wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 07:56 AM GMT

PDB ID	:	3CMW
Title	:	Mechanism of homologous recombination from the RecA-ssDNA/dsDNA structures
Authors	:	Pavletich, N.P.
Deposited on	:	2008-03-24
Resolution	:	2.80 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:

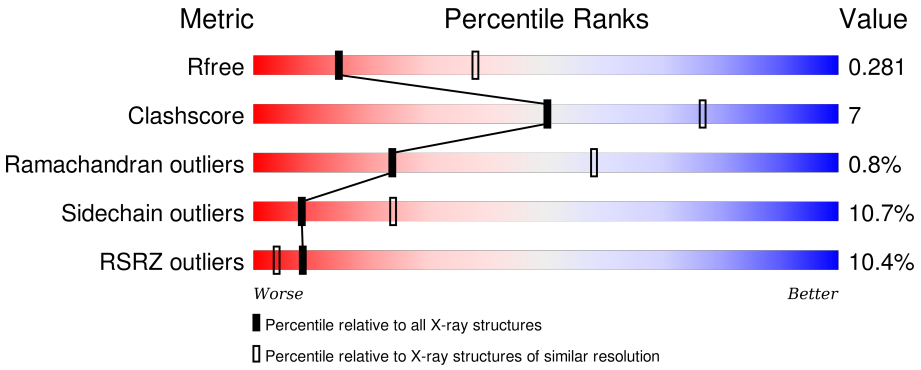
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	B	15	20% 60% 20%
1	D	15	7% 27% 53% 20%
2	A	1706	10% 77% 15% • 6%
2	C	1706	9% 77% 14% • 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 25046 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 DNA chain called DNA (5'-D(*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DT)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	12	Total	C	N	O	P	0	0	0
			237	120	24	82	11			
1	D	12	Total	C	N	O	P	0	0	0
			237	120	24	82	11			

- Molecule 2 is a protein called Protein recA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	1609	Total	C	N	O	S	0	0	0
			12125	7622	2100	2347	56			
2	C	1608	Total	C	N	O	S	0	0	0
			12117	7617	2100	2344	56			

There are 130 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
A	995	GLY	-	linker	UNP P0A7G6
A	996	SER	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
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
A	3986	THR	-	linker	UNP P0A7G6
A	3987	GLY	-	linker	UNP P0A7G6
A	3988	SER	-	linker	UNP P0A7G6
A	3989	THR	-	linker	UNP P0A7G6
A	3990	GLY	-	linker	UNP P0A7G6
A	3991	SER	-	linker	UNP P0A7G6
A	3992	MET	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	3993	SER	-	linker	UNP P0A7G6
A	3994	GLY	-	linker	UNP P0A7G6
A	3995	ARG	-	linker	UNP P0A7G6
A	3996	THR	-	linker	UNP P0A7G6
A	3997	GLY	-	linker	UNP P0A7G6
A	3998	SER	-	linker	UNP P0A7G6
A	3999	MET	-	linker	UNP P0A7G6
A	4000	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

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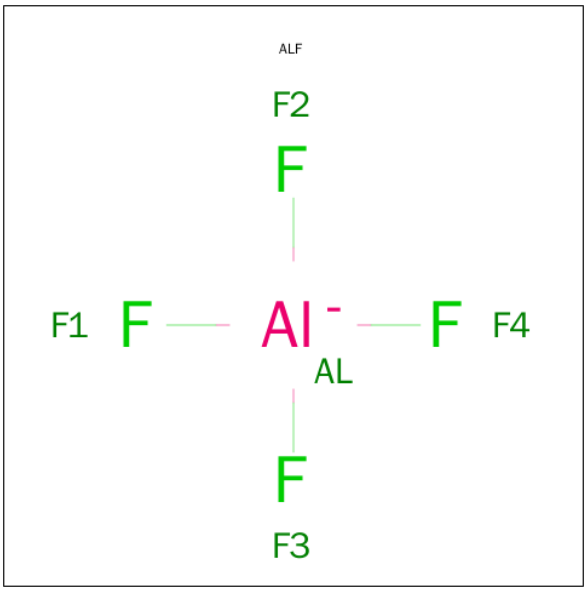
Chain	Residue	Modelled	Actual	Comment	Reference
C	2985	THR	-	linker	UNP P0A7G6
C	2986	GLY	-	linker	UNP P0A7G6
C	2987	SER	-	linker	UNP P0A7G6
C	2988	THR	-	linker	UNP P0A7G6
C	2989	GLY	-	linker	UNP P0A7G6
C	2990	SER	-	linker	UNP P0A7G6
C	2991	ALA	-	linker	UNP P0A7G6
C	2992	SER	-	linker	UNP P0A7G6
C	2993	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
C	3986	THR	-	linker	UNP P0A7G6
C	3987	GLY	-	linker	UNP P0A7G6
C	3988	SER	-	linker	UNP P0A7G6
C	3989	THR	-	linker	UNP P0A7G6
C	3990	GLY	-	linker	UNP P0A7G6
C	3991	SER	-	linker	UNP P0A7G6
C	3992	MET	-	linker	UNP P0A7G6
C	3993	SER	-	linker	UNP P0A7G6
C	3994	GLY	-	linker	UNP P0A7G6
C	3995	ARG	-	linker	UNP P0A7G6
C	3996	THR	-	linker	UNP P0A7G6
C	3997	GLY	-	linker	UNP P0A7G6
C	3998	SER	-	linker	UNP P0A7G6
C	3999	MET	-	linker	UNP P0A7G6
C	4000	SER	-	linker	UNP P0A7G6

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

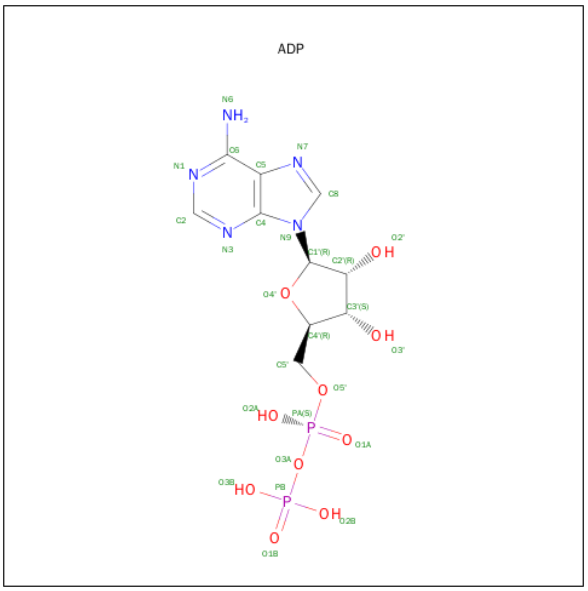
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total Mg 5 5	0	0
3	C	5	Total Mg 5 5	0	0

- Molecule 4 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Al F 5 1 4	0	0
4	A	1	Total Al F 5 1 4	0	0
4	A	1	Total Al F 5 1 4	0	0
4	A	1	Total Al F 5 1 4	0	0
4	A	1	Total Al F 5 1 4	0	0
4	C	1	Total Al F 5 1 4	0	0
4	C	1	Total Al F 5 1 4	0	0
4	C	1	Total Al F 5 1 4	0	0
4	C	1	Total Al F 5 1 4	0	0
4	C	1	Total Al F 5 1 4	0	0

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



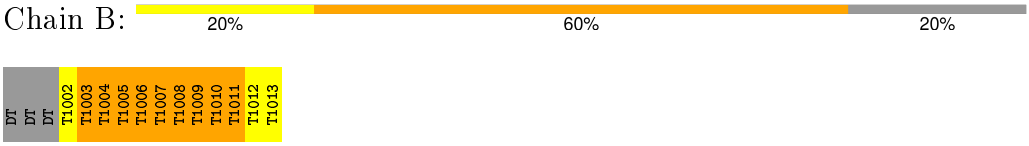
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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.

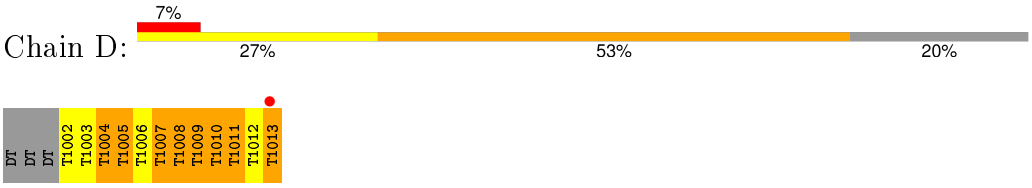
• Molecule 1: DNA (5'-D(*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DT)-3')

Chain B:



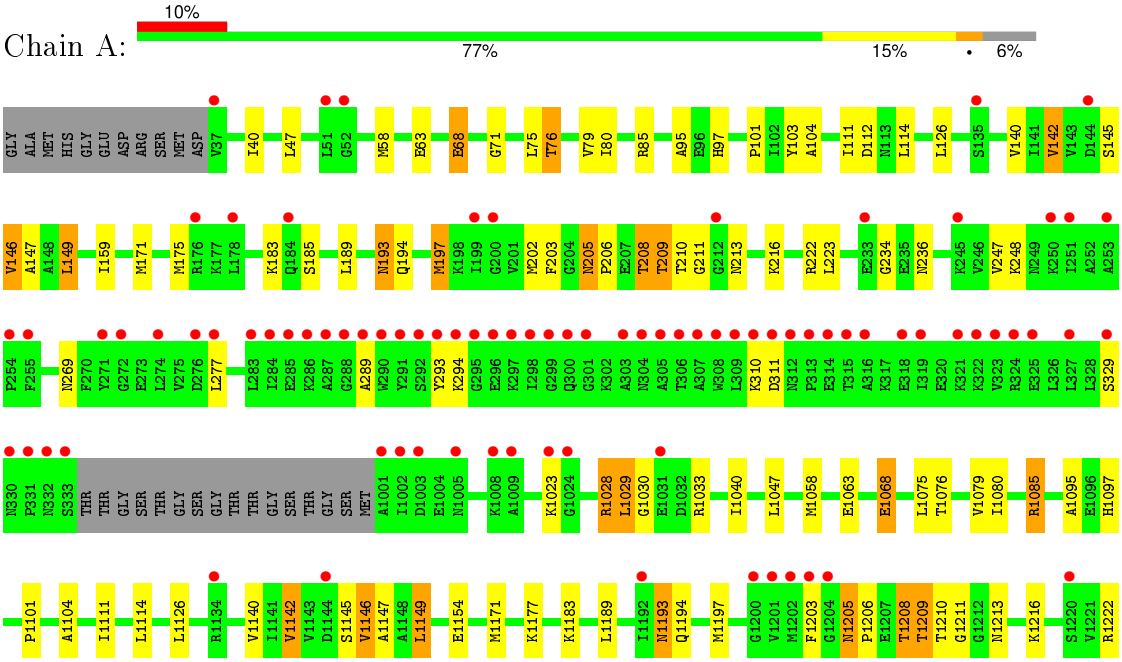
• Molecule 1: DNA (5'-D(*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DT)-3')

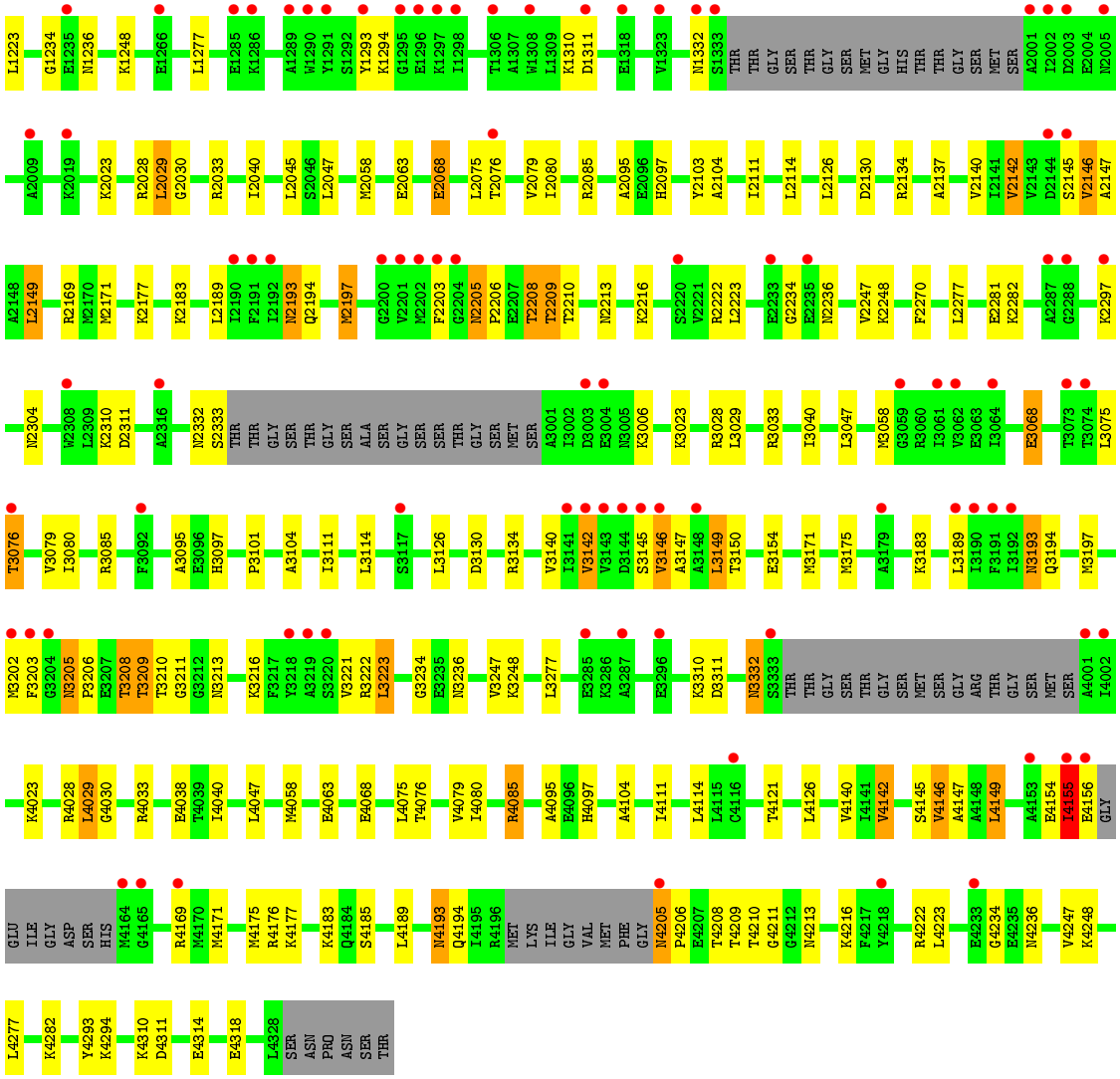
Chain D:



• Molecule 2: Protein recA

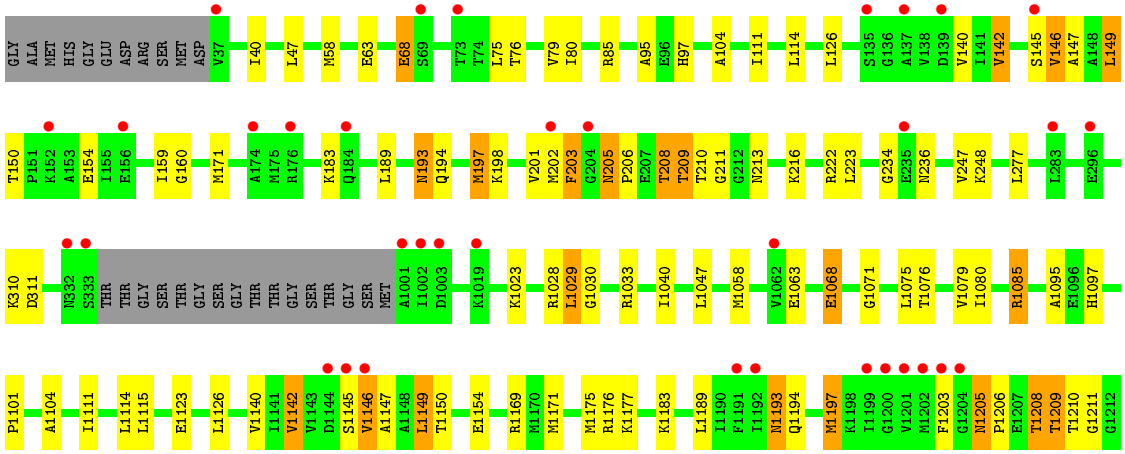
Chain A:

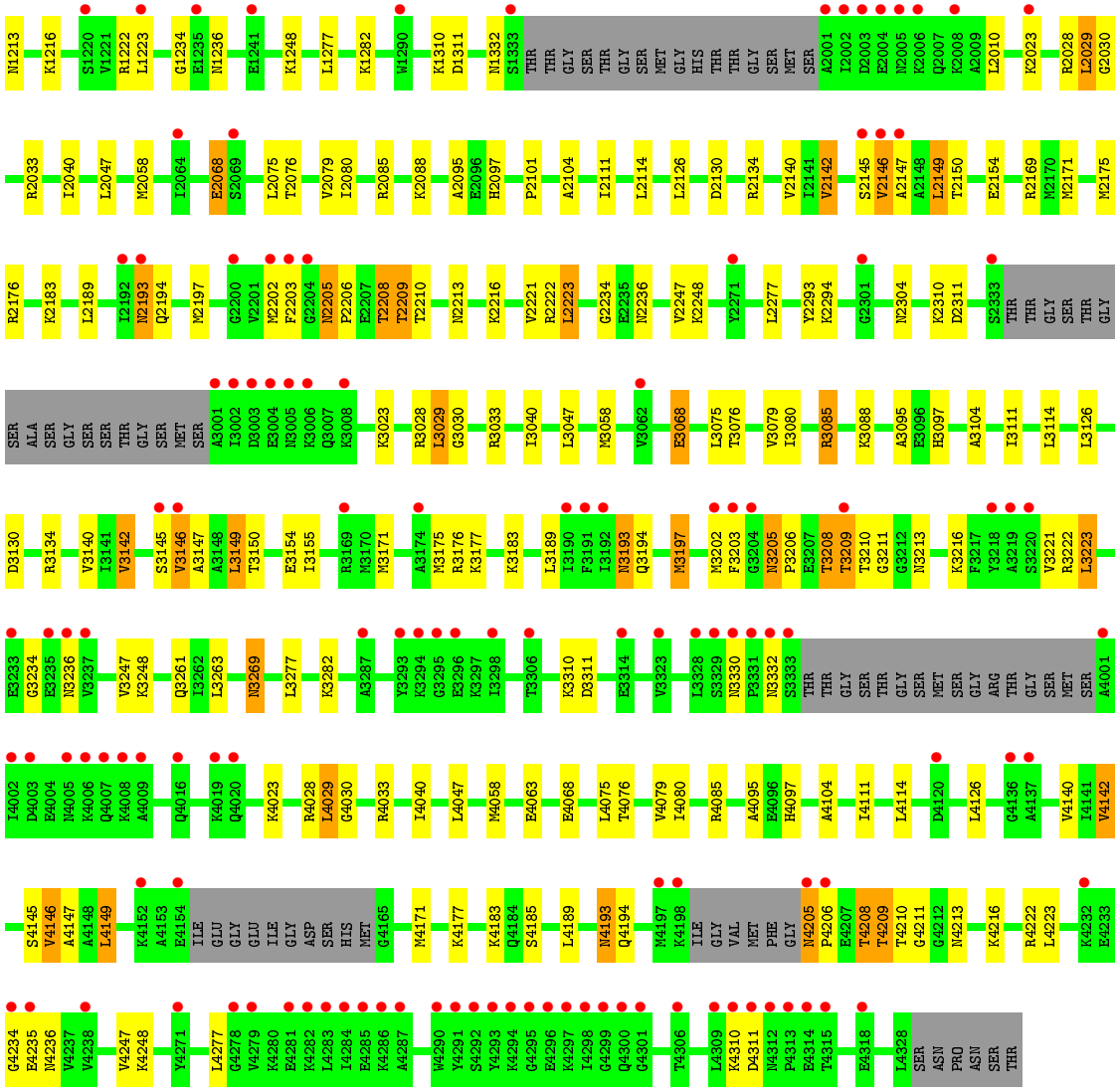




- Molecule 2: Protein recA

Chain C:




N1213 K1216 S1220 V1221 R1222 L1223 G1234 E1235 N1236 E1241 K1248 L1277 K1282 W1290 K1310 D1311 N1332 S1333 THR THR GLY SER THR GLY SER MET GLY HIS THR THR GLY SER MET SER A2001 I2002 D2003 E2004 N2005 K2006 Q2007 K2008 A2009 L2010 K2023 R2028 L2029 G2030
R2033 I2040 L2047 M2058 I2064 E2068 S2069 L2075 T2076 V2079 I2080 R2085 K2088 A2095 E2096 H2097 P2101 A2104 I2111 L2114 L2126 D2130 R2134 V2140 I2141 V2142 S2145 V2146 A2147 A2148 L2149 T2150 E2154 R2169 M2170 M2171 M2175
R2176 K2183 L2189 I2192 N2193 Q2194 M2197 G2200 V2201 M2202 F2203 G2204 N2205 P2206 E2207 T2208 T2209 T2210 N2213 K2216 V2221 R2222 L2223 G2234 E2235 N2236 V2247 K2248 Y2271 L2277 Y2293 K2294 G2301 N2304 K2310 D2311 S2333 THR THR GLY SER THR GLY
SER ALA SER GLY SER SER THR GLY SER MET SER A3001 I3002 D3003 E3004 N3005 K3006 Q3007 K3008 K3023 R3028 L3029 G3030 R3033 I3040 L3047 M3058 V3062 E3068 L3075 T3076 V3079 I3080 R3085 K3088 A3095 E3096 H3097 A3104 I3111 L3114 L3126
D3130 R3134 V3140 I3141 V3142 S3145 V3146 A3147 A3148 L3149 T3150 E3154 I3155 R3169 M3170 M3171 A3174 M3175 R3176 K3177 K3183 L3189 I3190 F3191 I3192 N3193 Q3194 M3197 M3202 F3203 G3204 N3205 P3206 E3207 T3208 T3209 T3210 G3211 G3212 N3213 K3216 F3217 Y3218 A3219 S3220 V3221 R3222 L3223
E3233 G3234 E3235 N3236 V3237 V3247 K3248 Q3261 I3262 L3263 N3269 L3277 K3282 A3287 Y3293 K3294 G3295 E3296 K3297 I3298 T3306 K3310 D3311 E3314 V3323 L3328 S3329 N3330 P3331 N3332 S3333 THR THR GLY SER THR GLY SER MET SER GLY ARG THR GLY SER MET SER A4001
I4002 D4003 E4004 N4005 K4006 Q4007 K4008 A4009 Q4016 K4019 Q4020 K4023 R4028 L4029 G4030 R4033 I4040 L4047 M4058 E4063 E4068 L4075 T4076 V4079 I4080 R4085 A4095 E4096 H4097 A4104 I4111 L4114 D4120 L4126 G4136 A4137 V4140 I4141 V4142
S4145 V4146 A4147 A4148 L4149 K4152 A4153 E4154 ILE GLU GLY GLU ILE GLY ASP SER HIS MET G4165 M4171 K4177 K4183 Q4184 S4185 L4189 N4193 Q4194 M4197 K4198 ILE GLY VAL MET PHE GLY N4205 P4206 E4207 T4208 T4209 T4210 G4211 G4212 N4213 K4216 R4222 L4223 K4232 E4233
G4234 E4235 N4236 V4237 V4238 V4247 K4248 Y4271 L4277 G4278 V4279 K4280 E4281 K4282 L4283 I4284 E4285 K4286 A4287 W4290 Y4291 S4292 Y4293 K4294 G4295 E4296 K4297 I4298 G4299 Q4300 G4301 T4306 L4309 K4310 D4311 N4312 P4313 E4314 T4315 E4318 L4328 SER ASN PRO ASN SER THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	159.00Å 300.50Å 80.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 39.41 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.0 (20.00-2.80) 87.9 (39.41-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.3.0036	Depositor
R, R_{free}	0.214 , 0.236 0.264 , 0.281	Depositor DCC
R_{free} test set	1693 reflections (2.01%)	DCC
Wilson B-factor (Å^2)	63.7	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 39.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 87028 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	25046	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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: ALF, MG, ADP

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	B	1.67	3/260 (1.2%)	2.31	18/400 (4.5%)
1	D	1.52	2/260 (0.8%)	2.15	17/400 (4.2%)
2	A	0.45	0/12264	0.59	0/16503
2	C	0.45	0/12256	0.59	0/16491
All	All	0.50	5/25040 (0.0%)	0.68	35/33794 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1010	DT	C3'-O3'	-6.92	1.34	1.44
1	B	1007	DT	C3'-O3'	-6.88	1.35	1.44
1	D	1010	DT	C3'-O3'	-6.23	1.35	1.44
1	D	1007	DT	C3'-O3'	-5.48	1.36	1.44
1	B	1009	DT	C1'-N1	5.14	1.55	1.49

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1013	DT	C1'-O4'-C4'	-12.89	97.21	110.10
1	B	1013	DT	O4'-C1'-N1	10.35	115.24	108.00
1	D	1013	DT	C1'-O4'-C4'	-9.35	100.75	110.10
1	D	1013	DT	O4'-C4'-C3'	-9.24	100.45	106.00
1	D	1007	DT	O4'-C1'-N1	8.29	113.80	108.00

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	B	237	0	146	11	0
1	D	237	0	146	19	0
2	A	12125	0	12452	174	2
2	C	12117	0	12447	175	1
3	A	5	0	0	0	0
3	C	5	0	0	0	0
4	A	25	0	0	0	0
4	C	25	0	0	0	0
5	A	135	0	60	3	0
5	C	135	0	60	1	0
All	All	25046	0	25311	351	2

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 7.

The worst 5 of 351 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:D:1013:DT:O4	2:A:3202:MET:HG2	1.49	1.10
2:A:2068:GLU:HG2	2:A:3216:LYS:HB3	1.33	1.08
2:A:68:GLU:HG2	2:A:1216:LYS:HB3	1.24	1.07
2:C:68:GLU:HG2	2:C:1216:LYS:HB3	1.42	0.99
2:A:3068:GLU:HG2	2:A:4216:LYS:HB3	1.48	0.95

All (2) 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)
2:A:4038:GLU:OE1	2:A:4318:GLU:OE2[2_555]	1.97	0.23
2:A:2297:LYS:NZ	2:C:4097:HIS:O[1_554]	2.15	0.05

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
2	A	1595/1706 (94%)	1545 (97%)	37 (2%)	13 (1%)	24 58
2	C	1594/1706 (93%)	1550 (97%)	33 (2%)	11 (1%)	26 62
All	All	3189/3412 (94%)	3095 (97%)	70 (2%)	24 (1%)	24 58

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	1023	LYS
2	A	2023	LYS
2	A	3023	LYS
2	A	3332	ASN
2	A	4023	LYS

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
2	A	1267/1339 (95%)	1128 (89%)	139 (11%)	8 23
2	C	1266/1339 (94%)	1134 (90%)	132 (10%)	9 25
All	All	2533/2678 (95%)	2262 (89%)	271 (11%)	8 24

5 of 271 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	4146	VAL

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Mol	Chain	Res	Type
2	C	189	LEU
2	C	4079	VAL
2	A	4185	SER
2	A	4311	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	4184	GLN
2	C	193	ASN
2	C	4181	ASN
2	A	4193	ASN
2	A	4304	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 30 ligands modelled in this entry, 10 are monoatomic - leaving 20 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	$\#\|Z\|>2$
4	ALF	A	1501	-	0,4,4	0.00	-	0,6,6	0.00	-
5	ADP	A	1502	3	22,29,29	0.83	1 (4%)	27,45,45	2.42	7 (25%)
4	ALF	A	2501	-	0,4,4	0.00	-	0,6,6	0.00	-
5	ADP	A	2502	3	22,29,29	0.97	1 (4%)	27,45,45	2.07	5 (18%)
4	ALF	A	3501	-	0,4,4	0.00	-	0,6,6	0.00	-
5	ADP	A	3502	3	22,29,29	1.00	2 (9%)	27,45,45	2.34	6 (22%)
4	ALF	A	4501	-	0,4,4	0.00	-	0,6,6	0.00	-
5	ADP	A	4502	3	22,29,29	1.24	2 (9%)	27,45,45	1.91	6 (22%)
4	ALF	A	501	-	0,4,4	0.00	-	0,6,6	0.00	-
5	ADP	A	502	3	22,29,29	1.07	1 (4%)	27,45,45	2.09	4 (14%)
4	ALF	C	1501	-	0,4,4	0.00	-	0,6,6	0.00	-
5	ADP	C	1502	3	22,29,29	0.89	1 (4%)	27,45,45	1.86	5 (18%)
4	ALF	C	2501	-	0,4,4	0.00	-	0,6,6	0.00	-
5	ADP	C	2502	3	22,29,29	0.98	1 (4%)	27,45,45	2.28	7 (25%)
4	ALF	C	3501	-	0,4,4	0.00	-	0,6,6	0.00	-
5	ADP	C	3502	3	22,29,29	0.90	1 (4%)	27,45,45	2.25	6 (22%)
4	ALF	C	4501	-	0,4,4	0.00	-	0,6,6	0.00	-
5	ADP	C	4502	3	22,29,29	1.06	1 (4%)	27,45,45	2.12	7 (25%)
4	ALF	C	501	-	0,4,4	0.00	-	0,6,6	0.00	-
5	ADP	C	502	3	22,29,29	0.90	1 (4%)	27,45,45	2.06	5 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ALF	A	1501	-	-	0/0/0/0	0/0/0/0
5	ADP	A	1502	3	-	0/12/32/32	0/3/3/3
4	ALF	A	2501	-	-	0/0/0/0	0/0/0/0
5	ADP	A	2502	3	-	0/12/32/32	0/3/3/3
4	ALF	A	3501	-	-	0/0/0/0	0/0/0/0
5	ADP	A	3502	3	-	0/12/32/32	0/3/3/3
4	ALF	A	4501	-	-	0/0/0/0	0/0/0/0
5	ADP	A	4502	3	-	0/12/32/32	0/3/3/3
4	ALF	A	501	-	-	0/0/0/0	0/0/0/0
5	ADP	A	502	3	-	0/12/32/32	0/3/3/3
4	ALF	C	1501	-	-	0/0/0/0	0/0/0/0
5	ADP	C	1502	3	-	0/12/32/32	0/3/3/3
4	ALF	C	2501	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ADP	C	2502	3	-	0/12/32/32	0/3/3/3
4	ALF	C	3501	-	-	0/0/0/0	0/0/0/0
5	ADP	C	3502	3	-	0/12/32/32	0/3/3/3
4	ALF	C	4501	-	-	0/0/0/0	0/0/0/0
5	ADP	C	4502	3	-	0/12/32/32	0/3/3/3
4	ALF	C	501	-	-	0/0/0/0	0/0/0/0
5	ADP	C	502	3	-	0/12/32/32	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	4502	ADP	O4'-C1'	2.35	1.44	1.41
5	A	3502	ADP	C5-C4	2.42	1.46	1.40
5	A	3502	ADP	O4'-C1'	2.45	1.44	1.41
5	C	1502	ADP	C5-C4	2.45	1.46	1.40
5	A	1502	ADP	C5-C4	2.57	1.46	1.40

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	3502	ADP	N3-C2-N1	-9.03	121.98	128.89
5	A	1502	ADP	N3-C2-N1	-8.11	122.69	128.89
5	C	3502	ADP	N3-C2-N1	-8.00	122.77	128.89
5	C	2502	ADP	N3-C2-N1	-7.54	123.12	128.89
5	C	4502	ADP	N3-C2-N1	-7.37	123.25	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2502	ADP	1	0
5	A	502	ADP	2	0
5	C	1502	ADP	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	B	12/15 (80%)	0.52	0 100 100	29, 56, 64, 65	0
1	D	12/15 (80%)	0.63	1 (8%) 14 7	22, 52, 61, 61	0
2	A	1609/1706 (94%)	0.71	176 (10%) 7 3	52, 62, 78, 107	0
2	C	1608/1706 (94%)	0.65	159 (9%) 9 4	50, 62, 79, 108	0
All	All	3241/3442 (94%)	0.68	336 (10%) 8 4	22, 62, 79, 108	0

The worst 5 of 336 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	1001	ALA	12.4
2	A	4164	MET	7.8
2	C	3330	ASN	7.7
2	C	4291	TYR	7.7
2	C	3202	MET	7.6

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
4	ALF	A	501	5/5	0.95	0.32	0.58	60,60,63,64	0
4	ALF	C	2501	5/5	0.95	0.33	0.53	45,47,50,50	0
4	ALF	C	3501	5/5	0.94	0.28	0.50	47,49,52,53	0
4	ALF	C	501	5/5	0.97	0.34	0.15	44,49,49,52	0
4	ALF	A	1501	5/5	0.94	0.28	0.13	45,47,50,53	0
4	ALF	C	1501	5/5	0.97	0.28	-0.02	40,42,46,47	0
4	ALF	A	3501	5/5	0.96	0.28	-0.17	42,46,49,51	0
4	ALF	A	2501	5/5	0.97	0.29	-0.19	40,44,45,47	0
5	ADP	A	502	27/27	0.93	0.22	-0.34	50,53,57,60	0
5	ADP	C	502	27/27	0.97	0.23	-0.64	37,40,43,47	0
5	ADP	C	4502	27/27	0.94	0.15	-0.89	54,56,61,63	0
5	ADP	A	1502	27/27	0.96	0.19	-0.95	33,40,44,46	0
5	ADP	A	4502	27/27	0.94	0.15	-0.97	47,62,63,68	0
5	ADP	C	3502	27/27	0.94	0.18	-1.03	40,50,52,53	0
5	ADP	C	2502	27/27	0.96	0.18	-1.03	41,46,49,49	0
5	ADP	C	1502	27/27	0.97	0.19	-1.10	32,36,39,41	0
5	ADP	A	2502	27/27	0.96	0.18	-1.13	37,42,45,47	0
4	ALF	A	4501	5/5	0.80	0.16	-1.14	78,79,81,82	0
4	ALF	C	4501	5/5	0.88	0.14	-1.15	67,71,73,75	0
5	ADP	A	3502	27/27	0.97	0.19	-1.16	28,35,39,40	0
3	MG	A	1500	1/1	0.88	0.39	-	47,47,47,47	0
3	MG	C	500	1/1	0.86	0.49	-	50,50,50,50	0
3	MG	C	2500	1/1	0.94	0.51	-	48,48,48,48	0
3	MG	A	4500	1/1	0.95	0.29	-	60,60,60,60	0
3	MG	C	3500	1/1	0.88	0.43	-	45,45,45,45	0
3	MG	C	4500	1/1	0.89	0.31	-	56,56,56,56	0
3	MG	A	500	1/1	0.95	0.55	-	57,57,57,57	0
3	MG	A	2500	1/1	0.82	0.42	-	42,42,42,42	0
3	MG	A	3500	1/1	0.90	0.50	-	46,46,46,46	0
3	MG	C	1500	1/1	0.95	0.46	-	45,45,45,45	0

6.5 Other polymers (i)

There are no such residues in this entry.