



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:12 PM GMT

PDB ID : 1EI1  
Title : DIMERIZATION OF E. COLI DNA GYRASE B PROVIDES A STRUCTURAL MECHANISM FOR ACTIVATING THE ATPASE CATALYTIC CENTER  
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Deposited on : 2000-02-23  
Resolution : 2.30 Å(reported)

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

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

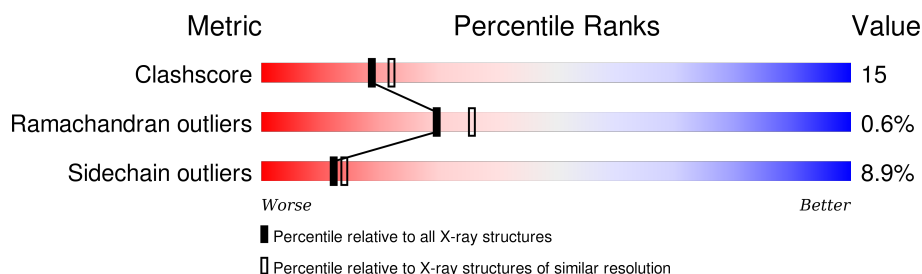
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	391	
1	B	391	

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	SO4	A	1081	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6674 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.

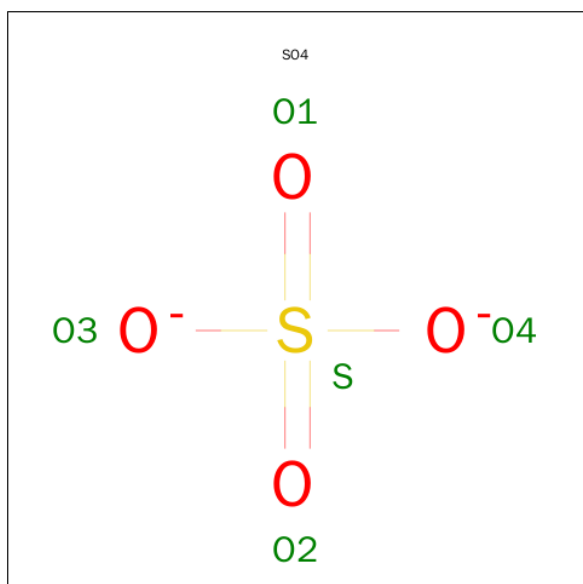
- Molecule 1 is a protein called DNA GYRASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	2	0
			3040	1901	537	592	10			
1	B	391	Total	C	N	O	S	0	2	0
			3040	1901	537	592	10			

There are 4 discrepancies between the modelled and reference sequences:

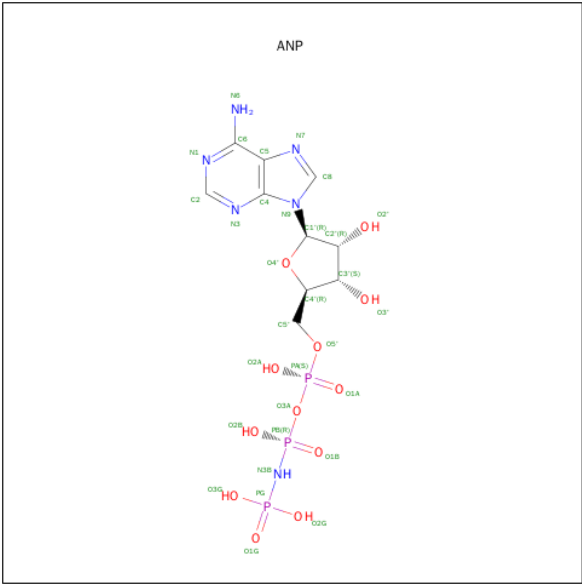
Chain	Residue	Modelled	Actual	Comment	Reference
A	5	SER	TYR	ENGINEERED	UNP P06982
A	198	ASP	ASN	CONFLICT	UNP P06982
B	405	SER	TYR	ENGINEERED	UNP P06982
B	598	ASP	ASN	CONFLICT	UNP P06982

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

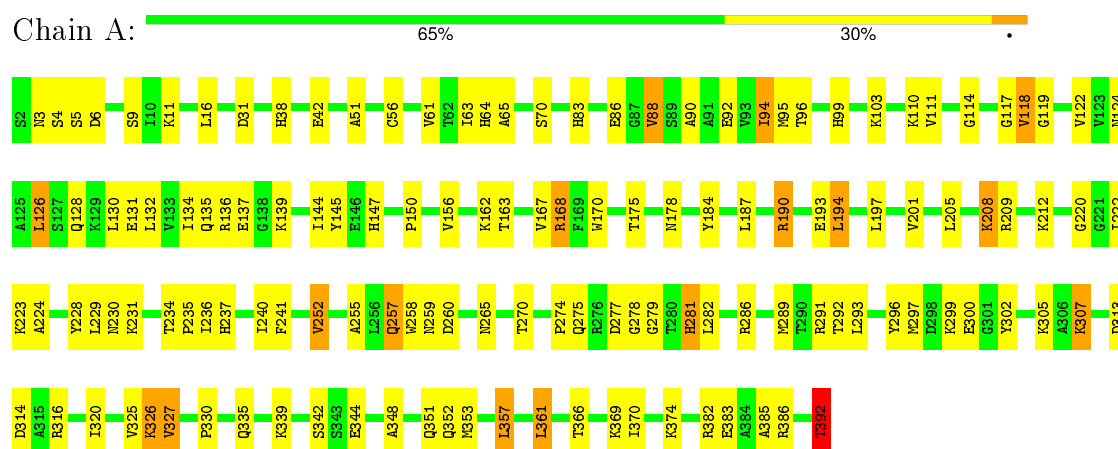
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	231	Total	O	0	0
			231	231		
5	B	274	Total	O	0	0
			274	274		

### 3 Residue-property plots

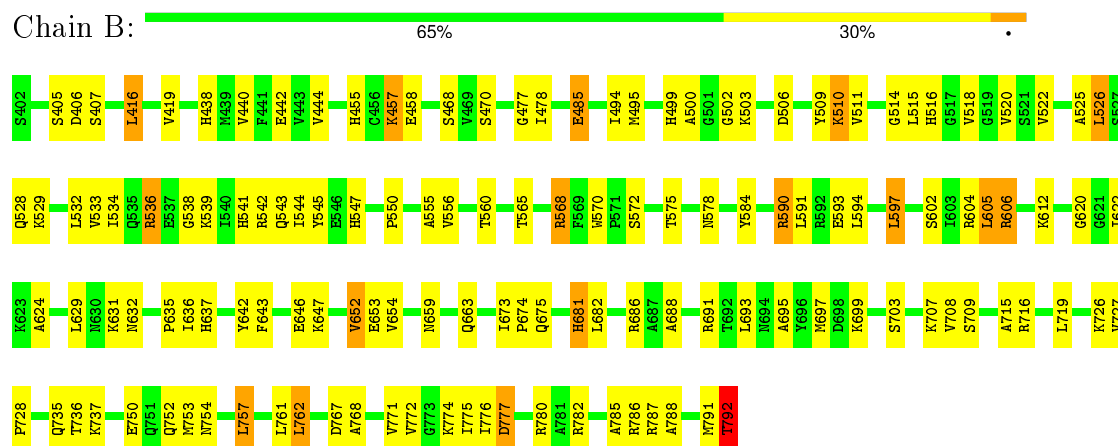
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

#### • Molecule 1: DNA GYRASE B



#### • Molecule 1: DNA GYRASE B



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.70 Å   137.40 Å   78.90 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	6.00 – 2.30	Depositor
% Data completeness (in resolution range)	65.1 (6.00-2.30)	Depositor
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.166 , 0.266	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6674	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ANP, SO4

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	0.53	1/3101 (0.0%)	0.65	0/4183
1	B	0.67	1/3101 (0.0%)	0.66	0/4183
All	All	0.60	2/6202 (0.0%)	0.66	0/8366

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	792	THR	C-OXT	30.20	1.80	1.23
1	A	392	THR	C-OXT	19.80	1.60	1.23

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	3040	0	3010	94	0
1	B	3040	0	3010	101	0
2	A	10	0	0	2	0
2	B	5	0	0	0	0
3	A	31	0	12	3	0
3	B	31	0	12	5	0
4	A	6	0	8	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	6	0	8	2	0
5	A	231	0	0	1	0
5	B	274	0	0	6	0
All	All	6674	0	6060	189	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 15.

All (189) 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:B:792:THR:C	1:B:792:THR:OXT	1.80	1.18
1:B:792:THR:CA	1:B:792:THR:OXT	1.95	1.14
1:B:792:THR:O	1:B:792:THR:OXT	1.67	1.08
1:B:792:THR:N	1:B:792:THR:OXT	2.08	0.86
1:A:327:VAL:HG22	1:A:330:PRO:HG3	1.58	0.83
1:B:792:THR:CB	1:B:792:THR:OXT	2.25	0.83
1:B:416:LEU:HG	1:B:525:ALA:HB2	1.60	0.81
1:B:470:SER:HB3	1:B:568:ARG:HG3	1.65	0.79
1:B:647:LYS:HG3	1:B:752:GLN:NE2	1.98	0.78
1:B:709:SER:HB3	1:B:782:ARG:HH22	1.48	0.77
1:B:528:GLN:HG3	1:B:572:SER:HA	1.66	0.76
1:A:111:VAL:HG11	1:A:326[A]:LYS:HG3	1.69	0.74
1:A:279:GLY:HA2	1:A:339:LYS:HE3	1.69	0.74
1:A:111:VAL:HG11	1:A:326[B]:LYS:HG3	1.69	0.73
1:A:168:ARG:HD2	1:A:170:TRP:CH2	2.26	0.71
1:A:220:GLY:HA3	1:A:224:ALA:HB2	1.71	0.71
1:B:568:ARG:HD2	1:B:570:TRP:CH2	2.26	0.70
1:A:234:THR:HB	1:A:260:ASP:OD1	1.91	0.70
1:B:715:ALA:HA	1:B:775:ILE:HD12	1.73	0.69
1:A:275:GLN:HE21	1:A:281:HIS:HE1	1.38	0.69
1:B:647:LYS:HG3	1:B:752:GLN:HE22	1.58	0.69
1:A:70:SER:HB3	1:A:168:ARG:CG	2.24	0.67
1:A:236:ILE:HD13	1:A:374:LYS:HD2	1.75	0.67
1:A:357:LEU:O	1:A:361:LEU:HD22	1.95	0.67
1:B:691:ARG:HE	1:B:754:ASN:ND2	1.94	0.65
1:A:237:HIS:HE1	1:A:258:TRP:H	1.45	0.63
1:A:132:LEU:HD21	1:A:134:ILE:HD11	1.82	0.62
1:A:126:LEU:HG	1:A:175:THR:HG21	1.81	0.61
4:A:2031:GOL:H31	1:B:405:SER:HB3	1.82	0.61
1:A:265:ASN:HB2	1:A:320:ILE:HG12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:545:TYR:HE1	1:B:550:PRO:HG3	1.65	0.61
1:A:228:TYR:O	1:A:231:LYS:HG2	2.01	0.61
1:A:145:TYR:CE1	1:A:150:PRO:HG3	2.36	0.60
1:B:494:ILE:HD12	1:B:520:VAL:HG11	1.83	0.60
1:A:383:GLU:HA	1:A:386:ARG:HB3	1.83	0.60
1:A:118:VAL:HG13	1:A:122:VAL:HG23	1.82	0.60
1:B:547:HIS:HD2	5:B:4133:HOH:O	1.84	0.60
1:B:591:LEU:HD12	1:B:605:LEU:HG	1.84	0.60
2:A:1081:SO4:O2	1:B:406:ASP:HA	2.01	0.60
1:A:6:ASP:O	1:A:9:SER:HB3	2.01	0.60
1:A:223:LYS:HE3	1:A:240:ILE:HB	1.84	0.60
1:B:675:GLN:NE2	1:B:681:HIS:HE1	1.99	0.60
1:A:353:MET:O	1:A:357:LEU:HB2	2.02	0.59
1:A:259:ASN:O	1:A:374:LYS:HE3	2.02	0.59
1:B:675:GLN:HE21	1:B:681:HIS:HE1	1.50	0.59
1:B:681:HIS:HD2	1:B:682:LEU:H	1.51	0.59
1:B:518:VAL:O	1:B:522:VAL:HG23	2.04	0.58
1:B:636:ILE:HD13	1:B:774:LYS:HD2	1.86	0.57
1:B:708:VAL:HG21	1:B:776:ILE:HG23	1.87	0.57
1:B:768:ALA:O	1:B:772:VAL:HG23	2.06	0.56
1:B:478:ILE:HB	1:B:534:ILE:HD13	1.87	0.56
1:A:366:THR:O	1:A:370:ILE:HG13	2.07	0.55
1:B:584:TYR:CZ	1:B:605:LEU:HD13	2.41	0.55
1:A:230:ASN:ND2	1:A:257:GLN:HG2	2.22	0.55
1:A:83:HIS:HB3	1:A:86:GLU:HB2	1.89	0.55
1:A:139:LYS:HD2	1:A:156:VAL:HG11	1.88	0.54
1:B:438:HIS:CD2	1:B:736:THR:HG22	2.42	0.54
1:A:135:GLN:O	1:A:163:THR:HA	2.08	0.54
1:B:777:ASP:HA	1:B:780:ARG:HD3	1.89	0.54
1:B:622:ILE:HD11	1:B:653:GLU:HG2	1.91	0.53
1:A:292:THR:HG21	1:A:357:LEU:HB3	1.91	0.53
1:A:70:SER:HB3	1:A:168:ARG:HG3	1.90	0.53
1:A:369:LYS:HG3	1:A:370:ILE:N	2.24	0.53
1:B:438:HIS:O	1:B:442:GLU:HG2	2.09	0.53
1:B:502:GLY:N	3:B:794:ANP:O3'	2.42	0.53
1:B:526:LEU:HG	1:B:575:THR:HG21	1.91	0.53
1:B:545:TYR:CE1	1:B:550:PRO:HG3	2.44	0.53
1:A:383:GLU:HB3	1:A:386:ARG:NH1	2.24	0.53
1:A:351:GLN:HB3	5:A:3191:HOH:O	2.07	0.53
1:B:485:GLU:HB3	5:B:1581:HOH:O	2.08	0.52
1:B:478:ILE:HB	1:B:534:ILE:CD1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:590:ARG:O	1:B:593:GLU:HG2	2.10	0.52
1:A:190:ARG:O	1:A:193:GLU:HG2	2.09	0.52
1:A:293:LEU:O	1:A:297:MET:HG3	2.10	0.52
1:B:478:ILE:HD13	1:B:494:ILE:HD11	1.91	0.51
1:A:83:HIS:ND1	1:A:86:GLU:HG2	2.24	0.51
1:A:385:ALA:HB1	1:B:785:ALA:HB1	1.90	0.51
1:B:771:VAL:O	1:B:775:ILE:HG12	2.11	0.51
1:A:135:GLN:OE1	1:A:162:LYS:HE3	2.12	0.50
1:A:94:ILE:HG13	1:A:95:MET:N	2.26	0.50
1:B:631:LYS:HE3	1:B:632:ASN:OD1	2.11	0.50
1:A:278:GLY:O	1:A:339:LYS:HA	2.11	0.50
1:A:90:ALA:O	1:A:94:ILE:HG23	2.11	0.50
1:B:534:ILE:O	1:B:541:HIS:HD2	1.95	0.50
1:A:16:LEU:HD21	1:A:96:THR:HA	1.94	0.50
1:B:604:ARG:HD2	5:B:4195:HOH:O	2.12	0.50
1:B:709:SER:HB3	1:B:782:ARG:NH2	2.23	0.49
1:B:514:GLY:CA	3:B:794:ANP:HNB1	2.25	0.49
1:B:538:GLY:HA2	1:B:560:THR:O	2.12	0.49
1:A:70:SER:HB3	1:A:168:ARG:HG2	1.92	0.49
1:B:543:GLN:NE2	1:B:545:TYR:OH	2.45	0.49
1:A:103:LYS:NZ	3:A:394:ANP:H3'	2.28	0.49
1:A:296:TYR:HA	1:A:299:LYS:HE2	1.94	0.49
1:A:5:SER:HB2	4:B:1031:GOL:O3	2.12	0.49
1:B:529:LYS:HA	1:B:545:TYR:O	2.13	0.48
1:A:51:ALA:HB1	1:A:201:VAL:HG21	1.95	0.48
1:B:631:LYS:HG3	1:B:632:ASN:N	2.28	0.48
1:A:118:VAL:HG13	1:A:122:VAL:CG2	2.43	0.48
1:B:635:PRO:HA	1:B:659:ASN:HA	1.95	0.48
1:B:681:HIS:CD2	1:B:682:LEU:H	2.31	0.48
1:B:542:ARG:CZ	1:B:544:ILE:HD11	2.43	0.48
1:A:124:ASN:HB2	1:A:130:LEU:HD13	1.95	0.48
1:A:281:HIS:HD2	1:A:282:LEU:H	1.60	0.48
1:A:128:GLN:HA	1:A:147:HIS:CD2	2.48	0.48
1:A:241:PHE:O	1:A:255:ALA:HA	2.14	0.48
1:B:642:TYR:HA	1:B:654:VAL:O	2.14	0.47
1:B:506:ASP:HB2	1:B:510:LYS:HA	1.95	0.47
1:A:70:SER:HA	1:A:167:VAL:O	2.15	0.47
1:A:65:ALA:HA	1:A:209:ARG:HG2	1.96	0.47
1:A:385:ALA:HA	1:B:788:ALA:HB3	1.97	0.47
1:A:99:HIS:N	1:A:117:GLY:O	2.48	0.47
1:A:252:VAL:HG11	1:A:352:GLN:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ASP:O	1:A:178:ASN:HB3	2.14	0.47
1:A:131:GLU:HG3	1:A:144:ILE:HD11	1.97	0.47
1:B:590:ARG:CZ	1:B:674:PRO:HD3	2.45	0.46
1:B:786:ARG:HH21	1:B:787:ARG:NE	2.12	0.46
1:B:637:HIS:HB2	1:B:767:ASP:OD1	2.16	0.46
1:A:300:GLU:HB2	1:A:302:TYR:CE1	2.51	0.46
1:B:695:ALA:O	1:B:699:LYS:HG2	2.15	0.46
1:A:277:ASP:HB2	1:A:339:LYS:HB2	1.98	0.46
1:B:542:ARG:NH1	1:B:544:ILE:HD11	2.31	0.46
3:B:794:ANP:H3'	3:B:794:ANP:O1B	2.16	0.45
1:B:503:LYS:HE3	3:B:794:ANP:H3'	1.98	0.45
1:B:688:ALA:HB2	1:B:750:GLU:HG3	1.99	0.45
1:A:327:VAL:HG22	1:A:330:PRO:CG	2.40	0.45
1:B:682:LEU:O	1:B:686:ARG:HG3	2.16	0.45
1:B:533:VAL:HA	1:B:541:HIS:O	2.16	0.45
1:B:539:LYS:HB3	1:B:556:VAL:HG13	1.98	0.45
1:B:686:ARG:HD2	1:B:716:ARG:CZ	2.46	0.45
1:A:342:SER:HB3	1:A:344:GLU:OE1	2.16	0.44
1:A:168:ARG:HD2	1:A:170:TRP:CZ2	2.52	0.44
2:A:1081:SO4:O3	1:B:407:SER:HB3	2.17	0.44
1:B:541:HIS:HA	1:B:555:ALA:O	2.17	0.44
1:B:511:VAL:HG11	1:B:726[A]:LYS:HG3	1.99	0.44
1:B:468:SER:HB3	1:B:570:TRP:CD1	2.53	0.44
1:A:392:THR:HG23	1:B:780:ARG:HH22	1.82	0.43
1:B:673:ILE:HG21	1:B:737:LYS:HB2	1.99	0.43
1:A:103:LYS:HD3	3:A:394:ANP:O1B	2.18	0.43
1:B:762:LEU:HD13	5:B:2573:HOH:O	2.18	0.43
1:A:353:MET:HE3	1:A:357:LEU:HD12	2.01	0.43
1:B:503:LYS:HE2	1:B:509:TYR:CE1	2.53	0.43
1:A:184:TYR:CG	1:A:212:LYS:HE3	2.54	0.43
1:A:190:ARG:NH1	1:A:274:PRO:HD3	2.33	0.43
1:A:190:ARG:HD3	1:A:194:LEU:HD22	2.00	0.43
1:B:675:GLN:HE21	1:B:681:HIS:CE1	2.35	0.43
1:A:5:SER:HB2	1:B:536:ARG:HH22	1.82	0.43
1:B:620:GLY:HA3	1:B:624:ALA:HB2	2.01	0.43
1:B:440:VAL:O	1:B:444:VAL:HG23	2.19	0.43
1:A:95:MET:HE3	1:A:132:LEU:HD22	2.01	0.43
1:B:532:LEU:O	1:B:542:ARG:HA	2.19	0.43
1:A:136:ARG:NH1	1:B:405:SER:HB2	2.33	0.42
1:B:455:HIS:O	1:B:457:LYS:HE2	2.19	0.42
1:A:237:HIS:CE1	1:A:258:TRP:H	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ARG:NH1	1:B:405:SER:O	2.52	0.42
1:A:63:ILE:HD11	1:A:187:LEU:HD12	2.01	0.42
1:A:275:GLN:HE21	1:A:281:HIS:CE1	2.27	0.42
1:A:11:LYS:O	1:B:500:ALA:HA	2.20	0.42
1:B:499:HIS:H	1:B:518:VAL:HG12	1.85	0.42
1:A:64:HIS:HA	1:A:208:LYS:HB2	2.02	0.42
1:A:114:GLY:CA	3:A:394:ANP:HNB1	2.32	0.42
1:B:503:LYS:HG2	5:B:2564:HOH:O	2.20	0.42
1:A:300:GLU:HB2	1:A:302:TYR:CD1	2.55	0.42
1:A:184:TYR:CZ	1:A:212:LYS:HG2	2.54	0.42
1:A:88:VAL:HG13	1:A:92:GLU:HB3	2.02	0.41
1:B:597:LEU:HD12	1:B:622:ILE:HG22	2.01	0.41
1:B:612:LYS:HD3	5:B:4087:HOH:O	2.20	0.41
1:A:270:THR:HA	1:A:325:VAL:HG23	2.02	0.41
4:A:2031:GOL:H31	1:B:405:SER:CB	2.50	0.41
1:B:516:HIS:HB2	3:B:794:ANP:O3G	2.21	0.41
1:A:275:GLN:NE2	1:A:281:HIS:HE1	2.13	0.41
1:B:697:MET:HG2	1:B:772:VAL:HG13	2.02	0.41
1:A:222:ILE:HG13	1:A:255:ALA:HB2	2.03	0.41
1:A:235:PRO:HA	1:A:259:ASN:HA	2.02	0.41
1:A:5:SER:HB3	4:B:1031:GOL:H31	2.03	0.41
1:B:693:LEU:HD23	1:B:693:LEU:HA	1.89	0.41
1:B:458:GLU:HA	1:B:602:SER:O	2.21	0.41
1:A:348:ALA:O	1:A:351:GLN:HG2	2.21	0.40
1:B:477:GLY:HA2	1:B:565:THR:OG1	2.21	0.40
1:B:606:ARG:N	1:B:606:ARG:HD2	2.35	0.40
1:B:703:SER:O	1:B:707:LYS:N	2.54	0.40
1:B:494:ILE:HG13	1:B:495:MET:N	2.36	0.40
1:A:252:VAL:CG1	1:A:352:GLN:HG3	2.52	0.40
1:A:38:HIS:O	1:A:42:GLU:HG2	2.21	0.40
1:B:643:PHE:CE2	1:B:652:VAL:HG22	2.57	0.40
1:A:286:ARG:HH11	1:A:316:ARG:NE	2.20	0.40
1:B:753:MET:O	1:B:757:LEU:HB2	2.21	0.40
1:A:131:GLU:HG3	1:A:144:ILE:CD1	2.52	0.40
1:B:727:VAL:HA	1:B:728:PRO:HD3	1.97	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	391/391 (100%)	365 (93%)	23 (6%)	3 (1%)	24	27
1	B	391/391 (100%)	374 (96%)	15 (4%)	2 (0%)	34	41
All	All	782/782 (100%)	739 (94%)	38 (5%)	5 (1%)	30	36

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	515	LEU
1	A	3	ASN
1	B	578	ASN
1	A	307	LYS
1	A	119	GLY

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	328/326 (101%)	295 (90%)	33 (10%)	9	11
1	B	328/326 (101%)	302 (92%)	26 (8%)	15	19
All	All	656/652 (101%)	597 (91%)	59 (9%)	12	14

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER

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Mol	Chain	Res	Type
1	A	56	CYS
1	A	61	VAL
1	A	88	VAL
1	A	94	ILE
1	A	110	LYS
1	A	118	VAL
1	A	126	LEU
1	A	137	GLU
1	A	168	ARG
1	A	190	ARG
1	A	194	LEU
1	A	197	LEU
1	A	205	LEU
1	A	208	LYS
1	A	229	LEU
1	A	252	VAL
1	A	257	GLN
1	A	281	HIS
1	A	289	MET
1	A	291	ARG
1	A	305	LYS
1	A	307	LYS
1	A	313	ASP
1	A	314	ASP
1	A	326[A]	LYS
1	A	326[B]	LYS
1	A	327	VAL
1	A	335	GLN
1	A	357	LEU
1	A	361	LEU
1	A	382	ARG
1	A	392	THR
1	B	416	LEU
1	B	419	VAL
1	B	457	LYS
1	B	485	GLU
1	B	510	LYS
1	B	526	LEU
1	B	536	ARG
1	B	568	ARG
1	B	590	ARG
1	B	594	LEU

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Mol	Chain	Res	Type
1	B	597	LEU
1	B	605	LEU
1	B	606	ARG
1	B	629	LEU
1	B	646	GLU
1	B	652	VAL
1	B	663	GLN
1	B	681	HIS
1	B	719	LEU
1	B	735	GLN
1	B	757	LEU
1	B	761	LEU
1	B	762	LEU
1	B	777	ASP
1	B	791	MET
1	B	792	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	GLN
1	A	217	HIS
1	A	237	HIS
1	A	275	GLN
1	A	281	HIS
1	A	354	ASN
1	B	403	ASN
1	B	528	GLN
1	B	541	HIS
1	B	543	GLN
1	B	657	GLN
1	B	675	GLN
1	B	681	HIS
1	B	754	ASN

### 5.3.3 RNA ⓘ

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](#)

7 ligands are modelled in this entry.

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	SO4	A	1081	-	4,4,4	1.53	0	6,6,6	0.15	0
4	GOL	A	2031	-	5,5,5	0.15	0	5,5,5	0.15	0
2	SO4	A	2081	-	4,4,4	1.11	0	6,6,6	0.13	0
3	ANP	A	394	-	27,33,33	2.52	8 (29%)	30,52,52	3.13	17 (56%)
4	GOL	B	1031	-	5,5,5	0.19	0	5,5,5	0.13	0
2	SO4	B	2101	-	4,4,4	1.37	0	6,6,6	0.18	0
3	ANP	B	794	-	27,33,33	2.26	7 (25%)	30,52,52	2.87	16 (53%)

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	SO4	A	1081	-	-	0/0/0/0	0/0/0/0
4	GOL	A	2031	-	-	0/4/4/4	0/0/0/0
2	SO4	A	2081	-	-	0/0/0/0	0/0/0/0
3	ANP	A	394	-	-	1/12/38/38	0/3/3/3
4	GOL	B	1031	-	-	0/4/4/4	0/0/0/0
2	SO4	B	2101	-	-	0/0/0/0	0/0/0/0
3	ANP	B	794	-	-	1/12/38/38	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	394	ANP	C5-N7	-5.47	1.20	1.39
3	B	794	ANP	C5-N7	-4.90	1.22	1.39
3	A	394	ANP	PB-O2B	-2.51	1.49	1.56
3	B	794	ANP	PB-O2B	-2.45	1.49	1.56
3	A	394	ANP	PG-O2G	-2.13	1.50	1.56
3	A	394	ANP	PB-O1B	2.25	1.48	1.46
3	B	794	ANP	PG-O1G	2.36	1.48	1.46
3	B	794	ANP	C2'-C3'	3.13	1.61	1.53
3	B	794	ANP	C2-N1	3.27	1.40	1.33
3	A	394	ANP	C2-N1	3.58	1.40	1.33
3	B	794	ANP	C2-N3	3.64	1.38	1.32
3	A	394	ANP	C2'-C3'	4.17	1.64	1.53
3	A	394	ANP	C2-N3	4.84	1.40	1.32
3	B	794	ANP	C3'-C4'	6.93	1.71	1.53
3	A	394	ANP	C3'-C4'	7.24	1.72	1.53

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	794	ANP	O3'-C3'-C4'	-7.67	88.05	111.05
3	A	394	ANP	O3'-C3'-C4'	-6.91	90.32	111.05
3	B	794	ANP	C2'-C1'-N9	-4.72	107.08	114.29
3	A	394	ANP	C2'-C1'-N9	-4.70	107.11	114.29
3	A	394	ANP	N6-C6-N1	-4.31	109.95	119.20
3	A	394	ANP	O3G-PG-O1G	-4.28	102.12	113.49
3	B	794	ANP	O5'-C5'-C4'	-4.27	93.38	109.12
3	B	794	ANP	O2A-PA-O1A	-4.09	90.33	112.53
3	B	794	ANP	N6-C6-N1	-3.97	110.69	119.20
3	A	394	ANP	C4-C5-N7	-3.75	106.03	109.48
3	A	394	ANP	O2A-PA-O1A	-3.55	93.29	112.53
3	B	794	ANP	O3G-PG-O1G	-3.45	104.31	113.49
3	B	794	ANP	C4-C5-N7	-3.37	106.38	109.48
3	A	394	ANP	O4'-C1'-N9	-3.02	101.78	108.10
3	B	794	ANP	O3G-PG-O2G	-2.93	98.90	107.58
3	B	794	ANP	N3-C2-N1	-2.85	126.71	128.89
3	A	394	ANP	C2'-C3'-C4'	-2.80	96.86	102.61
3	B	794	ANP	C1'-N9-C4	-2.30	123.47	126.94
3	A	394	ANP	O2A-PA-O5'	-2.22	97.27	108.46
3	A	394	ANP	O1B-PB-N3B	-2.11	108.67	111.90
3	A	394	ANP	C4'-O4'-C1'	2.01	111.93	109.72
3	B	794	ANP	C4'-O4'-C1'	2.26	112.20	109.72
3	A	394	ANP	O3'-C3'-C2'	2.38	119.56	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	794	ANP	C5'-C4'-C3'	2.43	124.86	115.21
3	B	794	ANP	O2G-PG-O1G	2.44	119.99	113.49
3	A	394	ANP	O2B-PB-O1B	2.77	115.78	110.00
3	A	394	ANP	O4'-C4'-C5'	3.29	121.09	109.32
3	B	794	ANP	O2A-PA-O3A	3.38	120.42	105.09
3	B	794	ANP	O1G-PG-N3B	3.40	117.12	111.90
3	B	794	ANP	O4'-C4'-C5'	3.43	121.61	109.32
3	A	394	ANP	O4'-C4'-C3'	3.48	112.17	105.15
3	A	394	ANP	O2A-PA-O3A	3.98	123.15	105.09
3	A	394	ANP	O1G-PG-N3B	7.71	123.72	111.90

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	794	ANP	O1G-PG-N3B-PB
3	A	394	ANP	O1G-PG-N3B-PB

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1081	SO4	2	0
4	A	2031	GOL	2	0
3	A	394	ANP	3	0
4	B	1031	GOL	2	0
3	B	794	ANP	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.