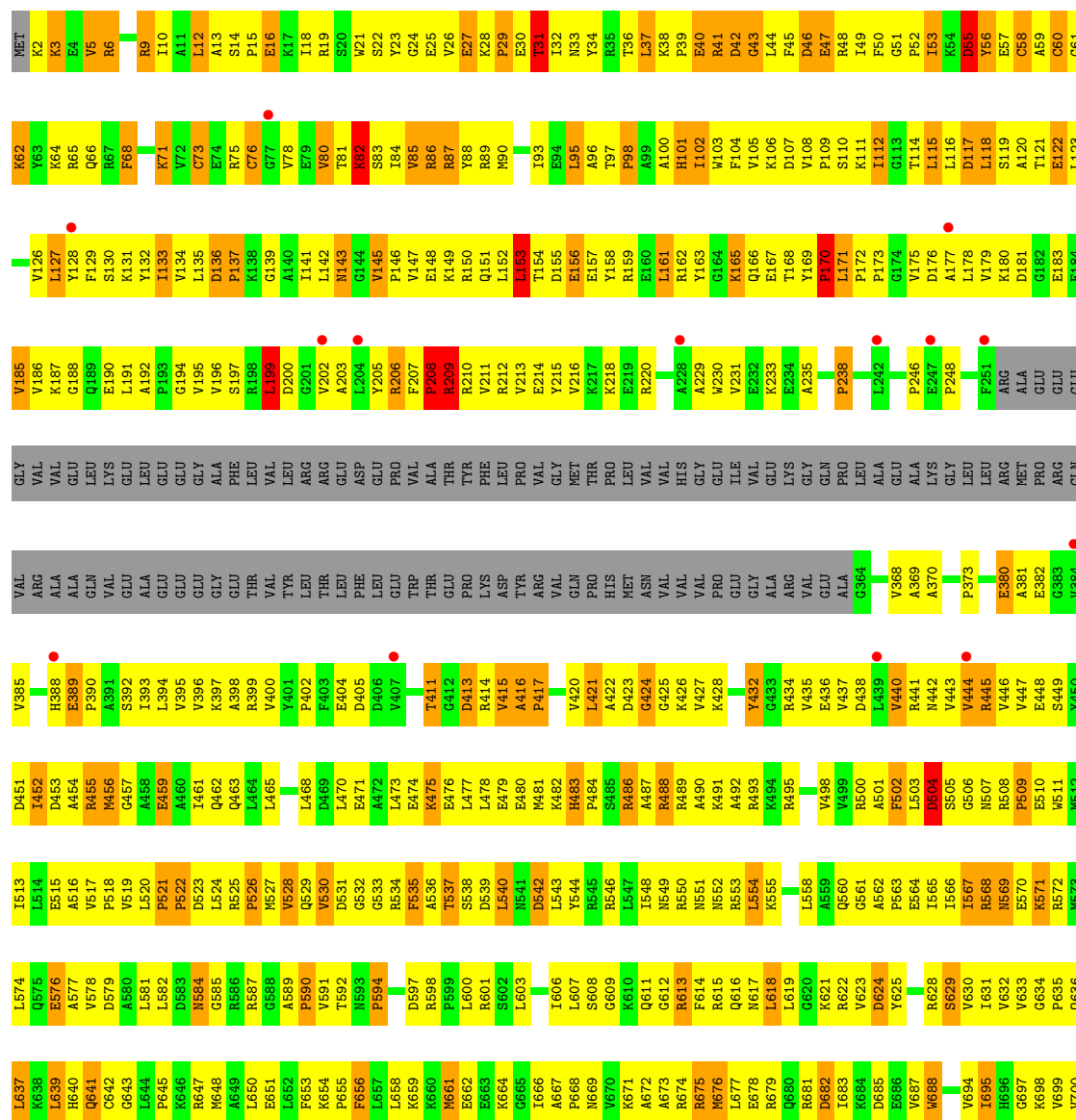


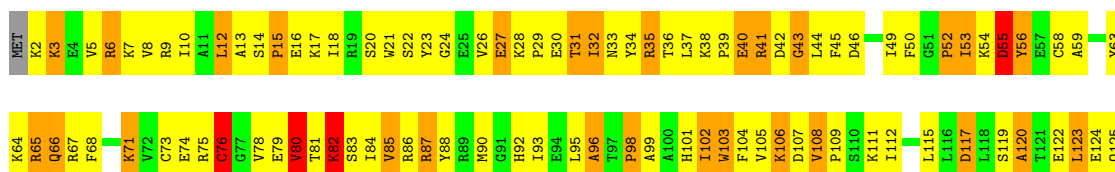
• Molecule 2: DNA-directed RNA polymerase beta chain



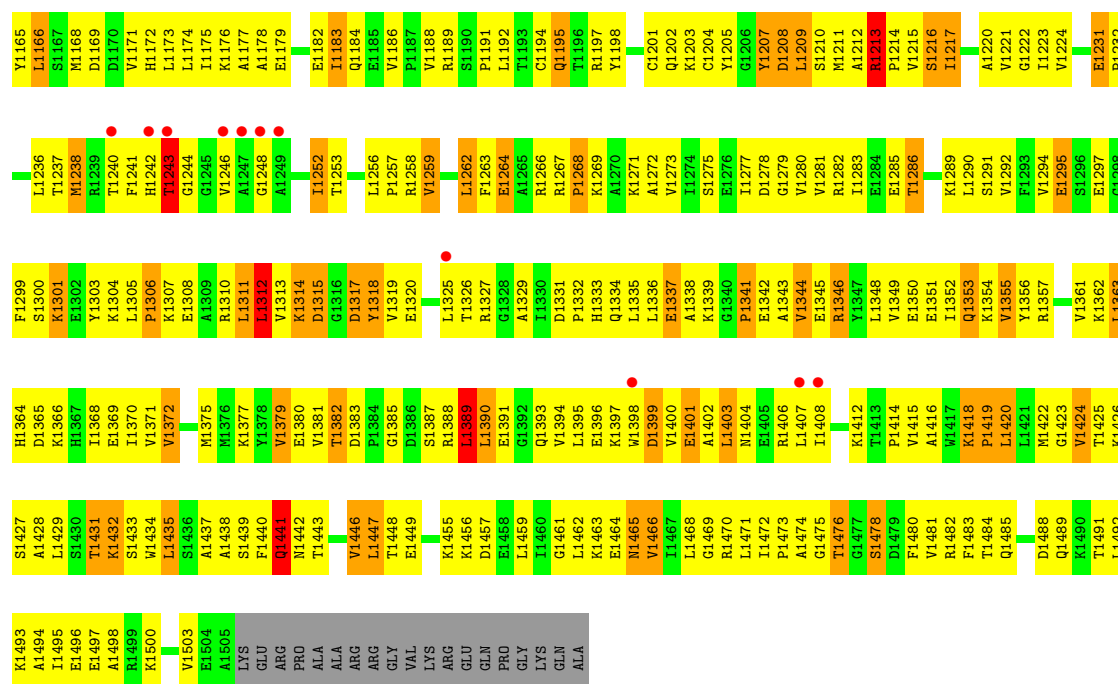


● Molecule 3: DNA-directed RNA polymerase beta' chain

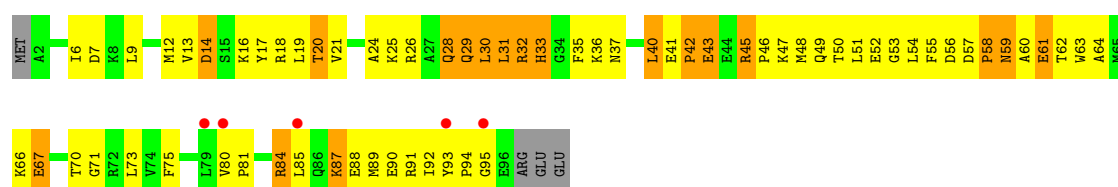




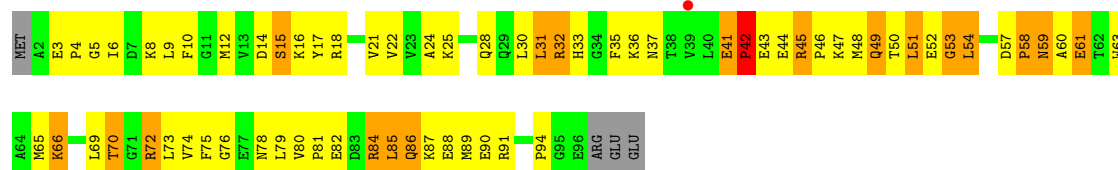




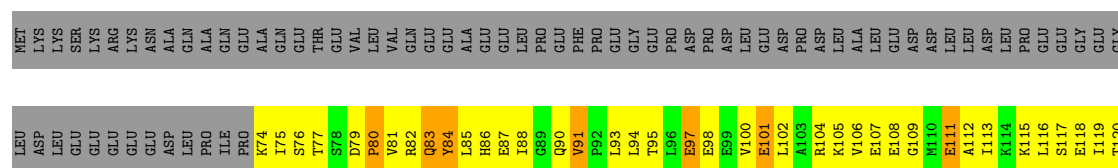
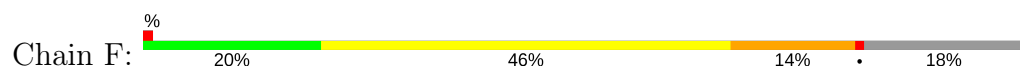
• Molecule 4: RNA polymerase omega chain

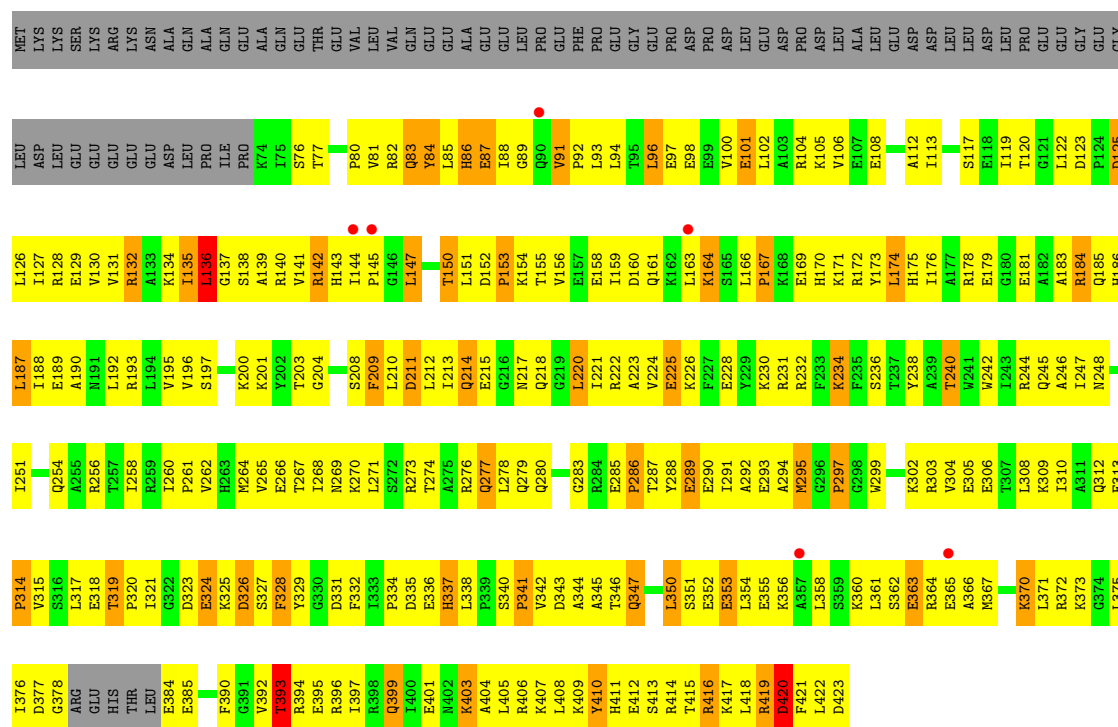


• Molecule 4: RNA polymerase omega chain



• Molecule 5: RNA polymerase sigma factor rpoD





4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	239.50Å 239.50Å 253.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.50 24.85 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.50) 92.5 (24.85-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.267 0.228 , 0.264	Depositor DCC
R_{free} test set	29710 reflections (6.10%)	DCC
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 76.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.499 for -h,-k,l 0.076 for h,-h-k,-l 0.076 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	60572	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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: MG, ZN, RPT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

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

All (4) bond length outliers are listed below:

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

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

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

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 60.

The worst 5 of 6470 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLN:HA	1:A:146:ARG:HH12	1.07	1.11
2:M:952:LEU:HD12	2:M:969:GLN:HE22	1.13	1.11
3:D:1087:ARG:HG2	3:D:1234:THR:HA	1.27	1.07
1:B:152:PRO:HD2	1:B:155:LYS:HD3	1.36	1.05
2:M:605:LYS:HB2	2:M:610:ARG:HH12	1.16	1.05

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	227/315 (72%)	201 (88%)	21 (9%)	5 (2%)	8	12
1	B	227/315 (72%)	198 (87%)	23 (10%)	6 (3%)	6	9
1	K	227/315 (72%)	200 (88%)	23 (10%)	4 (2%)	10	17
1	L	227/315 (72%)	203 (89%)	20 (9%)	4 (2%)	10	17

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

5 of 313 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	B	29	GLU
1	B	48	ILE
2	C	152	PRO
2	C	178	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	83/87 (95%)	62 (75%)	21 (25%)	0	1
4	O	83/87 (95%)	65 (78%)	18 (22%)	1	2
5	F	295/370 (80%)	233 (79%)	62 (21%)	1	2
5	P	295/370 (80%)	246 (83%)	49 (17%)	2	4
All	All	5692/6446 (88%)	4435 (78%)	1257 (22%)	1	2

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

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

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

Mol	Chain	Res	Type
5	F	218	GLN
2	M	117	HIS
4	O	86	GLN
5	F	337	HIS
1	K	229	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 493 ligands modelled in this entry, 491 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
7	RPT	C	8001	-	67,68,68	2.22	22 (32%)	96,101,101	1.19	10 (10%)
7	RPT	M	8002	-	67,68,68	2.31	21 (31%)	96,101,101	1.19	9 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	RPT	C	8001	-	-	0/64/96/96	0/2/6/6
7	RPT	M	8002	-	-	0/64/96/96	0/2/6/6

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	8002	RPT	O2-C8	-2.16	1.28	1.35
7	C	8001	RPT	C43-N2	2.08	1.32	1.27
7	M	8002	RPT	C32-C22	2.08	1.58	1.53
7	M	8002	RPT	C41-N3	2.21	1.51	1.46
7	C	8001	RPT	C41-N3	2.23	1.51	1.46

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	8002	RPT	C34-C26-C25	-2.96	105.97	111.43
7	M	8002	RPT	C31-C20-C19	-2.78	103.02	110.07
7	C	8001	RPT	C31-C20-C19	-2.62	103.44	110.07
7	M	8002	RPT	C4-C3-C43	-2.42	115.16	120.27
7	C	8001	RPT	C34-C26-C25	-2.31	107.18	111.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 13 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	229/315 (72%)	-0.31	1 (0%) 92 92	27, 63, 91, 115	0
1	B	229/315 (72%)	-0.11	12 (5%) 28 29	48, 93, 115, 119	0
1	K	229/315 (72%)	-0.30	2 (0%) 84 85	34, 65, 94, 134	0
1	L	229/315 (72%)	-0.21	6 (2%) 56 59	52, 92, 110, 131	0
2	C	1119/1119 (100%)	-0.34	14 (1%) 77 78	21, 75, 106, 118	0
2	M	1119/1119 (100%)	-0.31	15 (1%) 77 78	25, 79, 109, 122	0
3	D	1392/1524 (91%)	-0.27	24 (1%) 70 72	24, 65, 112, 132	0
3	N	1392/1524 (91%)	-0.25	31 (2%) 62 64	25, 69, 117, 138	0
4	E	95/99 (95%)	-0.27	5 (5%) 27 28	42, 83, 108, 126	0
4	O	95/99 (95%)	-0.39	1 (1%) 80 81	46, 80, 107, 114	0
5	F	345/423 (81%)	-0.36	6 (1%) 70 72	49, 84, 110, 127	0
5	P	345/423 (81%)	-0.28	6 (1%) 70 72	63, 89, 114, 124	0
All	All	6818/7590 (89%)	-0.29	123 (1%) 69 70	21, 75, 112, 138	0

The worst 5 of 123 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	802	ALA	7.6
3	D	1240	THR	5.8
3	N	1249	ALA	5.5
2	C	180	GLY	5.3
3	D	1245	GLY	5.3

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	RPT	C	8001	63/63	0.96	0.23	3.78	26,40,66,82	0
7	RPT	M	8002	63/63	0.96	0.22	2.23	33,45,55,57	0
8	ZN	N	7059	1/1	0.99	0.12	1.63	93,93,93,93	0
8	ZN	N	7113	1/1	0.99	0.13	1.62	84,84,84,84	0
6	MG	A	9002	1/1	0.99	0.17	0.54	31,31,31,31	0
6	MG	D	9095	1/1	0.97	0.15	0.49	30,30,30,30	0
6	MG	N	9199	1/1	0.99	0.11	0.44	35,35,35,35	0
6	MG	D	9038	1/1	0.99	0.14	0.36	39,39,39,39	0
6	MG	M	9260	1/1	0.99	0.12	0.24	36,36,36,36	0
6	MG	D	9330	1/1	0.92	0.14	0.22	39,39,39,39	0
6	MG	D	9011	1/1	0.99	0.12	0.16	33,33,33,33	0
6	MG	D	9024	1/1	0.98	0.14	0.14	36,36,36,36	0
6	MG	N	9398	1/1	0.99	0.15	0.13	48,48,48,48	0
6	MG	L	9183	1/1	0.99	0.13	0.12	37,37,37,37	0
6	MG	C	9003	1/1	0.99	0.13	0.07	38,38,38,38	0
6	MG	B	9033	1/1	0.99	0.14	0.07	33,33,33,33	0
6	MG	M	9400	1/1	0.99	0.12	-0.02	40,40,40,40	0
6	MG	K	9410	1/1	0.97	0.15	-0.02	36,36,36,36	0
6	MG	M	9407	1/1	0.98	0.14	-0.05	35,35,35,35	0
6	MG	D	9029	1/1	0.99	0.12	-0.11	33,33,33,33	0
6	MG	N	9207	1/1	0.99	0.13	-0.19	41,41,41,41	0
6	MG	A	9013	1/1	0.96	0.12	-0.24	44,44,44,44	0
6	MG	E	9007	1/1	0.98	0.11	-0.33	40,40,40,40	0
6	MG	C	9051	1/1	0.99	0.12	-0.45	37,37,37,37	0
6	MG	M	9242	1/1	0.99	0.11	-0.51	35,35,35,35	0
6	MG	P	9189	1/1	0.97	0.11	-0.58	49,49,49,49	0
6	MG	M	9208	1/1	0.99	0.10	-0.59	39,39,39,39	0
8	ZN	D	7112	1/1	0.99	0.10	-0.62	80,80,80,80	0
6	MG	M	9219	1/1	0.97	0.09	-0.74	47,47,47,47	0
6	MG	M	9247	1/1	0.98	0.07	-0.77	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	D	9329	1/1	0.99	0.12	-0.79	33,33,33,33	0
6	MG	M	9205	1/1	0.98	0.11	-0.79	38,38,38,38	0
6	MG	C	9031	1/1	0.99	0.10	-0.82	40,40,40,40	0
6	MG	D	9113	1/1	0.98	0.11	-0.83	34,34,34,34	0
6	MG	D	9028	1/1	0.98	0.13	-0.84	34,34,34,34	0
6	MG	A	9010	1/1	0.98	0.12	-0.85	30,30,30,30	0
6	MG	M	9434	1/1	0.98	0.11	-0.85	34,34,34,34	0
6	MG	N	9431	1/1	0.99	0.12	-0.91	39,39,39,39	0
6	MG	N	9200	1/1	0.95	0.10	-0.92	38,38,38,38	0
6	MG	F	9035	1/1	0.99	0.10	-0.92	40,40,40,40	0
6	MG	C	9053	1/1	0.99	0.12	-0.94	30,30,30,30	0
6	MG	D	9073	1/1	0.97	0.12	-0.96	34,34,34,34	0
6	MG	N	9184	1/1	0.98	0.10	-0.99	29,29,29,29	0
6	MG	M	9196	1/1	0.97	0.09	-1.03	42,42,42,42	0
6	MG	E	9074	1/1	0.96	0.09	-1.09	59,59,59,59	0
6	MG	C	9046	1/1	0.99	0.11	-1.16	38,38,38,38	0
6	MG	D	9062	1/1	0.96	0.08	-1.19	47,47,47,47	0
6	MG	N	9402	1/1	0.99	0.07	-1.23	45,45,45,45	0
6	MG	P	9228	1/1	0.98	0.09	-1.24	43,43,43,43	0
6	MG	D	9036	1/1	0.95	0.09	-1.36	44,44,44,44	0
6	MG	K	9180	1/1	1.00	0.11	-1.37	42,42,42,42	0
6	MG	K	9213	1/1	0.98	0.11	-1.38	43,43,43,43	0
6	MG	B	9032	1/1	0.99	0.06	-1.50	34,34,34,34	0
6	MG	N	9316	1/1	0.99	0.08	-1.51	37,37,37,37	0
6	MG	D	9089	1/1	0.99	0.09	-1.52	36,36,36,36	0
6	MG	N	9238	1/1	0.99	0.11	-1.53	43,43,43,43	0
6	MG	M	9300	1/1	0.99	0.09	-1.55	39,39,39,39	0
8	ZN	D	7058	1/1	0.87	0.07	-1.64	106,106,106,106	0
6	MG	D	9009	1/1	0.96	0.09	-1.67	43,43,43,43	0
6	MG	D	9001	1/1	0.93	0.10	-1.69	36,36,36,36	0
6	MG	B	9059	1/1	0.96	0.07	-1.72	48,48,48,48	0
6	MG	K	9188	1/1	0.97	0.12	-1.76	40,40,40,40	0
6	MG	C	9015	1/1	0.98	0.09	-1.81	38,38,38,38	0
6	MG	M	9299	1/1	0.99	0.09	-1.87	43,43,43,43	0
6	MG	D	9087	1/1	0.97	0.07	-1.88	43,43,43,43	0
6	MG	A	9354	1/1	0.99	0.09	-1.88	37,37,37,37	0
6	MG	C	9092	1/1	0.98	0.06	-1.97	44,44,44,44	0
6	MG	N	9467	1/1	0.99	0.12	-2.09	35,35,35,35	0
6	MG	N	9243	1/1	0.98	0.09	-2.11	35,35,35,35	0
6	MG	D	9054	1/1	0.96	0.08	-2.16	44,44,44,44	0
6	MG	C	9061	1/1	0.99	0.07	-2.18	34,34,34,34	0
6	MG	N	9211	1/1	0.97	0.10	-2.25	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	A	9027	1/1	0.98	0.08	-2.27	37,37,37,37	0
6	MG	D	9365	1/1	0.96	0.06	-2.31	41,41,41,41	0
6	MG	M	9195	1/1	0.99	0.08	-2.31	34,34,34,34	0
6	MG	M	9268	1/1	0.99	0.09	-2.31	32,32,32,32	0
6	MG	D	9333	1/1	0.99	0.07	-2.32	33,33,33,33	0
6	MG	A	9081	1/1	0.96	0.08	-2.37	40,40,40,40	0
6	MG	N	9214	1/1	0.98	0.10	-2.44	33,33,33,33	0
6	MG	F	9057	1/1	1.00	0.09	-2.53	30,30,30,30	0
6	MG	M	9239	1/1	0.98	0.07	-2.67	34,34,34,34	0
6	MG	N	9298	1/1	0.98	0.05	-2.92	55,55,55,55	0
6	MG	D	9017	1/1	0.97	0.10	-2.95	42,42,42,42	0
6	MG	L	9182	1/1	0.94	0.05	-3.10	47,47,47,47	0
6	MG	N	9271	1/1	1.00	0.07	-3.11	43,43,43,43	0
6	MG	A	9156	1/1	0.97	0.08	-3.12	43,43,43,43	0
6	MG	A	9088	1/1	0.99	0.07	-3.12	36,36,36,36	0
6	MG	D	9367	1/1	0.97	0.06	-3.45	31,31,31,31	0
6	MG	O	9197	1/1	0.98	0.04	-3.70	57,57,57,57	0
6	MG	C	9004	1/1	0.98	0.10	-3.73	39,39,39,39	0
6	MG	N	9293	1/1	0.98	0.15	-	42,42,42,42	0
6	MG	L	9421	1/1	0.98	0.12	-	53,53,53,53	0
6	MG	B	9110	1/1	0.99	0.12	-	49,49,49,49	0
6	MG	M	9486	1/1	0.99	0.07	-	48,48,48,48	0
6	MG	A	9124	1/1	0.99	0.12	-	39,39,39,39	0
6	MG	M	9248	1/1	1.00	0.08	-	48,48,48,48	0
6	MG	D	9364	1/1	0.99	0.12	-	47,47,47,47	0
6	MG	L	9252	1/1	0.97	0.09	-	45,45,45,45	0
6	MG	D	9039	1/1	0.99	0.12	-	44,44,44,44	0
6	MG	K	9290	1/1	0.98	0.12	-	51,51,51,51	0
6	MG	M	9295	1/1	0.99	0.08	-	42,42,42,42	0
6	MG	A	9345	1/1	0.99	0.12	-	41,41,41,41	0
6	MG	K	9264	1/1	0.98	0.08	-	42,42,42,42	0
6	MG	F	9008	1/1	0.98	0.09	-	40,40,40,40	0
6	MG	M	9220	1/1	0.99	0.11	-	51,51,51,51	0
6	MG	M	9440	1/1	0.98	0.10	-	50,50,50,50	0
6	MG	F	9356	1/1	0.98	0.14	-	37,37,37,37	0
6	MG	M	9256	1/1	0.89	0.17	-	56,56,56,56	0
6	MG	D	9351	1/1	0.99	0.06	-	43,43,43,43	0
6	MG	D	9058	1/1	0.99	0.08	-	38,38,38,38	0
6	MG	B	9358	1/1	0.99	0.07	-	39,39,39,39	0
6	MG	D	9084	1/1	0.99	0.11	-	37,37,37,37	0
6	MG	N	9292	1/1	0.96	0.12	-	56,56,56,56	0
6	MG	B	9359	1/1	0.96	0.10	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	C	9067	1/1	0.94	0.17	-	57,57,57,57	0
6	MG	C	9020	1/1	0.99	0.10	-	34,34,34,34	0
6	MG	K	9433	1/1	0.97	0.07	-	50,50,50,50	0
6	MG	F	9389	1/1	0.97	0.11	-	53,53,53,53	0
6	MG	C	9176	1/1	0.99	0.09	-	28,28,28,28	0
6	MG	C	9138	1/1	0.98	0.08	-	43,43,43,43	0
6	MG	M	9319	1/1	1.00	0.12	-	41,41,41,41	0
6	MG	D	9135	1/1	0.98	0.14	-	50,50,50,50	0
6	MG	A	9043	1/1	0.99	0.17	-	37,37,37,37	0
6	MG	C	9361	1/1	1.00	0.10	-	41,41,41,41	0
6	MG	K	9405	1/1	0.98	0.11	-	56,56,56,56	0
6	MG	D	9102	1/1	0.94	0.13	-	44,44,44,44	0
6	MG	B	9093	1/1	0.98	0.15	-	40,40,40,40	0
6	MG	B	9457	1/1	0.98	0.07	-	43,43,43,43	0
6	MG	D	9163	1/1	0.98	0.14	-	52,52,52,52	0
6	MG	N	9221	1/1	0.92	0.13	-	44,44,44,44	0
6	MG	D	9121	1/1	0.98	0.09	-	35,35,35,35	0
6	MG	A	9125	1/1	0.97	0.12	-	36,36,36,36	0
6	MG	C	9362	1/1	0.90	0.15	-	55,55,55,55	0
6	MG	C	9126	1/1	0.99	0.10	-	46,46,46,46	0
6	MG	C	9168	1/1	0.91	0.10	-	45,45,45,45	0
6	MG	F	9481	1/1	0.99	0.08	-	57,57,57,57	0
6	MG	D	9144	1/1	0.99	0.12	-	39,39,39,39	0
6	MG	C	9128	1/1	0.98	0.12	-	52,52,52,52	0
6	MG	D	9373	1/1	0.97	0.12	-	51,51,51,51	0
6	MG	C	9340	1/1	0.98	0.09	-	60,60,60,60	0
6	MG	P	9315	1/1	0.99	0.08	-	35,35,35,35	0
6	MG	L	9289	1/1	0.97	0.14	-	62,62,62,62	0
6	MG	D	9374	1/1	0.98	0.10	-	41,41,41,41	0
6	MG	C	9461	1/1	0.98	0.07	-	50,50,50,50	0
6	MG	D	9152	1/1	0.98	0.12	-	67,67,67,67	0
6	MG	D	9339	1/1	0.99	0.14	-	37,37,37,37	0
6	MG	D	9166	1/1	0.97	0.09	-	40,40,40,40	0
6	MG	C	9455	1/1	0.99	0.11	-	40,40,40,40	0
6	MG	D	9118	1/1	0.98	0.11	-	44,44,44,44	0
6	MG	A	9016	1/1	0.98	0.14	-	36,36,36,36	0
6	MG	M	9452	1/1	0.98	0.13	-	42,42,42,42	0
6	MG	C	9107	1/1	0.97	0.09	-	42,42,42,42	0
6	MG	D	9379	1/1	0.98	0.11	-	47,47,47,47	0
6	MG	C	9122	1/1	0.97	0.10	-	56,56,56,56	0
6	MG	N	9215	1/1	0.98	0.12	-	32,32,32,32	0
6	MG	N	9415	1/1	0.98	0.07	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	D	9348	1/1	0.97	0.14	-	57,57,57,57	0
6	MG	D	9023	1/1	0.99	0.14	-	34,34,34,34	0
6	MG	M	9412	1/1	0.97	0.14	-	43,43,43,43	0
6	MG	C	9044	1/1	0.99	0.14	-	34,34,34,34	0
6	MG	M	9320	1/1	1.00	0.11	-	34,34,34,34	0
6	MG	N	9419	1/1	0.98	0.11	-	51,51,51,51	0
6	MG	P	9235	1/1	0.98	0.16	-	40,40,40,40	0
6	MG	K	9432	1/1	0.99	0.13	-	49,49,49,49	0
6	MG	M	9409	1/1	0.99	0.10	-	36,36,36,36	0
6	MG	M	9284	1/1	0.98	0.14	-	54,54,54,54	0
6	MG	C	9154	1/1	0.98	0.07	-	43,43,43,43	0
6	MG	C	9055	1/1	0.99	0.11	-	38,38,38,38	0
6	MG	D	9120	1/1	0.99	0.08	-	31,31,31,31	0
6	MG	D	9331	1/1	0.99	0.18	-	43,43,43,43	0
6	MG	D	9069	1/1	0.98	0.12	-	48,48,48,48	0
6	MG	N	9303	1/1	0.99	0.08	-	54,54,54,54	0
6	MG	C	9464	1/1	0.98	0.06	-	48,48,48,48	0
6	MG	C	9021	1/1	0.98	0.09	-	37,37,37,37	0
6	MG	D	9158	1/1	0.97	0.12	-	60,60,60,60	0
6	MG	K	9438	1/1	0.98	0.10	-	52,52,52,52	0
6	MG	M	9305	1/1	0.98	0.09	-	46,46,46,46	0
6	MG	L	9314	1/1	0.98	0.07	-	56,56,56,56	0
6	MG	N	9435	1/1	0.98	0.23	-	53,53,53,53	0
6	MG	B	9080	1/1	0.98	0.10	-	56,56,56,56	0
6	MG	N	9472	1/1	0.99	0.15	-	56,56,56,56	0
6	MG	N	9404	1/1	0.98	0.12	-	55,55,55,55	0
6	MG	M	9442	1/1	0.99	0.07	-	59,59,59,59	0
6	MG	P	9216	1/1	0.97	0.13	-	48,48,48,48	0
6	MG	N	9313	1/1	0.94	0.10	-	43,43,43,43	0
6	MG	L	9414	1/1	0.94	0.13	-	51,51,51,51	0
6	MG	F	9159	1/1	0.98	0.15	-	57,57,57,57	0
6	MG	D	9336	1/1	0.99	0.10	-	53,53,53,53	0
6	MG	D	9386	1/1	0.99	0.11	-	40,40,40,40	0
6	MG	C	9022	1/1	0.97	0.12	-	37,37,37,37	0
6	MG	N	9181	1/1	0.98	0.16	-	47,47,47,47	0
6	MG	D	9091	1/1	1.00	0.13	-	27,27,27,27	0
6	MG	C	9360	1/1	0.97	0.13	-	53,53,53,53	0
6	MG	C	9119	1/1	0.97	0.07	-	43,43,43,43	0
6	MG	C	9042	1/1	0.99	0.07	-	47,47,47,47	0
6	MG	D	9174	1/1	0.97	0.12	-	47,47,47,47	0
6	MG	N	9276	1/1	0.97	0.08	-	61,61,61,61	0
6	MG	P	9285	1/1	0.98	0.09	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	F	9148	1/1	0.95	0.08	-	54,54,54,54	0
6	MG	M	9230	1/1	1.00	0.11	-	50,50,50,50	0
6	MG	D	9041	1/1	0.97	0.13	-	47,47,47,47	0
6	MG	C	9350	1/1	0.93	0.07	-	60,60,60,60	0
6	MG	C	9366	1/1	0.99	0.14	-	41,41,41,41	0
6	MG	M	9324	1/1	0.95	0.08	-	41,41,41,41	0
6	MG	N	9267	1/1	0.98	0.12	-	42,42,42,42	0
6	MG	D	9146	1/1	0.99	0.10	-	31,31,31,31	0
6	MG	D	9167	1/1	0.97	0.12	-	49,49,49,49	0
6	MG	D	9137	1/1	0.98	0.08	-	47,47,47,47	0
6	MG	D	9369	1/1	0.98	0.10	-	49,49,49,49	0
6	MG	F	9048	1/1	0.99	0.10	-	41,41,41,41	0
6	MG	D	9177	1/1	0.97	0.13	-	64,64,64,64	0
6	MG	B	9378	1/1	0.99	0.13	-	47,47,47,47	0
6	MG	D	9133	1/1	0.99	0.13	-	42,42,42,42	0
6	MG	F	9387	1/1	0.98	0.10	-	53,53,53,53	0
6	MG	N	9186	1/1	0.99	0.12	-	49,49,49,49	0
6	MG	D	9063	1/1	0.98	0.08	-	33,33,33,33	0
6	MG	F	9109	1/1	0.94	0.11	-	60,60,60,60	0
6	MG	L	9306	1/1	0.99	0.11	-	57,57,57,57	0
6	MG	N	9288	1/1	0.99	0.09	-	49,49,49,49	0
6	MG	M	9294	1/1	0.96	0.09	-	52,52,52,52	0
6	MG	D	9480	1/1	0.99	0.10	-	55,55,55,55	0
6	MG	F	9363	1/1	0.98	0.12	-	53,53,53,53	0
6	MG	N	9449	1/1	0.94	0.09	-	51,51,51,51	0
6	MG	A	9384	1/1	0.98	0.14	-	39,39,39,39	0
6	MG	M	9263	1/1	0.94	0.10	-	56,56,56,56	0
6	MG	D	9346	1/1	0.97	0.07	-	47,47,47,47	0
6	MG	D	9396	1/1	0.99	0.10	-	62,62,62,62	0
6	MG	N	9249	1/1	1.00	0.10	-	45,45,45,45	0
6	MG	D	9328	1/1	0.99	0.12	-	30,30,30,30	0
6	MG	M	9272	1/1	0.99	0.17	-	45,45,45,45	0
6	MG	A	9368	1/1	0.99	0.13	-	43,43,43,43	0
6	MG	N	9270	1/1	0.98	0.05	-	39,39,39,39	0
6	MG	C	9071	1/1	0.99	0.11	-	42,42,42,42	0
6	MG	B	9116	1/1	0.99	0.09	-	38,38,38,38	0
6	MG	D	9132	1/1	0.98	0.10	-	43,43,43,43	0
6	MG	M	9321	1/1	1.00	0.12	-	41,41,41,41	0
6	MG	D	9453	1/1	0.96	0.11	-	38,38,38,38	0
6	MG	N	9323	1/1	0.99	0.09	-	38,38,38,38	0
6	MG	K	9223	1/1	0.99	0.09	-	32,32,32,32	0
6	MG	D	9072	1/1	0.99	0.14	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	M	9222	1/1	0.99	0.10	-	35,35,35,35	0
6	MG	A	9357	1/1	0.94	0.11	-	54,54,54,54	0
6	MG	C	9065	1/1	0.98	0.10	-	37,37,37,37	0
6	MG	D	9385	1/1	0.99	0.13	-	35,35,35,35	0
6	MG	D	9129	1/1	0.99	0.14	-	42,42,42,42	0
6	MG	D	9005	1/1	0.99	0.11	-	40,40,40,40	0
6	MG	N	9187	1/1	0.99	0.18	-	33,33,33,33	0
6	MG	N	9465	1/1	0.98	0.08	-	49,49,49,49	0
6	MG	O	9296	1/1	0.98	0.11	-	42,42,42,42	0
6	MG	L	9307	1/1	0.99	0.10	-	35,35,35,35	0
6	MG	M	9424	1/1	0.98	0.13	-	34,34,34,34	0
6	MG	P	9280	1/1	0.98	0.10	-	51,51,51,51	0
6	MG	P	9325	1/1	0.97	0.12	-	49,49,49,49	0
6	MG	N	9444	1/1	0.99	0.15	-	49,49,49,49	0
6	MG	A	9342	1/1	0.99	0.12	-	39,39,39,39	0
6	MG	M	9310	1/1	0.98	0.07	-	46,46,46,46	0
6	MG	A	9078	1/1	0.93	0.13	-	66,66,66,66	0
6	MG	D	9151	1/1	0.99	0.15	-	57,57,57,57	0
6	MG	M	9401	1/1	1.00	0.10	-	37,37,37,37	0
6	MG	D	9165	1/1	0.97	0.07	-	32,32,32,32	0
6	MG	D	9070	1/1	0.99	0.07	-	33,33,33,33	0
6	MG	C	9047	1/1	0.96	0.12	-	53,53,53,53	0
6	MG	N	9317	1/1	0.99	0.09	-	43,43,43,43	0
6	MG	C	9143	1/1	0.99	0.10	-	35,35,35,35	0
6	MG	M	9471	1/1	0.95	0.08	-	47,47,47,47	0
6	MG	A	9460	1/1	0.98	0.07	-	55,55,55,55	0
6	MG	D	9127	1/1	0.97	0.14	-	48,48,48,48	0
6	MG	C	9086	1/1	0.99	0.14	-	39,39,39,39	0
6	MG	M	9224	1/1	0.99	0.13	-	40,40,40,40	0
6	MG	N	9287	1/1	0.98	0.09	-	53,53,53,53	0
6	MG	F	9123	1/1	0.97	0.09	-	37,37,37,37	0
6	MG	D	9014	1/1	0.95	0.10	-	41,41,41,41	0
6	MG	K	9413	1/1	0.99	0.10	-	54,54,54,54	0
6	MG	M	9411	1/1	0.94	0.09	-	47,47,47,47	0
6	MG	O	9198	1/1	0.96	0.12	-	36,36,36,36	0
6	MG	M	9474	1/1	0.99	0.14	-	49,49,49,49	0
6	MG	D	9392	1/1	0.98	0.12	-	52,52,52,52	0
6	MG	M	9406	1/1	0.96	0.15	-	67,67,67,67	0
6	MG	A	9352	1/1	0.97	0.10	-	46,46,46,46	0
6	MG	P	9258	1/1	1.00	0.14	-	51,51,51,51	0
6	MG	N	9448	1/1	0.99	0.09	-	51,51,51,51	0
6	MG	F	9393	1/1	0.99	0.12	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	K	9469	1/1	0.99	0.12	-	50,50,50,50	0
6	MG	O	9420	1/1	0.94	0.10	-	51,51,51,51	0
6	MG	N	9426	1/1	0.96	0.09	-	41,41,41,41	0
6	MG	D	9130	1/1	0.99	0.09	-	51,51,51,51	0
6	MG	D	9341	1/1	0.99	0.10	-	41,41,41,41	0
6	MG	K	9244	1/1	0.99	0.07	-	44,44,44,44	0
6	MG	C	9149	1/1	0.94	0.16	-	48,48,48,48	0
6	MG	C	9050	1/1	0.99	0.15	-	37,37,37,37	0
6	MG	N	9445	1/1	0.98	0.10	-	51,51,51,51	0
6	MG	O	9439	1/1	0.98	0.16	-	56,56,56,56	0
6	MG	M	9225	1/1	0.96	0.14	-	56,56,56,56	0
6	MG	C	9162	1/1	0.95	0.12	-	50,50,50,50	0
6	MG	M	9441	1/1	0.98	0.07	-	45,45,45,45	0
6	MG	D	9343	1/1	0.99	0.10	-	59,59,59,59	0
6	MG	M	9210	1/1	0.96	0.13	-	41,41,41,41	0
6	MG	D	9397	1/1	0.98	0.12	-	51,51,51,51	0
6	MG	D	9082	1/1	0.95	0.14	-	60,60,60,60	0
6	MG	M	9201	1/1	0.97	0.10	-	45,45,45,45	0
6	MG	N	9232	1/1	0.97	0.08	-	47,47,47,47	0
6	MG	L	9309	1/1	0.98	0.13	-	49,49,49,49	0
6	MG	A	9097	1/1	0.99	0.16	-	34,34,34,34	0
6	MG	A	9111	1/1	0.98	0.09	-	35,35,35,35	0
6	MG	C	9353	1/1	0.99	0.10	-	48,48,48,48	0
6	MG	C	9371	1/1	0.99	0.15	-	54,54,54,54	0
6	MG	F	9376	1/1	0.97	0.19	-	62,62,62,62	0
6	MG	M	9261	1/1	0.96	0.11	-	47,47,47,47	0
6	MG	C	9175	1/1	0.96	0.14	-	68,68,68,68	0
6	MG	B	9094	1/1	0.99	0.15	-	38,38,38,38	0
6	MG	P	9399	1/1	0.99	0.11	-	34,34,34,34	0
6	MG	P	9202	1/1	0.94	0.10	-	49,49,49,49	0
6	MG	B	9458	1/1	0.97	0.08	-	44,44,44,44	0
6	MG	N	9326	1/1	0.96	0.14	-	62,62,62,62	0
6	MG	A	9332	1/1	0.99	0.06	-	35,35,35,35	0
6	MG	A	9395	1/1	0.99	0.14	-	50,50,50,50	0
6	MG	D	9100	1/1	0.99	0.08	-	43,43,43,43	0
6	MG	N	9322	1/1	0.98	0.10	-	54,54,54,54	0
6	MG	N	9192	1/1	0.91	0.12	-	62,62,62,62	0
6	MG	N	9318	1/1	0.99	0.11	-	34,34,34,34	0
6	MG	N	9443	1/1	0.99	0.13	-	54,54,54,54	0
6	MG	F	9382	1/1	0.99	0.09	-	40,40,40,40	0
6	MG	C	9178	1/1	0.97	0.09	-	39,39,39,39	0
6	MG	N	9179	1/1	0.99	0.12	-	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	D	9349	1/1	0.98	0.13	-	33,33,33,33	0
6	MG	N	9217	1/1	0.95	0.15	-	48,48,48,48	0
6	MG	D	9338	1/1	0.98	0.10	-	42,42,42,42	0
6	MG	N	9253	1/1	0.98	0.12	-	42,42,42,42	0
6	MG	N	9262	1/1	0.99	0.09	-	51,51,51,51	0
6	MG	L	9437	1/1	0.99	0.06	-	40,40,40,40	0
6	MG	F	9139	1/1	0.99	0.10	-	38,38,38,38	0
6	MG	C	9355	1/1	0.96	0.12	-	58,58,58,58	0
6	MG	M	9234	1/1	0.96	0.12	-	53,53,53,53	0
6	MG	D	9335	1/1	0.99	0.06	-	52,52,52,52	0
6	MG	D	9006	1/1	0.97	0.12	-	40,40,40,40	0
6	MG	D	9052	1/1	0.98	0.07	-	65,65,65,65	0
6	MG	N	9231	1/1	0.98	0.11	-	52,52,52,52	0
6	MG	N	9429	1/1	0.98	0.10	-	45,45,45,45	0
6	MG	F	9390	1/1	0.93	0.07	-	46,46,46,46	0
6	MG	M	9275	1/1	0.97	0.12	-	55,55,55,55	0
6	MG	D	9173	1/1	0.98	0.07	-	48,48,48,48	0
6	MG	C	9372	1/1	0.96	0.09	-	61,61,61,61	0
6	MG	B	9083	1/1	0.99	0.13	-	40,40,40,40	0
6	MG	D	9134	1/1	0.99	0.13	-	47,47,47,47	0
6	MG	N	9417	1/1	0.99	0.09	-	39,39,39,39	0
6	MG	N	9302	1/1	0.99	0.10	-	31,31,31,31	0
6	MG	F	9172	1/1	0.96	0.11	-	51,51,51,51	0
6	MG	C	9142	1/1	0.98	0.15	-	48,48,48,48	0
6	MG	D	9108	1/1	0.98	0.15	-	51,51,51,51	0
6	MG	P	9436	1/1	0.99	0.11	-	49,49,49,49	0
6	MG	M	9227	1/1	0.99	0.12	-	35,35,35,35	0
6	MG	C	9145	1/1	0.99	0.13	-	66,66,66,66	0
6	MG	F	9101	1/1	1.00	0.12	-	44,44,44,44	0
6	MG	L	9246	1/1	0.98	0.12	-	52,52,52,52	0
6	MG	D	9030	1/1	0.97	0.09	-	48,48,48,48	0
6	MG	M	9190	1/1	0.99	0.16	-	29,29,29,29	0
6	MG	C	9115	1/1	0.99	0.11	-	36,36,36,36	0
6	MG	N	9204	1/1	0.98	0.19	-	44,44,44,44	0
6	MG	D	9334	1/1	0.99	0.10	-	54,54,54,54	0
6	MG	P	9277	1/1	0.99	0.09	-	41,41,41,41	0
6	MG	M	9212	1/1	0.98	0.08	-	32,32,32,32	0
6	MG	N	9468	1/1	0.99	0.10	-	55,55,55,55	0
6	MG	A	9106	1/1	0.99	0.12	-	38,38,38,38	0
6	MG	N	9185	1/1	0.98	0.14	-	56,56,56,56	0
6	MG	L	9278	1/1	0.96	0.11	-	44,44,44,44	0
6	MG	C	9026	1/1	0.99	0.13	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	D	9456	1/1	0.99	0.10	-	55,55,55,55	0
6	MG	N	9274	1/1	0.99	0.18	-	40,40,40,40	0
6	MG	C	9160	1/1	0.97	0.09	-	44,44,44,44	0
6	MG	F	9370	1/1	0.96	0.09	-	46,46,46,46	0
6	MG	C	9112	1/1	0.98	0.11	-	39,39,39,39	0
6	MG	C	9090	1/1	0.98	0.10	-	47,47,47,47	0
6	MG	D	9161	1/1	0.91	0.09	-	57,57,57,57	0
6	MG	B	9104	1/1	0.97	0.10	-	45,45,45,45	0
6	MG	N	9430	1/1	0.99	0.08	-	57,57,57,57	0
6	MG	L	9245	1/1	0.97	0.09	-	62,62,62,62	0
6	MG	B	9136	1/1	0.99	0.10	-	47,47,47,47	0
6	MG	A	9012	1/1	0.98	0.10	-	47,47,47,47	0
6	MG	P	9255	1/1	0.99	0.12	-	34,34,34,34	0
6	MG	F	9383	1/1	0.98	0.11	-	48,48,48,48	0
6	MG	C	9394	1/1	0.98	0.09	-	33,33,33,33	0
6	MG	N	9269	1/1	0.99	0.07	-	42,42,42,42	0
6	MG	P	9482	1/1	1.00	0.11	-	48,48,48,48	0
6	MG	E	9045	1/1	0.98	0.12	-	61,61,61,61	0
6	MG	K	9257	1/1	0.97	0.10	-	58,58,58,58	0
6	MG	O	9254	1/1	0.99	0.08	-	39,39,39,39	0
6	MG	L	9283	1/1	0.98	0.12	-	59,59,59,59	0
6	MG	N	9408	1/1	1.00	0.14	-	45,45,45,45	0
6	MG	N	9233	1/1	0.95	0.14	-	62,62,62,62	0
6	MG	M	9281	1/1	0.99	0.11	-	49,49,49,49	0
6	MG	O	9266	1/1	1.00	0.08	-	47,47,47,47	0
6	MG	N	9427	1/1	0.94	0.14	-	58,58,58,58	0
6	MG	N	9229	1/1	0.99	0.07	-	41,41,41,41	0
6	MG	C	9487	1/1	1.00	0.11	-	32,32,32,32	0
6	MG	A	9380	1/1	0.99	0.11	-	44,44,44,44	0
6	MG	M	9416	1/1	0.99	0.11	-	45,45,45,45	0
6	MG	F	9157	1/1	0.99	0.11	-	42,42,42,42	0
6	MG	N	9428	1/1	0.98	0.10	-	42,42,42,42	0
6	MG	L	9466	1/1	0.99	0.10	-	49,49,49,49	0
6	MG	L	9218	1/1	0.96	0.09	-	33,33,33,33	0
6	MG	N	9291	1/1	0.95	0.12	-	64,64,64,64	0
6	MG	K	9470	1/1	0.91	0.13	-	55,55,55,55	0
6	MG	N	9418	1/1	0.99	0.10	-	49,49,49,49	0
6	MG	N	9265	1/1	0.98	0.14	-	61,61,61,61	0
6	MG	F	9105	1/1	0.98	0.14	-	36,36,36,36	0
6	MG	B	9478	1/1	0.98	0.12	-	61,61,61,61	0
6	MG	C	9377	1/1	0.99	0.09	-	44,44,44,44	0
6	MG	D	9085	1/1	0.99	0.18	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	D	9459	1/1	0.98	0.05	-	54,54,54,54	0
6	MG	D	9117	1/1	1.00	0.13	-	48,48,48,48	0
6	MG	O	9483	1/1	0.99	0.09	-	63,63,63,63	0
6	MG	C	9037	1/1	0.98	0.16	-	51,51,51,51	0
6	MG	B	9056	1/1	0.98	0.13	-	43,43,43,43	0
6	MG	M	9447	1/1	0.94	0.07	-	64,64,64,64	0
6	MG	D	9347	1/1	0.99	0.09	-	49,49,49,49	0
6	MG	A	9477	1/1	0.98	0.18	-	52,52,52,52	0
6	MG	D	9337	1/1	0.99	0.15	-	53,53,53,53	0
6	MG	C	9025	1/1	0.98	0.14	-	39,39,39,39	0
6	MG	P	9297	1/1	0.95	0.09	-	45,45,45,45	0
6	MG	N	9484	1/1	0.99	0.07	-	37,37,37,37	0
6	MG	D	9388	1/1	0.97	0.09	-	37,37,37,37	0
6	MG	D	9096	1/1	0.96	0.15	-	60,60,60,60	0
6	MG	D	9064	1/1	0.98	0.14	-	44,44,44,44	0
6	MG	N	9206	1/1	0.99	0.16	-	31,31,31,31	0
6	MG	A	9153	1/1	0.97	0.15	-	66,66,66,66	0
6	MG	E	9155	1/1	0.99	0.14	-	44,44,44,44	0
6	MG	N	9451	1/1	0.99	0.06	-	41,41,41,41	0
6	MG	D	9077	1/1	0.99	0.11	-	35,35,35,35	0
6	MG	M	9203	1/1	0.99	0.11	-	32,32,32,32	0
6	MG	C	9049	1/1	0.94	0.10	-	46,46,46,46	0
6	MG	K	9191	1/1	0.98	0.15	-	32,32,32,32	0
6	MG	N	9311	1/1	1.00	0.10	-	39,39,39,39	0
6	MG	B	9103	1/1	0.97	0.12	-	43,43,43,43	0
6	MG	F	9098	1/1	0.98	0.11	-	54,54,54,54	0
6	MG	C	9463	1/1	0.99	0.09	-	55,55,55,55	0
6	MG	C	9114	1/1	0.99	0.09	-	30,30,30,30	0
6	MG	M	9273	1/1	0.97	0.12	-	44,44,44,44	0
6	MG	D	9018	1/1	0.98	0.11	-	39,39,39,39	0
6	MG	D	9140	1/1	0.99	0.13	-	40,40,40,40	0
6	MG	D	9344	1/1	0.98	0.11	-	55,55,55,55	0
6	MG	F	9060	1/1	0.97	0.10	-	41,41,41,41	0
6	MG	F	9375	1/1	0.98	0.13	-	36,36,36,36	0
6	MG	N	9240	1/1	0.99	0.14	-	46,46,46,46	0
6	MG	N	9423	1/1	0.98	0.17	-	58,58,58,58	0
6	MG	N	9476	1/1	0.99	0.09	-	54,54,54,54	0
6	MG	B	9131	1/1	0.99	0.08	-	33,33,33,33	0
6	MG	C	9381	1/1	0.96	0.08	-	53,53,53,53	0
6	MG	D	9150	1/1	0.99	0.14	-	31,31,31,31	0
6	MG	C	9391	1/1	0.96	0.06	-	60,60,60,60	0
6	MG	P	9209	1/1	0.96	0.15	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	N	9308	1/1	0.99	0.15	-	55,55,55,55	0
6	MG	N	9259	1/1	0.98	0.15	-	34,34,34,34	0
6	MG	N	9473	1/1	0.97	0.12	-	51,51,51,51	0
6	MG	M	9485	1/1	1.00	0.07	-	54,54,54,54	0
6	MG	A	9068	1/1	0.98	0.12	-	39,39,39,39	0
6	MG	N	9193	1/1	1.00	0.15	-	34,34,34,34	0
6	MG	N	9304	1/1	0.99	0.11	-	47,47,47,47	0
6	MG	C	9019	1/1	0.96	0.13	-	57,57,57,57	0
6	MG	M	9250	1/1	0.98	0.07	-	38,38,38,38	0
6	MG	N	9327	1/1	0.95	0.07	-	40,40,40,40	0
6	MG	N	9279	1/1	0.99	0.11	-	54,54,54,54	0
6	MG	M	9312	1/1	0.99	0.12	-	37,37,37,37	0
6	MG	C	9454	1/1	0.99	0.09	-	55,55,55,55	0
6	MG	D	9147	1/1	0.99	0.10	-	41,41,41,41	0
6	MG	N	9286	1/1	0.98	0.14	-	31,31,31,31	0
6	MG	C	9076	1/1	1.00	0.12	-	33,33,33,33	0
6	MG	P	9226	1/1	0.93	0.08	-	43,43,43,43	0
6	MG	F	9099	1/1	0.97	0.13	-	56,56,56,56	0
6	MG	D	9141	1/1	0.99	0.06	-	50,50,50,50	0
6	MG	C	9169	1/1	0.99	0.13	-	42,42,42,42	0
6	MG	K	9251	1/1	0.97	0.11	-	43,43,43,43	0
6	MG	K	9301	1/1	0.98	0.12	-	43,43,43,43	0
6	MG	D	9034	1/1	0.99	0.08	-	41,41,41,41	0
6	MG	N	9422	1/1	0.97	0.14	-	56,56,56,56	0
6	MG	N	9194	1/1	0.94	0.12	-	51,51,51,51	0
6	MG	N	9236	1/1	0.98	0.10	-	39,39,39,39	0
6	MG	C	9170	1/1	0.99	0.06	-	41,41,41,41	0
6	MG	P	9446	1/1	0.99	0.13	-	34,34,34,34	0
6	MG	N	9450	1/1	0.97	0.10	-	48,48,48,48	0
6	MG	C	9079	1/1	0.99	0.11	-	38,38,38,38	0
6	MG	N	9425	1/1	0.97	0.12	-	46,46,46,46	0
6	MG	E	9479	1/1	0.98	0.10	-	62,62,62,62	0
6	MG	M	9475	1/1	0.97	0.05	-	62,62,62,62	0
6	MG	N	9403	1/1	0.99	0.12	-	34,34,34,34	0
6	MG	M	9241	1/1	0.98	0.11	-	36,36,36,36	0
6	MG	A	9171	1/1	0.97	0.11	-	58,58,58,58	0
6	MG	C	9164	1/1	0.99	0.10	-	49,49,49,49	0
6	MG	B	9040	1/1	0.99	0.16	-	36,36,36,36	0
6	MG	M	9237	1/1	0.97	0.15	-	52,52,52,52	0
6	MG	P	9282	1/1	0.98	0.09	-	56,56,56,56	0
6	MG	A	9066	1/1	0.97	0.14	-	47,47,47,47	0
6	MG	A	9075	1/1	0.99	0.10	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	C	9462	1/1	0.99	0.08	-	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.