wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 07:57 AM GMT

PDB ID	:	3CMV
Title	:	Mechanism of homologous recombination from the RecA-ssDNA/dsDNA structures
Authors	:	Pavletich, N.P.
Deposited on	:	2008-03-24
Resolution	:	4.30 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:

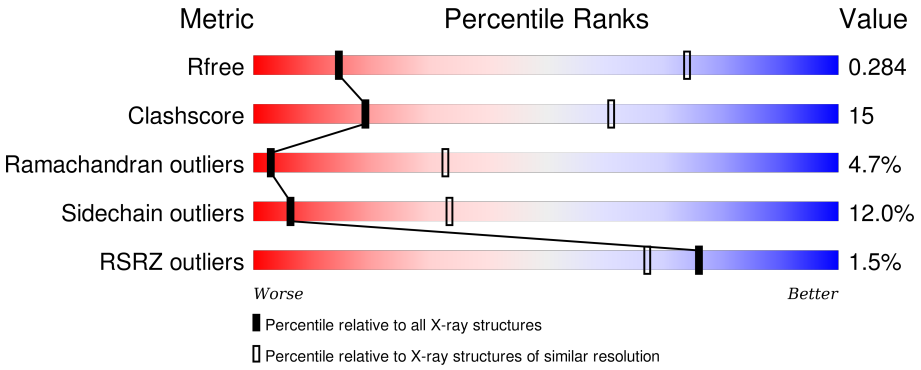
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 4.30 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	1059 (5.00-3.60)
Clashscore	102246	1166 (5.00-3.60)
Ramachandran outliers	100387	1106 (5.00-3.60)
Sidechain outliers	100360	1089 (5.00-3.60)
RSRZ outliers	91569	1062 (5.00-3.60)

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	1357	55% 27% 6% • 12%
1	B	1357	54% 27% 5% 14%
1	C	1357	54% 27% 5% 13%
1	D	1357	55% 27% 5% 13%
1	E	1357	53% 27% 5% 14%

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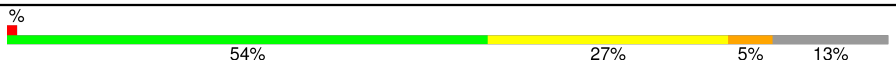
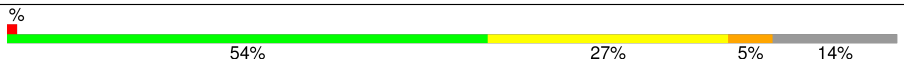
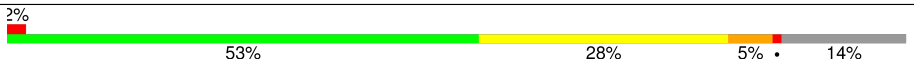
Mol	Chain	Length	Quality of chain
1	F	1357	
1	G	1357	
1	H	1357	

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
2	MG	D	2701	-	-	-	X
2	MG	E	701	-	-	-	X
2	MG	F	701	-	-	-	X
2	MG	G	2701	-	-	-	X
3	ANP	A	1400	X	-	-	-
3	ANP	A	2400	X	-	-	-
3	ANP	A	3400	X	-	-	-
3	ANP	A	400	X	-	-	-
3	ANP	B	1400	X	-	-	-
3	ANP	B	2400	X	-	-	-
3	ANP	B	3400	X	-	-	-
3	ANP	B	400	X	-	-	-
3	ANP	C	1400	X	-	-	-
3	ANP	C	2400	X	-	-	-
3	ANP	C	3400	X	-	-	-
3	ANP	C	400	X	-	-	-
3	ANP	D	1400	X	-	-	-
3	ANP	D	2400	X	-	-	-
3	ANP	D	3400	X	-	-	-
3	ANP	D	400	X	-	-	-
3	ANP	E	1400	X	-	-	-
3	ANP	E	2400	X	-	-	-
3	ANP	E	3400	X	-	-	-
3	ANP	E	400	X	-	-	-
3	ANP	F	1400	X	-	-	-
3	ANP	F	2400	X	-	-	X
3	ANP	F	3400	X	-	-	-
3	ANP	F	400	X	-	-	-
3	ANP	G	1400	X	-	-	-
3	ANP	G	2400	X	-	-	X
3	ANP	G	3400	X	-	-	-
3	ANP	G	400	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ANP	H	1400	X	-	-	-
3	ANP	H	2400	X	-	-	-
3	ANP	H	3400	X	-	-	-
3	ANP	H	400	X	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 71761 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 Protein recA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1190	Total	C	N	O	S	0	0	0
			8970	5660	1553	1719	38			
1	B	1163	Total	C	N	O	S	0	0	0
			8769	5538	1519	1677	35			
1	C	1175	Total	C	N	O	S	0	0	0
			8856	5587	1533	1700	36			
1	D	1175	Total	C	N	O	S	0	0	0
			8856	5587	1533	1700	36			
1	E	1165	Total	C	N	O	S	0	0	0
			8787	5548	1521	1683	35			
1	F	1175	Total	C	N	O	S	0	0	0
			8856	5587	1533	1700	36			
1	G	1167	Total	C	N	O	S	0	0	0
			8799	5554	1523	1687	35			
1	H	1173	Total	C	N	O	S	0	0	0
			8844	5581	1531	1696	36			

There are 400 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	GLY	-	linker	UNP P0A7G6
A	27	ALA	-	linker	UNP P0A7G6
A	28	MET	-	linker	UNP P0A7G6
A	29	HIS	-	linker	UNP P0A7G6
A	986	THR	-	linker	UNP P0A7G6
A	987	GLY	-	linker	UNP P0A7G6
A	988	SER	-	linker	UNP P0A7G6
A	989	THR	-	linker	UNP P0A7G6
A	990	GLY	-	linker	UNP P0A7G6
A	991	SER	-	linker	UNP P0A7G6
A	992	GLY	-	linker	UNP P0A7G6
A	993	THR	-	linker	UNP P0A7G6
A	994	THR	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	995	GLY	-	linker	UNP P0A7G6
A	996	SER	-	linker	UNP P0A7G6
A	997	THR	-	linker	UNP P0A7G6
A	998	GLY	-	linker	UNP P0A7G6
A	999	SER	-	linker	UNP P0A7G6
A	1000	MET	-	linker	UNP P0A7G6
A	1986	THR	-	linker	UNP P0A7G6
A	1987	GLY	-	linker	UNP P0A7G6
A	1988	SER	-	linker	UNP P0A7G6
A	1989	THR	-	linker	UNP P0A7G6
A	1990	GLY	-	linker	UNP P0A7G6
A	1991	SER	-	linker	UNP P0A7G6
A	1992	MET	-	linker	UNP P0A7G6
A	1993	GLY	-	linker	UNP P0A7G6
A	1994	HIS	-	linker	UNP P0A7G6
A	1995	THR	-	linker	UNP P0A7G6
A	1996	THR	-	linker	UNP P0A7G6
A	1997	GLY	-	linker	UNP P0A7G6
A	1998	SER	-	linker	UNP P0A7G6
A	1999	MET	-	linker	UNP P0A7G6
A	2000	SER	-	linker	UNP P0A7G6
A	2985	THR	-	linker	UNP P0A7G6
A	2986	GLY	-	linker	UNP P0A7G6
A	2987	SER	-	linker	UNP P0A7G6
A	2988	THR	-	linker	UNP P0A7G6
A	2989	GLY	-	linker	UNP P0A7G6
A	2990	SER	-	linker	UNP P0A7G6
A	2991	ALA	-	linker	UNP P0A7G6
A	2992	SER	-	linker	UNP P0A7G6
A	2993	GLY	-	linker	UNP P0A7G6
A	2994	SER	-	linker	UNP P0A7G6
A	2995	SER	-	linker	UNP P0A7G6
A	2996	THR	-	linker	UNP P0A7G6
A	2997	GLY	-	linker	UNP P0A7G6
A	2998	SER	-	linker	UNP P0A7G6
A	2999	MET	-	linker	UNP P0A7G6
A	3000	SER	-	linker	UNP P0A7G6
B	26	GLY	-	linker	UNP P0A7G6
B	27	ALA	-	linker	UNP P0A7G6
B	28	MET	-	linker	UNP P0A7G6
B	29	HIS	-	linker	UNP P0A7G6
B	986	THR	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	987	GLY	-	linker	UNP P0A7G6
B	988	SER	-	linker	UNP P0A7G6
B	989	THR	-	linker	UNP P0A7G6
B	990	GLY	-	linker	UNP P0A7G6
B	991	SER	-	linker	UNP P0A7G6
B	992	GLY	-	linker	UNP P0A7G6
B	993	THR	-	linker	UNP P0A7G6
B	994	THR	-	linker	UNP P0A7G6
B	995	GLY	-	linker	UNP P0A7G6
B	996	SER	-	linker	UNP P0A7G6
B	997	THR	-	linker	UNP P0A7G6
B	998	GLY	-	linker	UNP P0A7G6
B	999	SER	-	linker	UNP P0A7G6
B	1000	MET	-	linker	UNP P0A7G6
B	1986	THR	-	linker	UNP P0A7G6
B	1987	GLY	-	linker	UNP P0A7G6
B	1988	SER	-	linker	UNP P0A7G6
B	1989	THR	-	linker	UNP P0A7G6
B	1990	GLY	-	linker	UNP P0A7G6
B	1991	SER	-	linker	UNP P0A7G6
B	1992	MET	-	linker	UNP P0A7G6
B	1993	GLY	-	linker	UNP P0A7G6
B	1994	HIS	-	linker	UNP P0A7G6
B	1995	THR	-	linker	UNP P0A7G6
B	1996	THR	-	linker	UNP P0A7G6
B	1997	GLY	-	linker	UNP P0A7G6
B	1998	SER	-	linker	UNP P0A7G6
B	1999	MET	-	linker	UNP P0A7G6
B	2000	SER	-	linker	UNP P0A7G6
B	2985	THR	-	linker	UNP P0A7G6
B	2986	GLY	-	linker	UNP P0A7G6
B	2987	SER	-	linker	UNP P0A7G6
B	2988	THR	-	linker	UNP P0A7G6
B	2989	GLY	-	linker	UNP P0A7G6
B	2990	SER	-	linker	UNP P0A7G6
B	2991	ALA	-	linker	UNP P0A7G6
B	2992	SER	-	linker	UNP P0A7G6
B	2993	GLY	-	linker	UNP P0A7G6
B	2994	SER	-	linker	UNP P0A7G6
B	2995	SER	-	linker	UNP P0A7G6
B	2996	THR	-	linker	UNP P0A7G6
B	2997	GLY	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2998	SER	-	linker	UNP P0A7G6
B	2999	MET	-	linker	UNP P0A7G6
B	3000	SER	-	linker	UNP P0A7G6
C	26	GLY	-	linker	UNP P0A7G6
C	27	ALA	-	linker	UNP P0A7G6
C	28	MET	-	linker	UNP P0A7G6
C	29	HIS	-	linker	UNP P0A7G6
C	986	THR	-	linker	UNP P0A7G6
C	987	GLY	-	linker	UNP P0A7G6
C	988	SER	-	linker	UNP P0A7G6
C	989	THR	-	linker	UNP P0A7G6
C	990	GLY	-	linker	UNP P0A7G6
C	991	SER	-	linker	UNP P0A7G6
C	992	GLY	-	linker	UNP P0A7G6
C	993	THR	-	linker	UNP P0A7G6
C	994	THR	-	linker	UNP P0A7G6
C	995	GLY	-	linker	UNP P0A7G6
C	996	SER	-	linker	UNP P0A7G6
C	997	THR	-	linker	UNP P0A7G6
C	998	GLY	-	linker	UNP P0A7G6
C	999	SER	-	linker	UNP P0A7G6
C	1000	MET	-	linker	UNP P0A7G6
C	1986	THR	-	linker	UNP P0A7G6
C	1987	GLY	-	linker	UNP P0A7G6
C	1988	SER	-	linker	UNP P0A7G6
C	1989	THR	-	linker	UNP P0A7G6
C	1990	GLY	-	linker	UNP P0A7G6
C	1991	SER	-	linker	UNP P0A7G6
C	1992	MET	-	linker	UNP P0A7G6
C	1993	GLY	-	linker	UNP P0A7G6
C	1994	HIS	-	linker	UNP P0A7G6
C	1995	THR	-	linker	UNP P0A7G6
C	1996	THR	-	linker	UNP P0A7G6
C	1997	GLY	-	linker	UNP P0A7G6
C	1998	SER	-	linker	UNP P0A7G6
C	1999	MET	-	linker	UNP P0A7G6
C	2000	SER	-	linker	UNP P0A7G6
C	2985	THR	-	linker	UNP P0A7G6
C	2986	GLY	-	linker	UNP P0A7G6
C	2987	SER	-	linker	UNP P0A7G6
C	2988	THR	-	linker	UNP P0A7G6
C	2989	GLY	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2990	SER	-	linker	UNP P0A7G6
C	2991	ALA	-	linker	UNP P0A7G6
C	2992	SER	-	linker	UNP P0A7G6
C	2993	GLY	-	linker	UNP P0A7G6
C	2994	SER	-	linker	UNP P0A7G6
C	2995	SER	-	linker	UNP P0A7G6
C	2996	THR	-	linker	UNP P0A7G6
C	2997	GLY	-	linker	UNP P0A7G6
C	2998	SER	-	linker	UNP P0A7G6
C	2999	MET	-	linker	UNP P0A7G6
C	3000	SER	-	linker	UNP P0A7G6
D	26	GLY	-	linker	UNP P0A7G6
D	27	ALA	-	linker	UNP P0A7G6
D	28	MET	-	linker	UNP P0A7G6
D	29	HIS	-	linker	UNP P0A7G6
D	986	THR	-	linker	UNP P0A7G6
D	987	GLY	-	linker	UNP P0A7G6
D	988	SER	-	linker	UNP P0A7G6
D	989	THR	-	linker	UNP P0A7G6
D	990	GLY	-	linker	UNP P0A7G6
D	991	SER	-	linker	UNP P0A7G6
D	992	GLY	-	linker	UNP P0A7G6
D	993	THR	-	linker	UNP P0A7G6
D	994	THR	-	linker	UNP P0A7G6
D	995	GLY	-	linker	UNP P0A7G6
D	996	SER	-	linker	UNP P0A7G6
D	997	THR	-	linker	UNP P0A7G6
D	998	GLY	-	linker	UNP P0A7G6
D	999	SER	-	linker	UNP P0A7G6
D	1000	MET	-	linker	UNP P0A7G6
D	1986	THR	-	linker	UNP P0A7G6
D	1987	GLY	-	linker	UNP P0A7G6
D	1988	SER	-	linker	UNP P0A7G6
D	1989	THR	-	linker	UNP P0A7G6
D	1990	GLY	-	linker	UNP P0A7G6
D	1991	SER	-	linker	UNP P0A7G6
D	1992	MET	-	linker	UNP P0A7G6
D	1993	GLY	-	linker	UNP P0A7G6
D	1994	HIS	-	linker	UNP P0A7G6
D	1995	THR	-	linker	UNP P0A7G6
D	1996	THR	-	linker	UNP P0A7G6
D	1997	GLY	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1998	SER	-	linker	UNP P0A7G6
D	1999	MET	-	linker	UNP P0A7G6
D	2000	SER	-	linker	UNP P0A7G6
D	2985	THR	-	linker	UNP P0A7G6
D	2986	GLY	-	linker	UNP P0A7G6
D	2987	SER	-	linker	UNP P0A7G6
D	2988	THR	-	linker	UNP P0A7G6
D	2989	GLY	-	linker	UNP P0A7G6
D	2990	SER	-	linker	UNP P0A7G6
D	2991	ALA	-	linker	UNP P0A7G6
D	2992	SER	-	linker	UNP P0A7G6
D	2993	GLY	-	linker	UNP P0A7G6
D	2994	SER	-	linker	UNP P0A7G6
D	2995	SER	-	linker	UNP P0A7G6
D	2996	THR	-	linker	UNP P0A7G6
D	2997	GLY	-	linker	UNP P0A7G6
D	2998	SER	-	linker	UNP P0A7G6
D	2999	MET	-	linker	UNP P0A7G6
D	3000	SER	-	linker	UNP P0A7G6
E	26	GLY	-	linker	UNP P0A7G6
E	27	ALA	-	linker	UNP P0A7G6
E	28	MET	-	linker	UNP P0A7G6
E	29	HIS	-	linker	UNP P0A7G6
E	986	THR	-	linker	UNP P0A7G6
E	987	GLY	-	linker	UNP P0A7G6
E	988	SER	-	linker	UNP P0A7G6
E	989	THR	-	linker	UNP P0A7G6
E	990	GLY	-	linker	UNP P0A7G6
E	991	SER	-	linker	UNP P0A7G6
E	992	GLY	-	linker	UNP P0A7G6
E	993	THR	-	linker	UNP P0A7G6
E	994	THR	-	linker	UNP P0A7G6
E	995	GLY	-	linker	UNP P0A7G6
E	996	SER	-	linker	UNP P0A7G6
E	997	THR	-	linker	UNP P0A7G6
E	998	GLY	-	linker	UNP P0A7G6
E	999	SER	-	linker	UNP P0A7G6
E	1000	MET	-	linker	UNP P0A7G6
E	1986	THR	-	linker	UNP P0A7G6
E	1987	GLY	-	linker	UNP P0A7G6
E	1988	SER	-	linker	UNP P0A7G6
E	1989	THR	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1990	GLY	-	linker	UNP P0A7G6
E	1991	SER	-	linker	UNP P0A7G6
E	1992	MET	-	linker	UNP P0A7G6
E	1993	GLY	-	linker	UNP P0A7G6
E	1994	HIS	-	linker	UNP P0A7G6
E	1995	THR	-	linker	UNP P0A7G6
E	1996	THR	-	linker	UNP P0A7G6
E	1997	GLY	-	linker	UNP P0A7G6
E	1998	SER	-	linker	UNP P0A7G6
E	1999	MET	-	linker	UNP P0A7G6
E	2000	SER	-	linker	UNP P0A7G6
E	2985	THR	-	linker	UNP P0A7G6
E	2986	GLY	-	linker	UNP P0A7G6
E	2987	SER	-	linker	UNP P0A7G6
E	2988	THR	-	linker	UNP P0A7G6
E	2989	GLY	-	linker	UNP P0A7G6
E	2990	SER	-	linker	UNP P0A7G6
E	2991	ALA	-	linker	UNP P0A7G6
E	2992	SER	-	linker	UNP P0A7G6
E	2993	GLY	-	linker	UNP P0A7G6
E	2994	SER	-	linker	UNP P0A7G6
E	2995	SER	-	linker	UNP P0A7G6
E	2996	THR	-	linker	UNP P0A7G6
E	2997	GLY	-	linker	UNP P0A7G6
E	2998	SER	-	linker	UNP P0A7G6
E	2999	MET	-	linker	UNP P0A7G6
E	3000	SER	-	linker	UNP P0A7G6
F	26	GLY	-	linker	UNP P0A7G6
F	27	ALA	-	linker	UNP P0A7G6
F	28	MET	-	linker	UNP P0A7G6
F	29	HIS	-	linker	UNP P0A7G6
F	986	THR	-	linker	UNP P0A7G6
F	987	GLY	-	linker	UNP P0A7G6
F	988	SER	-	linker	UNP P0A7G6
F	989	THR	-	linker	UNP P0A7G6
F	990	GLY	-	linker	UNP P0A7G6
F	991	SER	-	linker	UNP P0A7G6
F	992	GLY	-	linker	UNP P0A7G6
F	993	THR	-	linker	UNP P0A7G6
F	994	THR	-	linker	UNP P0A7G6
F	995	GLY	-	linker	UNP P0A7G6
F	996	SER	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	997	THR	-	linker	UNP P0A7G6
F	998	GLY	-	linker	UNP P0A7G6
F	999	SER	-	linker	UNP P0A7G6
F	1000	MET	-	linker	UNP P0A7G6
F	1986	THR	-	linker	UNP P0A7G6
F	1987	GLY	-	linker	UNP P0A7G6
F	1988	SER	-	linker	UNP P0A7G6
F	1989	THR	-	linker	UNP P0A7G6
F	1990	GLY	-	linker	UNP P0A7G6
F	1991	SER	-	linker	UNP P0A7G6
F	1992	MET	-	linker	UNP P0A7G6
F	1993	GLY	-	linker	UNP P0A7G6
F	1994	HIS	-	linker	UNP P0A7G6
F	1995	THR	-	linker	UNP P0A7G6
F	1996	THR	-	linker	UNP P0A7G6
F	1997	GLY	-	linker	UNP P0A7G6
F	1998	SER	-	linker	UNP P0A7G6
F	1999	MET	-	linker	UNP P0A7G6
F	2000	SER	-	linker	UNP P0A7G6
F	2985	THR	-	linker	UNP P0A7G6
F	2986	GLY	-	linker	UNP P0A7G6
F	2987	SER	-	linker	UNP P0A7G6
F	2988	THR	-	linker	UNP P0A7G6
F	2989	GLY	-	linker	UNP P0A7G6
F	2990	SER	-	linker	UNP P0A7G6
F	2991	ALA	-	linker	UNP P0A7G6
F	2992	SER	-	linker	UNP P0A7G6
F	2993	GLY	-	linker	UNP P0A7G6
F	2994	SER	-	linker	UNP P0A7G6
F	2995	SER	-	linker	UNP P0A7G6
F	2996	THR	-	linker	UNP P0A7G6
F	2997	GLY	-	linker	UNP P0A7G6
F	2998	SER	-	linker	UNP P0A7G6
F	2999	MET	-	linker	UNP P0A7G6
F	3000	SER	-	linker	UNP P0A7G6
G	26	GLY	-	linker	UNP P0A7G6
G	27	ALA	-	linker	UNP P0A7G6
G	28	MET	-	linker	UNP P0A7G6
G	29	HIS	-	linker	UNP P0A7G6
G	986	THR	-	linker	UNP P0A7G6
G	987	GLY	-	linker	UNP P0A7G6
G	988	SER	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	989	THR	-	linker	UNP P0A7G6
G	990	GLY	-	linker	UNP P0A7G6
G	991	SER	-	linker	UNP P0A7G6
G	992	GLY	-	linker	UNP P0A7G6
G	993	THR	-	linker	UNP P0A7G6
G	994	THR	-	linker	UNP P0A7G6
G	995	GLY	-	linker	UNP P0A7G6
G	996	SER	-	linker	UNP P0A7G6
G	997	THR	-	linker	UNP P0A7G6
G	998	GLY	-	linker	UNP P0A7G6
G	999	SER	-	linker	UNP P0A7G6
G	1000	MET	-	linker	UNP P0A7G6
G	1986	THR	-	linker	UNP P0A7G6
G	1987	GLY	-	linker	UNP P0A7G6
G	1988	SER	-	linker	UNP P0A7G6
G	1989	THR	-	linker	UNP P0A7G6
G	1990	GLY	-	linker	UNP P0A7G6
G	1991	SER	-	linker	UNP P0A7G6
G	1992	MET	-	linker	UNP P0A7G6
G	1993	GLY	-	linker	UNP P0A7G6
G	1994	HIS	-	linker	UNP P0A7G6
G	1995	THR	-	linker	UNP P0A7G6
G	1996	THR	-	linker	UNP P0A7G6
G	1997	GLY	-	linker	UNP P0A7G6
G	1998	SER	-	linker	UNP P0A7G6
G	1999	MET	-	linker	UNP P0A7G6
G	2000	SER	-	linker	UNP P0A7G6
G	2985	THR	-	linker	UNP P0A7G6
G	2986	GLY	-	linker	UNP P0A7G6
G	2987	SER	-	linker	UNP P0A7G6
G	2988	THR	-	linker	UNP P0A7G6
G	2989	GLY	-	linker	UNP P0A7G6
G	2990	SER	-	linker	UNP P0A7G6
G	2991	ALA	-	linker	UNP P0A7G6
G	2992	SER	-	linker	UNP P0A7G6
G	2993	GLY	-	linker	UNP P0A7G6
G	2994	SER	-	linker	UNP P0A7G6
G	2995	SER	-	linker	UNP P0A7G6
G	2996	THR	-	linker	UNP P0A7G6
G	2997	GLY	-	linker	UNP P0A7G6
G	2998	SER	-	linker	UNP P0A7G6
G	2999	MET	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	3000	SER	-	linker	UNP P0A7G6
H	26	GLY	-	linker	UNP P0A7G6
H	27	ALA	-	linker	UNP P0A7G6
H	28	MET	-	linker	UNP P0A7G6
H	29	HIS	-	linker	UNP P0A7G6
H	986	THR	-	linker	UNP P0A7G6
H	987	GLY	-	linker	UNP P0A7G6
H	988	SER	-	linker	UNP P0A7G6
H	989	THR	-	linker	UNP P0A7G6
H	990	GLY	-	linker	UNP P0A7G6
H	991	SER	-	linker	UNP P0A7G6
H	992	GLY	-	linker	UNP P0A7G6
H	993	THR	-	linker	UNP P0A7G6
H	994	THR	-	linker	UNP P0A7G6
H	995	GLY	-	linker	UNP P0A7G6
H	996	SER	-	linker	UNP P0A7G6
H	997	THR	-	linker	UNP P0A7G6
H	998	GLY	-	linker	UNP P0A7G6
H	999	SER	-	linker	UNP P0A7G6
H	1000	MET	-	linker	UNP P0A7G6
H	1986	THR	-	linker	UNP P0A7G6
H	1987	GLY	-	linker	UNP P0A7G6
H	1988	SER	-	linker	UNP P0A7G6
H	1989	THR	-	linker	UNP P0A7G6
H	1990	GLY	-	linker	UNP P0A7G6
H	1991	SER	-	linker	UNP P0A7G6
H	1992	MET	-	linker	UNP P0A7G6
H	1993	GLY	-	linker	UNP P0A7G6
H	1994	HIS	-	linker	UNP P0A7G6
H	1995	THR	-	linker	UNP P0A7G6
H	1996	THR	-	linker	UNP P0A7G6
H	1997	GLY	-	linker	UNP P0A7G6
H	1998	SER	-	linker	UNP P0A7G6
H	1999	MET	-	linker	UNP P0A7G6
H	2000	SER	-	linker	UNP P0A7G6
H	2985	THR	-	linker	UNP P0A7G6
H	2986	GLY	-	linker	UNP P0A7G6
H	2987	SER	-	linker	UNP P0A7G6
H	2988	THR	-	linker	UNP P0A7G6
H	2989	GLY	-	linker	UNP P0A7G6
H	2990	SER	-	linker	UNP P0A7G6
H	2991	ALA	-	linker	UNP P0A7G6

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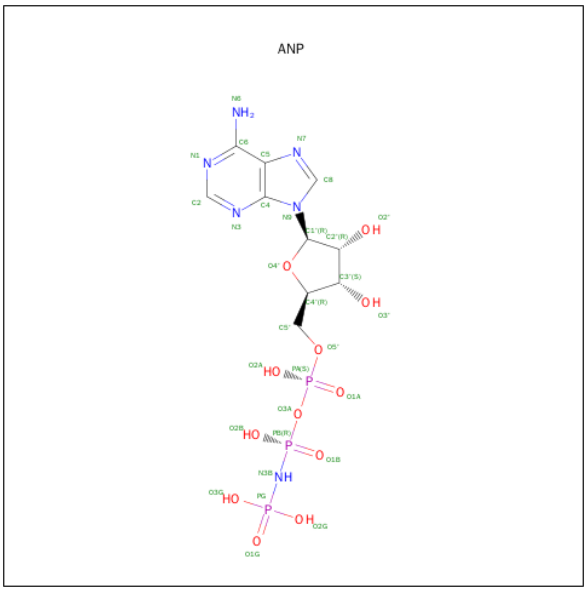
Chain	Residue	Modelled	Actual	Comment	Reference
H	2992	SER	-	linker	UNP P0A7G6
H	2993	GLY	-	linker	UNP P0A7G6
H	2994	SER	-	linker	UNP P0A7G6
H	2995	SER	-	linker	UNP P0A7G6
H	2996	THR	-	linker	UNP P0A7G6
H	2997	GLY	-	linker	UNP P0A7G6
H	2998	SER	-	linker	UNP P0A7G6
H	2999	MET	-	linker	UNP P0A7G6
H	3000	SER	-	linker	UNP P0A7G6

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	4	Total Mg 4 4	0	0
2	D	4	Total Mg 4 4	0	0
2	E	4	Total Mg 4 4	0	0
2	H	4	Total Mg 4 4	0	0
2	B	4	Total Mg 4 4	0	0
2	C	4	Total Mg 4 4	0	0
2	A	4	Total Mg 4 4	0	0
2	F	4	Total Mg 4 4	0	0

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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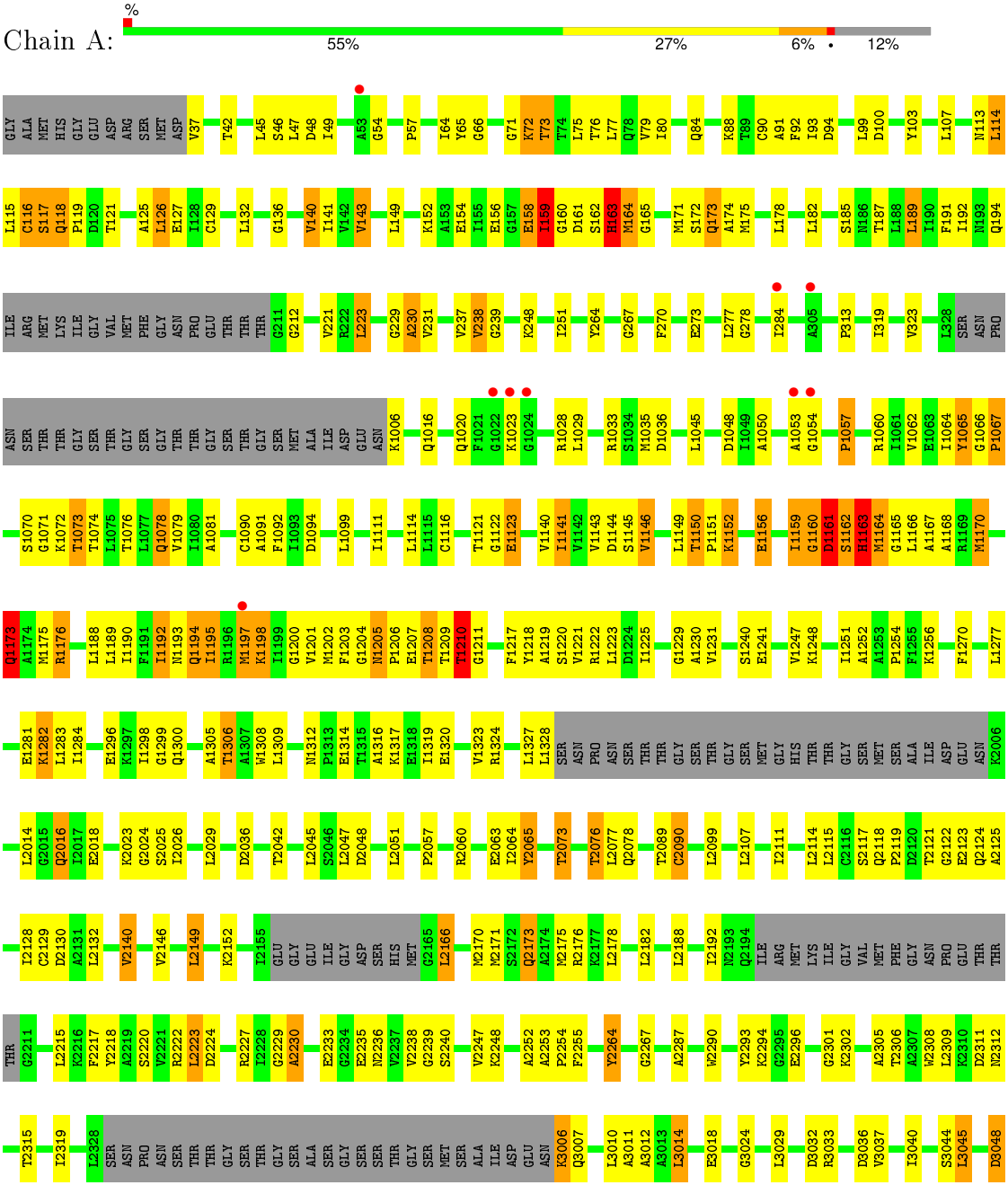
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	G	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	G	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	G	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	G	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	H	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	H	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	H	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	H	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

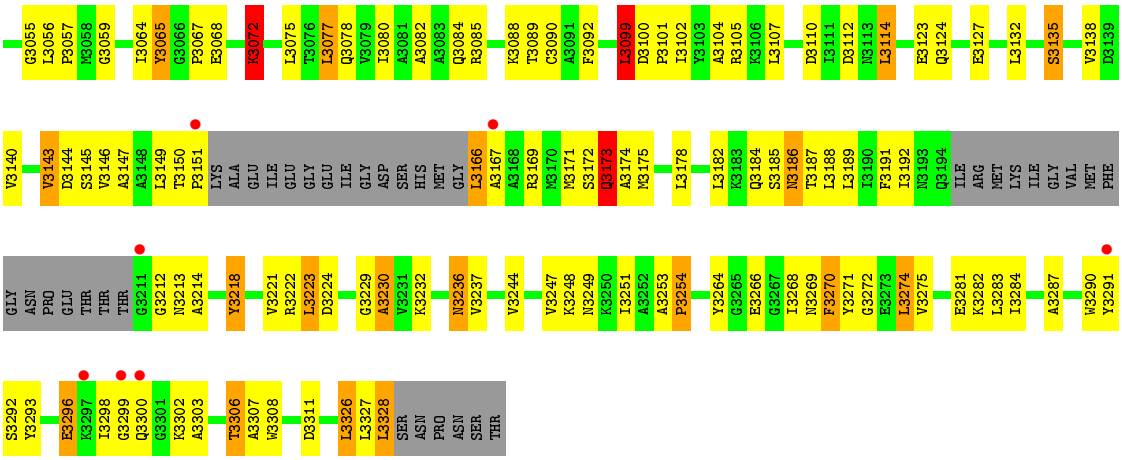
3 Residue-property plots (i)

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: Protein recA

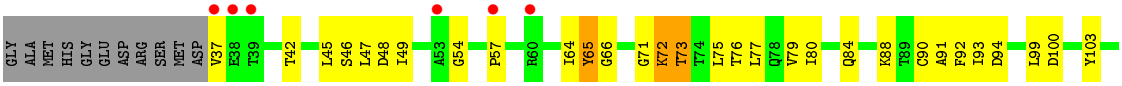
Chain A:

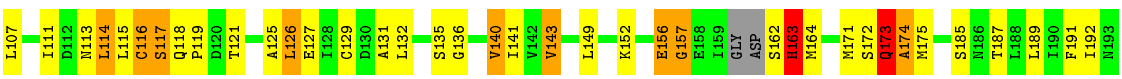


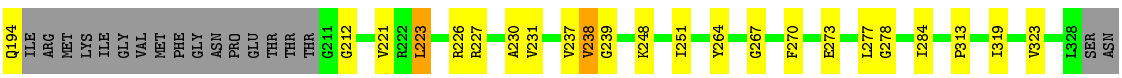


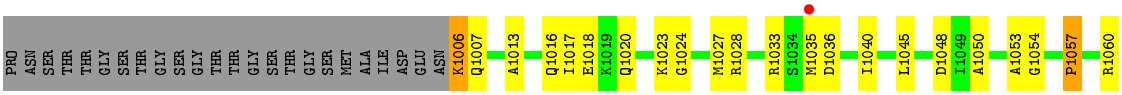
- Molecule 1: Protein recA

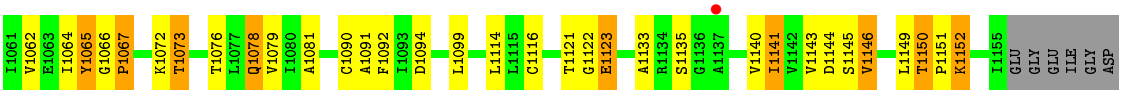
Chain B:

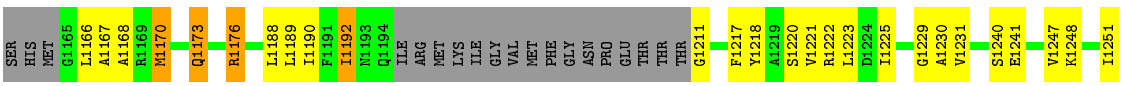


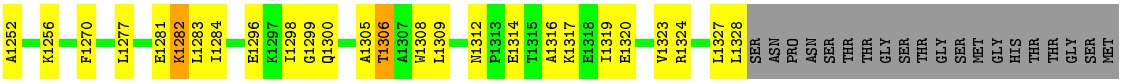


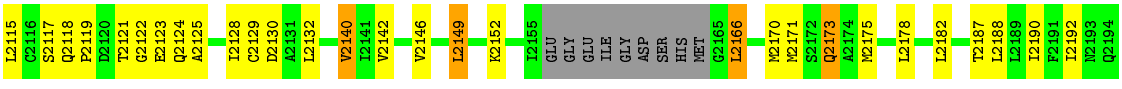


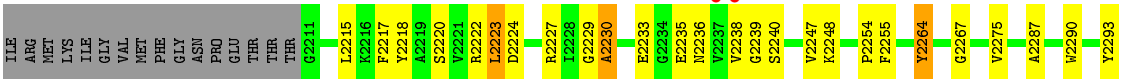


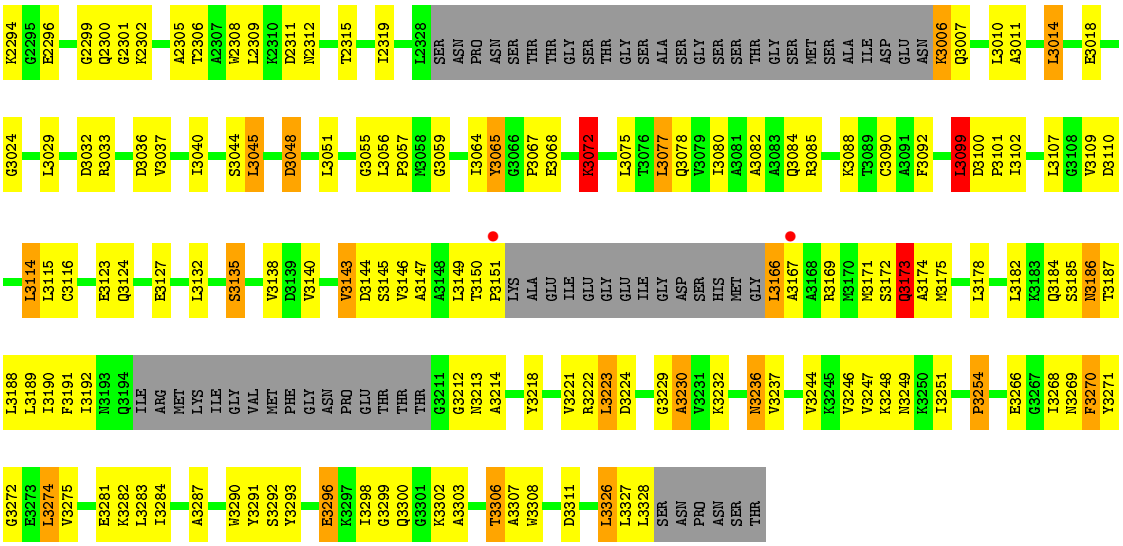






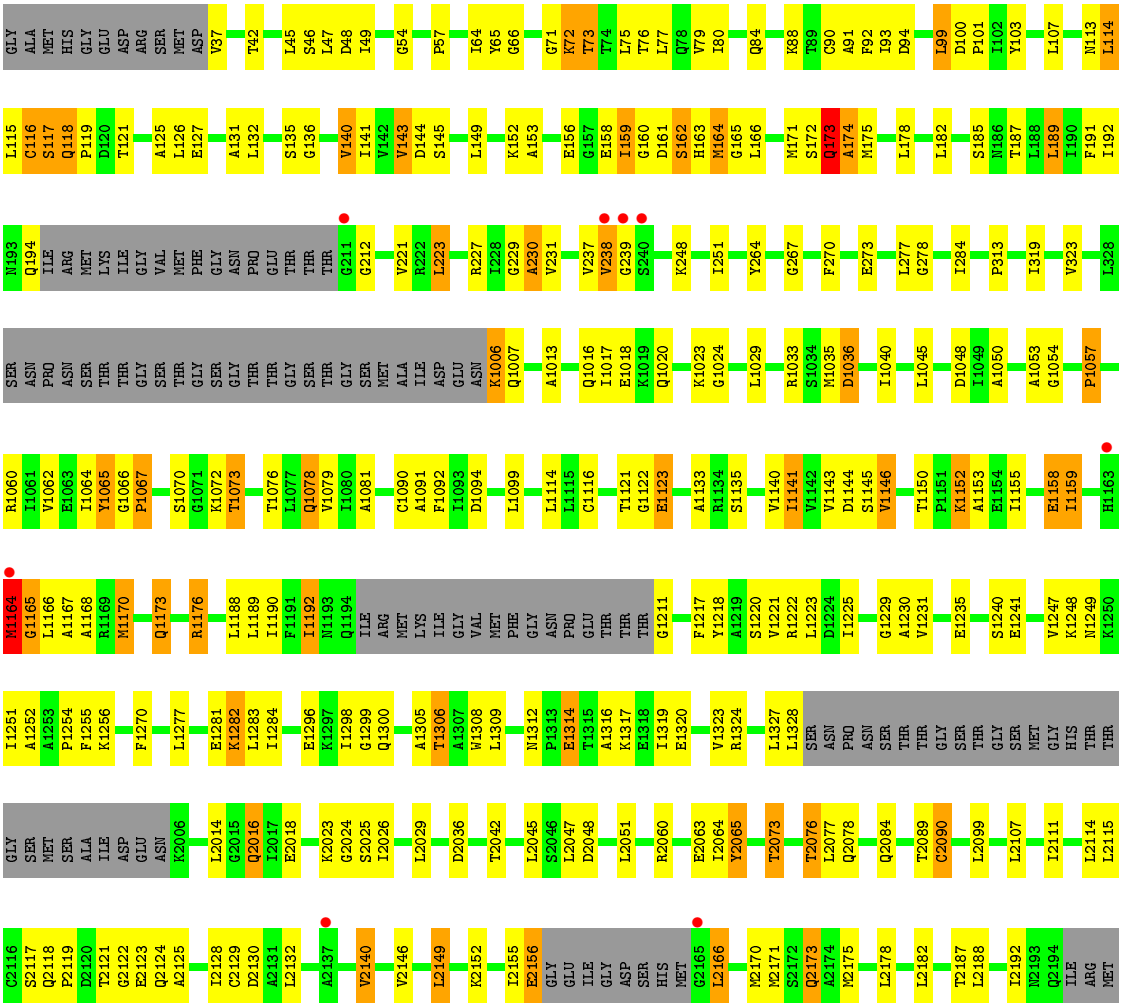


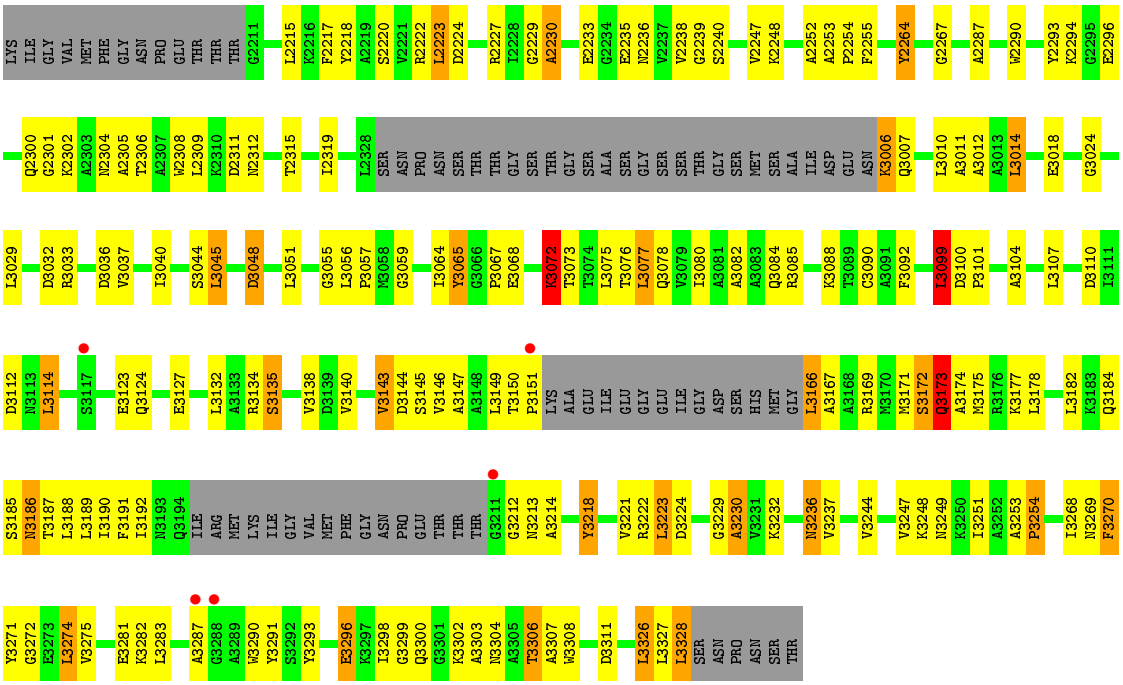




- Molecule 1: Protein recA

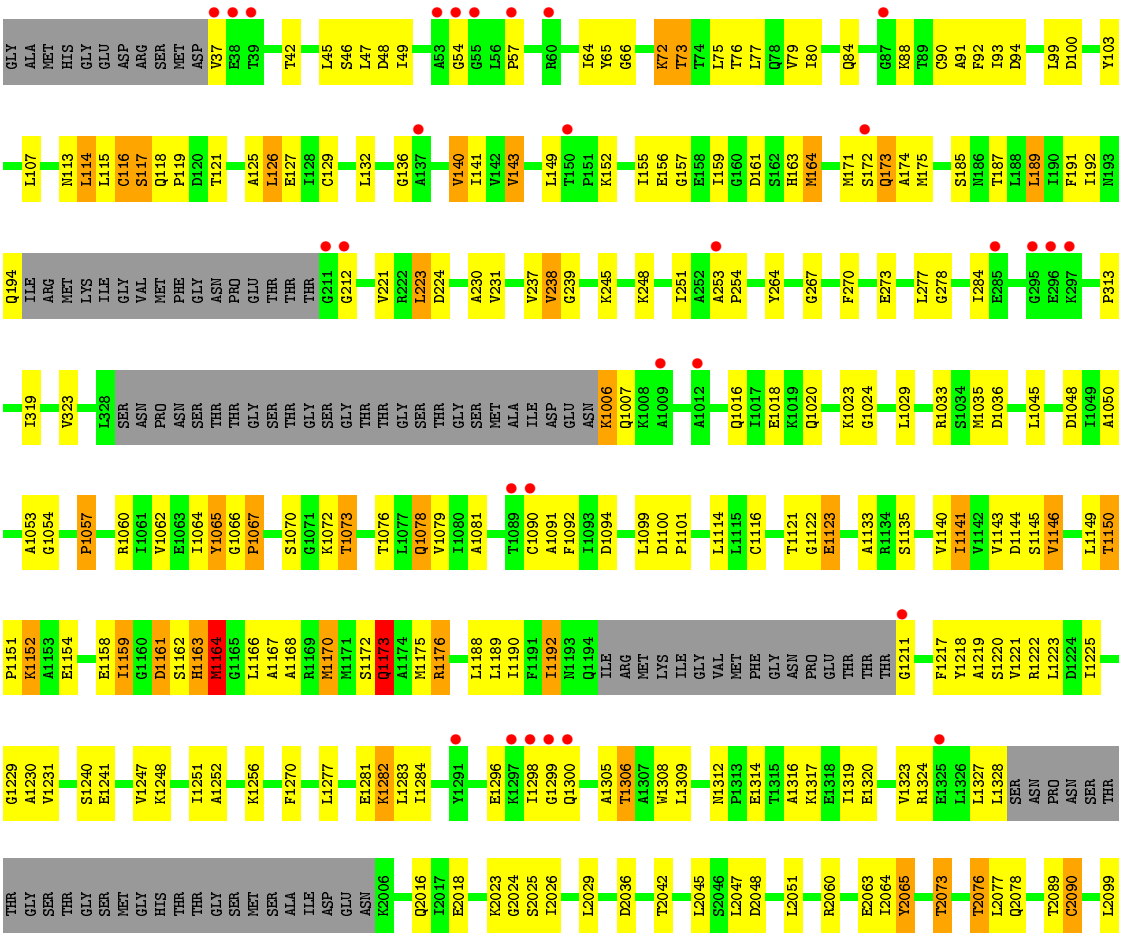
Chain C:

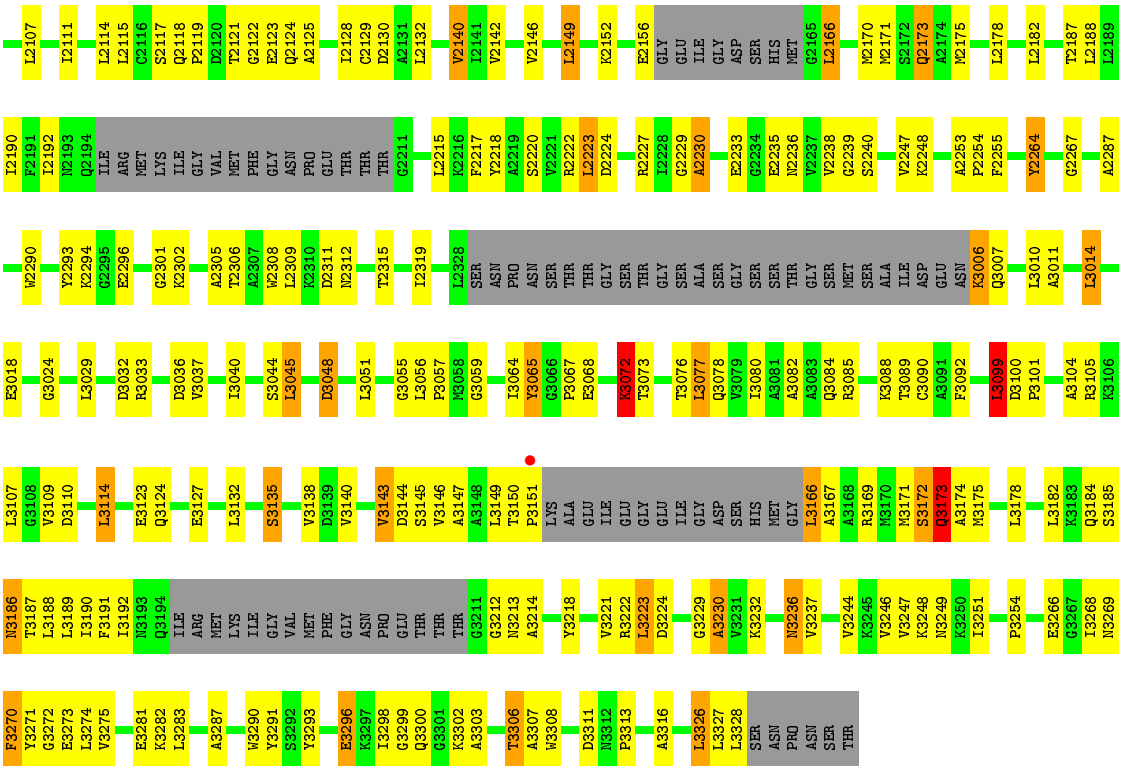




- Molecule 1: Protein recA

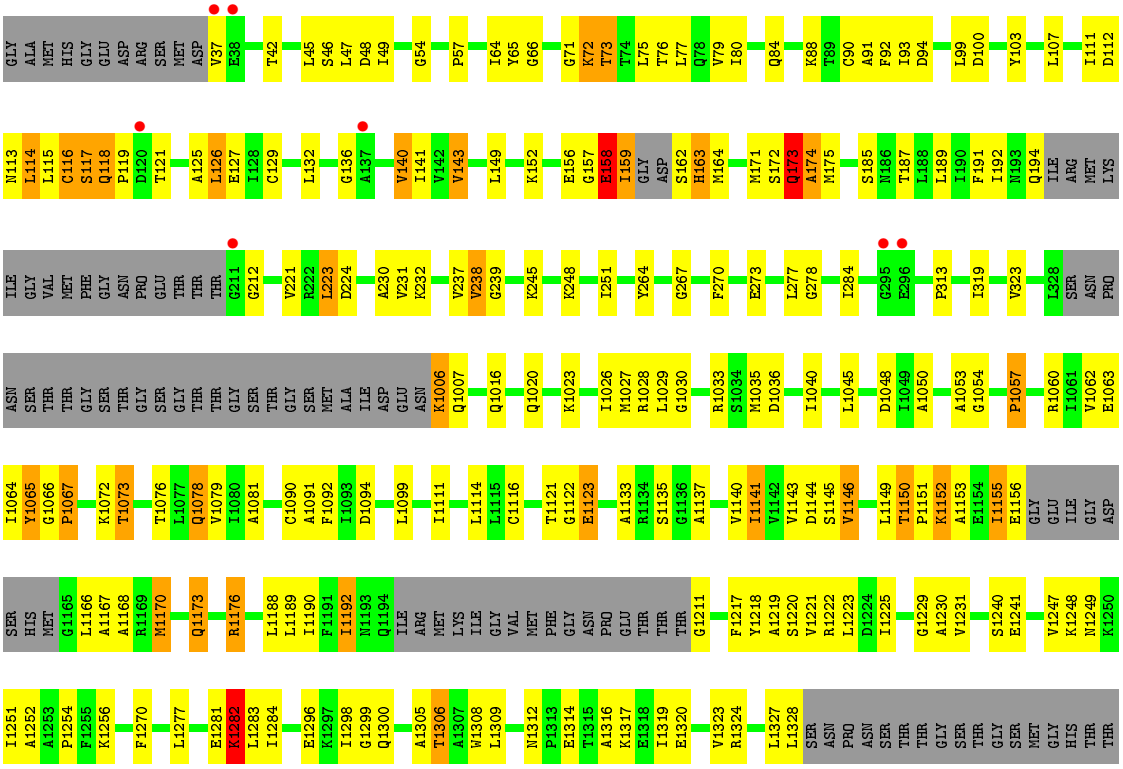
Chain D:

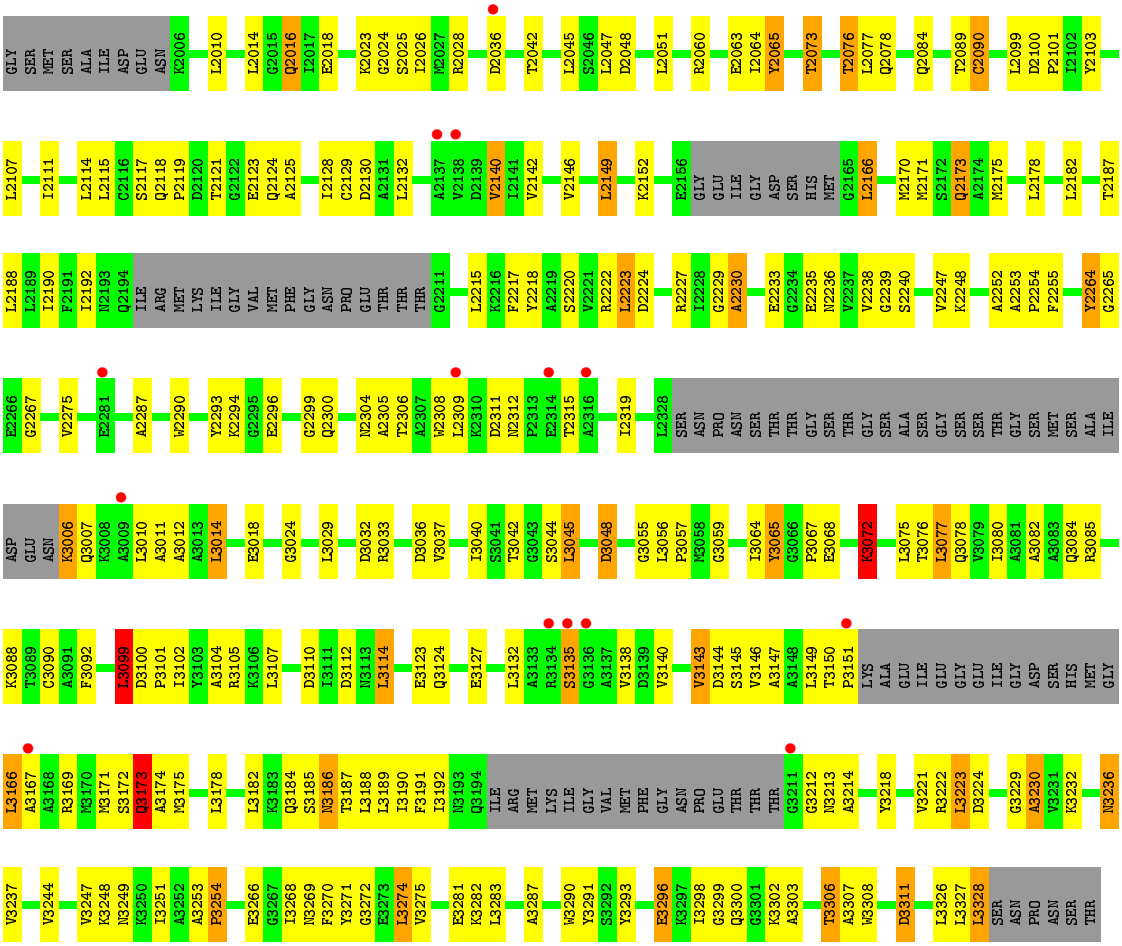




- Molecule 1: Protein recA

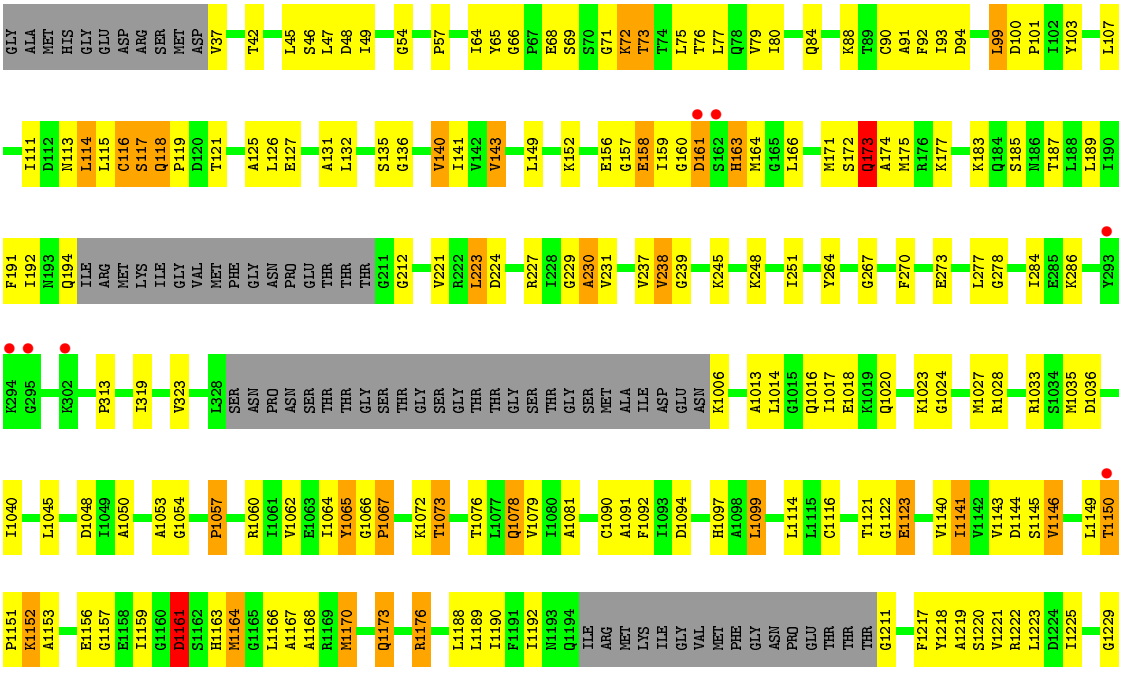
Chain E:

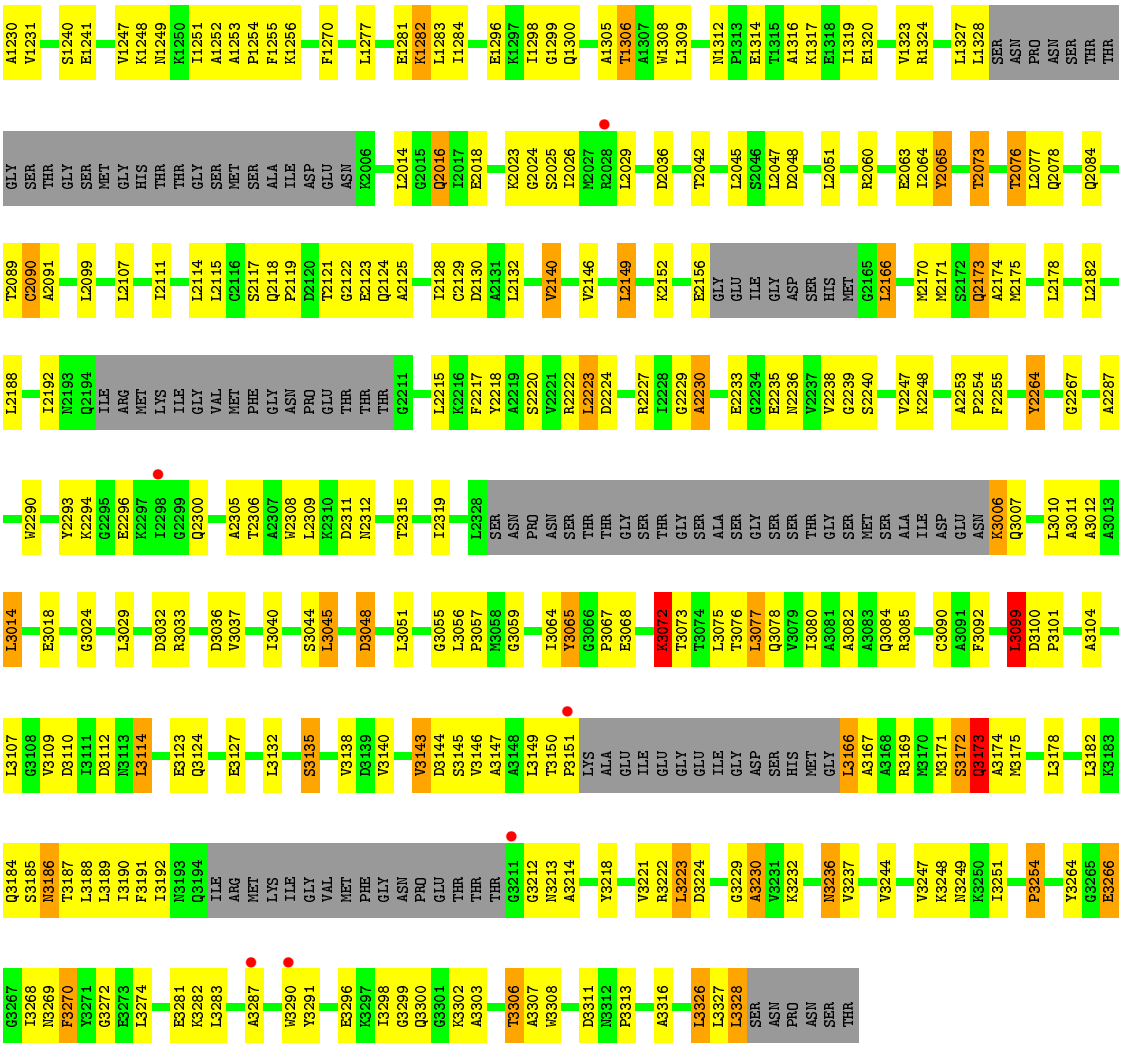




- Molecule 1: Protein recA

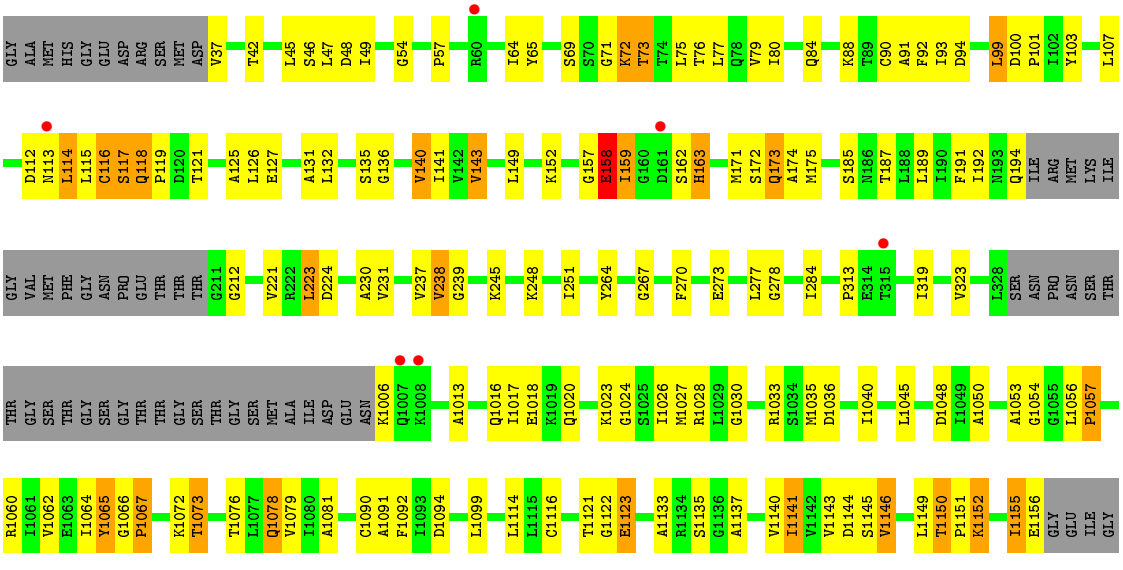
Chain F:

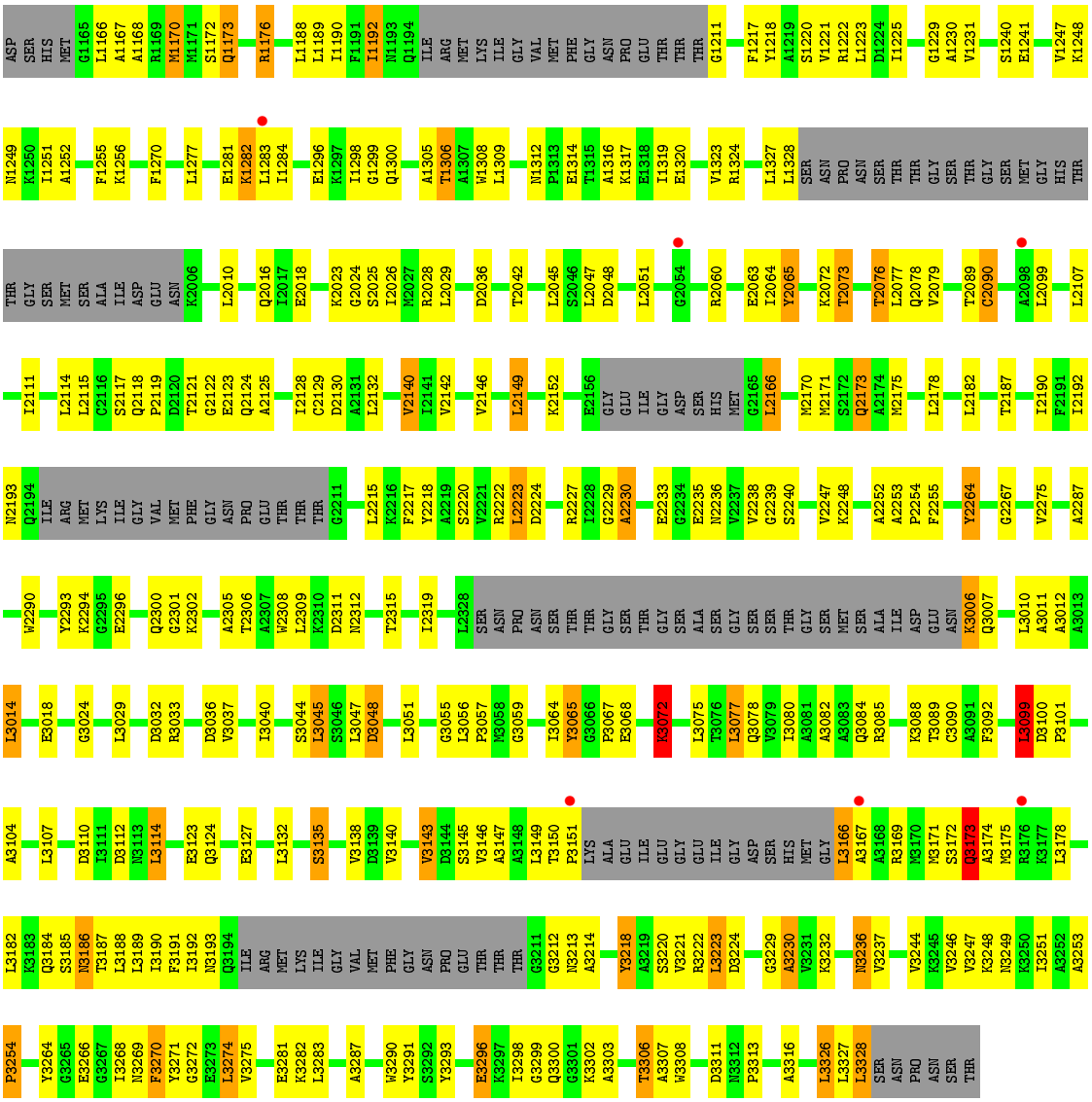




• Molecule 1: Protein recA

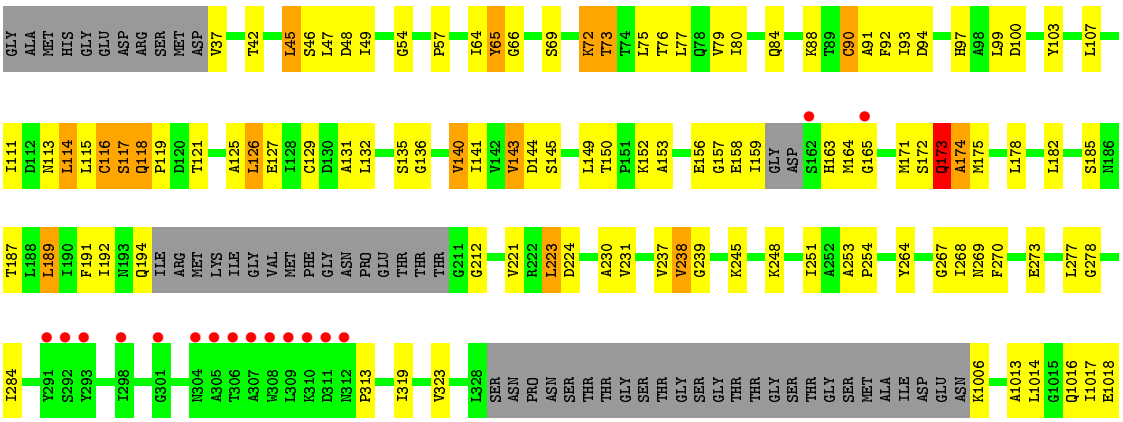
Chain G:

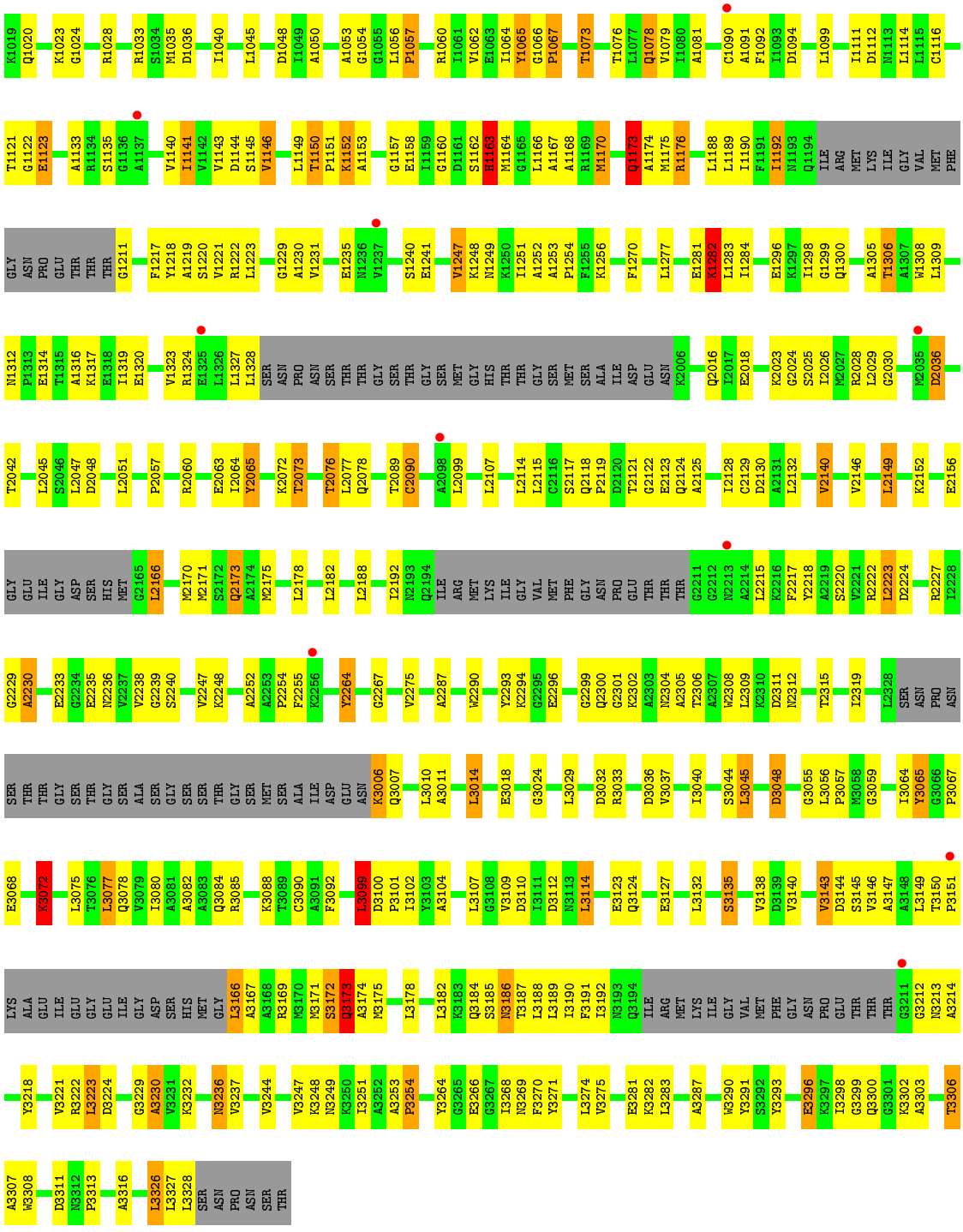




- Molecule 1: Protein recA

Chain H:




K1019 Q1020 K1023 G1024 R1028 R1033 S1034 M1035 D1036 I1040 L1045 D1048 I1049 A1050 A1053 G1054 G1055 L1056 P1057 R1060 I1061 V1062 E1063 I1064 Y1065 G1066 P1067 T1073 T1076 L1077 Q1078 V1079 I1080 A1081 C1090 A1091 F1092 I1093 D1094 L1099 I1111 D1112 N1113 L1114 L1115 C1116
T1121 G1122 E1123 A1133 R1134 S1135 G1136 A1137 V1140 I1141 V1142 V1143 D1144 S1145 V1146 L1149 T1150 P1151 K1152 A1153 G1157 E1158 I1159 G1160 D1161 S1162 H1163 M1164 G1165 L1166 A1167 A1168 R1169 M1170 Q1173 A1174 M1175 R1176 L1188 L1189 I1190 F1191 I1192 N1193 Q1194 ILE ARG MET LYS ILE GLY VAL MET PHE
GLY ASN PRO GLU THR THR THR G1211 F1217 Y1218 A1219 S1220 V1221 R1222 L1223 G1229 A1230 V1231 E1235 N1236 V1237 S1240 E1241 V1247 K1248 N1249 K1250 I1251 A1252 A1253 P1254 F1255 K1256 F1270 L1277 E1281 K1282 L1283 I1284 E1296 K1297 I1298 G1299 Q1300 A1305 T1306 A1307 W1308 L1309
N1312 P1313 E1314 T1315 A1316 K1317 E1318 I1319 E1320 V1323 R1324 E1325 L1326 L1327 L1328 SER ASN PRO ASN SER THR THR GLY SER THR GLY SER MET GLY HIS THR THR GLY SER MET SER ALA ILE ASP GLU ASN K2006 Q2016 I2017 E2018 K2023 G2024 S2025 I2026 M2027 R2028 L2029 G2030 M2035 D2036
T2042 L2045 S2046 L2047 D2048 L2051 P2057 R2060 E2063 I2064 Y2065 K2072 T2073 T2076 L2077 Q2078 T2089 C2090 A2098 L2099 L2107 L2114 L2115 C2116 S2117 Q2118 P2119 D2120 T2121 G2122 E2123 Q2124 A2125 I2128 C2129 D2130 A2131 L2132 V2140 V2146 L2149 K2152 E2156
GLY GLU ILE GLY ASP SER HIS MET G2165 L2166 M2170 M2171 S2172 Q2173 A2174 M2175 L2178 L2182 L2188 I2192 N2193 Q2194 ILE ARG MET LYS ILE GLY VAL MET PHE GLY ASN PRO GLU THR THR THR G2211 G2212 N2213 A2214 L2215 K2216 F2217 Y2218 A2219 S2220 V2221 R2222 L2223 D2224 R2227 I2228
G2229 A2230 E2233 G2234 E2235 N2236 V2237 V2238 G2239 S2240 V2247 K2248 A2252 A2253 P2254 F2255 K2256 Y2264 G2267 V2275 A2287 W2290 Y2293 K2294 G2295 E2296 G2299 Q2300 G2301 K2302 A2303 N2304 A2305 T2306 A2307 W2308 L2309 K2310 D2311 N2312 T2315 I2319 L2328 SER ASN PRO ASN
SER THR THR GLY SER THR GLY SER ALA SER GLY SER SER THR GLY SER MET SER ALA ILE ASP GLU ASN K3006 Q3007 L3010 A3011 L3014 E3018 G3024 L3029 D3032 R3033 D3036 V3037 I3040 S3044 L3045 D3048 G3055 L3056 P3057 M3058 G3059 I3064 Y3065 G3066 P3067
E3068 K3072 L3075 T3076 L3077 Q3078 V3079 I3080 A3081 A3082 A3083 Q3084 R3085 K3088 T3089 C3090 A3091 F3092 L3099 D3100 P3101 I3102 Y3103 A3104 L3107 G3108 V3109 D3110 I3111 D3112 N3113 L3114 E3123 Q3124 E3127 L3132 S3135 V3138 D3139 V3140 V3143 D3144 S3145 V3146 A3147 A3148 L3149 T3150 P3151
LYS ALA GLU ILE GLU GLY GLU ILE GLY ASP SER HIS MET GLY L3166 A3167 A3168 R3169 M3170 M3171 S3172 Q3173 A3174 M3175 L3178 L3182 K3183 Q3184 S3185 N3186 T3187 L3188 L3189 I3190 F3191 I3192 N3193 Q3194 ILE ARG MET LYS ILE GLY VAL MET PHE GLY ASN PRO GLU THR THR THR G3211 G3212 N3213 A3214
Y3218 V3221 R3222 I3223 D3224 G3229 A3230 Y3231 K3232 N3236 V3237 V3244 V3247 K3248 N3249 K3250 I3251 A3252 A3253 P3254 Y3264 G3265 E3266 G3267 I3268 N3269 F3270 Y3271 L3274 V3275 E3281 K3282 L3283 A3287 W3290 Y3291 S3292 Y3293 E3296 K3297 I3298 G3299 Q3300 G3301 K3302 A3303 T3306
A3307 W3308 D3311 N3312 P3313 A3316 I3326 L3327 L3328 SER ASN PRO ASN SER THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	176.60Å 189.80Å 424.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 4.30 39.93 – 4.30	Depositor EDS
% Data completeness (in resolution range)	92.7 (20.00-4.30) 92.7 (39.93-4.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 4.28Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.243 , 0.261 0.271 , 0.284	Depositor DCC
R_{free} test set	1841 reflections (2.02%)	DCC
Wilson B-factor (Å^2)	170.2	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.21 , 116.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	1 of 96833 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	71761	wwPDB-VP
Average B, all atoms (Å^2)	220.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: MG, ANP

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	6/9068 (0.1%)	0.80	10/12192 (0.1%)
1	B	0.76	4/8861 (0.0%)	0.76	1/11910 (0.0%)
1	C	0.77	0/8951	0.77	4/12033 (0.0%)
1	D	0.74	3/8951 (0.0%)	0.75	4/12033 (0.0%)
1	E	0.72	1/8879 (0.0%)	0.75	2/11934 (0.0%)
1	F	0.77	4/8951 (0.0%)	0.77	2/12033 (0.0%)
1	G	0.77	2/8892 (0.0%)	0.76	3/11953 (0.0%)
1	H	0.72	2/8938 (0.0%)	0.75	3/12014 (0.0%)
All	All	0.76	22/71491 (0.0%)	0.77	29/96102 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	11
1	B	0	3
1	C	0	4
1	D	0	7
1	E	0	6
1	F	0	6
1	G	0	5
1	H	0	4
All	All	0	46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	163	HIS	N-CA	7.46	1.61	1.46
1	B	3266	GLU	CG-CD	6.68	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1164	MET	CB-CG	6.66	1.72	1.51
1	D	156	GLU	CG-CD	5.97	1.60	1.51
1	F	3270	PHE	CE1-CZ	5.74	1.48	1.37

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1164	MET	C-N-CA	-8.01	105.48	122.30
1	D	2166	LEU	CA-CB-CG	7.24	131.94	115.30
1	G	2166	LEU	CA-CB-CG	7.23	131.93	115.30
1	H	2166	LEU	CA-CB-CG	7.23	131.93	115.30
1	E	2166	LEU	CA-CB-CG	7.21	131.89	115.30

There are no chirality outliers.

5 of 46 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1161	ASP	Peptide
1	A	1163	HIS	Peptide
1	A	158	GLU	Peptide
1	A	161	ASP	Peptide
1	A	163	HIS	Peptide

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	8970	0	9264	308	1
1	B	8769	0	9070	275	0
1	C	8856	0	9139	294	1
1	D	8856	0	9139	268	0
1	E	8787	0	9082	304	0
1	F	8856	0	9139	314	0
1	G	8799	0	9090	269	0
1	H	8844	0	9131	304	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	4	0	0	0	0
2	G	4	0	0	0	0
2	H	4	0	0	0	0
3	A	124	0	52	7	0
3	B	124	0	52	2	0
3	C	124	0	52	3	0
3	D	124	0	52	2	0
3	E	124	0	52	3	0
3	F	124	0	52	9	0
3	G	124	0	52	4	0
3	H	124	0	52	4	0
All	All	71761	0	73470	2200	1

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 15.

The worst 5 of 2200 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:1204:GLY:HA2	1:B:3115:LEU:CD2	1.50	1.42
1:A:1194:GLN:O	1:A:1195:ILE:CG2	1.73	1.37
1:A:162:SER:O	1:A:165:GLY:CA	1.71	1.35
1:A:1194:GLN:O	1:A:1195:ILE:CB	1.81	1.27
1:A:1194:GLN:O	1:A:1195:ILE:HG22	1.25	1.22

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1161:ASP:OD1	1:C:1314:GLU:OE2[4_456]	2.05	0.15

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	1172/1357 (86%)	923 (79%)	191 (16%)	58 (5%)	3 32
1	B	1139/1357 (84%)	915 (80%)	172 (15%)	52 (5%)	3 33
1	C	1155/1357 (85%)	919 (80%)	178 (15%)	58 (5%)	3 31
1	D	1155/1357 (85%)	923 (80%)	179 (16%)	53 (5%)	3 33
1	E	1141/1357 (84%)	910 (80%)	178 (16%)	53 (5%)	3 33
1	F	1155/1357 (85%)	913 (79%)	188 (16%)	54 (5%)	3 33
1	G	1145/1357 (84%)	914 (80%)	179 (16%)	52 (4%)	3 34
1	H	1151/1357 (85%)	914 (79%)	180 (16%)	57 (5%)	3 31
All	All	9213/10856 (85%)	7331 (80%)	1445 (16%)	437 (5%)	3 33

5 of 437 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	88	LYS
1	A	99	LEU
1	A	238	VAL
1	A	1099	LEU
1	A	1146	VAL

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	930/1065 (87%)	813 (87%)	117 (13%)	5 31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	908/1065 (85%)	801 (88%)	107 (12%)	6	35
1	C	917/1065 (86%)	805 (88%)	112 (12%)	6	33
1	D	917/1065 (86%)	810 (88%)	107 (12%)	7	35
1	E	910/1065 (85%)	801 (88%)	109 (12%)	6	33
1	F	917/1065 (86%)	812 (88%)	105 (12%)	7	35
1	G	911/1065 (86%)	800 (88%)	111 (12%)	6	33
1	H	916/1065 (86%)	806 (88%)	110 (12%)	6	33
All	All	7326/8520 (86%)	6448 (88%)	878 (12%)	6	33

5 of 878 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	2089	THR
1	E	1282	LYS
1	H	1221	VAL
1	D	2264	TYR
1	E	65	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 117 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	2300	GLN
1	E	2236	ASN
1	H	2020	GLN
1	D	3181	ASN
1	E	173	GLN

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 64 ligands modelled in this entry, 32 are monoatomic - leaving 32 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	$\#\|Z\| > 2$
3	ANP	A	1400	-	27,33,33	2.17	7 (25%)	30,52,52	2.26	6 (20%)
3	ANP	A	2400	-	27,33,33	2.29	8 (29%)	30,52,52	2.31	6 (20%)
3	ANP	A	3400	-	27,33,33	2.15	7 (25%)	30,52,52	2.61	9 (30%)
3	ANP	A	400	-	27,33,33	2.30	9 (33%)	30,52,52	2.12	5 (16%)
3	ANP	B	1400	-	27,33,33	2.25	8 (29%)	30,52,52	2.33	7 (23%)
3	ANP	B	2400	-	27,33,33	2.25	8 (29%)	30,52,52	2.28	6 (20%)
3	ANP	B	3400	-	27,33,33	2.10	7 (25%)	30,52,52	2.70	9 (30%)
3	ANP	B	400	-	27,33,33	2.26	8 (29%)	30,52,52	2.12	6 (20%)
3	ANP	C	1400	-	27,33,33	2.38	8 (29%)	30,52,52	2.32	7 (23%)
3	ANP	C	2400	-	27,33,33	2.18	8 (29%)	30,52,52	2.29	7 (23%)
3	ANP	C	3400	-	27,33,33	2.33	6 (22%)	30,52,52	2.65	9 (30%)
3	ANP	C	400	-	27,33,33	2.06	7 (25%)	30,52,52	2.17	6 (20%)
3	ANP	D	1400	-	27,33,33	2.23	7 (25%)	30,52,52	2.29	6 (20%)
3	ANP	D	2400	-	27,33,33	2.25	8 (29%)	30,52,52	2.26	6 (20%)
3	ANP	D	3400	-	27,33,33	2.14	7 (25%)	30,52,52	2.69	9 (30%)
3	ANP	D	400	-	27,33,33	2.31	7 (25%)	30,52,52	2.10	6 (20%)
3	ANP	E	1400	-	27,33,33	2.29	7 (25%)	30,52,52	2.33	6 (20%)
3	ANP	E	2400	-	27,33,33	2.31	9 (33%)	30,52,52	2.29	6 (20%)
3	ANP	E	3400	2	27,33,33	1.99	6 (22%)	30,52,52	2.68	9 (30%)
3	ANP	E	400	-	27,33,33	2.22	9 (33%)	30,52,52	2.15	5 (16%)
3	ANP	F	1400	-	27,33,33	2.34	8 (29%)	30,52,52	2.30	6 (20%)
3	ANP	F	2400	-	27,33,33	2.11	8 (29%)	30,52,52	2.32	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	ANP	F	3400	-	27,33,33	2.18	9 (33%)	30,52,52	2.65	9 (30%)
3	ANP	F	400	-	27,33,33	2.16	7 (25%)	30,52,52	2.07	6 (20%)
3	ANP	G	1400	-	27,33,33	2.26	8 (29%)	30,52,52	2.26	6 (20%)
3	ANP	G	2400	-	27,33,33	2.31	8 (29%)	30,52,52	2.29	7 (23%)
3	ANP	G	3400	-	27,33,33	2.34	7 (25%)	30,52,52	2.71	10 (33%)
3	ANP	G	400	-	27,33,33	2.20	7 (25%)	30,52,52	2.12	6 (20%)
3	ANP	H	1400	-	27,33,33	2.34	8 (29%)	30,52,52	2.23	7 (23%)
3	ANP	H	2400	-	27,33,33	2.24	8 (29%)	30,52,52	2.31	7 (23%)
3	ANP	H	3400	-	27,33,33	2.23	6 (22%)	30,52,52	2.81	9 (30%)
3	ANP	H	400	-	27,33,33	2.18	8 (29%)	30,52,52	2.11	5 (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
3	ANP	A	1400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	A	2400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	A	3400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	A	400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	B	1400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	B	2400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	B	3400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	B	400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	C	1400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	C	2400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	C	3400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	C	400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	D	1400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	D	2400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	D	3400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	D	400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	E	1400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	E	2400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	E	3400	2	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	E	400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	F	1400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	F	2400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	F	3400	-	1/1/7/8	0/12/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	F	400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	G	1400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	G	2400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	G	3400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	G	400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	H	1400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	H	2400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	H	3400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	H	400	-	1/1/7/8	0/12/38/38	0/3/3/3

The worst 5 of 243 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	3400	ANP	PB-O2B	-2.46	1.49	1.56
3	A	3400	ANP	PB-O2B	-2.46	1.49	1.56
3	A	400	ANP	PG-O2G	-2.32	1.50	1.56
3	C	400	ANP	PG-O2G	-2.21	1.50	1.56
3	G	400	ANP	PG-O2G	-2.21	1.50	1.56

The worst 5 of 220 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	2400	ANP	N3-C2-N1	-8.07	122.72	128.89
3	H	2400	ANP	N3-C2-N1	-7.90	122.84	128.89
3	A	2400	ANP	N3-C2-N1	-7.90	122.85	128.89
3	E	1400	ANP	N3-C2-N1	-7.80	122.92	128.89
3	E	2400	ANP	N3-C2-N1	-7.78	122.94	128.89

5 of 32 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	G	3400	ANP	C4'
3	D	3400	ANP	C4'
3	E	400	ANP	C4'
3	F	3400	ANP	C4'
3	E	2400	ANP	C4'

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1400	ANP	3	0
3	A	3400	ANP	3	0
3	A	400	ANP	1	0
3	B	3400	ANP	1	0
3	B	400	ANP	1	0
3	C	3400	ANP	2	0
3	C	400	ANP	1	0
3	D	3400	ANP	2	0
3	E	1400	ANP	1	0
3	E	3400	ANP	1	0
3	E	400	ANP	1	0
3	F	3400	ANP	3	0
3	F	400	ANP	6	0
3	G	3400	ANP	2	0
3	G	400	ANP	2	0
3	H	3400	ANP	3	0
3	H	400	ANP	1	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	1190/1357 (87%)	-0.13	16 (1%)	79	71	181, 217, 253, 285	0
1	B	1163/1357 (85%)	-0.28	12 (1%)	84	77	175, 217, 254, 286	0
1	C	1175/1357 (86%)	-0.20	13 (1%)	82	76	187, 216, 253, 284	0
1	D	1175/1357 (86%)	-0.11	31 (2%)	59	49	181, 218, 256, 286	0
1	E	1165/1357 (85%)	-0.14	21 (1%)	71	62	186, 218, 255, 288	0
1	F	1175/1357 (86%)	-0.16	13 (1%)	82	76	185, 217, 255, 285	0
1	G	1167/1357 (85%)	-0.18	12 (1%)	84	77	185, 216, 254, 291	0
1	H	1173/1357 (86%)	-0.17	26 (2%)	65	56	186, 218, 255, 288	0
All	All	9383/10856 (86%)	-0.17	144 (1%)	76	67	175, 217, 255, 291	0

The worst 5 of 144 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	3151	PRO	6.6
1	A	3151	PRO	5.9
1	C	3151	PRO	5.1
1	C	2137	ALA	4.8
1	D	211	GLY	4.7

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands (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
2	MG	E	701	1/1	0.58	1.16	7.93	204,204,204,204	0
2	MG	F	701	1/1	0.94	0.55	4.64	189,189,189,189	0
2	MG	E	2701	1/1	0.87	0.34	1.08	228,228,228,228	0
3	ANP	G	2400	31/31	0.72	0.41	1.02	303,308,315,315	0
3	ANP	H	400	31/31	0.83	0.42	0.90	254,263,265,265	0
3	ANP	E	1400	31/31	0.79	0.32	0.83	287,293,296,296	0
3	ANP	D	400	31/31	0.84	0.29	0.78	263,273,274,274	0
3	ANP	B	1400	31/31	0.86	0.30	0.76	275,286,290,290	0
3	ANP	F	1400	31/31	0.82	0.34	0.70	271,280,286,286	0
2	MG	D	2701	1/1	0.67	0.41	0.69	237,237,237,237	0
3	ANP	F	2400	31/31	0.72	0.44	0.68	286,303,310,310	0
3	ANP	D	1400	31/31	0.75	0.38	0.66	287,290,294,294	0
3	ANP	A	2400	31/31	0.86	0.34	0.65	308,311,315,315	0
3	ANP	H	2400	31/31	0.73	0.38	0.59	298,312,316,316	0
3	ANP	B	2400	31/31	0.79	0.34	0.40	306,312,314,314	0
3	ANP	A	1400	31/31	0.75	0.36	0.40	267,280,283,283	0
3	ANP	B	400	31/31	0.80	0.33	0.32	242,255,259,260	0
3	ANP	H	1400	31/31	0.83	0.32	0.31	296,299,304,304	0
3	ANP	G	400	31/31	0.84	0.28	0.26	253,262,264,265	0
3	ANP	C	1400	31/31	0.84	0.25	0.26	288,291,293,294	0
2	MG	G	2701	1/1	0.93	0.45	0.24	192,192,192,192	0
3	ANP	F	400	31/31	0.86	0.33	0.11	243,257,263,263	0
2	MG	F	2701	1/1	0.80	0.37	0.10	232,232,232,232	0
3	ANP	D	2400	31/31	0.85	0.30	0.07	305,310,315,315	0
2	MG	H	2701	1/1	0.83	0.36	0.01	271,271,271,271	0
3	ANP	E	2400	31/31	0.90	0.25	-0.05	307,317,320,320	0
2	MG	B	3701	1/1	0.96	0.18	-0.07	69,69,69,69	0
3	ANP	A	400	31/31	0.88	0.27	-0.09	246,250,255,256	0
3	ANP	E	400	31/31	0.89	0.26	-0.15	256,261,264,265	0
3	ANP	C	2400	31/31	0.89	0.28	-0.25	296,309,314,315	0
2	MG	E	3701	1/1	0.86	0.20	-0.29	131,131,131,131	0
3	ANP	C	400	31/31	0.84	0.29	-0.30	226,245,250,250	0
3	ANP	G	1400	31/31	0.81	0.25	-0.45	279,285,289,290	0
3	ANP	G	3400	31/31	0.91	0.19	-0.46	153,176,191,192	0
3	ANP	H	3400	31/31	0.90	0.18	-0.54	180,187,196,197	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	ANP	F	3400	31/31	0.92	0.20	-0.57	148,171,183,183	0
2	MG	B	2701	1/1	0.71	0.26	-0.71	238,238,238,238	0
2	MG	C	2701	1/1	0.93	0.26	-0.74	211,211,211,211	0
3	ANP	E	3400	31/31	0.94	0.19	-0.79	163,180,187,187	0
2	MG	C	3701	1/1	0.83	0.14	-0.83	140,140,140,140	0
3	ANP	B	3400	31/31	0.93	0.18	-0.86	143,159,176,178	0
3	ANP	C	3400	31/31	0.93	0.14	-0.87	176,190,200,200	0
2	MG	D	3701	1/1	0.95	0.14	-0.90	108,108,108,108	0
3	ANP	D	3400	31/31	0.92	0.16	-0.93	149,170,188,189	0
2	MG	G	3701	1/1	0.97	0.10	-1.30	100,100,100,100	0
2	MG	A	2701	1/1	0.89	0.15	-1.44	247,247,247,247	0
3	ANP	A	3400	31/31	0.94	0.17	-1.47	152,165,180,181	0
2	MG	H	3701	1/1	0.95	0.15	-1.55	121,121,121,121	0
2	MG	A	3701	1/1	0.97	0.09	-3.54	116,116,116,116	0
2	MG	F	3701	1/1	0.98	0.09	-4.18	77,77,77,77	0
2	MG	B	701	1/1	0.84	1.12	-	184,184,184,184	0
2	MG	E	1701	1/1	0.83	0.48	-	190,190,190,190	0
2	MG	D	701	1/1	0.76	0.65	-	261,261,261,261	0
2	MG	D	1701	1/1	0.75	1.11	-	212,212,212,212	0
2	MG	F	1701	1/1	0.86	0.59	-	175,175,175,175	0
2	MG	A	701	1/1	0.86	0.63	-	143,143,143,143	0
2	MG	C	1701	1/1	0.96	0.18	-	132,132,132,132	0
2	MG	C	701	1/1	0.58	0.61	-	177,177,177,177	0
2	MG	A	1701	1/1	0.87	0.86	-	181,181,181,181	0
2	MG	G	1701	1/1	0.89	0.53	-	191,191,191,191	0
2	MG	H	1701	1/1	0.83	0.67	-	188,188,188,188	0
2	MG	H	701	1/1	0.92	0.17	-	200,200,200,200	0
2	MG	G	701	1/1	0.54	0.96	-	215,215,215,215	0
2	MG	B	1701	1/1	0.74	0.41	-	214,214,214,214	0

6.5 Other polymers (i)

There are no such residues in this entry.