wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 12:26 AM GMT

PDB ID	:	2A68
Title	:	Crystal structure of the T. thermophilus RNA polymerase holoenzyme in complex with antibiotic rifabutin
Authors	:	Artsimovitch, I.; Vassylyeva, M.N.; Svetlov, D.; Svetlov, V.; Perederina, A.; Igarashi, N.; Matsugaki, N.; Wakatsuki, S.; Tahirov, T.H.; Vassylyev, D.G.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2005-07-01
Resolution	:	2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

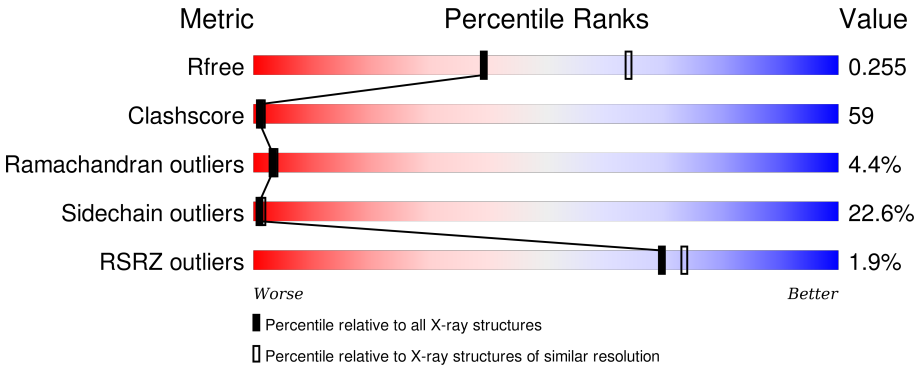
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	14% 44% 14% 27%
1	B	315	5% 20% 41% 11% 27%
1	K	315	% 17% 40% 15% 27%
1	L	315	3% 20% 42% 11% 27%
2	C	1119	% 23% 59% 17%

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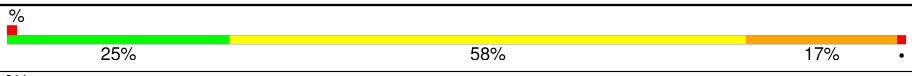
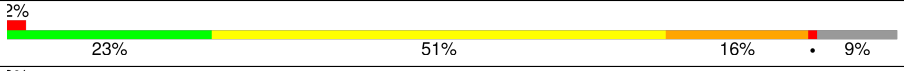
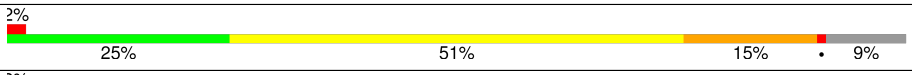
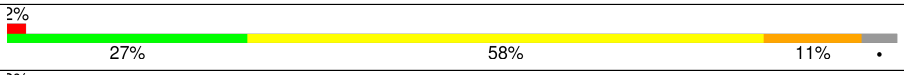
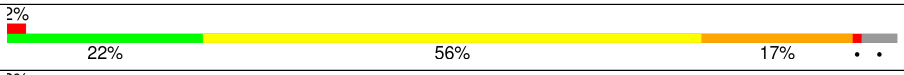
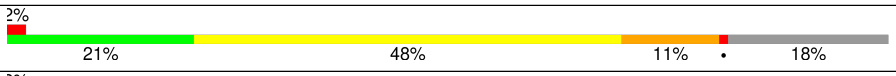
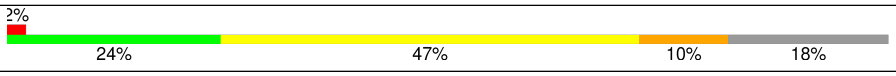
Mol	Chain	Length	Quality of chain
2	M	1119	
3	D	1524	
3	N	1524	
4	E	99	
4	O	99	
5	F	423	
5	P	423	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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 hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

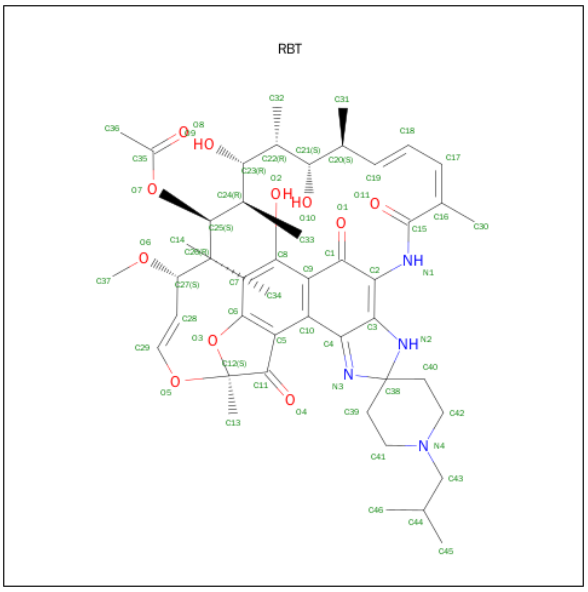
- Molecule 5 is a protein called RNA polymerase sigma factor rpoD.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	P	20	Total	Mg	0	0
			20	20		
6	D	137	Total	Mg	0	0
			137	137		
6	K	21	Total	Mg	0	0
			21	21		
6	E	10	Total	Mg	0	0
			10	10		
6	B	23	Total	Mg	0	0
			23	23		
6	C	81	Total	Mg	0	0
			81	81		
6	A	31	Total	Mg	0	0
			31	31		
6	N	108	Total	Mg	0	0
			108	108		
6	O	6	Total	Mg	0	0
			6	6		
6	L	25	Total	Mg	0	0
			25	25		
6	F	31	Total	Mg	0	0
			31	31		
6	M	69	Total	Mg	0	0
			69	69		

- Molecule 7 is RIFABUTIN (three-letter code: RBT) (formula: $C_{46}H_{62}N_4O_{11}$).



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

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

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

- Molecule 9 is water.

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

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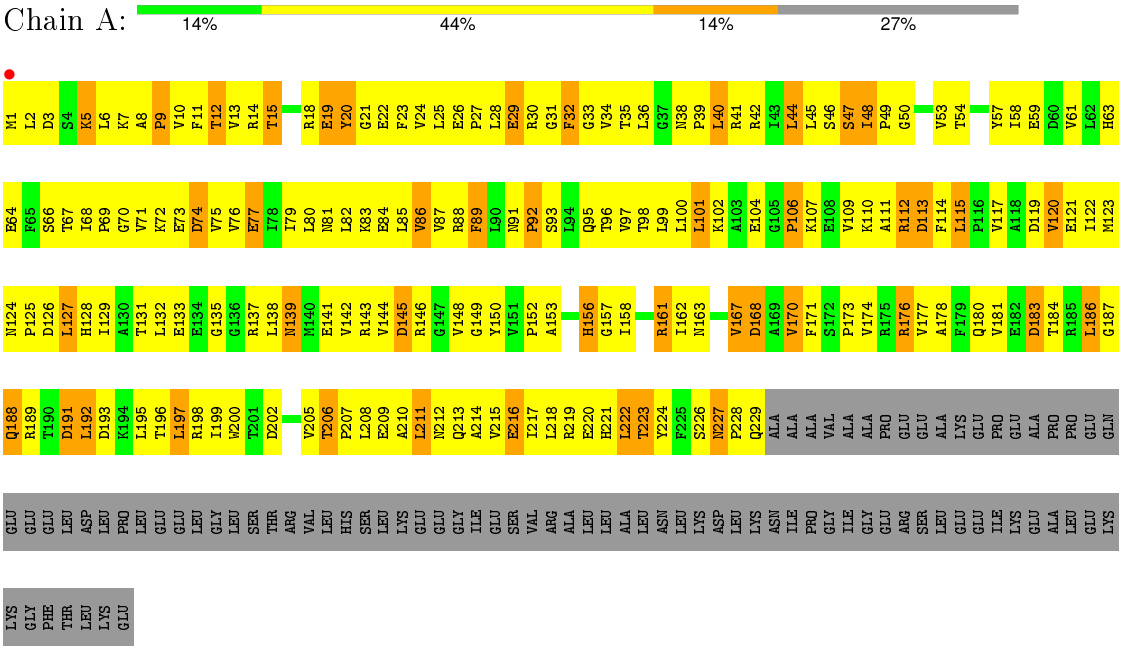
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	F	456	Total O 456 456	0	0
9	K	213	Total O 213 213	0	0
9	L	237	Total O 237 237	0	0
9	M	998	Total O 998 998	0	0
9	N	1357	Total O 1357 1357	0	0
9	O	117	Total O 117 117	0	0
9	P	377	Total O 377 377	0	0

3 Residue-property plots (i)

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.

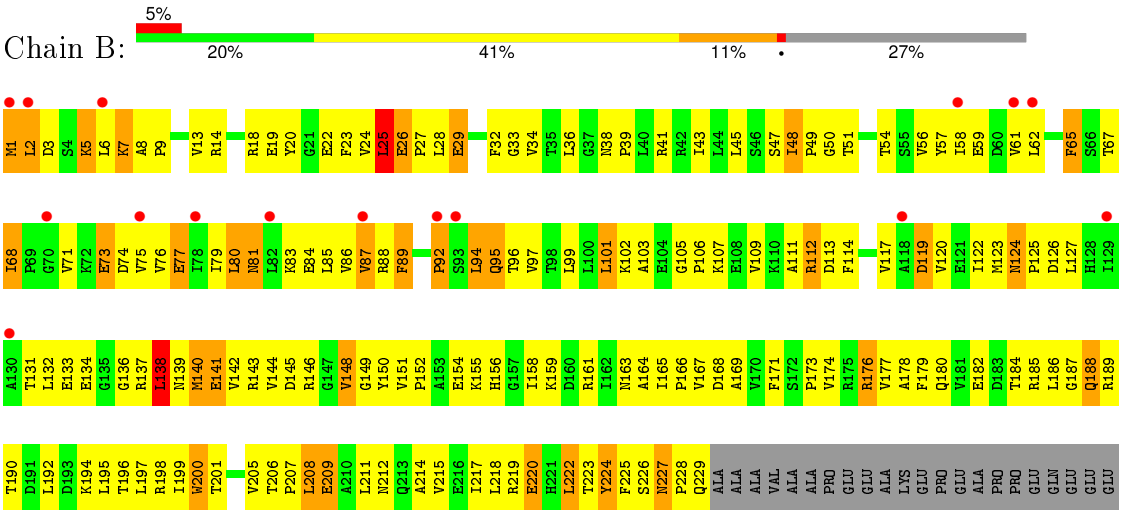
- Molecule 1: DNA-directed RNA polymerase alpha chain

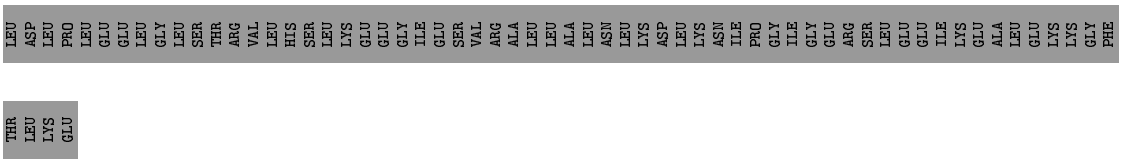
Chain A:



- Molecule 1: DNA-directed RNA polymerase alpha chain

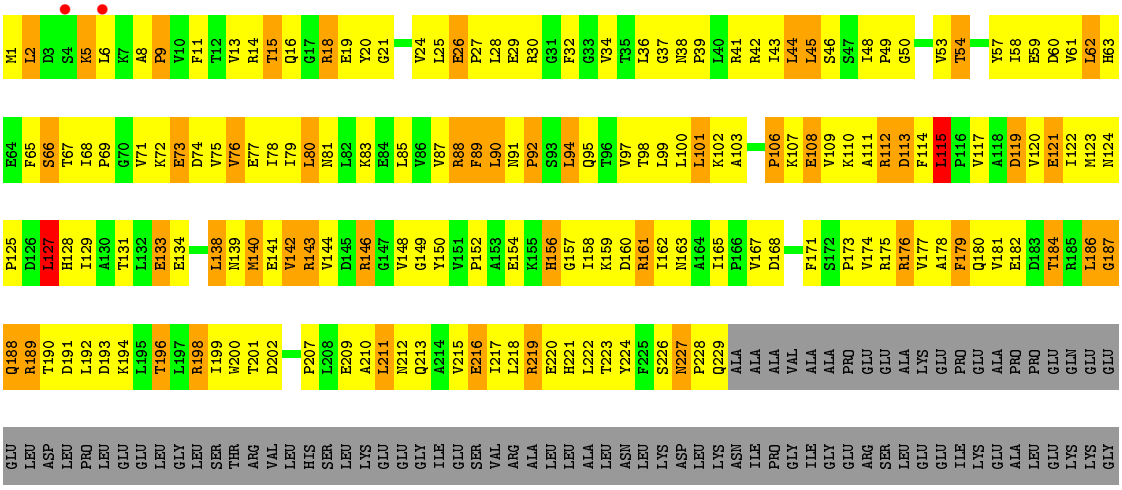
Chain B:





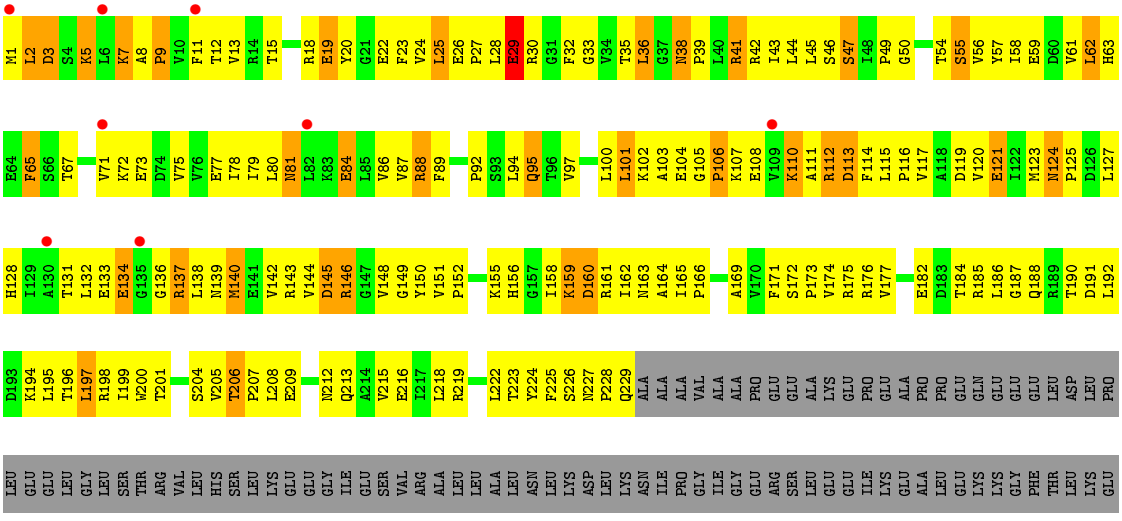
• Molecule 1: DNA-directed RNA polymerase alpha chain

Chain K:



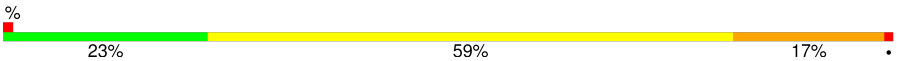
• Molecule 1: DNA-directed RNA polymerase alpha chain

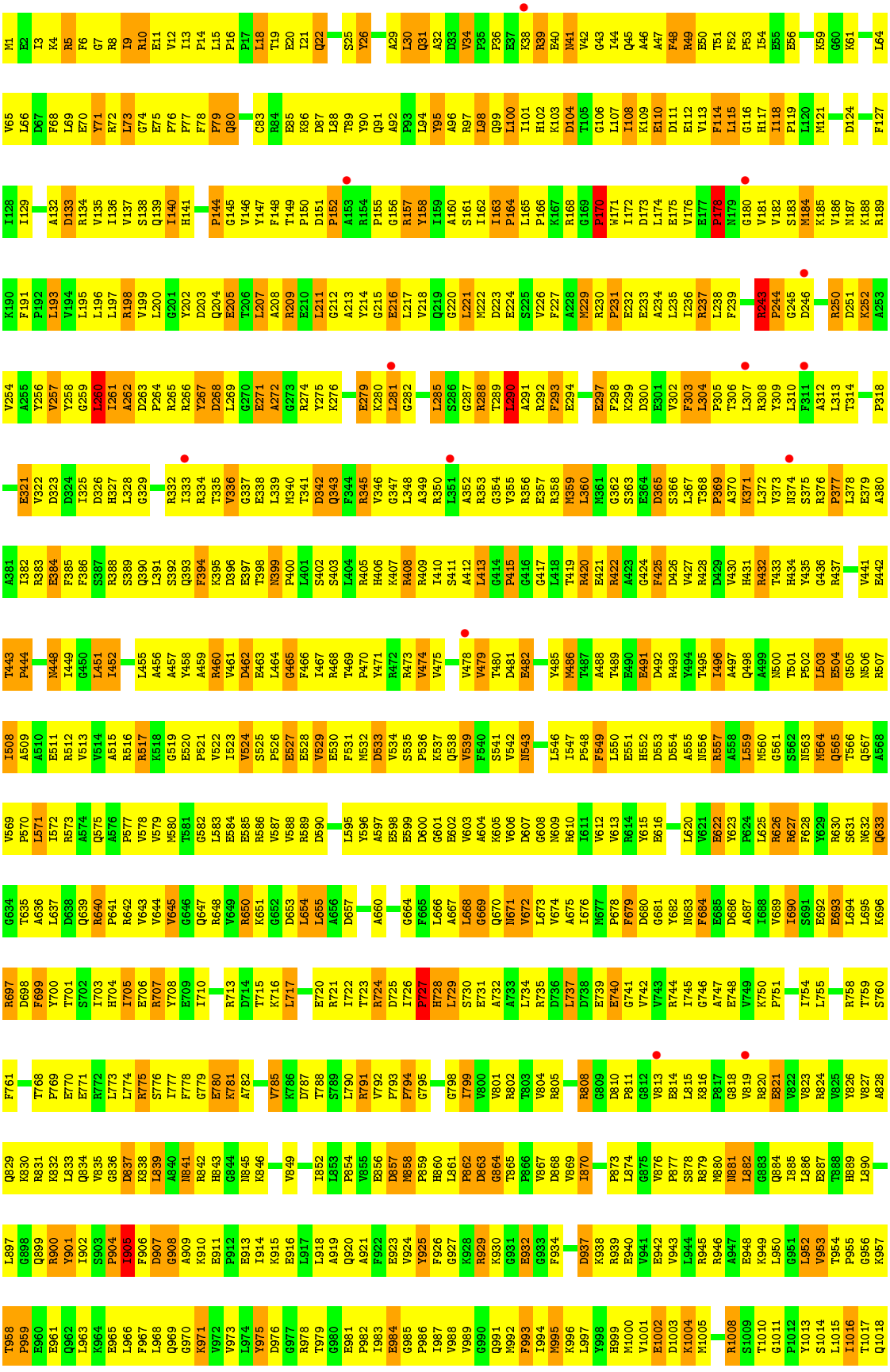
Chain L:

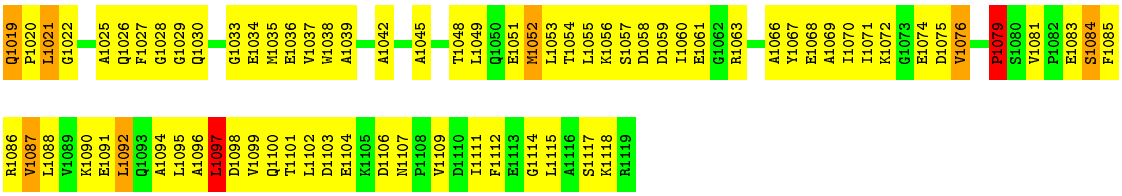


• Molecule 2: DNA-directed RNA polymerase beta chain

Chain C:

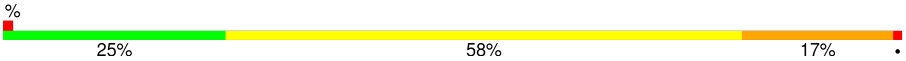


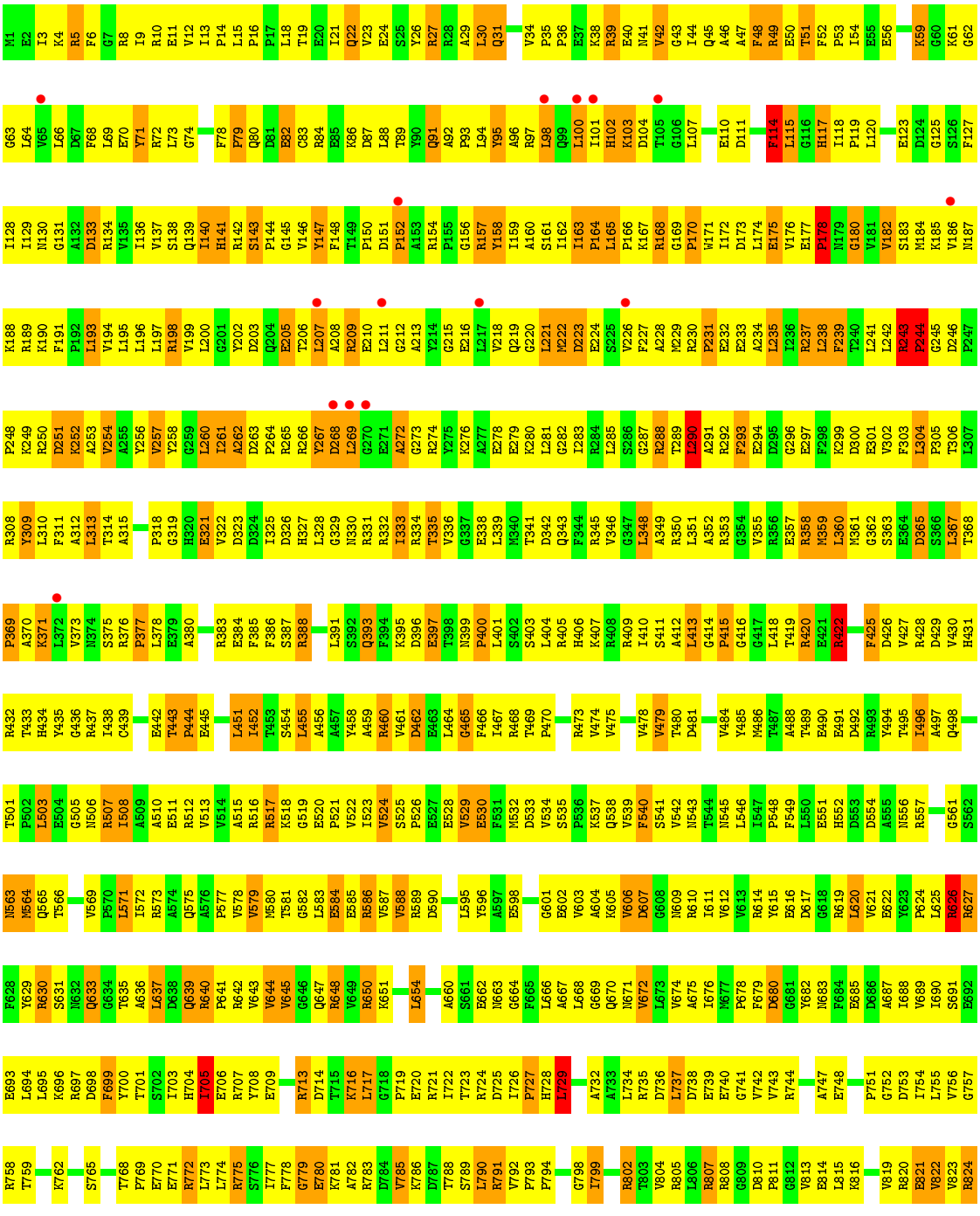


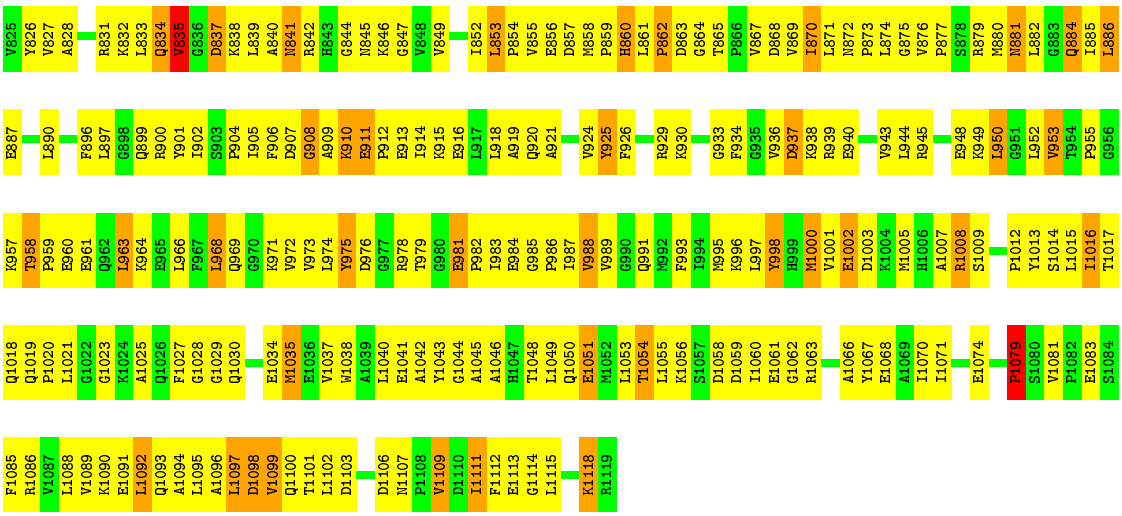


• Molecule 2: DNA-directed RNA polymerase beta chain

Chain M:

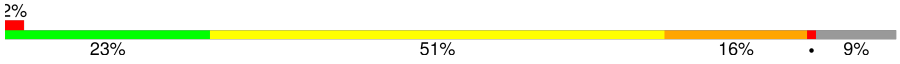


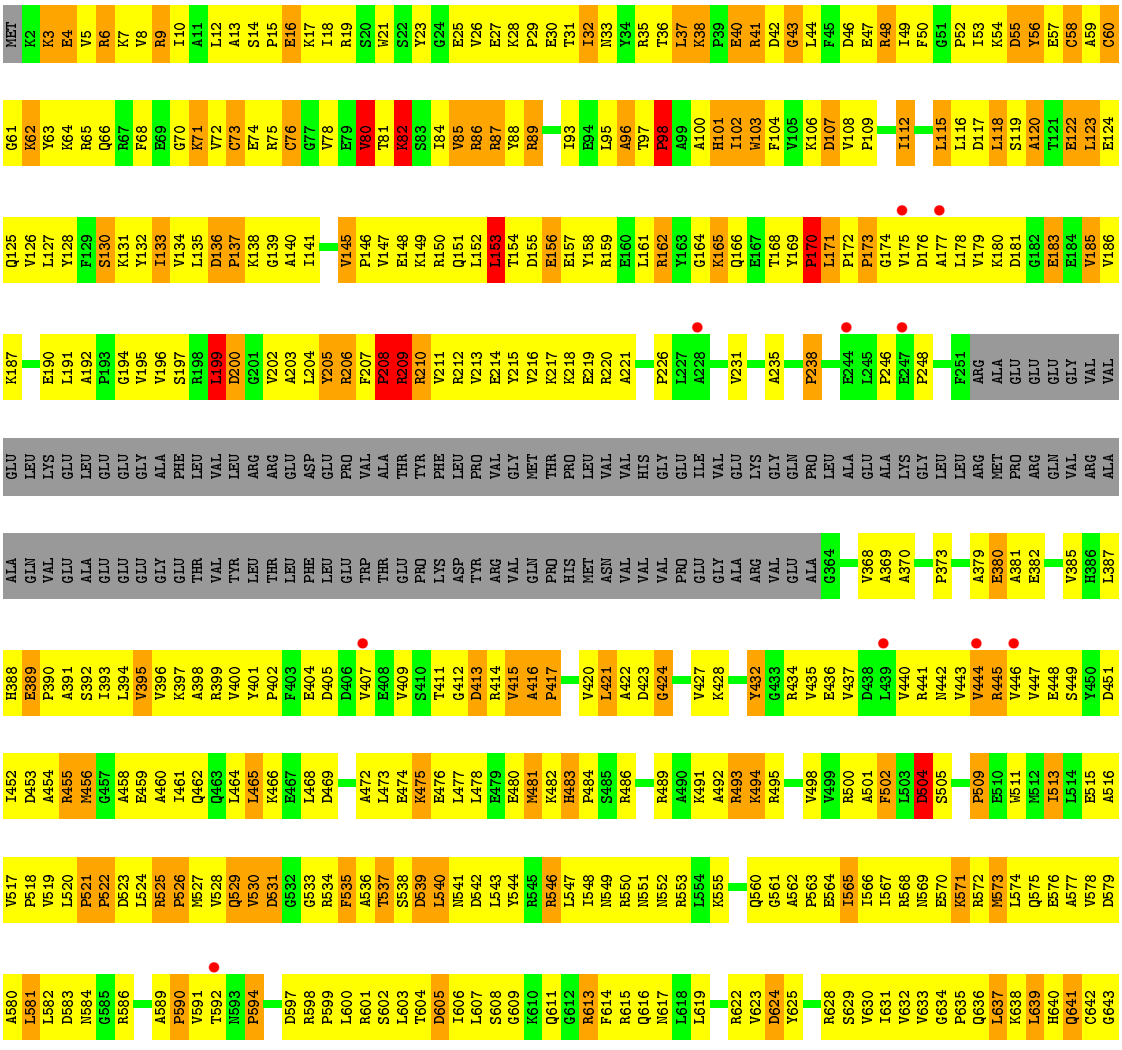


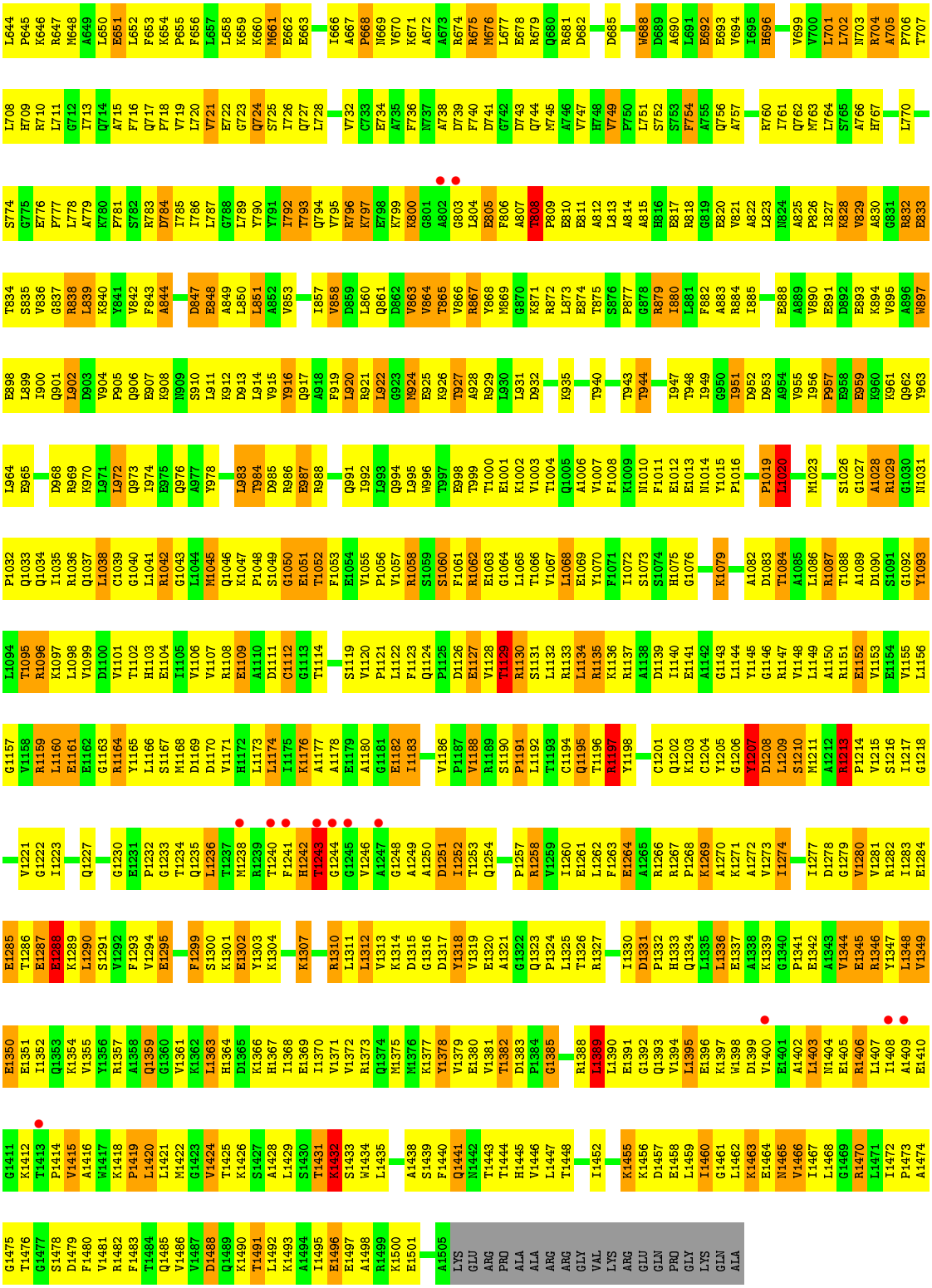


• Molecule 3: DNA-directed RNA polymerase beta' chain

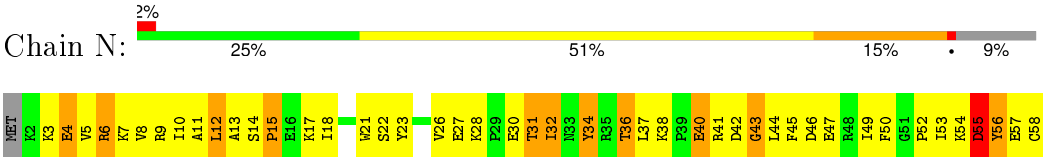
Chain D:

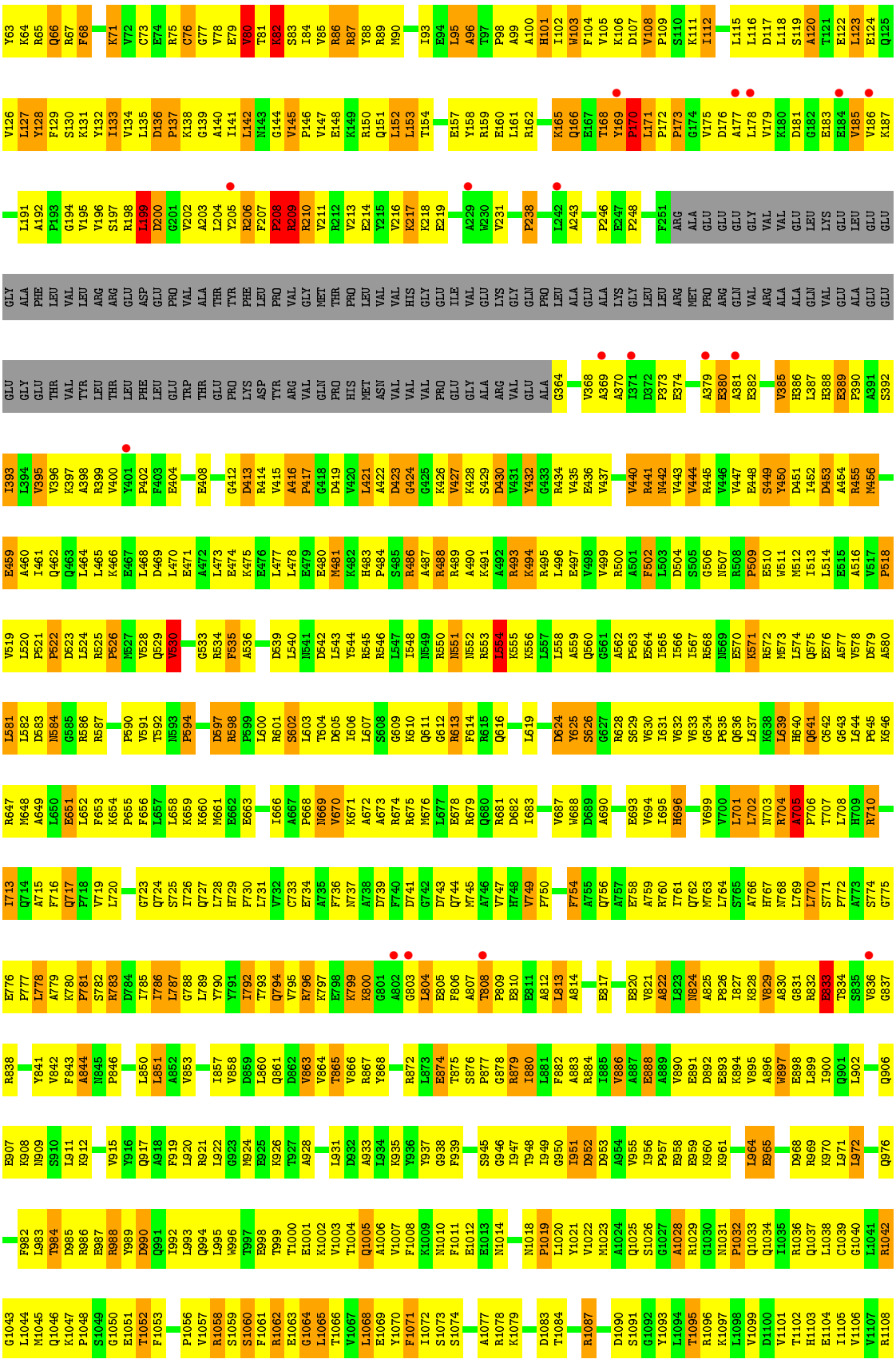


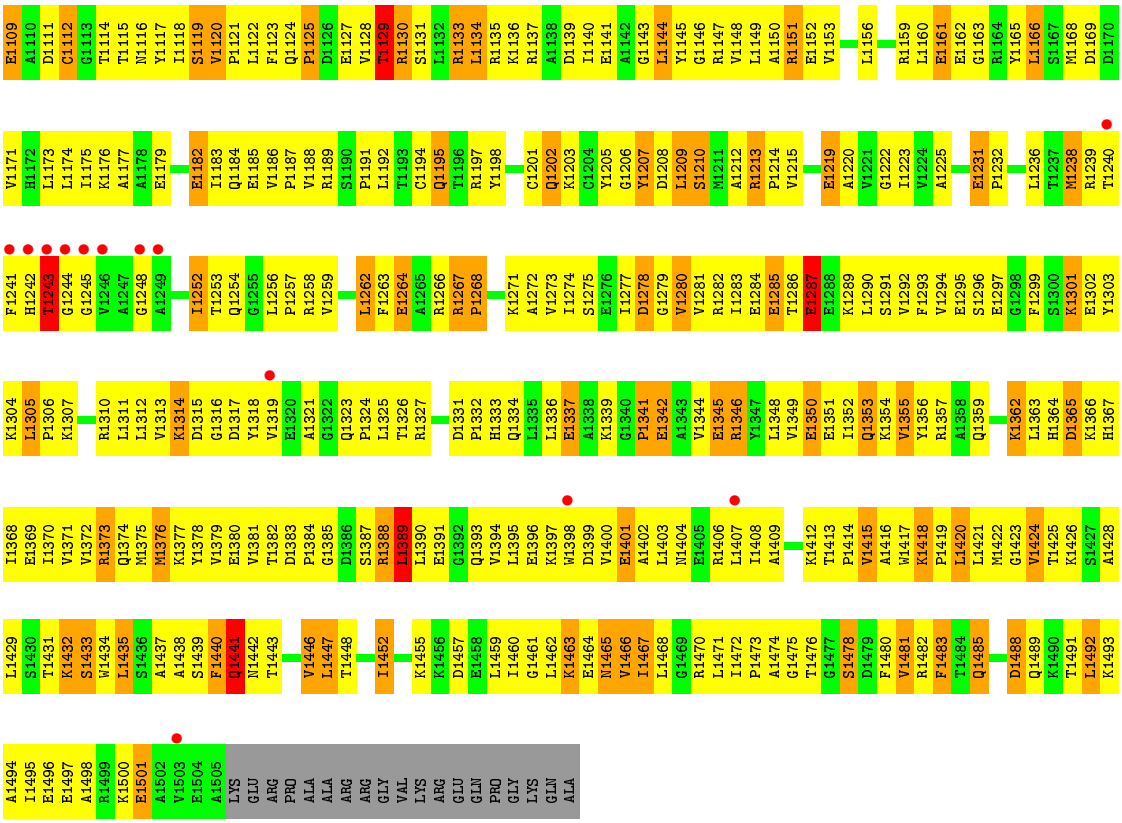




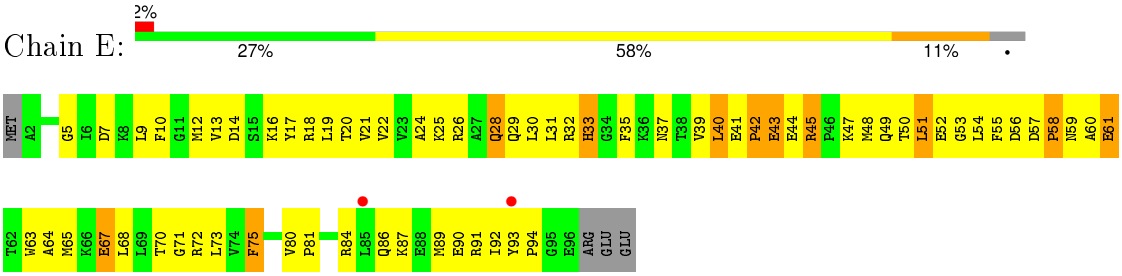
• Molecule 3: DNA-directed RNA polymerase beta' chain



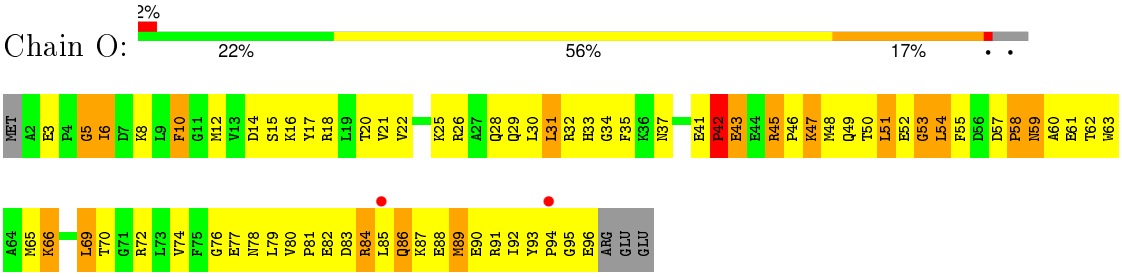




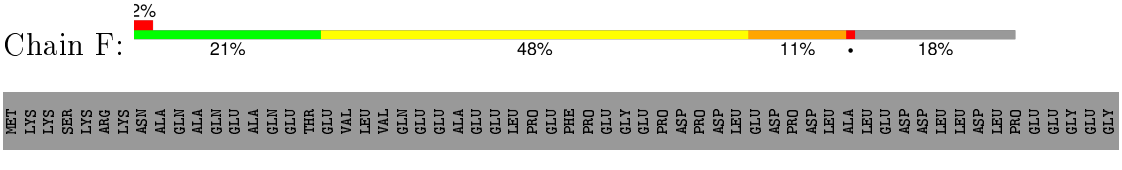
• Molecule 4: RNA polymerase omega chain

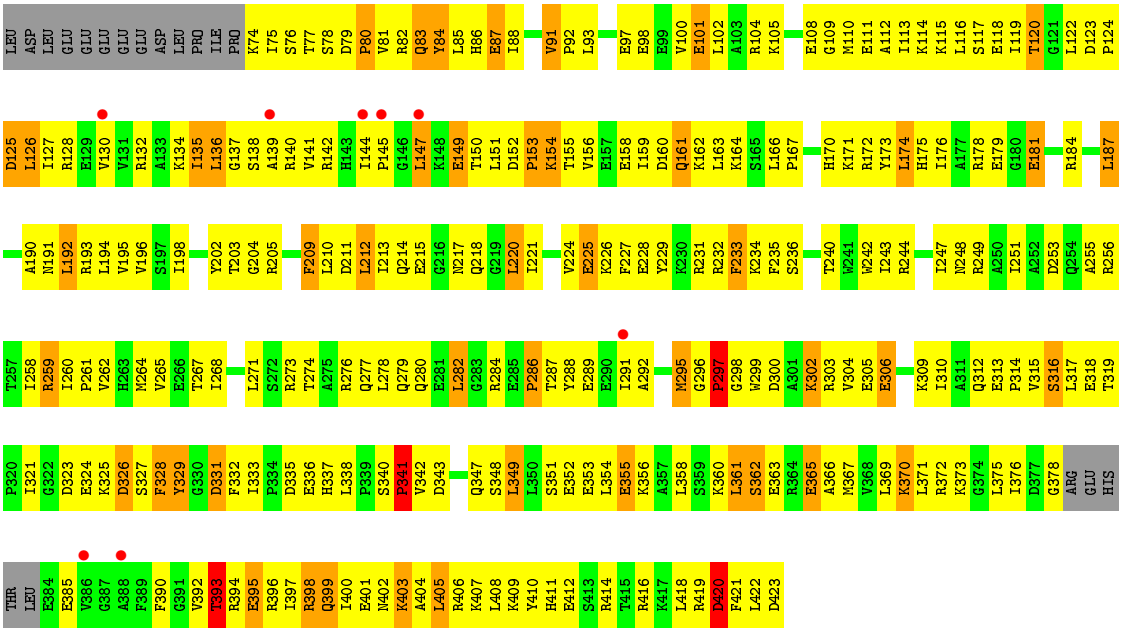


• Molecule 4: RNA polymerase omega chain



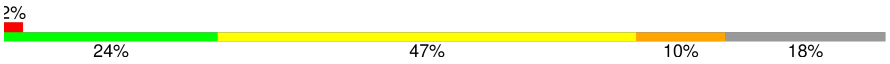
• Molecule 5: RNA polymerase sigma factor rpoD

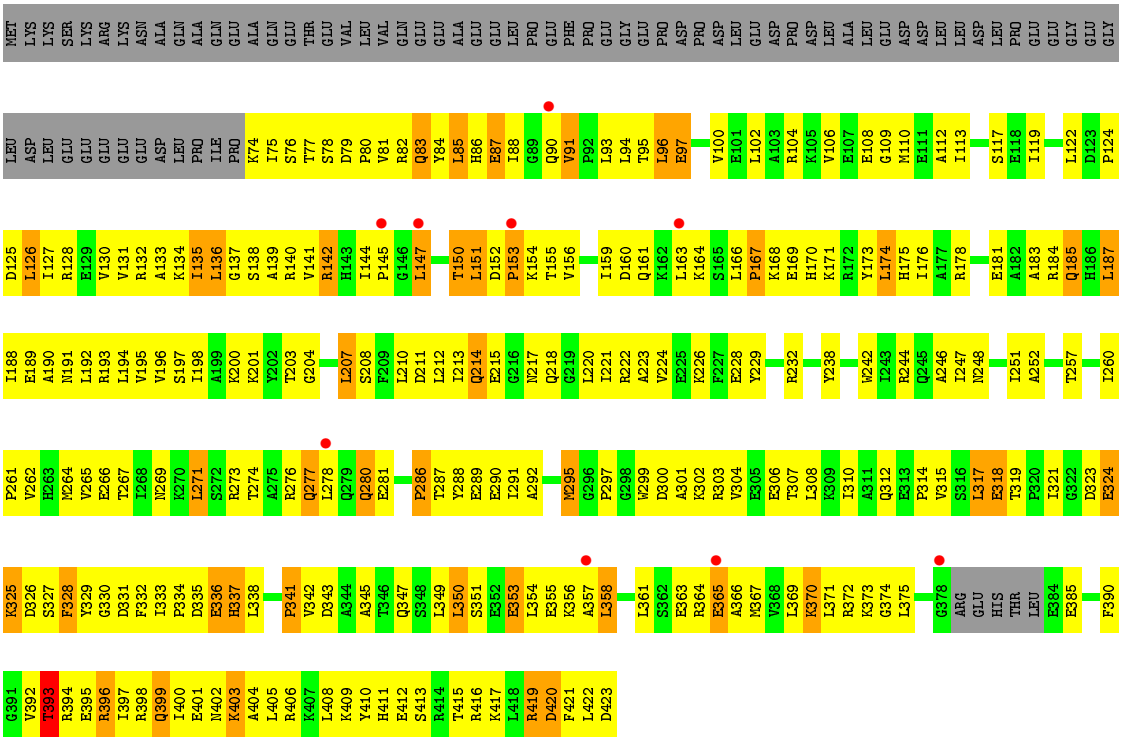




• Molecule 5: RNA polymerase sigma factor rpoD

Chain P:





4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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)	0.27 , 77.1	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[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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(^{o})	Ideal(^{o})
1	B	138	LEU	CA-CB-CG	8.26	134.29	115.30
3	D	199	LEU	CA-CB-CG	-8.08	96.72	115.30
3	N	199	LEU	CA-CB-CG	-7.83	97.28	115.30
3	N	1389	LEU	CA-CB-CG	7.33	132.15	115.30
5	F	361	LEU	CA-CB-CG	7.04	131.49	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1806	0	1861	231	0
1	B	1806	0	1861	211	0
1	K	1806	0	1861	199	0
1	L	1806	0	1861	202	0
2	C	8829	0	8933	1201	0
2	M	8829	0	8933	1179	0
3	D	10797	0	10873	1404	0
3	N	10797	0	10873	1285	0
4	E	769	0	775	92	0
4	O	769	0	775	99	0
5	F	2771	0	2844	340	0
5	P	2771	0	2844	315	0
6	A	31	0	0	0	0
6	B	23	0	0	0	0
6	C	81	0	0	0	0
6	D	137	0	0	0	0
6	E	10	0	0	0	0
6	F	31	0	0	0	0
6	K	21	0	0	0	0
6	L	25	0	0	0	0
6	M	69	0	0	0	0
6	N	108	0	0	0	0
6	O	6	0	0	0	0
6	P	20	0	0	0	0
7	C	61	0	61	3	0
7	M	61	0	61	3	0
8	D	2	0	0	0	0
8	N	2	0	0	0	0
9	A	253	0	0	49	0
9	B	307	0	0	49	0
9	C	1000	0	0	202	0
9	D	1418	0	0	282	0
9	E	112	0	0	22	0
9	F	456	0	0	98	0

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 59.

The worst 5 of 6365 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ARG:HH12	2:C:857:ASP:HB3	1.08	1.12
2:M:1054:THR:HG21	2:M:1079:PRO:HB3	1.27	1.11
3:N:1045:MET:HG2	3:N:1073:SER:HA	1.35	1.08
2:C:630:ARG:HH21	2:C:705:ILE:HG22	1.18	1.07
3:N:52:PRO:HB2	3:N:80:VAL:HG13	1.34	1.06

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	227/315 (72%)	204 (90%)	19 (8%)	4 (2%)	11 18
1	B	227/315 (72%)	201 (88%)	21 (9%)	5 (2%)	8 13
1	K	227/315 (72%)	204 (90%)	19 (8%)	4 (2%)	11 18
1	L	227/315 (72%)	205 (90%)	18 (8%)	4 (2%)	11 18
2	C	1117/1119 (100%)	911 (82%)	153 (14%)	53 (5%)	3 3

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

5 of 301 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	B	29	GLU
1	B	48	ILE
2	C	152	PRO
2	C	156	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	202/273 (74%)	148 (73%)	54 (27%)	0 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 1
4	E	83/87 (95%)	67 (81%)	16 (19%)	2 3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	O	83/87 (95%)	61 (74%)	22 (26%)	0 1
5	F	295/370 (80%)	235 (80%)	60 (20%)	1 2
5	P	295/370 (80%)	247 (84%)	48 (16%)	3 5
All	All	5692/6446 (88%)	4406 (77%)	1286 (23%)	1 1

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

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

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

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	59,66,66	2.71	21 (35%)	84,101,101	1.84	18 (21%)
7	RBT	M	8002	-	59,66,66	2.66	21 (35%)	84,101,101	1.81	14 (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	0/2/6/6
7	RBT	M	8002	-	-	0/59/116/116	0/2/6/6

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	8002	RBT	O2-C8	-3.53	1.28	1.37
7	C	8001	RBT	O2-C8	-2.69	1.30	1.37
7	C	8001	RBT	C32-C22	2.02	1.58	1.53
7	M	8002	RBT	C9-C1	2.17	1.52	1.46
7	C	8001	RBT	O6-C37	2.18	1.50	1.42

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	8001	RBT	O3-C6-C5	-3.82	111.08	114.28
7	M	8002	RBT	O3-C6-C5	-3.76	111.13	114.28
7	C	8001	RBT	C9-C10-C5	-3.53	116.06	119.97
7	M	8002	RBT	C9-C10-C5	-3.39	116.21	119.97
7	M	8002	RBT	C31-C20-C19	-2.91	102.95	110.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

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

5.7 Other polymers

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, 95^{th} 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%)	-0.36	1 (0%) 93 93	29, 60, 84, 110	0
1	B	229/315 (72%)	-0.07	16 (6%) 19 22	44, 89, 114, 118	0
1	K	229/315 (72%)	-0.36	2 (0%) 85 88	33, 58, 89, 120	0
1	L	229/315 (72%)	-0.21	8 (3%) 48 53	49, 89, 109, 119	0
2	C	1119/1119 (100%)	-0.34	13 (1%) 81 83	14, 74, 102, 117	0
2	M	1119/1119 (100%)	-0.34	15 (1%) 79 82	19, 71, 103, 119	0
3	D	1392/1524 (91%)	-0.31	23 (1%) 73 76	19, 62, 107, 125	0
3	N	1392/1524 (91%)	-0.32	30 (2%) 65 69	23, 65, 107, 131	0
4	E	95/99 (95%)	-0.35	2 (2%) 67 71	41, 77, 107, 120	0
4	O	95/99 (95%)	-0.40	2 (2%) 67 71	33, 72, 94, 103	0
5	F	345/423 (81%)	-0.35	8 (2%) 64 67	46, 81, 104, 118	0
5	P	345/423 (81%)	-0.26	9 (2%) 59 63	53, 81, 108, 123	0
All	All	6818/7590 (89%)	-0.32	129 (1%) 70 73	14, 70, 105, 131	0

The worst 5 of 129 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	P	145	PRO	6.1
3	N	1243	THR	6.0
2	M	269	LEU	5.4
3	D	1244	GLY	5.1
3	D	1240	THR	5.0

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 (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, 95^{th} 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	RBT	C	8001	61/61	0.97	0.19	2.48	25,37,42,48	0
6	MG	C	9121	1/1	0.99	0.15	1.86	43,43,43,43	0
7	RBT	M	8002	61/61	0.96	0.18	1.80	28,39,48,54	0
6	MG	K	9214	1/1	0.98	0.20	1.47	31,31,31,31	0
8	ZN	D	7112	1/1	0.99	0.13	1.30	72,72,72,72	0
6	MG	A	9001	1/1	0.98	0.18	1.13	26,26,26,26	0
6	MG	D	9002	1/1	0.98	0.16	0.83	29,29,29,29	0
8	ZN	N	7113	1/1	0.99	0.11	0.15	79,79,79,79	0
6	MG	N	9218	1/1	0.99	0.12	0.05	32,32,32,32	0
8	ZN	N	7059	1/1	1.00	0.12	0.04	83,83,83,83	0
6	MG	M	9220	1/1	0.96	0.13	-0.12	45,45,45,45	0
6	MG	D	9008	1/1	0.99	0.13	-0.13	37,37,37,37	0
6	MG	D	9015	1/1	0.98	0.12	-0.32	37,37,37,37	0
6	MG	F	9421	1/1	1.00	0.13	-0.32	30,30,30,30	0
6	MG	D	9042	1/1	0.97	0.12	-0.33	47,47,47,47	0
6	MG	D	9021	1/1	0.99	0.12	-0.45	34,34,34,34	0
6	MG	K	9265	1/1	0.99	0.13	-0.47	37,37,37,37	0
6	MG	D	9049	1/1	0.99	0.14	-0.53	31,31,31,31	0
6	MG	D	9123	1/1	0.98	0.14	-0.55	37,37,37,37	0
6	MG	C	9020	1/1	0.99	0.14	-0.58	28,28,28,28	0
6	MG	D	9036	1/1	0.98	0.13	-0.62	41,41,41,41	0
6	MG	N	9215	1/1	0.99	0.10	-0.83	40,40,40,40	0
6	MG	D	9172	1/1	0.98	0.10	-0.88	35,35,35,35	0
6	MG	N	9277	1/1	0.99	0.09	-0.91	37,37,37,37	0
6	MG	D	9449	1/1	0.98	0.07	-0.92	29,29,29,29	0
6	MG	A	9024	1/1	0.99	0.10	-0.94	29,29,29,29	0
6	MG	C	9004	1/1	0.99	0.09	-0.96	30,30,30,30	0
6	MG	D	9453	1/1	1.00	0.12	-0.98	31,31,31,31	0
6	MG	P	9275	1/1	0.99	0.09	-1.00	32,32,32,32	0
6	MG	D	9069	1/1	1.00	0.12	-1.01	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	MG	K	9487	1/1	0.99	0.12	-1.05	36,36,36,36	0
6	MG	N	9335	1/1	0.99	0.10	-1.10	33,33,33,33	0
6	MG	D	9026	1/1	0.97	0.12	-1.14	37,37,37,37	0
6	MG	M	9323	1/1	0.99	0.10	-1.15	37,37,37,37	0
6	MG	B	9163	1/1	0.92	0.07	-1.20	44,44,44,44	0
6	MG	C	9025	1/1	0.99	0.10	-1.22	39,39,39,39	0
6	MG	N	9526	1/1	0.98	0.10	-1.22	30,30,30,30	0
6	MG	C	9161	1/1	0.99	0.07	-1.24	40,40,40,40	0
6	MG	F	9053	1/1	0.99	0.10	-1.25	34,34,34,34	0
6	MG	M	9312	1/1	0.97	0.10	-1.26	37,37,37,37	0
6	MG	P	9536	1/1	0.99	0.07	-1.29	41,41,41,41	0
6	MG	C	9005	1/1	0.99	0.08	-1.30	31,31,31,31	0
6	MG	C	9398	1/1	0.95	0.10	-1.31	44,44,44,44	0
6	MG	C	9011	1/1	0.99	0.10	-1.35	39,39,39,39	0
6	MG	N	9221	1/1	0.99	0.10	-1.39	30,30,30,30	0
6	MG	C	9144	1/1	0.99	0.09	-1.40	39,39,39,39	0
6	MG	D	9441	1/1	0.98	0.10	-1.43	46,46,46,46	0
6	MG	N	9475	1/1	0.99	0.07	-1.51	43,43,43,43	0
6	MG	N	9226	1/1	0.99	0.07	-1.55	30,30,30,30	0
6	MG	N	9280	1/1	0.99	0.09	-1.73	34,34,34,34	0
6	MG	N	9263	1/1	0.99	0.08	-1.74	37,37,37,37	0
6	MG	L	9272	1/1	0.99	0.10	-1.79	29,29,29,29	0
6	MG	C	9046	1/1	0.99	0.09	-1.80	31,31,31,31	0
8	ZN	D	7058	1/1	0.96	0.07	-1.80	100,100,100,100	0
6	MG	D	9181	1/1	0.99	0.06	-1.86	36,36,36,36	0
6	MG	B	9101	1/1	0.98	0.08	-1.86	40,40,40,40	0
6	MG	F	9465	1/1	0.99	0.06	-1.88	36,36,36,36	0
6	MG	M	9372	1/1	0.99	0.09	-1.98	47,47,47,47	0
6	MG	D	9105	1/1	0.99	0.07	-1.99	48,48,48,48	0
6	MG	K	9212	1/1	1.00	0.08	-2.00	33,33,33,33	0
6	MG	N	9207	1/1	0.98	0.10	-2.11	30,30,30,30	0
6	MG	D	9179	1/1	1.00	0.09	-2.27	30,30,30,30	0
6	MG	D	9037	1/1	1.00	0.08	-2.30	31,31,31,31	0
6	MG	C	9056	1/1	0.99	0.06	-2.42	34,34,34,34	0
6	MG	C	9515	1/1	0.98	0.08	-2.42	41,41,41,41	0
6	MG	N	9509	1/1	0.99	0.11	-2.51	31,31,31,31	0
6	MG	F	9407	1/1	0.99	0.07	-2.54	32,32,32,32	0
6	MG	D	9013	1/1	1.00	0.09	-2.55	34,34,34,34	0
6	MG	M	9478	1/1	0.98	0.06	-2.56	35,35,35,35	0
6	MG	D	9129	1/1	0.99	0.09	-2.67	38,38,38,38	0
6	MG	N	9248	1/1	0.99	0.06	-2.80	47,47,47,47	0
6	MG	F	9032	1/1	0.99	0.09	-3.07	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	MG	C	9414	1/1	0.97	0.07	-3.10	41,41,41,41	0
6	MG	D	9147	1/1	0.96	0.09	-3.13	40,40,40,40	0
6	MG	C	9431	1/1	0.99	0.06	-3.17	42,42,42,42	0
6	MG	N	9531	1/1	1.00	0.10	-3.20	38,38,38,38	0
6	MG	C	9420	1/1	0.99	0.07	-3.36	37,37,37,37	0
6	MG	C	9047	1/1	0.97	0.06	-3.48	47,47,47,47	0
6	MG	D	9017	1/1	0.99	0.07	-3.80	37,37,37,37	0
6	MG	N	9349	1/1	0.96	0.06	-3.81	37,37,37,37	0
6	MG	D	9012	1/1	0.98	0.06	-4.27	39,39,39,39	0
6	MG	D	9120	1/1	0.99	0.07	-4.76	34,34,34,34	0
6	MG	D	9003	1/1	0.98	0.06	-4.97	43,43,43,43	0
6	MG	D	9451	1/1	0.98	0.09	-5.59	37,37,37,37	0
6	MG	K	9217	1/1	0.98	0.06	-5.86	36,36,36,36	0
6	MG	N	9282	1/1	0.99	0.06	-6.78	38,38,38,38	0
6	MG	D	9055	1/1	0.98	0.09	-	51,51,51,51	0
6	MG	F	9437	1/1	0.98	0.09	-	47,47,47,47	0
6	MG	D	9087	1/1	1.00	0.09	-	27,27,27,27	0
6	MG	C	9156	1/1	0.97	0.12	-	43,43,43,43	0
6	MG	N	9303	1/1	0.99	0.12	-	35,35,35,35	0
6	MG	C	9098	1/1	0.99	0.09	-	52,52,52,52	0
6	MG	L	9530	1/1	0.99	0.10	-	58,58,58,58	0
6	MG	D	9452	1/1	0.99	0.10	-	32,32,32,32	0
6	MG	K	9367	1/1	0.98	0.08	-	38,38,38,38	0
6	MG	C	9171	1/1	0.99	0.09	-	33,33,33,33	0
6	MG	D	9182	1/1	1.00	0.07	-	46,46,46,46	0
6	MG	D	9436	1/1	0.99	0.09	-	46,46,46,46	0
6	MG	A	9062	1/1	0.96	0.11	-	45,45,45,45	0
6	MG	N	9286	1/1	0.99	0.12	-	46,46,46,46	0
6	MG	N	9498	1/1	0.98	0.09	-	45,45,45,45	0
6	MG	A	9116	1/1	0.99	0.12	-	47,47,47,47	0
6	MG	C	9031	1/1	0.99	0.12	-	43,43,43,43	0
6	MG	N	9371	1/1	0.99	0.10	-	30,30,30,30	0
6	MG	F	9542	1/1	0.99	0.19	-	50,50,50,50	0
6	MG	L	9480	1/1	0.99	0.13	-	36,36,36,36	0
6	MG	N	9342	1/1	0.98	0.06	-	48,48,48,48	0
6	MG	M	9223	1/1	0.99	0.10	-	48,48,48,48	0
6	MG	A	9097	1/1	0.98	0.09	-	41,41,41,41	0
6	MG	A	9117	1/1	0.99	0.07	-	32,32,32,32	0
6	MG	K	9370	1/1	0.99	0.06	-	46,46,46,46	0
6	MG	K	9477	1/1	1.00	0.11	-	38,38,38,38	0
6	MG	D	9543	1/1	0.97	0.12	-	46,46,46,46	0
6	MG	M	9347	1/1	0.98	0.11	-	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	MG	C	9027	1/1	1.00	0.12	-	28,28,28,28	0
6	MG	P	9304	1/1	0.97	0.10	-	57,57,57,57	0
6	MG	M	9254	1/1	0.99	0.08	-	34,34,34,34	0
6	MG	N	9301	1/1	0.98	0.08	-	50,50,50,50	0
6	MG	D	9162	1/1	0.99	0.11	-	44,44,44,44	0
6	MG	L	9278	1/1	1.00	0.08	-	46,46,46,46	0
6	MG	E	9131	1/1	0.98	0.08	-	47,47,47,47	0
6	MG	C	9086	1/1	0.99	0.10	-	34,34,34,34	0
6	MG	D	9517	1/1	0.99	0.09	-	45,45,45,45	0
6	MG	N	9297	1/1	0.98	0.13	-	48,48,48,48	0
6	MG	D	9446	1/1	0.99	0.10	-	36,36,36,36	0
6	MG	B	9092	1/1	0.98	0.11	-	50,50,50,50	0
6	MG	A	9078	1/1	0.98	0.13	-	34,34,34,34	0
6	MG	M	9340	1/1	0.99	0.10	-	43,43,43,43	0
6	MG	M	9259	1/1	0.97	0.17	-	57,57,57,57	0
6	MG	L	9330	1/1	0.99	0.09	-	41,41,41,41	0
6	MG	C	9457	1/1	0.98	0.10	-	40,40,40,40	0
6	MG	F	9054	1/1	0.99	0.07	-	37,37,37,37	0
6	MG	C	9422	1/1	0.99	0.13	-	41,41,41,41	0
6	MG	D	9155	1/1	0.97	0.12	-	56,56,56,56	0
6	MG	C	9455	1/1	0.97	0.12	-	61,61,61,61	0
6	MG	N	9244	1/1	0.97	0.08	-	37,37,37,37	0
6	MG	M	9336	1/1	0.99	0.10	-	31,31,31,31	0
6	MG	D	9463	1/1	0.99	0.11	-	32,32,32,32	0
6	MG	A	9514	1/1	0.96	0.12	-	42,42,42,42	0
6	MG	D	9122	1/1	0.99	0.10	-	31,31,31,31	0
6	MG	K	9553	1/1	0.98	0.09	-	50,50,50,50	0
6	MG	D	9077	1/1	0.99	0.10	-	32,32,32,32	0
6	MG	N	9356	1/1	0.99	0.14	-	29,29,29,29	0
6	MG	E	9151	1/1	0.98	0.05	-	48,48,48,48	0
6	MG	N	9327	1/1	0.97	0.11	-	54,54,54,54	0
6	MG	D	9174	1/1	0.99	0.10	-	35,35,35,35	0
6	MG	D	9393	1/1	0.99	0.13	-	35,35,35,35	0
6	MG	D	9095	1/1	0.97	0.06	-	40,40,40,40	0
6	MG	F	9164	1/1	0.99	0.11	-	29,29,29,29	0
6	MG	A	9559	1/1	0.97	0.12	-	45,45,45,45	0
6	MG	D	9112	1/1	0.98	0.13	-	39,39,39,39	0
6	MG	D	9159	1/1	0.99	0.11	-	35,35,35,35	0
6	MG	N	9246	1/1	0.97	0.13	-	49,49,49,49	0
6	MG	D	9100	1/1	0.99	0.07	-	31,31,31,31	0
6	MG	M	9251	1/1	0.99	0.13	-	33,33,33,33	0
6	MG	P	9502	1/1	0.99	0.07	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	MG	N	9307	1/1	0.99	0.09	-	38,38,38,38	0
6	MG	M	9481	1/1	0.99	0.09	-	37,37,37,37	0
6	MG	C	9546	1/1	0.98	0.06	-	49,49,49,49	0
6	MG	D	9203	1/1	0.99	0.09	-	46,46,46,46	0
6	MG	C	9023	1/1	0.97	0.09	-	44,44,44,44	0
6	MG	A	9139	1/1	0.99	0.10	-	35,35,35,35	0
6	MG	C	9456	1/1	0.99	0.07	-	37,37,37,37	0
6	MG	K	9344	1/1	0.98	0.12	-	55,55,55,55	0
6	MG	C	9191	1/1	0.98	0.13	-	44,44,44,44	0
6	MG	N	9534	1/1	0.99	0.09	-	54,54,54,54	0
6	MG	M	9472	1/1	0.99	0.06	-	51,51,51,51	0
6	MG	D	9417	1/1	0.99	0.11	-	35,35,35,35	0
6	MG	P	9296	1/1	0.99	0.07	-	42,42,42,42	0
6	MG	M	9219	1/1	0.98	0.10	-	39,39,39,39	0
6	MG	A	9050	1/1	0.97	0.10	-	41,41,41,41	0
6	MG	A	9394	1/1	0.99	0.10	-	46,46,46,46	0
6	MG	C	9141	1/1	0.97	0.12	-	45,45,45,45	0
6	MG	C	9028	1/1	0.99	0.07	-	41,41,41,41	0
6	MG	N	9499	1/1	0.98	0.08	-	38,38,38,38	0
6	MG	M	9285	1/1	0.98	0.13	-	43,43,43,43	0
6	MG	F	9045	1/1	0.99	0.10	-	40,40,40,40	0
6	MG	D	9016	1/1	0.99	0.07	-	38,38,38,38	0
6	MG	M	9540	1/1	0.98	0.16	-	63,63,63,63	0
6	MG	D	9110	1/1	0.98	0.13	-	38,38,38,38	0
6	MG	N	9508	1/1	0.97	0.11	-	41,41,41,41	0
6	MG	O	9231	1/1	1.00	0.15	-	41,41,41,41	0
6	MG	L	9346	1/1	0.97	0.14	-	52,52,52,52	0
6	MG	L	9311	1/1	0.98	0.07	-	33,33,33,33	0
6	MG	C	9083	1/1	0.98	0.11	-	48,48,48,48	0
6	MG	F	9048	1/1	0.96	0.16	-	50,50,50,50	0
6	MG	P	9353	1/1	0.99	0.11	-	44,44,44,44	0
6	MG	D	9057	1/1	0.98	0.11	-	33,33,33,33	0
6	MG	M	9216	1/1	0.99	0.12	-	44,44,44,44	0
6	MG	B	9512	1/1	0.99	0.20	-	53,53,53,53	0
6	MG	D	9405	1/1	0.99	0.10	-	38,38,38,38	0
6	MG	B	9427	1/1	0.98	0.11	-	42,42,42,42	0
6	MG	C	9157	1/1	0.98	0.16	-	44,44,44,44	0
6	MG	N	9266	1/1	0.98	0.08	-	36,36,36,36	0
6	MG	K	9264	1/1	1.00	0.09	-	36,36,36,36	0
6	MG	D	9403	1/1	0.99	0.16	-	30,30,30,30	0
6	MG	P	9240	1/1	0.99	0.11	-	38,38,38,38	0
6	MG	A	9440	1/1	0.99	0.10	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	MG	D	9418	1/1	0.99	0.08	-	47,47,47,47	0
6	MG	M	9224	1/1	0.99	0.06	-	38,38,38,38	0
6	MG	C	9170	1/1	0.99	0.10	-	36,36,36,36	0
6	MG	C	9185	1/1	0.99	0.18	-	60,60,60,60	0
6	MG	M	9380	1/1	1.00	0.08	-	32,32,32,32	0
6	MG	N	9506	1/1	0.98	0.10	-	56,56,56,56	0
6	MG	D	9128	1/1	0.99	0.11	-	35,35,35,35	0
6	MG	N	9474	1/1	0.96	0.13	-	56,56,56,56	0
6	MG	N	9305	1/1	0.99	0.09	-	42,42,42,42	0
6	MG	M	9255	1/1	0.96	0.13	-	58,58,58,58	0
6	MG	L	9234	1/1	0.99	0.07	-	41,41,41,41	0
6	MG	N	9550	1/1	0.99	0.09	-	34,34,34,34	0
6	MG	M	9267	1/1	0.96	0.11	-	41,41,41,41	0
6	MG	N	9501	1/1	0.99	0.08	-	47,47,47,47	0
6	MG	M	9382	1/1	0.99	0.09	-	33,33,33,33	0
6	MG	N	9529	1/1	0.98	0.08	-	55,55,55,55	0
6	MG	D	9067	1/1	0.97	0.12	-	49,49,49,49	0
6	MG	M	9227	1/1	0.98	0.10	-	44,44,44,44	0
6	MG	C	9113	1/1	0.99	0.16	-	47,47,47,47	0
6	MG	B	9434	1/1	0.99	0.11	-	35,35,35,35	0
6	MG	B	9150	1/1	0.98	0.10	-	43,43,43,43	0
6	MG	M	9366	1/1	0.99	0.10	-	41,41,41,41	0
6	MG	M	9298	1/1	0.98	0.12	-	43,43,43,43	0
6	MG	M	9318	1/1	0.99	0.14	-	51,51,51,51	0
6	MG	M	9328	1/1	0.99	0.09	-	48,48,48,48	0
6	MG	M	9210	1/1	0.99	0.13	-	35,35,35,35	0
6	MG	C	9549	1/1	0.98	0.11	-	48,48,48,48	0
6	MG	N	9503	1/1	0.96	0.12	-	52,52,52,52	0
6	MG	M	9334	1/1	0.97	0.09	-	44,44,44,44	0
6	MG	D	9562	1/1	0.99	0.17	-	49,49,49,49	0
6	MG	N	9238	1/1	0.99	0.16	-	29,29,29,29	0
6	MG	C	9007	1/1	0.98	0.11	-	34,34,34,34	0
6	MG	D	9094	1/1	0.99	0.10	-	35,35,35,35	0
6	MG	M	9241	1/1	1.00	0.09	-	35,35,35,35	0
6	MG	D	9401	1/1	0.98	0.12	-	40,40,40,40	0
6	MG	N	9533	1/1	0.99	0.12	-	33,33,33,33	0
6	MG	D	9149	1/1	1.00	0.13	-	42,42,42,42	0
6	MG	F	9089	1/1	0.99	0.10	-	48,48,48,48	0
6	MG	M	9283	1/1	0.98	0.14	-	35,35,35,35	0
6	MG	M	9361	1/1	0.99	0.10	-	51,51,51,51	0
6	MG	D	9058	1/1	0.99	0.11	-	41,41,41,41	0
6	MG	D	9202	1/1	0.98	0.18	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	MG	L	9299	1/1	1.00	0.07	-	36,36,36,36	0
6	MG	N	9358	1/1	0.97	0.12	-	48,48,48,48	0
6	MG	D	9445	1/1	0.98	0.13	-	48,48,48,48	0
6	MG	N	9387	1/1	0.99	0.07	-	28,28,28,28	0
6	MG	P	9558	1/1	0.98	0.09	-	44,44,44,44	0
6	MG	N	9230	1/1	0.97	0.09	-	40,40,40,40	0
6	MG	C	9444	1/1	0.99	0.09	-	40,40,40,40	0
6	MG	B	9450	1/1	0.99	0.08	-	46,46,46,46	0
6	MG	E	9467	1/1	0.97	0.12	-	52,52,52,52	0
6	MG	D	9075	1/1	0.99	0.11	-	39,39,39,39	0
6	MG	M	9325	1/1	0.97	0.10	-	44,44,44,44	0
6	MG	P	9541	1/1	0.98	0.10	-	44,44,44,44	0
6	MG	N	9528	1/1	0.99	0.10	-	40,40,40,40	0
6	MG	C	9201	1/1	0.99	0.08	-	45,45,45,45	0
6	MG	N	9365	1/1	0.98	0.12	-	43,43,43,43	0
6	MG	D	9143	1/1	1.00	0.14	-	35,35,35,35	0
6	MG	C	9521	1/1	0.99	0.12	-	45,45,45,45	0
6	MG	D	9466	1/1	0.98	0.10	-	57,57,57,57	0
6	MG	D	9168	1/1	0.98	0.06	-	38,38,38,38	0
6	MG	F	9547	1/1	1.00	0.09	-	52,52,52,52	0
6	MG	N	9381	1/1	0.97	0.07	-	35,35,35,35	0
6	MG	N	9256	1/1	0.99	0.09	-	41,41,41,41	0
6	MG	A	9430	1/1	0.97	0.11	-	35,35,35,35	0
6	MG	N	9314	1/1	0.98	0.11	-	38,38,38,38	0
6	MG	F	9135	1/1	0.99	0.14	-	42,42,42,42	0
6	MG	N	9379	1/1	0.99	0.06	-	56,56,56,56	0
6	MG	L	9300	1/1	0.99	0.07	-	58,58,58,58	0
6	MG	C	9088	1/1	0.99	0.12	-	36,36,36,36	0
6	MG	N	9235	1/1	0.95	0.12	-	63,63,63,63	0
6	MG	D	9038	1/1	0.99	0.11	-	35,35,35,35	0
6	MG	M	9261	1/1	0.96	0.10	-	45,45,45,45	0
6	MG	C	9462	1/1	0.99	0.12	-	50,50,50,50	0
6	MG	N	9245	1/1	0.98	0.12	-	28,28,28,28	0
6	MG	M	9377	1/1	0.98	0.12	-	39,39,39,39	0
6	MG	M	9469	1/1	1.00	0.14	-	39,39,39,39	0
6	MG	B	9391	1/1	0.99	0.12	-	27,27,27,27	0
6	MG	D	9052	1/1	0.99	0.09	-	36,36,36,36	0
6	MG	F	9197	1/1	0.99	0.10	-	39,39,39,39	0
6	MG	N	9295	1/1	0.98	0.05	-	48,48,48,48	0
6	MG	B	9180	1/1	0.99	0.09	-	36,36,36,36	0
6	MG	C	9029	1/1	0.99	0.12	-	36,36,36,36	0
6	MG	N	9273	1/1	0.99	0.17	-	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	MG	N	9504	1/1	0.98	0.10	-	32,32,32,32	0
6	MG	F	9435	1/1	0.99	0.08	-	40,40,40,40	0
6	MG	N	9376	1/1	0.99	0.13	-	31,31,31,31	0
6	MG	D	9158	1/1	0.99	0.08	-	31,31,31,31	0
6	MG	N	9490	1/1	0.98	0.12	-	41,41,41,41	0
6	MG	N	9320	1/1	0.99	0.11	-	41,41,41,41	0
6	MG	D	9548	1/1	0.97	0.12	-	51,51,51,51	0
6	MG	E	9186	1/1	0.99	0.10	-	35,35,35,35	0
6	MG	D	9154	1/1	0.99	0.11	-	31,31,31,31	0
6	MG	O	9359	1/1	0.96	0.08	-	57,57,57,57	0
6	MG	D	9169	1/1	0.99	0.12	-	45,45,45,45	0
6	MG	L	9471	1/1	0.99	0.10	-	33,33,33,33	0
6	MG	M	9384	1/1	0.99	0.10	-	35,35,35,35	0
6	MG	P	9333	1/1	0.99	0.07	-	28,28,28,28	0
6	MG	D	9189	1/1	0.99	0.10	-	34,34,34,34	0
6	MG	D	9423	1/1	0.97	0.09	-	44,44,44,44	0
6	MG	M	9287	1/1	0.99	0.08	-	36,36,36,36	0
6	MG	P	9322	1/1	0.96	0.12	-	43,43,43,43	0
6	MG	L	9505	1/1	0.98	0.10	-	58,58,58,58	0
6	MG	D	9510	1/1	1.00	0.12	-	51,51,51,51	0
6	MG	D	9043	1/1	1.00	0.11	-	28,28,28,28	0
6	MG	L	9258	1/1	0.94	0.10	-	47,47,47,47	0
6	MG	N	9527	1/1	1.00	0.14	-	42,42,42,42	0
6	MG	D	9424	1/1	0.98	0.14	-	50,50,50,50	0
6	MG	B	9103	1/1	0.99	0.09	-	37,37,37,37	0
6	MG	N	9313	1/1	0.98	0.09	-	39,39,39,39	0
6	MG	C	9439	1/1	0.99	0.10	-	35,35,35,35	0
6	MG	N	9368	1/1	0.99	0.09	-	41,41,41,41	0
6	MG	P	9326	1/1	0.99	0.08	-	39,39,39,39	0
6	MG	M	9321	1/1	0.99	0.13	-	40,40,40,40	0
6	MG	L	9260	1/1	0.99	0.09	-	41,41,41,41	0
6	MG	D	9519	1/1	0.99	0.12	-	55,55,55,55	0
6	MG	A	9560	1/1	0.99	0.13	-	49,49,49,49	0
6	MG	C	9044	1/1	0.99	0.08	-	37,37,37,37	0
6	MG	D	9084	1/1	0.96	0.10	-	47,47,47,47	0
6	MG	M	9383	1/1	0.96	0.09	-	46,46,46,46	0
6	MG	C	9196	1/1	0.99	0.13	-	30,30,30,30	0
6	MG	C	9205	1/1	0.99	0.12	-	53,53,53,53	0
6	MG	F	9206	1/1	0.98	0.12	-	33,33,33,33	0
6	MG	M	9331	1/1	1.00	0.08	-	49,49,49,49	0
6	MG	C	9127	1/1	1.00	0.10	-	41,41,41,41	0
6	MG	N	9242	1/1	0.98	0.12	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	MG	A	9145	1/1	0.97	0.11	-	45,45,45,45	0
6	MG	B	9146	1/1	0.99	0.09	-	44,44,44,44	0
6	MG	E	9511	1/1	1.00	0.12	-	42,42,42,42	0
6	MG	D	9397	1/1	0.98	0.12	-	31,31,31,31	0
6	MG	N	9319	1/1	0.98	0.11	-	41,41,41,41	0
6	MG	E	9115	1/1	0.99	0.08	-	39,39,39,39	0
6	MG	C	9124	1/1	0.98	0.08	-	33,33,33,33	0
6	MG	D	9175	1/1	0.99	0.09	-	40,40,40,40	0
6	MG	F	9010	1/1	0.97	0.17	-	57,57,57,57	0
6	MG	N	9486	1/1	0.97	0.09	-	44,44,44,44	0
6	MG	P	9329	1/1	0.99	0.07	-	46,46,46,46	0
6	MG	M	9233	1/1	0.98	0.15	-	38,38,38,38	0
6	MG	D	9523	1/1	0.97	0.11	-	41,41,41,41	0
6	MG	C	9415	1/1	0.99	0.11	-	38,38,38,38	0
6	MG	B	9395	1/1	0.98	0.11	-	56,56,56,56	0
6	MG	N	9208	1/1	0.97	0.12	-	35,35,35,35	0
6	MG	N	9375	1/1	0.99	0.10	-	43,43,43,43	0
6	MG	A	9178	1/1	0.99	0.09	-	28,28,28,28	0
6	MG	P	9317	1/1	0.98	0.18	-	53,53,53,53	0
6	MG	A	9411	1/1	0.99	0.10	-	31,31,31,31	0
6	MG	K	9257	1/1	0.96	0.12	-	57,57,57,57	0
6	MG	D	9561	1/1	0.99	0.06	-	38,38,38,38	0
6	MG	A	9194	1/1	0.99	0.09	-	40,40,40,40	0
6	MG	D	9416	1/1	0.99	0.09	-	48,48,48,48	0
6	MG	D	9136	1/1	0.99	0.10	-	41,41,41,41	0
6	MG	D	9073	1/1	0.99	0.15	-	38,38,38,38	0
6	MG	N	9289	1/1	0.99	0.09	-	35,35,35,35	0
6	MG	N	9225	1/1	0.99	0.08	-	40,40,40,40	0
6	MG	D	9166	1/1	0.99	0.08	-	49,49,49,49	0
6	MG	B	9389	1/1	0.98	0.10	-	37,37,37,37	0
6	MG	N	9352	1/1	0.99	0.05	-	44,44,44,44	0
6	MG	F	9072	1/1	0.99	0.07	-	40,40,40,40	0
6	MG	A	9107	1/1	0.97	0.07	-	40,40,40,40	0
6	MG	C	9074	1/1	0.99	0.13	-	30,30,30,30	0
6	MG	O	9355	1/1	0.99	0.14	-	36,36,36,36	0
6	MG	D	9443	1/1	0.99	0.07	-	47,47,47,47	0
6	MG	C	9071	1/1	0.99	0.13	-	39,39,39,39	0
6	MG	D	9039	1/1	0.98	0.11	-	40,40,40,40	0
6	MG	B	9137	1/1	0.99	0.09	-	35,35,35,35	0
6	MG	D	9520	1/1	0.96	0.14	-	46,46,46,46	0
6	MG	D	9059	1/1	0.98	0.10	-	40,40,40,40	0
6	MG	E	9187	1/1	0.99	0.12	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	MG	N	9491	1/1	1.00	0.11	-	43,43,43,43	0
6	MG	A	9018	1/1	0.99	0.14	-	31,31,31,31	0
6	MG	D	9065	1/1	0.99	0.14	-	44,44,44,44	0
6	MG	D	9454	1/1	0.99	0.08	-	42,42,42,42	0
6	MG	D	9518	1/1	0.97	0.11	-	55,55,55,55	0
6	MG	E	9438	1/1	0.99	0.10	-	38,38,38,38	0
6	MG	P	9274	1/1	0.99	0.11	-	45,45,45,45	0
6	MG	C	9106	1/1	1.00	0.09	-	37,37,37,37	0
6	MG	D	9447	1/1	0.98	0.09	-	50,50,50,50	0
6	MG	K	9363	1/1	0.97	0.09	-	47,47,47,47	0
6	MG	M	9364	1/1	0.94	0.08	-	37,37,37,37	0
6	MG	C	9545	1/1	0.99	0.10	-	45,45,45,45	0
6	MG	C	9428	1/1	0.99	0.12	-	42,42,42,42	0
6	MG	C	9081	1/1	0.97	0.13	-	52,52,52,52	0
6	MG	D	9090	1/1	0.99	0.11	-	48,48,48,48	0
6	MG	F	9035	1/1	0.99	0.10	-	40,40,40,40	0
6	MG	F	9153	1/1	0.98	0.07	-	39,39,39,39	0
6	MG	D	9544	1/1	0.99	0.11	-	49,49,49,49	0
6	MG	L	9271	1/1	0.99	0.09	-	39,39,39,39	0
6	MG	B	9033	1/1	0.99	0.10	-	44,44,44,44	0
6	MG	F	9429	1/1	0.98	0.12	-	57,57,57,57	0
6	MG	N	9316	1/1	0.99	0.09	-	32,32,32,32	0
6	MG	N	9354	1/1	0.95	0.07	-	42,42,42,42	0
6	MG	F	9030	1/1	1.00	0.11	-	36,36,36,36	0
6	MG	N	9476	1/1	0.99	0.06	-	44,44,44,44	0
6	MG	D	9099	1/1	0.98	0.07	-	38,38,38,38	0
6	MG	C	9063	1/1	0.98	0.10	-	32,32,32,32	0
6	MG	D	9516	1/1	0.98	0.05	-	51,51,51,51	0
6	MG	D	9140	1/1	0.98	0.13	-	43,43,43,43	0
6	MG	N	9470	1/1	1.00	0.15	-	27,27,27,27	0
6	MG	C	9014	1/1	0.98	0.14	-	45,45,45,45	0
6	MG	D	9119	1/1	0.99	0.09	-	44,44,44,44	0
6	MG	N	9281	1/1	0.98	0.09	-	50,50,50,50	0
6	MG	L	9249	1/1	0.97	0.07	-	51,51,51,51	0
6	MG	A	9102	1/1	0.98	0.09	-	38,38,38,38	0
6	MG	M	9268	1/1	0.99	0.11	-	37,37,37,37	0
6	MG	M	9385	1/1	0.99	0.10	-	29,29,29,29	0
6	MG	C	9130	1/1	0.99	0.14	-	42,42,42,42	0
6	MG	L	9345	1/1	0.99	0.12	-	42,42,42,42	0
6	MG	D	9460	1/1	0.99	0.14	-	38,38,38,38	0
6	MG	C	9190	1/1	0.96	0.07	-	40,40,40,40	0
6	MG	F	9513	1/1	0.99	0.14	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	MG	D	9096	1/1	0.97	0.14	-	43,43,43,43	0
6	MG	N	9538	1/1	0.92	0.10	-	42,42,42,42	0
6	MG	N	9291	1/1	0.99	0.15	-	55,55,55,55	0
6	MG	M	9348	1/1	0.97	0.11	-	63,63,63,63	0
6	MG	O	9209	1/1	0.96	0.11	-	37,37,37,37	0
6	MG	D	9060	1/1	0.99	0.11	-	35,35,35,35	0
6	MG	N	9310	1/1	0.98	0.08	-	36,36,36,36	0
6	MG	D	9091	1/1	0.99	0.14	-	47,47,47,47	0
6	MG	F	9525	1/1	0.99	0.08	-	54,54,54,54	0
6	MG	N	9555	1/1	0.97	0.11	-	56,56,56,56	0
6	MG	D	9425	1/1	0.99	0.09	-	44,44,44,44	0
6	MG	C	9396	1/1	0.98	0.14	-	57,57,57,57	0
6	MG	M	9290	1/1	0.98	0.12	-	48,48,48,48	0
6	MG	N	9247	1/1	0.97	0.08	-	29,29,29,29	0
6	MG	N	9270	1/1	0.99	0.13	-	47,47,47,47	0
6	MG	N	9308	1/1	1.00	0.12	-	31,31,31,31	0
6	MG	M	9489	1/1	0.99	0.09	-	43,43,43,43	0
6	MG	O	9337	1/1	1.00	0.08	-	34,34,34,34	0
6	MG	A	9126	1/1	0.99	0.10	-	39,39,39,39	0
6	MG	N	9324	1/1	0.99	0.08	-	39,39,39,39	0
6	MG	N	9468	1/1	1.00	0.11	-	35,35,35,35	0
6	MG	C	9524	1/1	0.99	0.08	-	45,45,45,45	0
6	MG	D	9125	1/1	0.99	0.10	-	35,35,35,35	0
6	MG	A	9200	1/1	0.99	0.10	-	49,49,49,49	0
6	MG	N	9360	1/1	1.00	0.05	-	39,39,39,39	0
6	MG	N	9262	1/1	0.98	0.13	-	49,49,49,49	0
6	MG	C	9193	1/1	0.99	0.09	-	37,37,37,37	0
6	MG	M	9373	1/1	0.99	0.12	-	38,38,38,38	0
6	MG	D	9432	1/1	0.98	0.10	-	47,47,47,47	0
6	MG	E	9402	1/1	0.99	0.12	-	39,39,39,39	0
6	MG	M	9497	1/1	0.99	0.12	-	43,43,43,43	0
6	MG	L	9479	1/1	0.99	0.10	-	48,48,48,48	0
6	MG	M	9211	1/1	0.98	0.10	-	28,28,28,28	0
6	MG	D	9019	1/1	0.98	0.15	-	35,35,35,35	0
6	MG	C	9068	1/1	0.95	0.12	-	37,37,37,37	0
6	MG	F	9133	1/1	0.99	0.10	-	42,42,42,42	0
6	MG	D	9111	1/1	0.96	0.09	-	43,43,43,43	0
6	MG	K	9493	1/1	0.99	0.09	-	38,38,38,38	0
6	MG	D	9066	1/1	0.97	0.11	-	49,49,49,49	0
6	MG	F	9410	1/1	0.94	0.12	-	47,47,47,47	0
6	MG	M	9276	1/1	0.98	0.13	-	54,54,54,54	0
6	MG	B	9199	1/1	0.95	0.10	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	MG	B	9419	1/1	0.98	0.12	-	46,46,46,46	0
6	MG	B	9079	1/1	0.98	0.11	-	28,28,28,28	0
6	MG	M	9485	1/1	0.98	0.06	-	42,42,42,42	0
6	MG	D	9041	1/1	0.98	0.10	-	32,32,32,32	0
6	MG	D	9070	1/1	0.99	0.10	-	46,46,46,46	0
6	MG	N	9228	1/1	0.98	0.08	-	49,49,49,49	0
6	MG	C	9408	1/1	0.99	0.12	-	38,38,38,38	0
6	MG	K	9492	1/1	0.99	0.10	-	40,40,40,40	0
6	MG	A	9173	1/1	0.99	0.10	-	41,41,41,41	0
6	MG	N	9343	1/1	0.99	0.09	-	45,45,45,45	0
6	MG	N	9237	1/1	0.99	0.14	-	40,40,40,40	0
6	MG	L	9483	1/1	0.97	0.15	-	44,44,44,44	0
6	MG	B	9442	1/1	0.99	0.12	-	47,47,47,47	0
6	MG	M	9293	1/1	0.98	0.11	-	43,43,43,43	0
6	MG	N	9386	1/1	0.99	0.08	-	46,46,46,46	0
6	MG	A	9522	1/1	0.98	0.11	-	57,57,57,57	0
6	MG	L	9374	1/1	0.99	0.09	-	47,47,47,47	0
6	MG	D	9459	1/1	0.99	0.10	-	33,33,33,33	0
6	MG	D	9009	1/1	0.98	0.12	-	53,53,53,53	0
6	MG	D	9082	1/1	0.99	0.11	-	30,30,30,30	0
6	MG	P	9284	1/1	0.97	0.10	-	51,51,51,51	0
6	MG	C	9177	1/1	0.96	0.09	-	40,40,40,40	0
6	MG	M	9557	1/1	0.98	0.09	-	54,54,54,54	0
6	MG	N	9554	1/1	0.97	0.11	-	45,45,45,45	0
6	MG	C	9458	1/1	0.98	0.09	-	38,38,38,38	0
6	MG	N	9253	1/1	0.96	0.08	-	39,39,39,39	0
6	MG	L	9213	1/1	0.98	0.23	-	49,49,49,49	0
6	MG	N	9357	1/1	0.99	0.09	-	41,41,41,41	0
6	MG	C	9076	1/1	0.99	0.11	-	37,37,37,37	0
6	MG	D	9152	1/1	0.97	0.11	-	32,32,32,32	0
6	MG	D	9142	1/1	0.99	0.11	-	40,40,40,40	0
6	MG	M	9252	1/1	0.99	0.12	-	37,37,37,37	0
6	MG	D	9104	1/1	0.98	0.09	-	35,35,35,35	0
6	MG	D	9433	1/1	0.99	0.12	-	46,46,46,46	0
6	MG	D	9051	1/1	0.99	0.07	-	36,36,36,36	0
6	MG	N	9315	1/1	0.98	0.11	-	41,41,41,41	0
6	MG	L	9532	1/1	0.98	0.08	-	51,51,51,51	0
6	MG	A	9413	1/1	0.96	0.10	-	46,46,46,46	0
6	MG	D	9132	1/1	0.99	0.10	-	33,33,33,33	0
6	MG	K	9507	1/1	0.99	0.14	-	45,45,45,45	0
6	MG	N	9341	1/1	0.98	0.13	-	38,38,38,38	0
6	MG	M	9473	1/1	0.97	0.11	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	MG	D	9006	1/1	1.00	0.14	-	30,30,30,30	0
6	MG	P	9239	1/1	1.00	0.11	-	33,33,33,33	0
6	MG	D	9034	1/1	0.98	0.16	-	37,37,37,37	0
6	MG	O	9362	1/1	0.98	0.04	-	49,49,49,49	0
6	MG	K	9496	1/1	0.99	0.09	-	42,42,42,42	0
6	MG	N	9294	1/1	0.99	0.07	-	49,49,49,49	0
6	MG	B	9148	1/1	0.98	0.15	-	54,54,54,54	0
6	MG	M	9369	1/1	0.99	0.09	-	35,35,35,35	0
6	MG	N	9302	1/1	1.00	0.14	-	48,48,48,48	0
6	MG	M	9222	1/1	0.99	0.09	-	33,33,33,33	0
6	MG	L	9236	1/1	0.99	0.08	-	41,41,41,41	0
6	MG	C	9204	1/1	0.99	0.12	-	41,41,41,41	0
6	MG	C	9160	1/1	1.00	0.12	-	46,46,46,46	0
6	MG	N	9551	1/1	0.97	0.08	-	40,40,40,40	0
6	MG	D	9138	1/1	0.99	0.12	-	38,38,38,38	0
6	MG	N	9338	1/1	0.98	0.12	-	42,42,42,42	0
6	MG	K	9279	1/1	0.99	0.11	-	36,36,36,36	0
6	MG	P	9388	1/1	0.99	0.08	-	45,45,45,45	0
6	MG	A	9404	1/1	1.00	0.16	-	55,55,55,55	0
6	MG	E	9184	1/1	0.97	0.16	-	48,48,48,48	0
6	MG	D	9134	1/1	0.99	0.10	-	40,40,40,40	0
6	MG	K	9484	1/1	0.98	0.11	-	30,30,30,30	0
6	MG	C	9183	1/1	0.98	0.16	-	44,44,44,44	0
6	MG	M	9535	1/1	0.99	0.12	-	40,40,40,40	0
6	MG	M	9332	1/1	0.97	0.13	-	54,54,54,54	0
6	MG	M	9537	1/1	0.99	0.13	-	38,38,38,38	0
6	MG	D	9108	1/1	0.98	0.11	-	51,51,51,51	0
6	MG	D	9118	1/1	0.99	0.12	-	34,34,34,34	0
6	MG	D	9085	1/1	0.99	0.10	-	32,32,32,32	0
6	MG	F	9167	1/1	0.98	0.12	-	59,59,59,59	0
6	MG	M	9488	1/1	0.98	0.12	-	42,42,42,42	0
6	MG	K	9351	1/1	0.97	0.09	-	37,37,37,37	0
6	MG	C	9390	1/1	1.00	0.12	-	30,30,30,30	0
6	MG	B	9176	1/1	1.00	0.09	-	41,41,41,41	0
6	MG	A	9109	1/1	0.98	0.09	-	33,33,33,33	0
6	MG	D	9061	1/1	0.99	0.11	-	35,35,35,35	0
6	MG	M	9350	1/1	0.98	0.09	-	37,37,37,37	0
6	MG	D	9195	1/1	1.00	0.08	-	32,32,32,32	0
6	MG	P	9269	1/1	0.99	0.09	-	41,41,41,41	0
6	MG	L	9378	1/1	0.98	0.14	-	47,47,47,47	0
6	MG	F	9448	1/1	0.98	0.10	-	38,38,38,38	0
6	MG	N	9482	1/1	0.99	0.14	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	MG	D	9464	1/1	0.99	0.12	-	38,38,38,38	0
6	MG	C	9426	1/1	0.99	0.06	-	47,47,47,47	0
6	MG	M	9500	1/1	0.99	0.09	-	46,46,46,46	0
6	MG	P	9494	1/1	0.99	0.10	-	50,50,50,50	0
6	MG	N	9552	1/1	0.99	0.11	-	46,46,46,46	0
6	MG	N	9292	1/1	0.98	0.16	-	52,52,52,52	0
6	MG	D	9114	1/1	0.99	0.10	-	32,32,32,32	0
6	MG	C	9198	1/1	0.99	0.11	-	36,36,36,36	0
6	MG	M	9309	1/1	0.98	0.15	-	35,35,35,35	0
6	MG	C	9406	1/1	0.98	0.10	-	47,47,47,47	0
6	MG	N	9539	1/1	0.97	0.10	-	57,57,57,57	0
6	MG	C	9192	1/1	0.97	0.10	-	55,55,55,55	0
6	MG	L	9556	1/1	0.98	0.09	-	58,58,58,58	0
6	MG	D	9392	1/1	0.99	0.09	-	46,46,46,46	0
6	MG	N	9250	1/1	0.95	0.16	-	61,61,61,61	0
6	MG	A	9412	1/1	0.99	0.12	-	33,33,33,33	0
6	MG	B	9040	1/1	0.99	0.16	-	29,29,29,29	0
6	MG	M	9229	1/1	0.98	0.09	-	35,35,35,35	0
6	MG	C	9399	1/1	0.96	0.10	-	43,43,43,43	0
6	MG	D	9093	1/1	0.99	0.11	-	34,34,34,34	0
6	MG	N	9306	1/1	0.99	0.13	-	30,30,30,30	0
6	MG	N	9339	1/1	0.99	0.11	-	34,34,34,34	0
6	MG	C	9400	1/1	0.99	0.12	-	49,49,49,49	0
6	MG	D	9064	1/1	0.99	0.11	-	41,41,41,41	0
6	MG	D	9188	1/1	0.99	0.09	-	37,37,37,37	0
6	MG	K	9495	1/1	0.99	0.10	-	35,35,35,35	0
6	MG	M	9243	1/1	0.98	0.11	-	45,45,45,45	0
6	MG	F	9461	1/1	0.97	0.12	-	52,52,52,52	0
6	MG	F	9080	1/1	0.99	0.12	-	30,30,30,30	0
6	MG	N	9232	1/1	0.98	0.10	-	33,33,33,33	0
6	MG	C	9022	1/1	0.99	0.12	-	28,28,28,28	0
6	MG	A	9165	1/1	0.98	0.11	-	65,65,65,65	0
6	MG	C	9409	1/1	0.99	0.12	-	49,49,49,49	0
6	MG	N	9288	1/1	0.98	0.10	-	33,33,33,33	0

6.5 Other polymers (i)

There are no such residues in this entry.