wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 02:31 PM GMT

PDB ID	:	3ZKB
Title	:	CRYSTAL STRUCTURE OF THE ATPASE REGION OF Mycobacterium tuberculosis GyrB WITH AMPPNP
Authors	:	Agrawal, A.; Roue, M.; Spitzfaden, C.; Petrella, S.; Aubry, A.; Volker, C.; Mossakowska, D.; Hann, M.; Bax, B.; Mayer, C.
Deposited on	:	2013-01-22
Resolution	:	2.90 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:

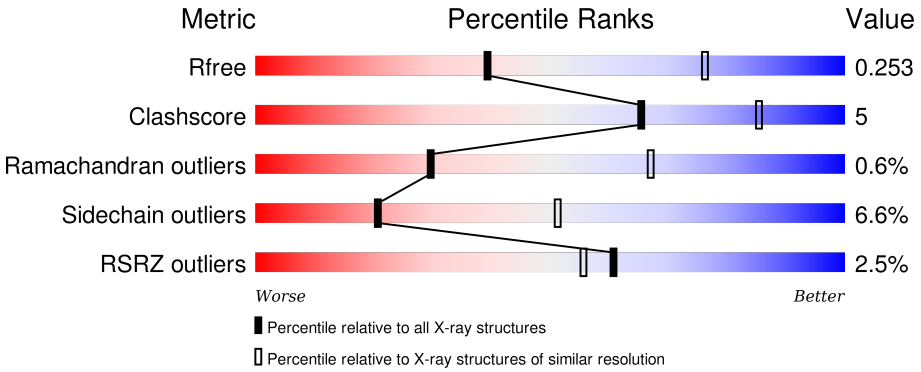
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	432	2% 71% 16% • 12%
1	B	432	% 76% 13% 12%
1	C	432	74% 15% • 10%
1	D	432	2% 75% 15% 9%
1	E	432	% 72% 16% • 11%

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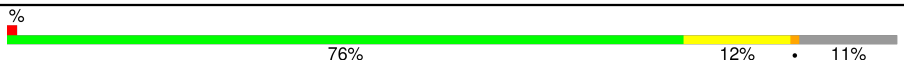
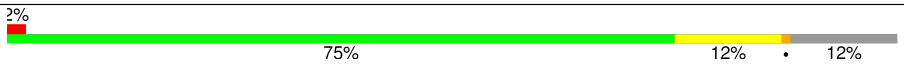
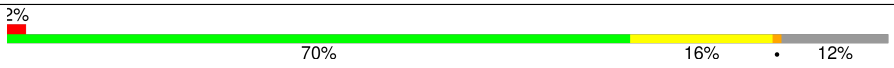
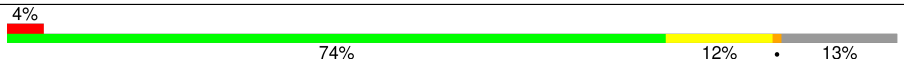
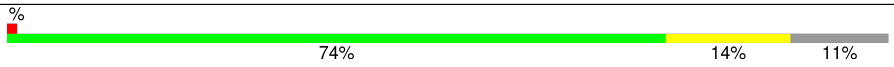
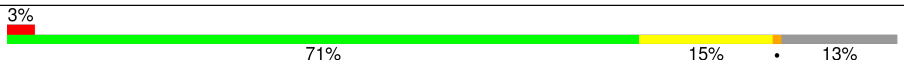
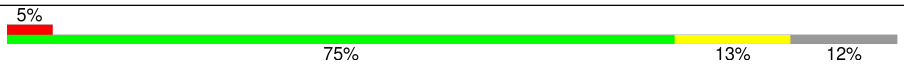
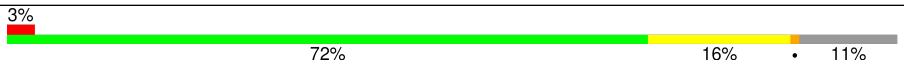
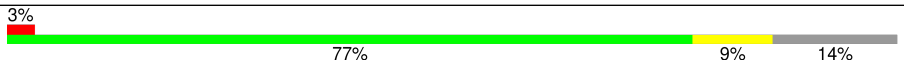
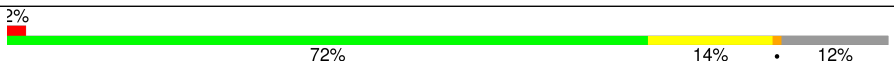
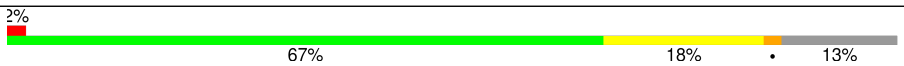
Mol	Chain	Length	Quality of chain
1	F	432	
1	G	432	
1	H	432	
1	I	432	
1	J	432	
1	K	432	
1	L	432	
1	M	432	
1	N	432	
1	O	432	
1	P	432	

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
3	MG	A	602	-	-	-	X
3	MG	C	1001	-	-	-	X
3	MG	I	602	-	-	-	X
3	MG	J	602	-	-	-	X
3	MG	L	602	-	-	-	X
3	MG	O	602	-	-	-	X
3	MG	P	602	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 46952 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 GYRASE SUBUNIT B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	380	Total	C	N	O	S	0	0	0
			2887	1809	509	563	6			
1	B	382	Total	C	N	O	S	0	0	0
			2874	1798	505	565	6			
1	C	387	Total	C	N	O	S	0	0	0
			2938	1842	516	574	6			
1	D	392	Total	C	N	O	S	0	0	0
			2954	1844	518	586	6			
1	E	386	Total	C	N	O	S	0	0	0
			2912	1821	511	574	6			
1	F	383	Total	C	N	O	S	0	0	0
			2888	1807	505	570	6			
1	G	381	Total	C	N	O	S	0	0	0
			2864	1796	502	560	6			
1	H	379	Total	C	N	O	S	0	0	0
			2866	1794	502	564	6			
1	I	375	Total	C	N	O	S	0	0	0
			2827	1768	494	559	6			
1	J	384	Total	C	N	O	S	0	0	0
			2884	1806	506	566	6			
1	K	376	Total	C	N	O	S	0	0	0
			2838	1778	497	557	6			
1	L	382	Total	C	N	O	S	0	0	0
			2862	1791	501	564	6			
1	M	383	Total	C	N	O	S	0	0	0
			2888	1808	509	565	6			
1	N	373	Total	C	N	O	S	0	0	0
			2816	1763	495	552	6			
1	O	379	Total	C	N	O	S	0	0	0
			2877	1803	506	562	6			
1	P	376	Total	C	N	O	S	0	0	0
			2822	1768	489	559	6			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	EXPRESSION TAG	UNP I6WX66
A	-3	PRO	-	EXPRESSION TAG	UNP I6WX66
A	-2	LEU	-	EXPRESSION TAG	UNP I6WX66
A	-1	GLY	-	EXPRESSION TAG	UNP I6WX66
A	0	SER	-	EXPRESSION TAG	UNP I6WX66
B	-4	GLY	-	EXPRESSION TAG	UNP I6WX66
B	-3	PRO	-	EXPRESSION TAG	UNP I6WX66
B	-2	LEU	-	EXPRESSION TAG	UNP I6WX66
B	-1	GLY	-	EXPRESSION TAG	UNP I6WX66
B	0	SER	-	EXPRESSION TAG	UNP I6WX66
C	-4	GLY	-	EXPRESSION TAG	UNP I6WX66
C	-3	PRO	-	EXPRESSION TAG	UNP I6WX66
C	-2	LEU	-	EXPRESSION TAG	UNP I6WX66
C	-1	GLY	-	EXPRESSION TAG	UNP I6WX66
C	0	SER	-	EXPRESSION TAG	UNP I6WX66
D	-4	GLY	-	EXPRESSION TAG	UNP I6WX66
D	-3	PRO	-	EXPRESSION TAG	UNP I6WX66
D	-2	LEU	-	EXPRESSION TAG	UNP I6WX66
D	-1	GLY	-	EXPRESSION TAG	UNP I6WX66
D	0	SER	-	EXPRESSION TAG	UNP I6WX66
E	-4	GLY	-	EXPRESSION TAG	UNP I6WX66
E	-3	PRO	-	EXPRESSION TAG	UNP I6WX66
E	-2	LEU	-	EXPRESSION TAG	UNP I6WX66
E	-1	GLY	-	EXPRESSION TAG	UNP I6WX66
E	0	SER	-	EXPRESSION TAG	UNP I6WX66
F	-4	GLY	-	EXPRESSION TAG	UNP I6WX66
F	-3	PRO	-	EXPRESSION TAG	UNP I6WX66
F	-2	LEU	-	EXPRESSION TAG	UNP I6WX66
F	-1	GLY	-	EXPRESSION TAG	UNP I6WX66
F	0	SER	-	EXPRESSION TAG	UNP I6WX66
G	-4	GLY	-	EXPRESSION TAG	UNP I6WX66
G	-3	PRO	-	EXPRESSION TAG	UNP I6WX66
G	-2	LEU	-	EXPRESSION TAG	UNP I6WX66
G	-1	GLY	-	EXPRESSION TAG	UNP I6WX66
G	0	SER	-	EXPRESSION TAG	UNP I6WX66
H	-4	GLY	-	EXPRESSION TAG	UNP I6WX66
H	-3	PRO	-	EXPRESSION TAG	UNP I6WX66
H	-2	LEU	-	EXPRESSION TAG	UNP I6WX66
H	-1	GLY	-	EXPRESSION TAG	UNP I6WX66
H	0	SER	-	EXPRESSION TAG	UNP I6WX66
I	-4	GLY	-	EXPRESSION TAG	UNP I6WX66
I	-3	PRO	-	EXPRESSION TAG	UNP I6WX66

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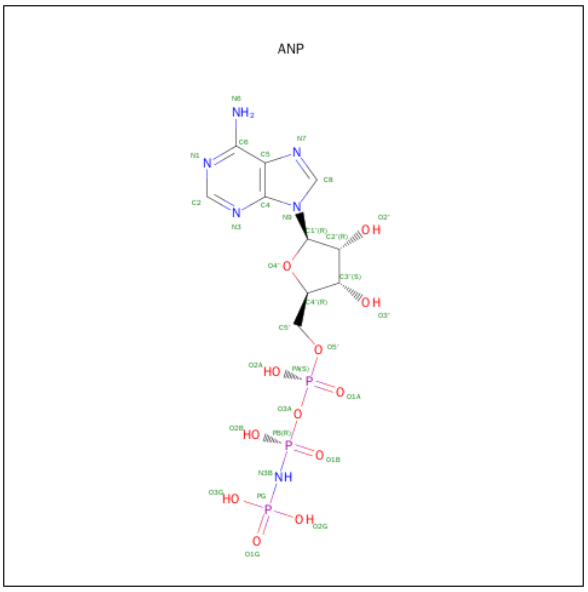
Chain	Residue	Modelled	Actual	Comment	Reference
I	-2	LEU	-	EXPRESSION TAG	UNP I6WX66
I	-1	GLY	-	EXPRESSION TAG	UNP I6WX66
I	0	SER	-	EXPRESSION TAG	UNP I6WX66
J	-4	GLY	-	EXPRESSION TAG	UNP I6WX66
J	-3	PRO	-	EXPRESSION TAG	UNP I6WX66
J	-2	LEU	-	EXPRESSION TAG	UNP I6WX66
J	-1	GLY	-	EXPRESSION TAG	UNP I6WX66
J	0	SER	-	EXPRESSION TAG	UNP I6WX66
K	-4	GLY	-	EXPRESSION TAG	UNP I6WX66
K	-3	PRO	-	EXPRESSION TAG	UNP I6WX66
K	-2	LEU	-	EXPRESSION TAG	UNP I6WX66
K	-1	GLY	-	EXPRESSION TAG	UNP I6WX66
K	0	SER	-	EXPRESSION TAG	UNP I6WX66
L	-4	GLY	-	EXPRESSION TAG	UNP I6WX66
L	-3	PRO	-	EXPRESSION TAG	UNP I6WX66
L	-2	LEU	-	EXPRESSION TAG	UNP I6WX66
L	-1	GLY	-	EXPRESSION TAG	UNP I6WX66
L	0	SER	-	EXPRESSION TAG	UNP I6WX66
M	-4	GLY	-	EXPRESSION TAG	UNP I6WX66
M	-3	PRO	-	EXPRESSION TAG	UNP I6WX66
M	-2	LEU	-	EXPRESSION TAG	UNP I6WX66
M	-1	GLY	-	EXPRESSION TAG	UNP I6WX66
M	0	SER	-	EXPRESSION TAG	UNP I6WX66
N	-4	GLY	-	EXPRESSION TAG	UNP I6WX66
N	-3	PRO	-	EXPRESSION TAG	UNP I6WX66
N	-2	LEU	-	EXPRESSION TAG	UNP I6WX66
N	-1	GLY	-	EXPRESSION TAG	UNP I6WX66
N	0	SER	-	EXPRESSION TAG	UNP I6WX66
O	-4	GLY	-	EXPRESSION TAG	UNP I6WX66
O	-3	PRO	-	EXPRESSION TAG	UNP I6WX66
O	-2	LEU	-	EXPRESSION TAG	UNP I6WX66
O	-1	GLY	-	EXPRESSION TAG	UNP I6WX66
O	0	SER	-	EXPRESSION TAG	UNP I6WX66
P	-4	GLY	-	EXPRESSION TAG	UNP I6WX66
P	-3	PRO	-	EXPRESSION TAG	UNP I6WX66
P	-2	LEU	-	EXPRESSION TAG	UNP I6WX66
P	-1	GLY	-	EXPRESSION TAG	UNP I6WX66
P	0	SER	-	EXPRESSION TAG	UNP I6WX66

- Molecule 2 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
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	G	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	H	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	I	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	J	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	K	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	L	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	M	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	N	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	1	Total	Mg	0	0
			1	1		
3	G	2	Total	Mg	0	0
			2	2		
3	J	1	Total	Mg	0	0
			1	1		
3	D	2	Total	Mg	0	0
			2	2		
3	K	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		
3	B	2	Total	Mg	0	0
			2	2		
3	I	1	Total	Mg	0	0
			1	1		
3	C	2	Total	Mg	0	0
			2	2		
3	A	1	Total	Mg	0	0
			1	1		
3	N	1	Total	Mg	0	0
			1	1		
3	O	1	Total	Mg	0	0
			1	1		
3	L	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		
3	M	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

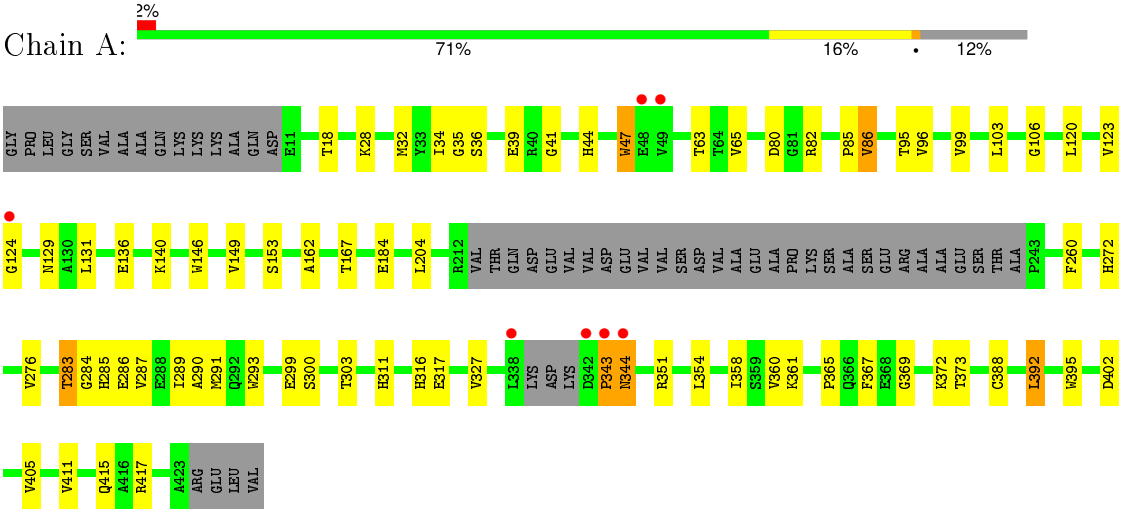
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	44	Total O 44 44	0	0
4	B	31	Total O 31 31	0	0
4	C	62	Total O 62 62	0	0
4	D	40	Total O 40 40	0	0
4	E	45	Total O 45 45	0	0
4	F	26	Total O 26 26	0	0
4	G	25	Total O 25 25	0	0
4	H	29	Total O 29 29	0	0
4	I	24	Total O 24 24	0	0
4	J	33	Total O 33 33	0	0
4	K	11	Total O 11 11	0	0
4	L	13	Total O 13 13	0	0
4	M	16	Total O 16 16	0	0
4	N	14	Total O 14 14	0	0
4	O	12	Total O 12 12	0	0
4	P	14	Total O 14 14	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.

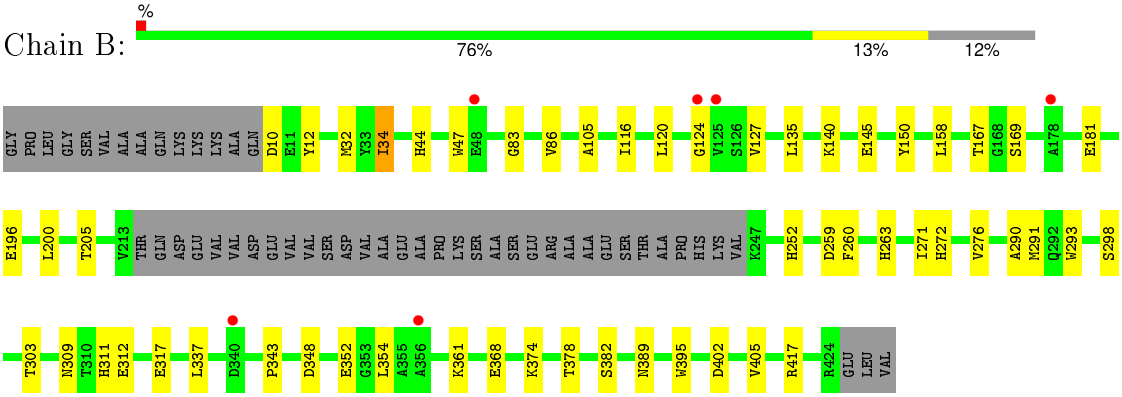
- Molecule 1: DNA GYRASE SUBUNIT B

Chain A:



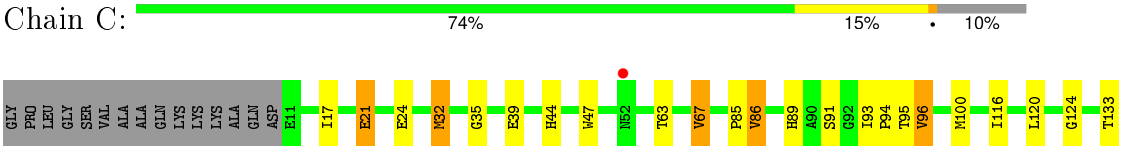
- Molecule 1: DNA GYRASE SUBUNIT B

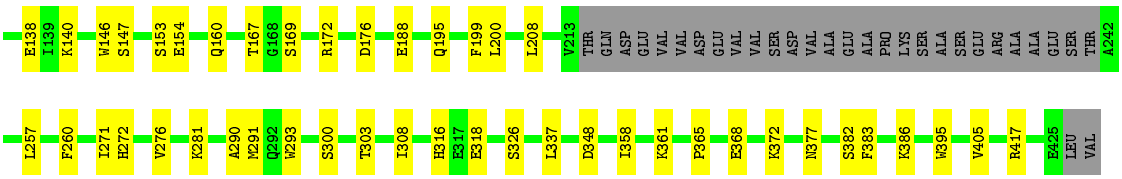
Chain B:



- Molecule 1: DNA GYRASE SUBUNIT B

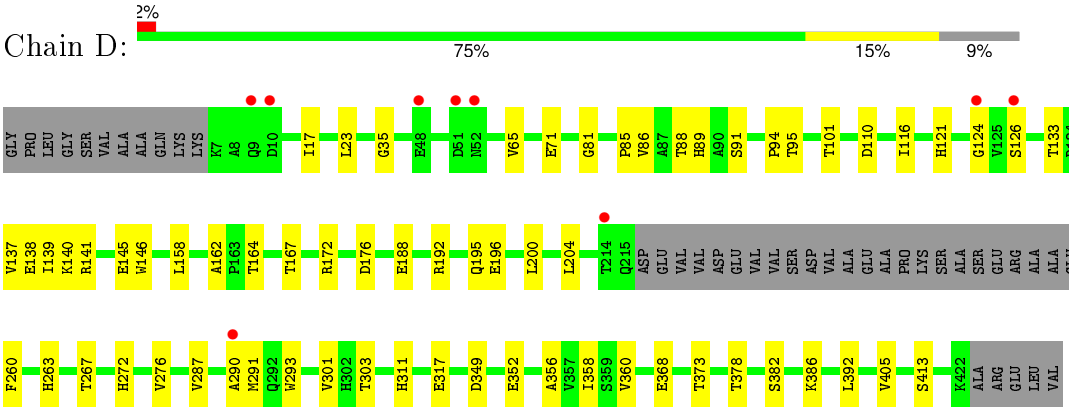
Chain C:





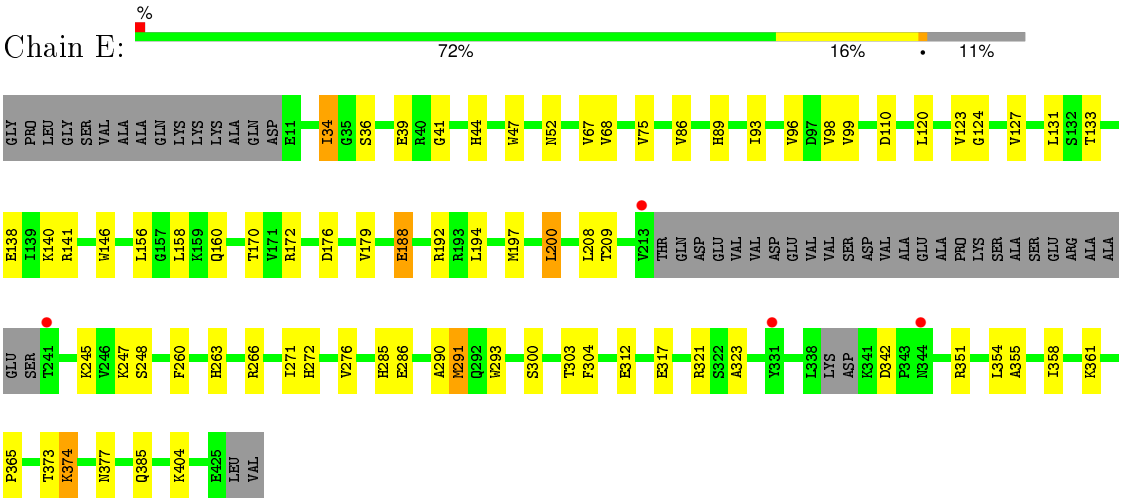
• Molecule 1: DNA GYRASE SUBUNIT B

Chain D:



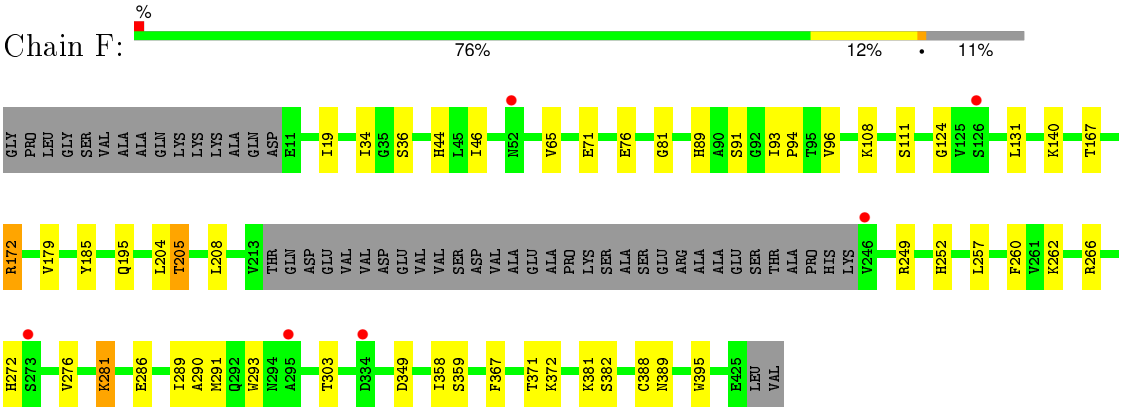
• Molecule 1: DNA GYRASE SUBUNIT B

Chain E:



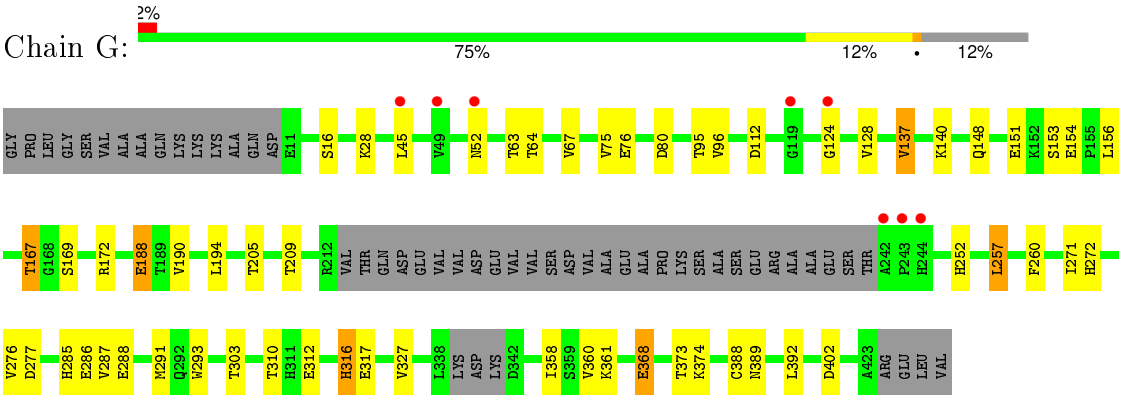
• Molecule 1: DNA GYRASE SUBUNIT B

Chain F:



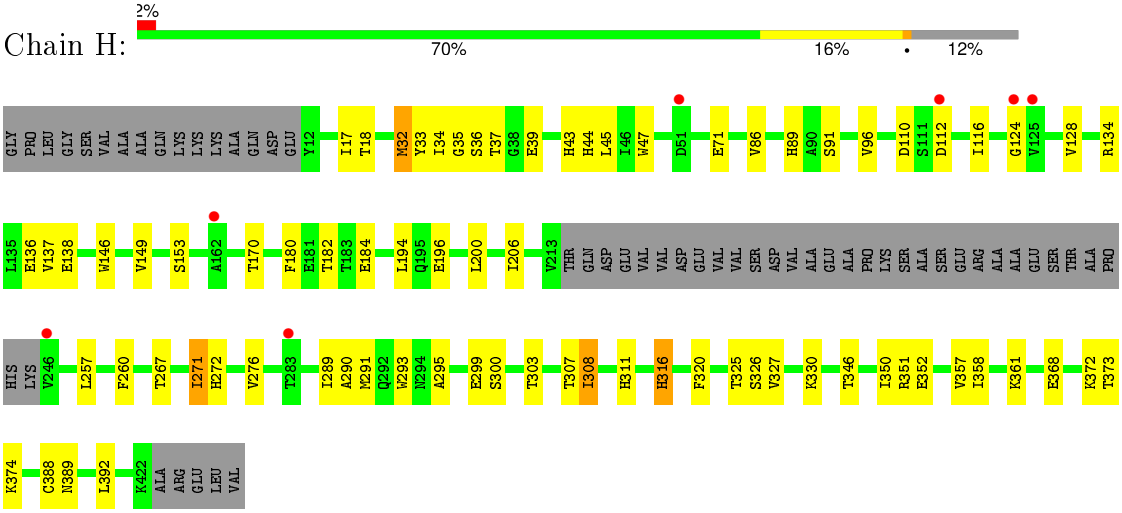
• Molecule 1: DNA GYRASE SUBUNIT B

Chain G:



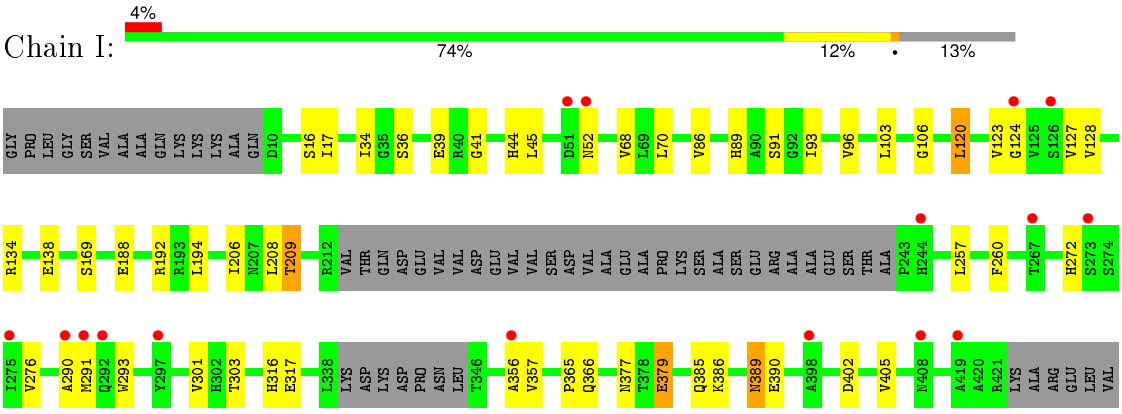
• Molecule 1: DNA GYRASE SUBUNIT B

Chain H:



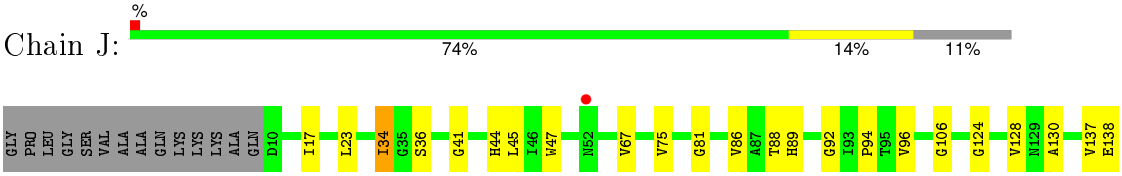
• Molecule 1: DNA GYRASE SUBUNIT B

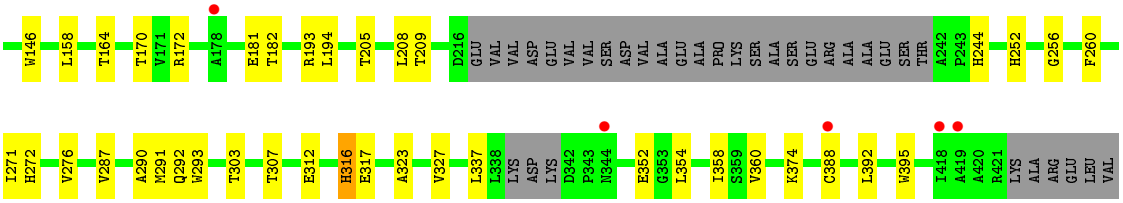
Chain I:



• Molecule 1: DNA GYRASE SUBUNIT B

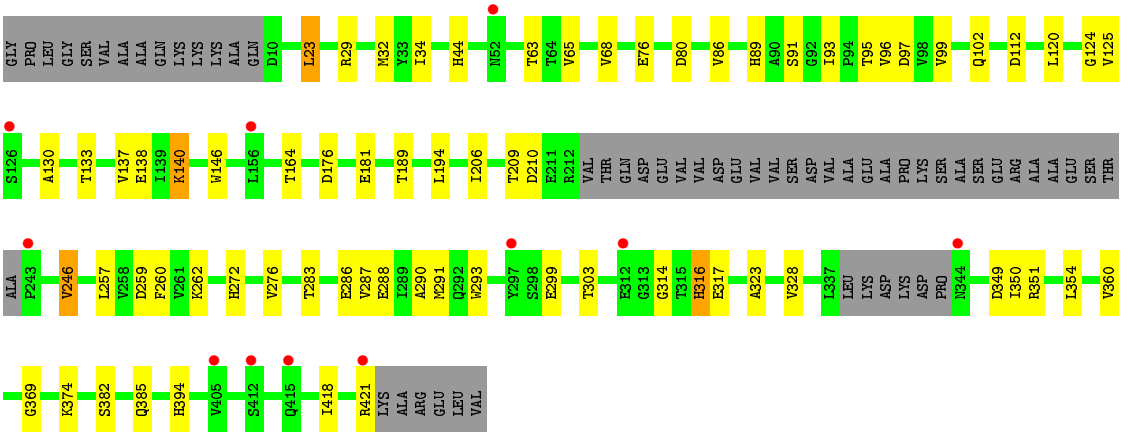
Chain J:





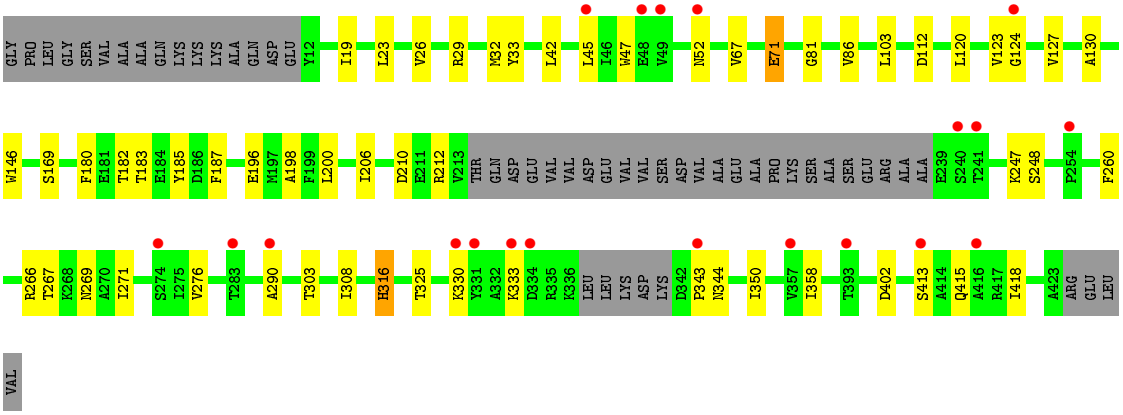
• Molecule 1: DNA GYRASE SUBUNIT B

Chain K:



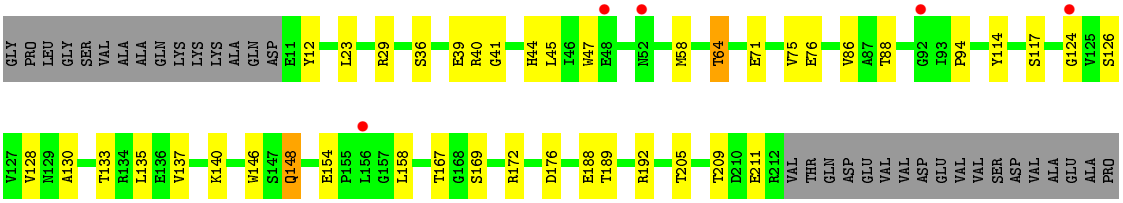
• Molecule 1: DNA GYRASE SUBUNIT B

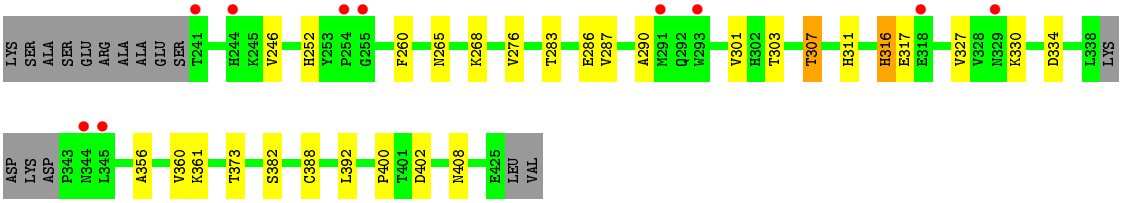
Chain L:



• Molecule 1: DNA GYRASE SUBUNIT B

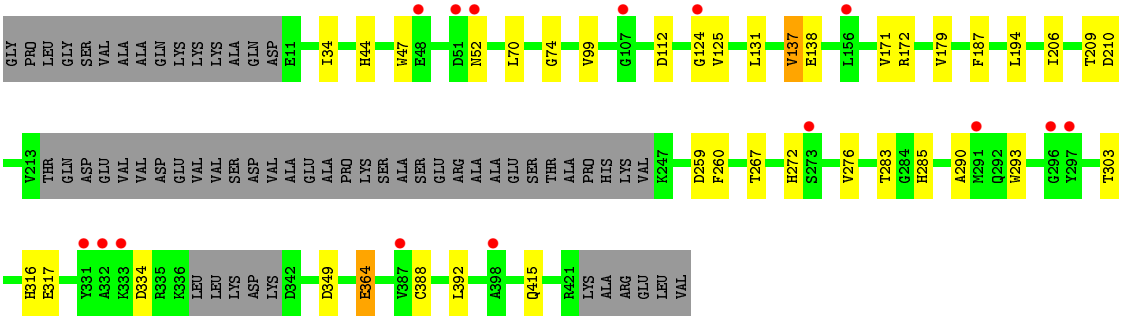
Chain M:





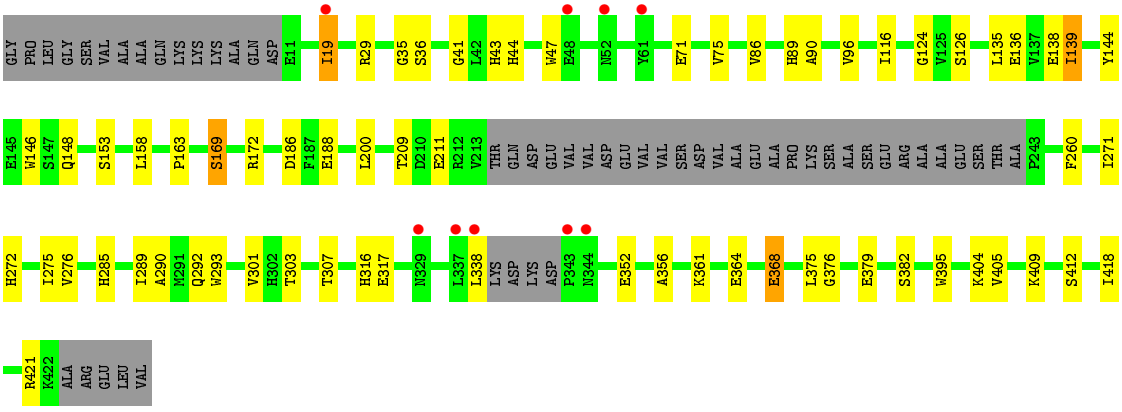
• Molecule 1: DNA GYRASE SUBUNIT B

Chain N:



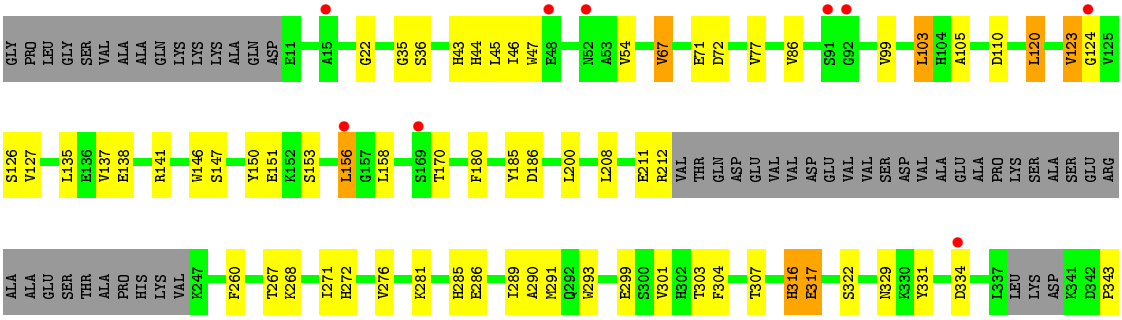
• Molecule 1: DNA GYRASE SUBUNIT B

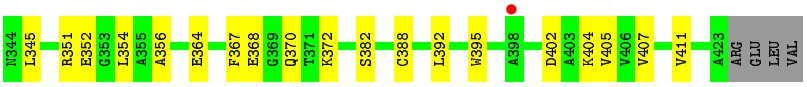
Chain O:



• Molecule 1: DNA GYRASE SUBUNIT B

Chain P:




N344
L345
R351
E352
G353
L354
A355
A356
E364
F367
E368
G369
Q370
T371
K372
S382
C388
L392
W395
A398
D402
A403
K404
V405
V406
V407
V411
A423
ARG
GLU
LEU
VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	101.36Å 138.20Å 147.69Å 105.28° 92.31° 107.23°	Depositor
Resolution (Å)	24.94 – 2.90 24.94 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.2 (24.94-2.90) 88.3 (24.94-2.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 2.89Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.182 , 0.240 0.195 , 0.253	Depositor DCC
R_{free} test set	7966 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	66.0	Xtriage
Anisotropy	0.668	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 46.4	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 159161 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	46952	wwPDB-VP
Average B, all atoms (Å^2)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.69% 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	0.45	0/2942	0.68	0/3991
1	B	0.44	0/2928	0.66	0/3978
1	C	0.46	0/2994	0.69	0/4062
1	D	0.44	0/3010	0.67	0/4091
1	E	0.46	0/2967	0.69	0/4030
1	F	0.43	0/2942	0.64	0/3997
1	G	0.42	0/2919	0.65	0/3967
1	H	0.43	0/2920	0.66	0/3966
1	I	0.41	0/2881	0.65	0/3913
1	J	0.44	0/2938	0.69	0/3993
1	K	0.44	0/2892	0.65	0/3927
1	L	0.47	0/2916	0.65	0/3963
1	M	0.43	0/2943	0.65	0/3995
1	N	0.43	0/2869	0.65	0/3896
1	O	0.42	0/2931	0.65	0/3975
1	P	0.43	0/2875	0.65	0/3907
All	All	0.44	0/46867	0.66	0/63651

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2887	0	2803	35	0
1	B	2874	0	2760	26	0
1	C	2938	0	2857	33	0
1	D	2954	0	2823	30	0
1	E	2912	0	2795	39	0
1	F	2888	0	2772	20	0
1	G	2864	0	2755	28	0
1	H	2866	0	2764	33	0
1	I	2827	0	2701	25	0
1	J	2884	0	2769	33	0
1	K	2838	0	2730	34	0
1	L	2862	0	2749	21	0
1	M	2888	0	2784	30	0
1	N	2816	0	2714	15	0
1	O	2877	0	2791	32	0
1	P	2822	0	2700	39	0
2	A	31	0	13	1	0
2	B	31	0	13	0	0
2	C	31	0	13	0	0
2	D	31	0	13	0	0
2	E	31	0	13	1	0
2	F	31	0	13	1	0
2	G	31	0	13	1	0
2	H	31	0	13	0	0
2	I	31	0	13	2	0
2	J	31	0	13	1	0
2	K	31	0	13	1	0
2	L	31	0	13	1	0
2	M	31	0	13	0	0
2	N	31	0	13	0	0
2	O	31	0	13	2	0
2	P	31	0	13	0	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	2	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
4	A	44	0	0	0	0
4	B	31	0	0	0	0
4	C	62	0	0	0	0
4	D	40	0	0	1	0
4	E	45	0	0	0	0
4	F	26	0	0	0	0
4	G	25	0	0	1	0
4	H	29	0	0	0	0
4	I	24	0	0	0	0
4	J	33	0	0	0	0
4	K	11	0	0	0	0
4	L	13	0	0	0	0
4	M	16	0	0	0	0
4	N	14	0	0	0	0
4	O	12	0	0	1	0
4	P	14	0	0	0	0
All	All	46952	0	44475	450	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 5.

The worst 5 of 450 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)
2:O:601:ANP:H5'2	2:O:601:ANP:H8	1.55	0.87
1:P:272:HIS:HE1	1:P:293:TRP:H	1.22	0.85
1:A:287:VAL:HG23	1:A:360:VAL:HG12	1.61	0.82
1:C:89:HIS:HD2	1:C:91:SER:HB2	1.44	0.81
1:H:272:HIS:HE1	1:H:293:TRP:H	1.28	0.80

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	374/432 (87%)	354 (95%)	17 (4%)	3 (1%)	24	60
1	B	378/432 (88%)	362 (96%)	13 (3%)	3 (1%)	24	60
1	C	383/432 (89%)	368 (96%)	13 (3%)	2 (0%)	34	71
1	D	388/432 (90%)	375 (97%)	11 (3%)	2 (0%)	34	71
1	E	380/432 (88%)	365 (96%)	14 (4%)	1 (0%)	46	79
1	F	379/432 (88%)	366 (97%)	11 (3%)	2 (0%)	34	71
1	G	375/432 (87%)	361 (96%)	13 (4%)	1 (0%)	46	79
1	H	375/432 (87%)	360 (96%)	13 (4%)	2 (0%)	34	71
1	I	369/432 (85%)	355 (96%)	12 (3%)	2 (0%)	34	71
1	J	378/432 (88%)	360 (95%)	13 (3%)	5 (1%)	15	46
1	K	370/432 (86%)	351 (95%)	17 (5%)	2 (0%)	34	71
1	L	376/432 (87%)	356 (95%)	17 (4%)	3 (1%)	24	60
1	M	377/432 (87%)	358 (95%)	18 (5%)	1 (0%)	46	79
1	N	367/432 (85%)	350 (95%)	16 (4%)	1 (0%)	46	79
1	O	373/432 (86%)	358 (96%)	14 (4%)	1 (0%)	46	79
1	P	370/432 (86%)	353 (95%)	14 (4%)	3 (1%)	24	60
All	All	6012/6912 (87%)	5752 (96%)	226 (4%)	34 (1%)	30	67

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	344	ASN
1	L	343	PRO
1	B	124	GLY
1	D	124	GLY
1	E	124	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	302/350 (86%)	283 (94%)	19 (6%)	22	54
1	B	297/350 (85%)	285 (96%)	12 (4%)	38	74
1	C	307/350 (88%)	283 (92%)	24 (8%)	16	41
1	D	306/350 (87%)	287 (94%)	19 (6%)	23	55
1	E	302/350 (86%)	283 (94%)	19 (6%)	22	54
1	F	299/350 (85%)	280 (94%)	19 (6%)	22	53
1	G	296/350 (85%)	275 (93%)	21 (7%)	18	47
1	H	299/350 (85%)	277 (93%)	22 (7%)	17	44
1	I	293/350 (84%)	274 (94%)	19 (6%)	21	52
1	J	298/350 (85%)	283 (95%)	15 (5%)	30	65
1	K	295/350 (84%)	278 (94%)	17 (6%)	25	58
1	L	297/350 (85%)	275 (93%)	22 (7%)	17	44
1	M	299/350 (85%)	277 (93%)	22 (7%)	17	44
1	N	293/350 (84%)	278 (95%)	15 (5%)	29	65
1	O	301/350 (86%)	281 (93%)	20 (7%)	21	51
1	P	292/350 (83%)	263 (90%)	29 (10%)	10	29
All	All	4776/5600 (85%)	4462 (93%)	314 (7%)	21	51

5 of 314 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	196	GLU
1	J	67	VAL
1	P	123	VAL
1	H	300	SER
1	I	93	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 83 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	44	HIS
1	I	408	ASN
1	O	415	GLN
1	H	89	HIS
1	I	89	HIS

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 36 ligands modelled in this entry, 20 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
2	ANP	A	601	3	27,33,33	4.12	11 (40%)	30,52,52	2.33	4 (13%)
2	ANP	B	601	3	27,33,33	4.27	11 (40%)	30,52,52	2.73	6 (20%)
2	ANP	C	601	3	27,33,33	4.14	11 (40%)	30,52,52	2.43	7 (23%)
2	ANP	D	601	3	27,33,33	4.02	11 (40%)	30,52,52	2.40	4 (13%)
2	ANP	E	601	3	27,33,33	4.19	11 (40%)	30,52,52	2.67	3 (10%)
2	ANP	F	601	3	27,33,33	4.10	11 (40%)	30,52,52	2.30	4 (13%)
2	ANP	G	601	3	27,33,33	4.12	11 (40%)	30,52,52	2.33	4 (13%)
2	ANP	H	601	3	27,33,33	4.19	10 (37%)	30,52,52	2.40	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	ANP	I	601	3	27,33,33	4.13	11 (40%)	30,52,52	2.50	5 (16%)
2	ANP	J	601	3	27,33,33	4.07	10 (37%)	30,52,52	2.44	5 (16%)
2	ANP	K	601	3	27,33,33	4.07	11 (40%)	30,52,52	2.39	5 (16%)
2	ANP	L	601	3	27,33,33	4.09	9 (33%)	30,52,52	2.27	7 (23%)
2	ANP	M	601	3	27,33,33	4.23	12 (44%)	30,52,52	2.47	7 (23%)
2	ANP	N	601	3	27,33,33	4.20	10 (37%)	30,52,52	2.38	4 (13%)
2	ANP	O	601	3	27,33,33	4.14	11 (40%)	30,52,52	2.40	7 (23%)
2	ANP	P	601	3	27,33,33	4.19	10 (37%)	30,52,52	2.55	7 (23%)

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
2	ANP	A	601	3	-	1/12/38/38	0/3/3/3
2	ANP	B	601	3	-	0/12/38/38	0/3/3/3
2	ANP	C	601	3	-	0/12/38/38	0/3/3/3
2	ANP	D	601	3	-	0/12/38/38	0/3/3/3
2	ANP	E	601	3	-	0/12/38/38	0/3/3/3
2	ANP	F	601	3	-	0/12/38/38	0/3/3/3
2	ANP	G	601	3	-	0/12/38/38	0/3/3/3
2	ANP	H	601	3	-	0/12/38/38	0/3/3/3
2	ANP	I	601	3	-	0/12/38/38	0/3/3/3
2	ANP	J	601	3	-	1/12/38/38	0/3/3/3
2	ANP	K	601	3	-	0/12/38/38	0/3/3/3
2	ANP	L	601	3	-	0/12/38/38	0/3/3/3
2	ANP	M	601	3	-	0/12/38/38	0/3/3/3
2	ANP	N	601	3	-	0/12/38/38	0/3/3/3
2	ANP	O	601	3	-	0/12/38/38	0/3/3/3
2	ANP	P	601	3	-	0/12/38/38	0/3/3/3

The worst 5 of 171 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	601	ANP	PG-N3B	-4.21	1.52	1.63
2	M	601	ANP	PG-N3B	-4.16	1.52	1.63
2	A	601	ANP	PG-N3B	-4.16	1.52	1.63
2	C	601	ANP	PG-N3B	-4.11	1.52	1.63
2	N	601	ANP	PG-N3B	-4.09	1.52	1.63

The worst 5 of 84 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	ANP	N3-C2-N1	-13.11	118.86	128.89
2	E	601	ANP	N3-C2-N1	-12.57	119.27	128.89
2	J	601	ANP	N3-C2-N1	-11.68	119.95	128.89
2	H	601	ANP	N3-C2-N1	-11.50	120.09	128.89
2	I	601	ANP	N3-C2-N1	-11.39	120.17	128.89

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	601	ANP	O1G-PG-N3B-PB
2	A	601	ANP	O1G-PG-N3B-PB

There are no ring outliers.

9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	ANP	1	0
2	E	601	ANP	1	0
2	F	601	ANP	1	0
2	G	601	ANP	1	0
2	I	601	ANP	2	0
2	J	601	ANP	1	0
2	K	601	ANP	1	0
2	L	601	ANP	1	0
2	O	601	ANP	2	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	380/432 (87%)	-0.31	7 (1%)	71	68	53, 85, 146, 167	0
1	B	382/432 (88%)	-0.23	6 (1%)	74	72	49, 93, 147, 176	0
1	C	387/432 (89%)	-0.38	1 (0%)	94	94	50, 72, 122, 151	0
1	D	392/432 (90%)	-0.30	9 (2%)	64	59	51, 79, 132, 170	0
1	E	386/432 (89%)	-0.37	4 (1%)	84	82	50, 78, 132, 161	0
1	F	383/432 (88%)	-0.24	6 (1%)	74	72	65, 96, 138, 156	0
1	G	381/432 (88%)	-0.27	8 (2%)	67	62	67, 93, 122, 156	0
1	H	379/432 (87%)	-0.23	7 (1%)	71	68	64, 91, 122, 137	0
1	I	375/432 (86%)	-0.06	16 (4%)	39	32	66, 101, 176, 192	0
1	J	384/432 (88%)	-0.37	6 (1%)	74	72	56, 83, 144, 172	0
1	K	376/432 (87%)	-0.02	11 (2%)	55	49	71, 104, 176, 190	0
1	L	382/432 (88%)	0.13	20 (5%)	31	24	74, 112, 180, 195	0
1	M	383/432 (88%)	-0.10	15 (3%)	43	36	78, 108, 145, 166	0
1	N	373/432 (86%)	-0.03	15 (4%)	42	35	74, 109, 152, 173	0
1	O	379/432 (87%)	-0.18	9 (2%)	62	57	78, 100, 131, 161	0
1	P	376/432 (87%)	-0.13	10 (2%)	58	52	76, 108, 139, 151	0
All	All	6098/6912 (88%)	-0.19	150 (2%)	61	55	49, 96, 149, 195	0

The worst 5 of 150 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	246	VAL	5.4
1	F	246	VAL	5.3
1	O	338	LEU	4.9
1	A	343	PRO	4.6
1	I	356	ALA	4.5

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
3	MG	C	1001	1/1	0.92	0.42	3.87	85,85,85,85	0
3	MG	I	602	1/1	0.99	0.66	3.82	82,82,82,82	0
3	MG	J	602	1/1	0.98	0.47	2.43	60,60,60,60	0
3	MG	P	602	1/1	0.95	0.44	1.81	97,97,97,97	0
2	ANP	E	601	31/31	0.98	0.27	1.41	62,69,73,76	0
3	MG	A	602	1/1	0.99	0.41	1.24	50,50,50,50	0
2	ANP	O	601	31/31	0.95	0.32	1.07	98,102,105,106	0
3	MG	L	602	1/1	0.93	0.43	1.06	74,74,74,74	0
3	MG	O	602	1/1	0.96	0.44	0.96	76,76,76,76	0
2	ANP	F	601	31/31	0.96	0.27	0.89	72,90,100,102	0
3	MG	F	602	1/1	0.98	0.33	0.89	53,53,53,53	0
2	ANP	P	601	31/31	0.96	0.28	0.81	94,98,108,111	0
2	ANP	I	601	31/31	0.96	0.28	0.79	70,75,80,83	0
2	ANP	C	601	31/31	0.98	0.26	0.75	43,56,63,65	0
2	ANP	J	601	31/31	0.98	0.25	0.71	49,63,68,69	0
2	ANP	A	601	31/31	0.98	0.27	0.63	56,65,76,81	0
2	ANP	N	601	31/31	0.98	0.29	0.59	81,89,95,97	0
2	ANP	M	601	31/31	0.98	0.28	0.56	76,87,92,93	0
2	ANP	K	601	31/31	0.96	0.25	0.53	90,96,104,106	0
2	ANP	H	601	31/31	0.97	0.24	0.50	69,77,80,83	0
2	ANP	L	601	31/31	0.97	0.25	0.24	74,92,98,99	0
2	ANP	B	601	31/31	0.96	0.23	0.23	56,81,90,93	0
3	MG	H	602	1/1	0.99	0.30	0.20	58,58,58,58	0
2	ANP	D	601	31/31	0.97	0.23	0.06	58,64,68,74	0
2	ANP	G	601	31/31	0.97	0.22	0.06	63,78,82,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	MG	K	602	1/1	0.96	0.29	0.06	54,54,54,54	0
3	MG	N	602	1/1	0.99	0.32	-0.13	75,75,75,75	0
3	MG	D	602	1/1	0.90	0.30	-0.15	58,58,58,58	0
3	MG	C	602	1/1	0.98	0.29	-0.23	51,51,51,51	0
3	MG	M	602	1/1	0.98	0.30	-0.24	51,51,51,51	0
3	MG	G	602	1/1	0.96	0.24	-0.60	63,63,63,63	0
3	MG	E	602	1/1	0.98	0.22	-0.83	56,56,56,56	0
3	MG	G	1001	1/1	0.97	0.10	-0.89	76,76,76,76	0
3	MG	D	1001	1/1	0.96	0.07	-	78,78,78,78	0
3	MG	B	1001	1/1	0.86	0.17	-	83,83,83,83	0
3	MG	B	602	1/1	0.95	0.29	-	57,57,57,57	0

6.5 Other polymers (i)

There are no such residues in this entry.