



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:54 am BST

PDB ID : 6GAU  
Title : Extremely 'open' clamp structure of DNA gyrase: role of the Corynebacteriales GyrB specific insert  
Authors : Petrella, S.; Capton, E.; Alzari, P.M.; Aubry, A.; Mayer, C.  
Deposited on : 2018-04-12  
Resolution : 3.30 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

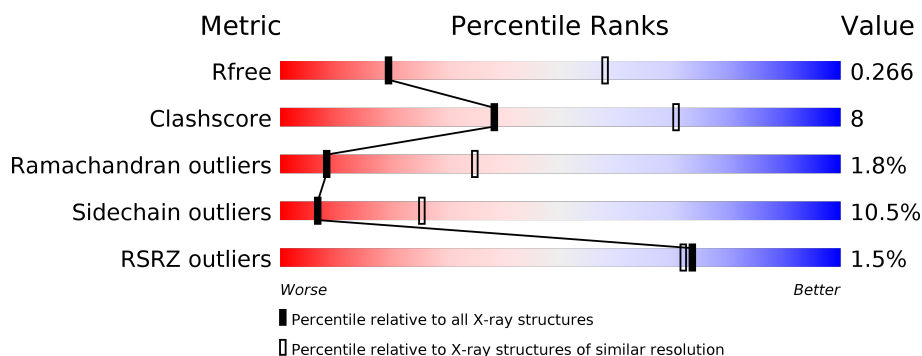
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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))
$R_{free}$	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 respectively. 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.

Mol	Chain	Length	Quality of chain
1	A	1179	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>20%</div> <div>•</div> <div>8%</div> </div> </div>
1	B	1179	<div> <div>67%</div> <div>21%</div> <div>•</div> <div>9%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16872 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.

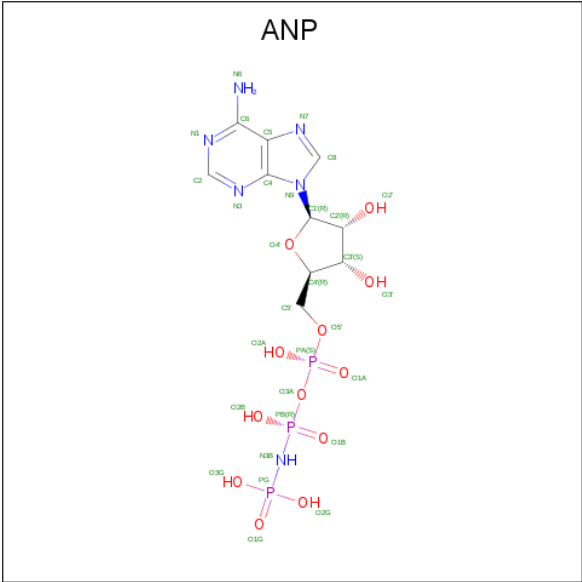
- Molecule 1 is a protein called DNA gyrase subunit B,DNA gyrase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1088	Total	C	N	O	S	0	0	0
			8485	5299	1529	1631	26			
1	B	1068	Total	C	N	O	S	0	0	0
			8323	5197	1493	1608	25			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP F6N7X0
A	999	GLY	-	linker	UNP F6N7X0
A	1000	ASP	-	linker	UNP F6N7X0
A	1001	LEU	-	linker	UNP F6N7X0
B	0	MET	-	initiating methionine	UNP F6N7X0
B	999	GLY	-	linker	UNP F6N7X0
B	1000	ASP	-	linker	UNP F6N7X0
B	1001	LEU	-	linker	UNP F6N7X0

- Molecule 2 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
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		

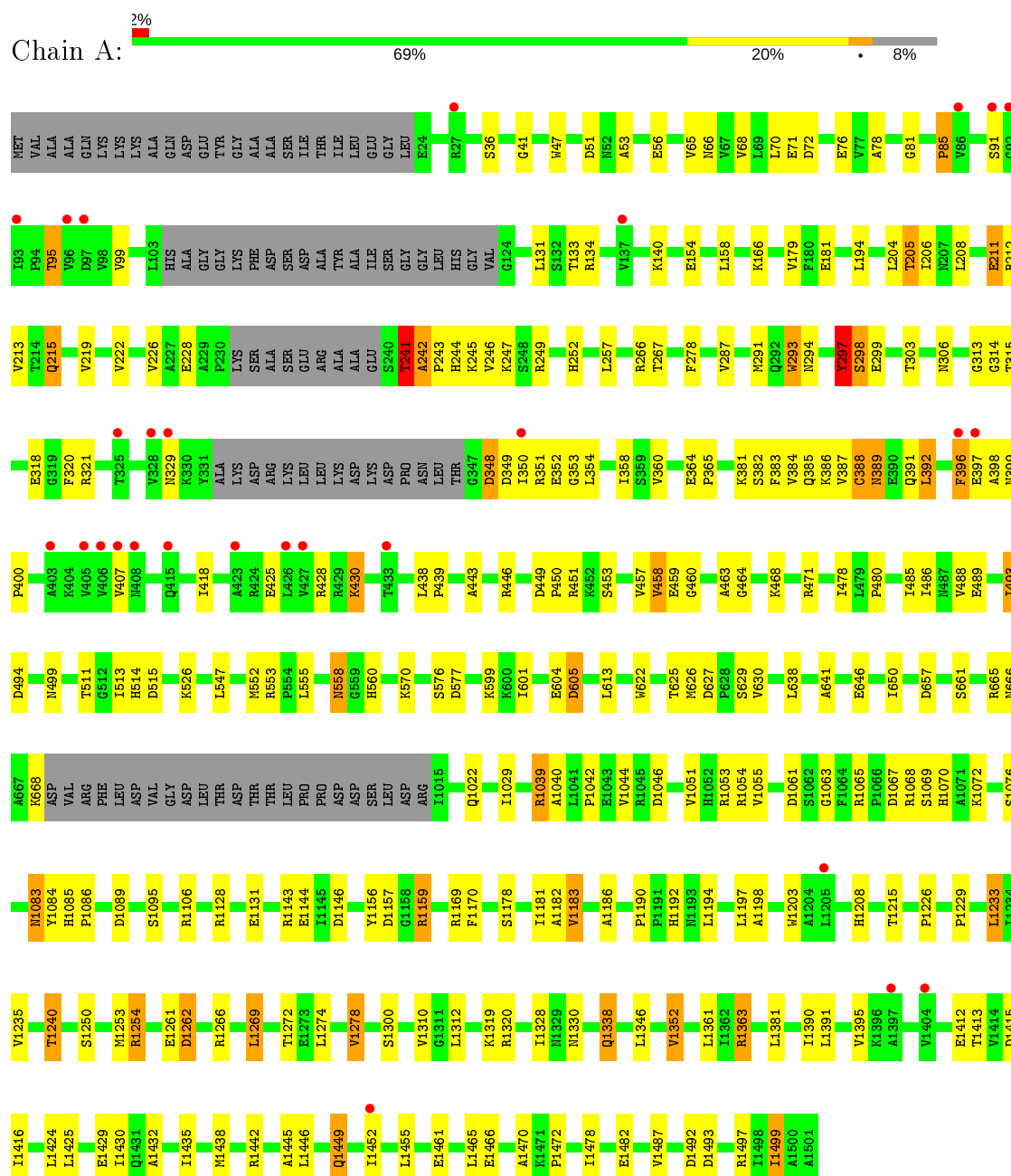
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

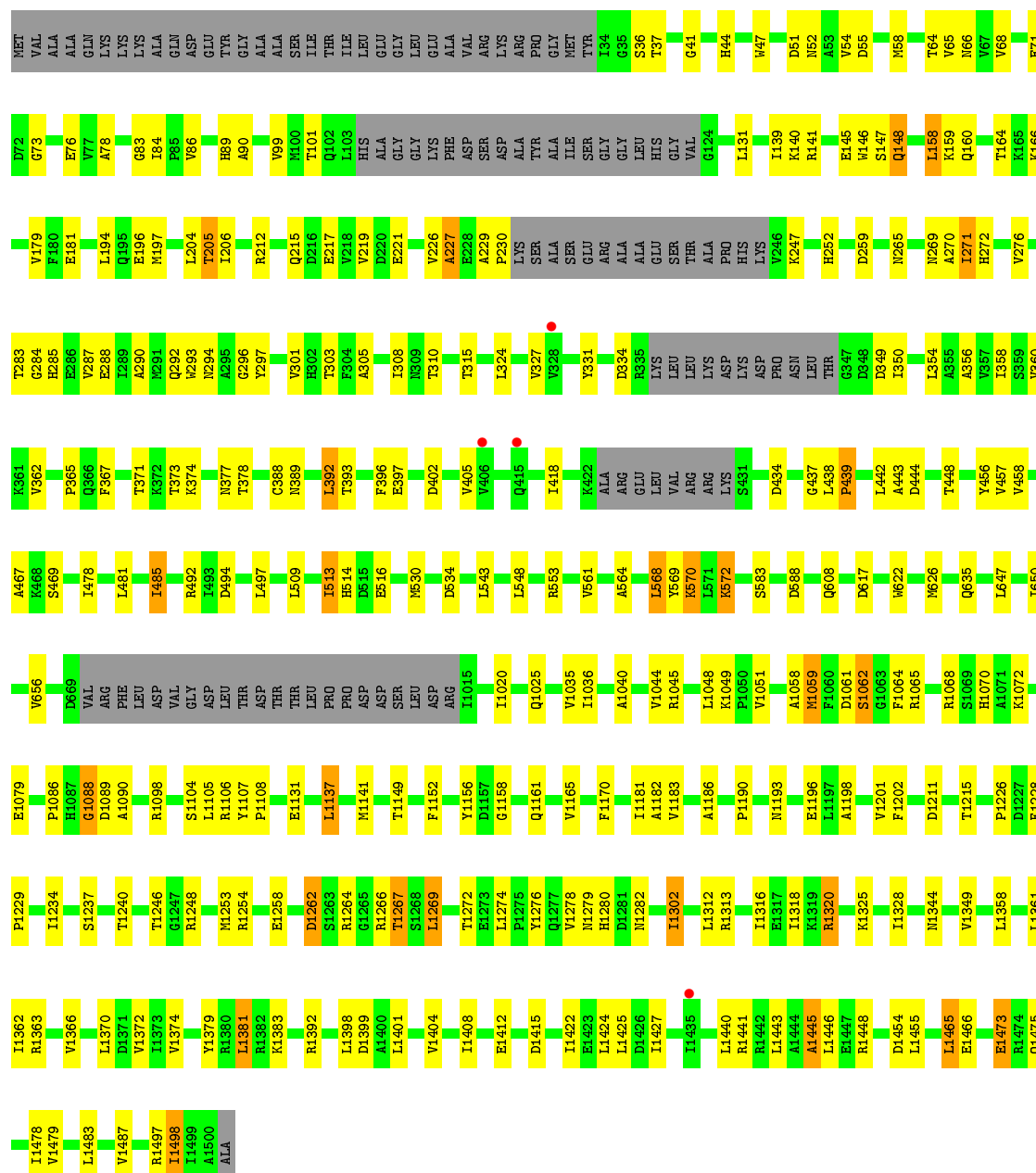
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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,DNA gyrase subunit A



- Chain B:  67% 21% • 9%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.52Å 96.78Å 105.79Å 75.64° 64.44° 65.80°	Depositor
Resolution (Å)	48.35 – 3.30 47.54 – 3.29	Depositor EDS
% Data completeness (in resolution range)	98.1 (48.35-3.30) 98.1 (47.54-3.29)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 3.33Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, $R_{free}$	0.173 , 0.251 0.189 , 0.266	Depositor DCC
$R_{free}$ test set	2235 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	86.4	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 80.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	16872	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.52	0/8622	0.74	0/11665
1	B	0.52	0/8455	0.75	0/11440
All	All	0.52	0/17077	0.75	0/23105

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	8485	0	8478	122	0
1	B	8323	0	8298	140	0
2	A	31	0	13	1	0
2	B	31	0	13	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	16872	0	16802	255	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 8.

All (255) 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:383:PHE:O	1:A:387:VAL:HG23	1.39	1.20
1:B:442:LEU:HD23	1:B:443:ALA:N	1.70	1.05
1:A:382:SER:O	1:A:386:LYS:HG3	1.58	1.02
1:B:1040:ALA:HB2	1:B:1182:ALA:HB3	1.51	0.92
1:A:382:SER:O	1:A:386:LYS:CG	2.26	0.83
1:B:52:ASN:HD22	2:B:1601:ANP:H8	1.45	0.79
1:A:1412:GLU:HA	1:B:1445:ALA:HB3	1.66	0.78
1:A:278:PHE:CZ	1:A:392:LEU:CD2	2.67	0.77
1:B:442:LEU:HD23	1:B:443:ALA:CA	2.14	0.77
1:A:1445:ALA:HB3	1:B:1412:GLU:HA	1.67	0.75
1:B:442:LEU:CD2	1:B:444:ASP:N	2.50	0.74
1:B:1044:VAL:HG21	1:B:1349:VAL:HG22	1.69	0.74
1:A:242:ALA:H	1:A:243:PRO:HD3	1.53	0.74
1:A:278:PHE:CZ	1:A:392:LEU:HD21	2.25	0.72
1:A:1254:ARG:HB3	1:A:1338:GLN:HG3	1.72	0.71
1:A:1040:ALA:HB2	1:A:1182:ALA:HB3	1.72	0.70
1:A:299:GLU:HG3	1:A:351:ARG:HB3	1.73	0.70
1:A:1143:ARG:HB3	1:A:1169:ARG:HG3	1.74	0.70
1:A:297:TYR:HA	1:A:353:GLY:HA2	1.74	0.69
1:B:276:VAL:O	1:B:290:ALA:HA	1.92	0.69
1:A:213:VAL:HG21	1:A:247:LYS:HB2	1.73	0.69
1:A:1274:LEU:HD22	1:A:1278:VAL:HG21	1.76	0.67
1:B:373:THR:HG22	1:B:374:LYS:H	1.59	0.67
1:A:278:PHE:HZ	1:A:392:LEU:HD21	1.57	0.67
1:A:397:GLU:O	1:A:400:PRO:HG3	1.95	0.66
1:B:1370:LEU:HD23	1:B:1479:VAL:HG21	1.78	0.65
1:A:1063:GLY:HA2	1:A:1065:ARG:NH1	2.12	0.64
1:A:1266:ARG:HD3	1:A:1320:ARG:HG2	1.80	0.64
1:A:398:ALA:O	1:A:400:PRO:HD3	1.98	0.64
1:A:303:THR:HG22	1:A:358:ILE:HB	1.79	0.64
1:B:1266:ARG:HG2	1:B:1320:ARG:HD2	1.81	0.63
1:B:1404:VAL:O	1:B:1408:ILE:HG12	1.98	0.63
1:A:384:VAL:HG12	1:A:388:CYS:SG	2.39	0.63
1:A:293:TRP:HZ3	1:A:350:ILE:O	1.82	0.63
1:B:442:LEU:C	1:B:442:LEU:HD23	2.19	0.62
1:B:442:LEU:CD2	1:B:443:ALA:N	2.56	0.62
1:A:1390:ILE:HD11	1:A:1430:ILE:HG22	1.82	0.62
1:A:381:LYS:O	1:A:385:GLN:HB2	2.00	0.62
1:B:1381:LEU:HD12	1:B:1465:LEU:HB2	1.80	0.61
1:A:627:ASP:HB3	1:A:630:VAL:HG22	1.83	0.61
1:B:442:LEU:HD23	1:B:444:ASP:N	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1381:LEU:HD11	1:A:1466:GLU:HG3	1.82	0.60
1:B:442:LEU:HD23	1:B:443:ALA:C	2.21	0.60
1:A:383:PHE:O	1:A:387:VAL:CG2	2.33	0.60
1:B:1105:LEU:HD12	1:B:1108:PRO:HA	1.84	0.60
1:A:1203:TRP:HZ3	1:A:1215:THR:HG22	1.67	0.59
1:A:389:ASN:HD22	1:A:389:ASN:C	2.06	0.59
1:B:388:CYS:O	1:B:392:LEU:HB2	2.03	0.59
1:A:1086:PRO:HG3	1:A:1156:TYR:CD2	2.39	0.58
1:A:1470:ALA:O	1:A:1472:PRO:HD3	2.04	0.58
1:A:471:ARG:HD3	1:A:478:ILE:HG12	1.84	0.58
1:B:36:SER:HB3	1:B:41:GLY:H	1.69	0.58
1:B:1475:GLN:HA	1:B:1478:ILE:HD12	1.85	0.58
1:B:1398:LEU:HA	1:B:1401:LEU:HG	1.86	0.58
1:A:1226:PRO:HD3	1:A:1240:THR:HG23	1.86	0.57
1:B:458:VAL:HG12	1:B:530:MET:HB2	1.86	0.57
1:B:1058:ALA:HB1	1:B:1079:GLU:HG3	1.86	0.57
1:B:622:TRP:HA	1:B:626:MET:HB2	1.86	0.57
1:B:1211:ASP:O	1:B:1215:THR:HG23	2.04	0.57
1:A:622:TRP:HA	1:A:626:MET:HB2	1.87	0.57
1:A:1054:ARG:HD3	1:A:1085:HIS:HB2	1.87	0.56
1:A:1083:ASN:HA	1:A:1156:TYR:HE1	1.69	0.56
1:B:65:VAL:HG23	1:B:204:LEU:HD11	1.86	0.56
1:B:310:THR:HA	1:B:373:THR:CG2	2.35	0.56
1:A:552:MET:HG2	1:A:555:LEU:HD12	1.87	0.56
1:A:287:VAL:HG23	1:A:360:VAL:HG12	1.88	0.55
1:B:55:ASP:HA	1:B:58:MET:HB3	1.88	0.55
1:A:205:THR:HG23	1:A:252:HIS:HB2	1.89	0.55
1:B:1267:THR:HB	1:B:1318:ILE:HD11	1.89	0.55
1:A:242:ALA:N	1:A:243:PRO:HD3	2.22	0.55
1:B:1141:MET:HG2	1:B:1170:PHE:HE2	1.72	0.55
1:A:1198:ALA:HB2	1:A:1487:VAL:HG11	1.89	0.54
1:B:1274:LEU:HD22	1:B:1278:VAL:HG21	1.88	0.54
1:A:140:LYS:HB3	1:A:166:LYS:O	2.08	0.53
1:B:1181:ILE:HG23	1:B:1186:ALA:HB2	1.90	0.53
1:B:1445:ALA:HA	1:B:1448:ARG:HD3	1.90	0.53
1:A:1072:LYS:HD3	1:A:1128:ARG:O	2.08	0.53
1:B:1059:MET:HG3	1:B:1064:PHE:HD2	1.73	0.53
1:A:1070:HIS:HB3	1:A:1131:GLU:HB3	1.90	0.52
1:B:272:HIS:HB2	1:B:402:ASP:CG	2.29	0.52
1:B:227:ALA:HA	1:B:1246:THR:O	2.09	0.52
1:A:1272:THR:O	1:A:1312:LEU:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:GLN:HB2	1:B:158:LEU:HB3	1.92	0.52
1:A:241:THR:HG23	1:A:243:PRO:HD3	1.91	0.52
1:B:44:HIS:HA	1:B:47:TRP:CD1	2.44	0.52
1:B:1190:PRO:HB2	1:B:1226:PRO:HB3	1.91	0.52
1:A:1042:PRO:HG3	1:A:1178:SER:HB3	1.92	0.52
1:B:327:VAL:HG11	1:B:392:LEU:HB3	1.90	0.52
1:A:68:VAL:HB	1:A:76:GLU:HB3	1.92	0.51
1:B:301:VAL:HG13	1:B:356:ALA:HB3	1.91	0.51
1:B:310:THR:HA	1:B:373:THR:HG23	1.91	0.51
1:B:1070:HIS:HB3	1:B:1131:GLU:HB3	1.92	0.51
1:B:66:ASN:HB2	1:B:78:ALA:HB3	1.92	0.51
1:A:99:VAL:HB	2:A:1601:ANP:H5'1	1.90	0.51
1:B:1065:ARG:HD2	1:B:1068:ARG:NH2	2.26	0.51
1:B:497:LEU:HD21	1:B:513:ILE:HG21	1.93	0.51
1:B:1269:LEU:HD13	1:B:1328:ILE:HG13	1.93	0.51
1:B:442:LEU:HD21	1:B:444:ASP:N	2.26	0.51
1:B:1058:ALA:O	1:B:1062:SER:HB2	2.11	0.51
1:A:1194:LEU:HG	1:A:1487:VAL:HG12	1.93	0.50
1:A:1412:GLU:HG3	1:B:1446:LEU:HB2	1.93	0.50
1:B:1424:LEU:HG	1:B:1425:LEU:HG	1.94	0.50
1:B:194:LEU:HB3	1:B:206:ILE:HG21	1.92	0.50
1:A:1192:HIS:HB2	1:A:1197:LEU:HD11	1.94	0.50
1:A:1438:MET:HE2	1:A:1442:ARG:HD2	1.93	0.50
1:B:569:TYR:HA	1:B:608:GLN:O	2.12	0.50
1:A:131:LEU:HD22	1:A:179:VAL:HG11	1.94	0.50
1:A:450:PRO:HA	1:A:453:SER:HB2	1.93	0.49
1:B:1035:VAL:HG12	1:B:1182:ALA:HB1	1.94	0.49
1:A:1233:LEU:H	1:A:1233:LEU:HD13	1.77	0.49
1:A:1391:LEU:O	1:A:1395:VAL:HG23	2.11	0.49
1:A:486:ILE:HB	1:A:499:ASN:HD22	1.78	0.49
1:A:1183:VAL:HG13	1:A:1183:VAL:O	2.13	0.49
1:B:140:LYS:HG2	1:B:145:GLU:HB3	1.95	0.49
1:B:362:VAL:HB	1:B:365:PRO:HB3	1.95	0.49
1:B:572:LYS:HE2	1:B:608:GLN:HB2	1.95	0.49
1:B:530:MET:HG2	1:B:564:ALA:HB2	1.95	0.49
1:A:211:GLU:HA	1:A:246:VAL:HG22	1.95	0.48
1:A:293:TRP:CE3	1:A:354:LEU:HB2	2.48	0.48
1:B:1401:LEU:HD11	1:B:1443:LEU:HD22	1.93	0.48
1:A:463:ALA:HB2	1:A:613:LEU:HB3	1.96	0.48
1:B:293:TRP:HH2	1:B:350:ILE:HG22	1.78	0.48
1:B:64:THR:HG23	1:B:205:THR:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:647:LEU:HD11	1:B:1025:GLN:HG3	1.96	0.48
1:B:1198:ALA:HB2	1:B:1487:VAL:HG21	1.96	0.48
1:A:291:MET:HB3	1:A:354:LEU:HD21	1.96	0.48
1:B:287:VAL:HG23	1:B:360:VAL:HG12	1.96	0.48
1:A:1413:THR:H	1:A:1416:ILE:HD12	1.78	0.48
1:B:51:ASP:HA	1:B:54:VAL:HG12	1.96	0.48
1:A:1040:ALA:HB2	1:A:1182:ALA:CB	2.43	0.47
1:B:1279:ASN:HB3	1:B:1282:ASN:HB2	1.96	0.47
1:B:148:GLN:H	1:B:158:LEU:HA	1.79	0.47
1:B:1272:THR:O	1:B:1312:LEU:HB3	2.13	0.47
1:B:227:ALA:HB2	1:B:1246:THR:HG22	1.96	0.47
1:A:1461:GLU:O	1:A:1465:LEU:HG	2.14	0.47
1:A:1395:VAL:HG13	1:A:1452:ILE:HG22	1.96	0.47
1:A:443:ALA:HB2	1:A:468:LYS:HE2	1.96	0.47
1:B:229:ALA:HB1	1:B:230:PRO:HD2	1.95	0.47
1:A:1424:LEU:HD23	1:A:1425:LEU:HG	1.97	0.47
1:A:460:GLY:HA2	1:A:464:GLY:HA3	1.97	0.47
1:B:89:HIS:CG	1:B:90:ALA:H	2.33	0.47
1:A:1438:MET:HB3	1:B:1440:LEU:HD12	1.96	0.47
1:B:303:THR:HG22	1:B:358:ILE:HB	1.96	0.47
1:A:1478:ILE:O	1:A:1482:GLU:HB2	2.15	0.47
1:B:1379:TYR:CZ	1:B:1383:LYS:HG3	2.50	0.47
1:A:1381:LEU:HD12	1:A:1465:LEU:HB2	1.96	0.47
1:A:249:ARG:HH22	1:A:665:ARG:HD3	1.80	0.47
1:B:84:ILE:HB	1:B:139:ILE:HG12	1.96	0.47
1:A:194:LEU:HD12	1:A:208:LEU:HD22	1.96	0.46
1:B:570:LYS:HB3	1:B:608:GLN:HB3	1.96	0.46
1:B:1137:LEU:HD23	1:B:1137:LEU:HA	1.84	0.46
1:A:315:THR:O	1:A:381:LYS:HA	2.15	0.46
1:B:1098:ARG:HG3	1:B:1104:SER:HB3	1.97	0.46
1:B:1392:ARG:HG3	1:B:1455:LEU:HD11	1.96	0.46
1:A:71:GLU:HA	1:A:212:ARG:HG2	1.96	0.46
1:A:36:SER:O	1:A:41:GLY:HA3	2.16	0.46
1:B:1215:THR:HG21	1:B:1363:ARG:HE	1.80	0.46
1:A:458:VAL:HG11	1:A:463:ALA:HB3	1.98	0.46
1:B:147:SER:HB3	1:B:159:LYS:H	1.81	0.45
1:A:1300:SER:HB3	1:A:1319:LYS:HG3	1.98	0.45
1:A:1449:GLN:HA	1:A:1452:ILE:HG12	1.97	0.45
1:A:352:GLU:C	1:A:354:LEU:H	2.20	0.45
1:A:646:GLU:O	1:A:650:ILE:HD12	2.17	0.45
1:B:1228:PHE:HB3	1:B:1276:TYR:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1234:ILE:HB	1:B:1498:ILE:HG23	1.99	0.45
1:A:1235:VAL:HA	1:A:1499:ILE:HG22	1.98	0.45
1:A:398:ALA:C	1:A:400:PRO:HD3	2.37	0.45
1:B:1193:ASN:HB3	1:B:1196:GLU:HG3	1.98	0.45
1:B:131:LEU:HD22	1:B:179:VAL:HG11	1.97	0.45
1:B:36:SER:HB3	1:B:41:GLY:N	2.32	0.45
1:B:1045:ARG:NH2	1:B:1165:VAL:HG11	2.32	0.45
1:B:467:ALA:HB1	1:B:478:ILE:HD12	1.99	0.45
1:B:1202:PHE:CE1	1:B:1483:LEU:HD23	2.52	0.44
1:B:485:ILE:HD13	1:B:485:ILE:N	2.31	0.44
1:A:65:VAL:O	1:A:206:ILE:HA	2.17	0.44
1:A:1046:ASP:OD2	1:A:1053:ARG:HD3	2.18	0.44
1:B:1201:VAL:HG13	1:B:1366:VAL:HG22	1.99	0.44
1:B:1107:TYR:HB3	1:B:1137:LEU:HD12	2.00	0.44
1:B:146:TRP:CZ3	1:B:160:GLN:HB2	2.53	0.44
1:A:66:ASN:HB2	1:A:78:ALA:HB3	2.00	0.44
1:B:54:VAL:HG21	1:B:197:MET:HE3	2.00	0.44
1:A:638:LEU:HD21	1:A:641:ALA:HB2	2.01	0.43
1:B:1044:VAL:CG2	1:B:1349:VAL:HG22	2.46	0.43
1:B:99:VAL:HB	2:B:1601:ANP:H5'1	2.01	0.43
1:B:315:THR:HG21	1:B:378:THR:HA	1.99	0.43
1:B:37:THR:HG22	1:B:181:GLU:HG3	2.00	0.43
1:A:278:PHE:CZ	1:A:392:LEU:HD23	2.51	0.43
1:A:668:LYS:HG2	1:A:1352:VAL:HG12	2.01	0.43
1:B:485:ILE:H	1:B:485:ILE:HD13	1.84	0.43
1:A:1254:ARG:HB3	1:A:1338:GLN:CG	2.46	0.43
1:B:1106:ARG:HA	1:B:1229:PRO:HB3	2.01	0.43
1:B:164:THR:HG22	1:B:166:LYS:H	1.84	0.43
1:B:442:LEU:C	1:B:442:LEU:CD2	2.84	0.43
1:A:1183:VAL:CG1	1:A:1183:VAL:O	2.67	0.43
1:B:1149:THR:HB	1:B:1372:VAL:HG13	2.01	0.43
1:A:1157:ASP:HB3	1:B:1072:LYS:HG3	2.00	0.43
1:A:396:PHE:HA	1:A:396:PHE:HD1	1.66	0.43
1:B:265:ASN:ND2	1:B:292:GLN:HB3	2.34	0.43
1:A:493:ILE:HD13	1:A:514:HIS:CD2	2.54	0.42
1:B:1253:MET:HE1	1:B:1276:TYR:N	2.34	0.42
1:B:270:ALA:HA	1:B:294:ASN:HA	2.01	0.42
1:B:219:VAL:HG12	1:B:247:LYS:HG3	2.00	0.42
1:A:449:ASP:OD2	1:A:451:ARG:HB2	2.19	0.42
1:B:1358:LEU:O	1:B:1362:ILE:HG12	2.20	0.42
1:B:438:LEU:HA	1:B:439:PRO:HD2	1.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:VAL:HG21	1:A:547:LEU:HA	2.01	0.42
1:B:1473:GLU:CD	1:B:1473:GLU:H	2.22	0.42
1:A:1190:PRO:HB2	1:A:1226:PRO:HB3	2.00	0.42
1:B:1398:LEU:HD22	1:B:1448:ARG:HG2	2.00	0.42
1:A:53:ALA:O	1:A:56:GLU:HB2	2.19	0.42
1:B:1152:PHE:HB3	1:B:1161:GLN:HB3	2.02	0.42
1:A:1072:LYS:CD	1:A:1128:ARG:O	2.67	0.42
1:A:1089:ASP:OD1	1:B:1088:GLY:HA2	2.20	0.42
1:B:327:VAL:HG22	1:B:393:THR:HG23	2.00	0.42
1:B:68:VAL:HB	1:B:76:GLU:HB3	2.02	0.42
1:A:306:ASN:ND2	1:A:365:PRO:HG3	2.34	0.42
1:B:140:LYS:HD3	1:B:164:THR:HG21	2.02	0.42
1:B:226:VAL:HB	1:B:227:ALA:H	1.65	0.42
1:B:305:ALA:O	1:B:308:ILE:HB	2.20	0.42
1:A:1106:ARG:HA	1:A:1229:PRO:HB3	2.02	0.42
1:A:1432:ALA:HA	1:A:1435:ILE:HD12	2.01	0.42
1:A:293:TRP:CD1	1:A:293:TRP:N	2.88	0.42
1:B:438:LEU:HA	1:B:438:LEU:HD23	1.77	0.42
1:B:297:TYR:CZ	1:B:492:ARG:HB3	2.55	0.41
1:A:389:ASN:ND2	1:A:389:ASN:O	2.50	0.41
1:B:1086:PRO:HG3	1:B:1156:TYR:CD2	2.56	0.41
1:A:1054:ARG:HG2	1:A:1084:TYR:HB3	2.03	0.41
1:A:389:ASN:ND2	1:A:389:ASN:C	2.72	0.41
1:A:558:ASN:HB2	1:A:560:HIS:CD2	2.56	0.41
1:A:1181:ILE:HG12	1:A:1186:ALA:HB2	2.01	0.41
1:A:468:LYS:HE3	1:A:480:PRO:HG3	2.02	0.41
1:A:1269:LEU:HD13	1:A:1328:ILE:HG13	2.02	0.41
1:B:1258:GLU:OE2	1:B:1272:THR:HG21	2.21	0.41
1:B:373:THR:HG22	1:B:374:LYS:N	2.29	0.41
1:B:83:GLY:HA3	1:B:141:ARG:HB3	2.03	0.41
1:A:85:PRO:HB2	1:A:95:THR:HB	2.03	0.41
1:B:456:TYR:HD2	1:B:530:MET:SD	2.44	0.41
1:A:1083:ASN:HB3	1:A:1159:ARG:HH22	1.86	0.40
1:B:392:LEU:HD23	1:B:396:PHE:HE2	1.86	0.40
1:A:297:TYR:HA	1:A:353:GLY:CA	2.47	0.40
1:B:1422:ILE:HG23	1:B:1427:ILE:O	2.21	0.40
1:B:205:THR:HG23	1:B:252:HIS:HB2	2.02	0.40
1:B:548:LEU:HD13	1:B:561:VAL:HG11	2.02	0.40
1:B:568:LEU:HB3	1:B:569:TYR:CD2	2.56	0.40
1:A:443:ALA:HB3	1:A:478:ILE:HB	2.03	0.40
1:B:1302:ILE:HG23	1:B:1316:ILE:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:ILE:HG12	1:B:543:LEU:HD13	2.04	0.40
1:A:1051:VAL:O	1:A:1055:VAL:HG23	2.21	0.40
1:A:1208:HIS:HA	1:A:1363:ARG:HH12	1.87	0.40
1:A:298:SER:H	1:A:353:GLY:H	1.69	0.40
1:B:1141:MET:HG2	1:B:1170:PHE:CE2	2.54	0.40
1:A:446:ARG:HE	1:B:1313:ARG:HH22	1.69	0.40
1:B:1443:LEU:O	1:B:1448:ARG:HD2	2.20	0.40
1:B:1475:GLN:O	1:B:1479:VAL:HG23	2.21	0.40
1:B:1483:LEU:O	1:B:1487:VAL:HG23	2.21	0.40

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	1078/1179 (91%)	943 (88%)	116 (11%)	19 (2%)	8	35
1	B	1056/1179 (90%)	944 (89%)	92 (9%)	20 (2%)	8	34
All	All	2134/2358 (90%)	1887 (88%)	208 (10%)	39 (2%)	8	35

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	GLY
1	A	297	TYR
1	A	298	SER
1	A	599	LYS
1	B	148	GLN
1	B	227	ALA
1	B	354	LEU
1	B	439	PRO
1	A	241	THR

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Mol	Chain	Res	Type
1	A	242	ALA
1	A	314	GLY
1	A	489	GLU
1	A	1039	ARG
1	B	217	GLU
1	B	377	ASN
1	B	514	HIS
1	B	1088	GLY
1	B	1089	ASP
1	B	1262	ASP
1	A	85	PRO
1	A	215	GLN
1	A	313	GLY
1	A	348	ASP
1	A	430	LYS
1	B	215	GLN
1	B	437	GLY
1	A	244	HIS
1	A	439	PRO
1	B	269	ASN
1	B	284	GLY
1	B	1090	ALA
1	B	1158	GLY
1	A	605	ASP
1	A	1261	GLU
1	A	1262	ASP
1	B	73	GLY
1	B	1445	ALA
1	B	271	ILE
1	B	296	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	905/976 (93%)	796 (88%)	109 (12%)	5 20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	889/976 (91%)	809 (91%)	80 (9%)	9	32
All	All	1794/1952 (92%)	1605 (90%)	189 (10%)	7	25

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	TRP
1	A	51	ASP
1	A	70	LEU
1	A	72	ASP
1	A	91	SER
1	A	95	THR
1	A	133	THR
1	A	134	ARG
1	A	154	GLU
1	A	158	LEU
1	A	181	GLU
1	A	204	LEU
1	A	205	THR
1	A	211	GLU
1	A	215	GLN
1	A	219	VAL
1	A	222	VAL
1	A	226	VAL
1	A	228	GLU
1	A	241	THR
1	A	245	LYS
1	A	257	LEU
1	A	266	ARG
1	A	267	THR
1	A	293	TRP
1	A	294	ASN
1	A	297	TYR
1	A	318	GLU
1	A	320	PHE
1	A	321	ARG
1	A	329	ASN
1	A	348	ASP
1	A	349	ASP
1	A	364	GLU
1	A	388	CYS
1	A	389	ASN

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Mol	Chain	Res	Type
1	A	391	GLN
1	A	392	LEU
1	A	396	PHE
1	A	399	ASN
1	A	407	VAL
1	A	418	ILE
1	A	425	GLU
1	A	428	ARG
1	A	430	LYS
1	A	438	LEU
1	A	457	VAL
1	A	458	VAL
1	A	459	GLU
1	A	485	ILE
1	A	493	ILE
1	A	494	ASP
1	A	511	THR
1	A	513	ILE
1	A	515	ASP
1	A	526	LYS
1	A	553	ARG
1	A	558	ASN
1	A	570	LYS
1	A	576	SER
1	A	577	ASP
1	A	601	ILE
1	A	604	GLU
1	A	605	ASP
1	A	625	THR
1	A	629	SER
1	A	657	ASP
1	A	661	SER
1	A	666	ASN
1	A	1022	GLN
1	A	1029	ILE
1	A	1039	ARG
1	A	1044	VAL
1	A	1061	ASP
1	A	1067	ASP
1	A	1068	ARG
1	A	1069	SER
1	A	1076	SER

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Mol	Chain	Res	Type
1	A	1083	ASN
1	A	1095	SER
1	A	1144	GLU
1	A	1146	ASP
1	A	1159	ARG
1	A	1170	PHE
1	A	1183	VAL
1	A	1233	LEU
1	A	1240	THR
1	A	1250	SER
1	A	1253	MET
1	A	1254	ARG
1	A	1262	ASP
1	A	1269	LEU
1	A	1278	VAL
1	A	1310	VAL
1	A	1330	ASN
1	A	1338	GLN
1	A	1346	LEU
1	A	1352	VAL
1	A	1361	LEU
1	A	1363	ARG
1	A	1415	ASP
1	A	1429	GLU
1	A	1446	LEU
1	A	1449	GLN
1	A	1455	LEU
1	A	1492	ASP
1	A	1493	ASP
1	A	1497	ARG
1	A	1499	ILE
1	B	71	GLU
1	B	86	VAL
1	B	101	THR
1	B	158	LEU
1	B	196	GLU
1	B	205	THR
1	B	212	ARG
1	B	221	GLU
1	B	259	ASP
1	B	271	ILE
1	B	283	THR

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Mol	Chain	Res	Type
1	B	285	HIS
1	B	288	GLU
1	B	324	LEU
1	B	331	TYR
1	B	334	ASP
1	B	349	ASP
1	B	367	PHE
1	B	371	THR
1	B	389	ASN
1	B	392	LEU
1	B	397	GLU
1	B	405	VAL
1	B	418	ILE
1	B	434	ASP
1	B	448	THR
1	B	457	VAL
1	B	469	SER
1	B	481	LEU
1	B	485	ILE
1	B	494	ASP
1	B	509	LEU
1	B	513	ILE
1	B	516	GLU
1	B	534	ASP
1	B	553	ARG
1	B	568	LEU
1	B	570	LYS
1	B	572	LYS
1	B	583	SER
1	B	588	ASP
1	B	617	ASP
1	B	635	GLN
1	B	650	ILE
1	B	656	VAL
1	B	1020	ILE
1	B	1036	ILE
1	B	1048	LEU
1	B	1049	LYS
1	B	1051	VAL
1	B	1059	MET
1	B	1061	ASP
1	B	1062	SER

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Mol	Chain	Res	Type
1	B	1137	LEU
1	B	1183	VAL
1	B	1237	SER
1	B	1240	THR
1	B	1248	ARG
1	B	1254	ARG
1	B	1262	ASP
1	B	1264	ARG
1	B	1267	THR
1	B	1269	LEU
1	B	1280	HIS
1	B	1302	ILE
1	B	1320	ARG
1	B	1325	LYS
1	B	1344	ASN
1	B	1361	LEU
1	B	1374	VAL
1	B	1381	LEU
1	B	1399	ASP
1	B	1415	ASP
1	B	1441	ARG
1	B	1454	ASP
1	B	1465	LEU
1	B	1466	GLU
1	B	1473	GLU
1	B	1497	ARG
1	B	1498	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	265	ASN
1	A	389	ASN
1	A	399	ASN
1	A	514	HIS
1	A	560	HIS
1	A	1344	ASN
1	B	263	HIS
1	B	1022	GLN

### 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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	ANP	B	1601	3	29,33,33	1.68	2 (6%)	31,52,52	1.07	4 (12%)
2	ANP	A	1601	3	29,33,33	1.85	2 (6%)	31,52,52	0.95	2 (6%)

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	B	1601	3	-	1/14/38/38	0/3/3/3
2	ANP	A	1601	3	-	4/14/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1601	ANP	PG-O1G	8.56	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1601	ANP	PB-O1B	7.28	1.57	1.46
2	B	1601	ANP	PB-O2B	-4.05	1.45	1.56
2	A	1601	ANP	PG-O3G	-4.02	1.45	1.56

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1601	ANP	O1G-PG-N3B	-2.81	107.63	111.77
2	B	1601	ANP	O2B-PB-O3A	2.60	113.32	104.64
2	B	1601	ANP	C5-C6-N6	2.38	123.97	120.35
2	A	1601	ANP	C5-C6-N6	2.28	123.81	120.35
2	B	1601	ANP	O3G-PG-O1G	-2.19	107.95	113.45
2	B	1601	ANP	O1B-PB-N3B	-2.05	108.75	111.77

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1601	ANP	PB-N3B-PG-O1G
2	A	1601	ANP	PG-N3B-PB-O1B
2	A	1601	ANP	PB-O3A-PA-O2A
2	B	1601	ANP	PB-O3A-PA-O2A
2	A	1601	ANP	PB-O3A-PA-O1A

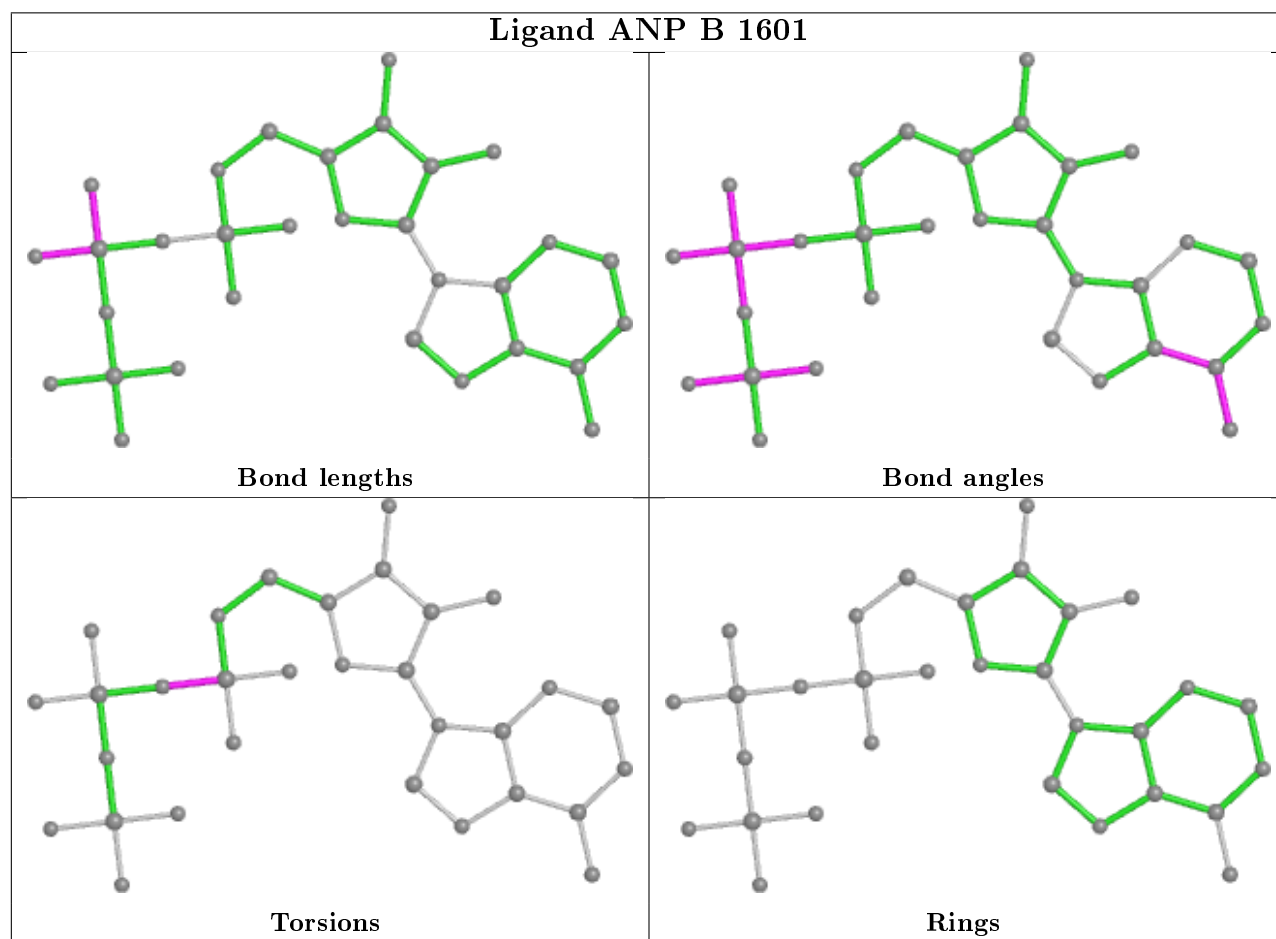
There are no ring outliers.

2 monomers are involved in 3 short contacts:

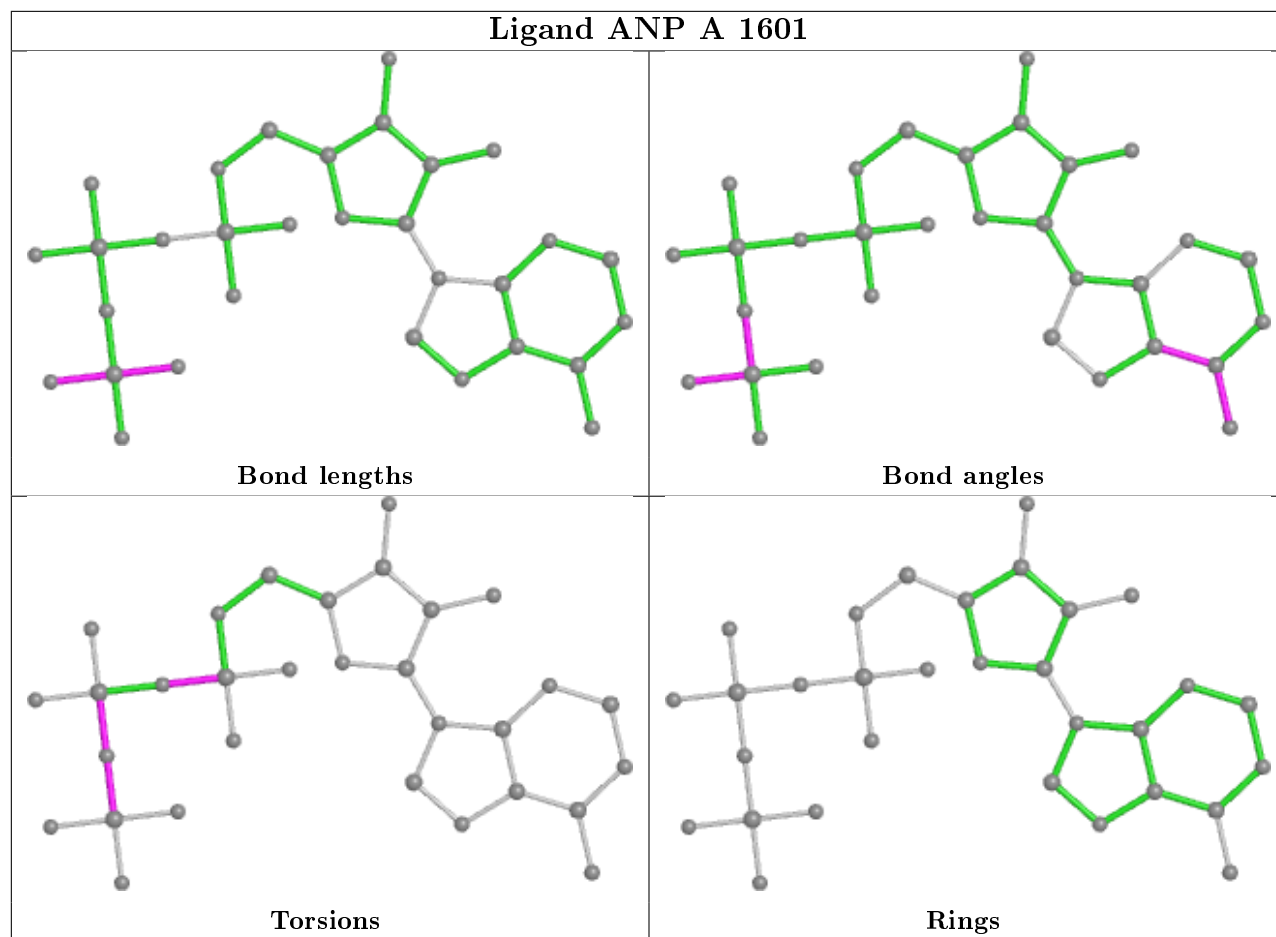
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1601	ANP	2	0
2	A	1601	ANP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 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

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1088/1179 (92%)	-0.15	28 (2%) 56 53	43, 98, 159, 195	0
1	B	1068/1179 (90%)	-0.24	4 (0%) 92 93	39, 96, 153, 175	0
All	All	2156/2358 (91%)	-0.19	32 (1%) 73 72	39, 97, 155, 195	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	328	VAL	3.9
1	A	408	ASN	3.7
1	A	93	ILE	3.4
1	A	91	SER	3.3
1	A	396	PHE	3.3
1	A	96	VAL	3.2
1	A	406	VAL	3.1
1	A	426	LEU	3.1
1	A	1452	ILE	3.1
1	A	27	ARG	3.1
1	A	92	GLY	3.1
1	A	415	GLN	2.9
1	A	405	VAL	2.9
1	A	97	ASP	2.9
1	A	325	THR	2.8
1	A	1397	ALA	2.7
1	B	1435	ILE	2.7
1	A	403	ALA	2.6
1	A	329	ASN	2.6
1	A	86	VAL	2.6
1	A	433	THR	2.6
1	A	137	VAL	2.4
1	A	407	VAL	2.4
1	A	397	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	328	VAL	2.3
1	B	406	VAL	2.3
1	A	350	ILE	2.2
1	A	423	ALA	2.2
1	A	1404	VAL	2.1
1	B	415	GLN	2.1
1	A	427	VAL	2.1
1	A	1205	LEU	2.0

## 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](#)

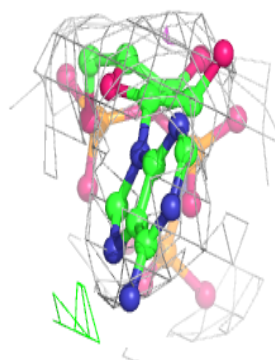
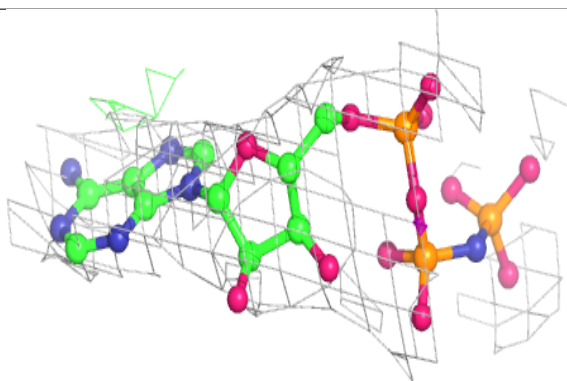
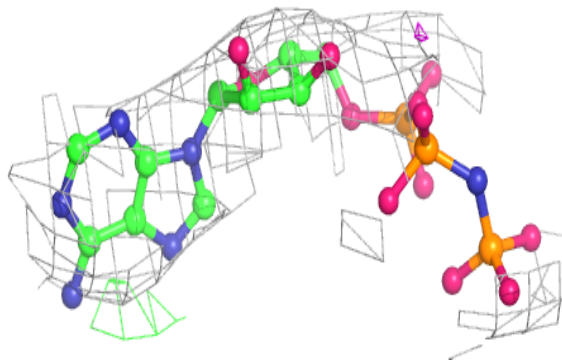
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ANP	B	1601	31/31	0.91	0.16	154,159,163,163	0
2	ANP	A	1601	31/31	0.93	0.14	131,139,147,148	0
3	MG	A	1602	1/1	0.97	0.09	102,102,102,102	0
3	MG	B	1602	1/1	0.98	0.08	123,123,123,123	0

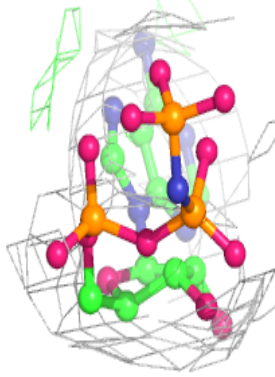
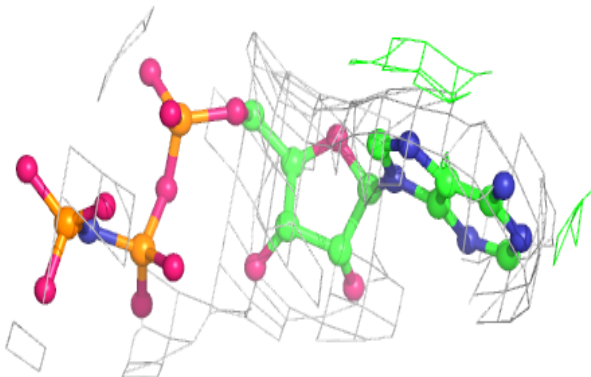
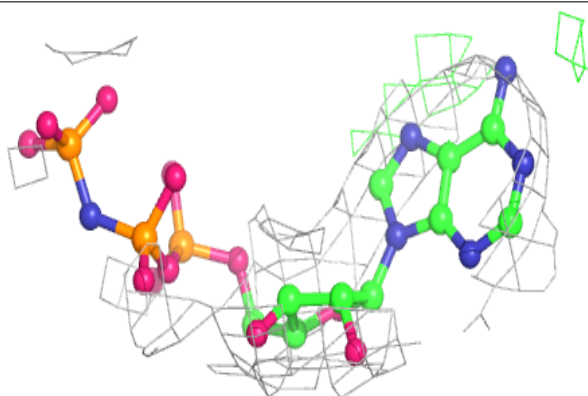
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around ANP B 1601:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around ANP A 1601:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.