



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:01 AM UTC

PDB ID : 4FCV / pdb\_00004fcv  
Title : Crystal structure of the C-terminal domain of ClpB  
Authors : Biter, A.B.; Lee, S.; Sung, N.; Tsai, F.T.F.  
Deposited on : 2012-05-25  
Resolution : 3.40 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

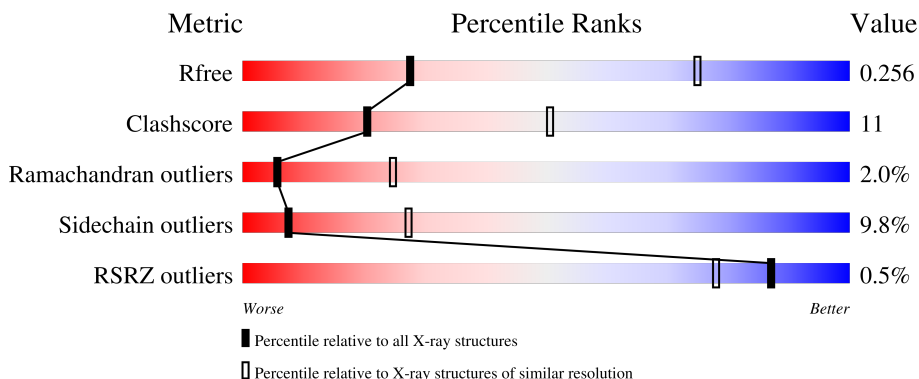
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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))
$R_{free}$	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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 of 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	311	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 68%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 28%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: red;"></div> </div> <p style="text-align: center;">68%                      28%                      .</p>
1	B	311	<div style="display: flex; align-items: center;"> <div style="width: 70%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 25%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: red;"></div> </div> <p style="text-align: center;">70%                      25%                      . .</p>
1	C	311	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 69%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 24%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 5%; height: 10px; background-color: orange;"></div> </div> <p style="text-align: center;">71%                      24%                      5%</p>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7527 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.

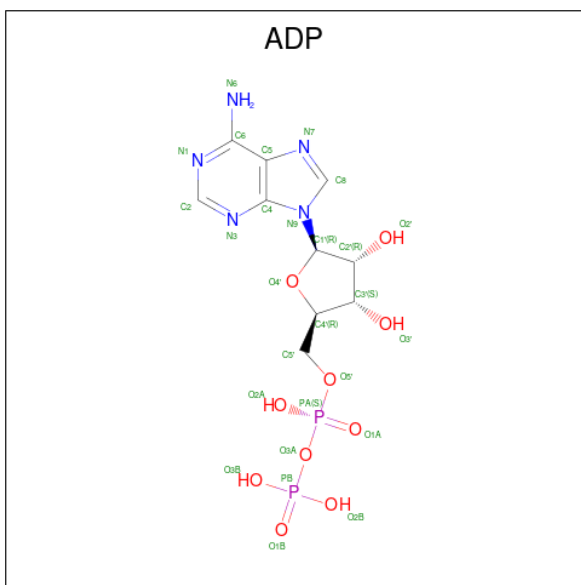
- Molecule 1 is a protein called Chaperone protein ClpB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	311	2482	1575	449	451	7	0	0	0
1	B	311	2482	1575	449	451	7	0	0	0
1	C	311	2482	1575	449	451	7	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	542	MSE	-	expression tag	UNP Q9RA63
A	543	LEU	-	expression tag	UNP Q9RA63
A	668	ALA	GLU	engineered mutation	UNP Q9RA63
A	683	MSE	ILE	engineered mutation	UNP Q9RA63
A	706	MSE	LEU	engineered mutation	UNP Q9RA63
A	770	MSE	LEU	engineered mutation	UNP Q9RA63
B	542	MSE	-	expression tag	UNP Q9RA63
B	543	LEU	-	expression tag	UNP Q9RA63
B	668	ALA	GLU	engineered mutation	UNP Q9RA63
B	683	MSE	ILE	engineered mutation	UNP Q9RA63
B	706	MSE	LEU	engineered mutation	UNP Q9RA63
B	770	MSE	LEU	engineered mutation	UNP Q9RA63
C	542	MSE	-	expression tag	UNP Q9RA63
C	543	LEU	-	expression tag	UNP Q9RA63
C	668	ALA	GLU	engineered mutation	UNP Q9RA63
C	683	MSE	ILE	engineered mutation	UNP Q9RA63
C	706	MSE	LEU	engineered mutation	UNP Q9RA63
C	770	MSE	LEU	engineered mutation	UNP Q9RA63

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).

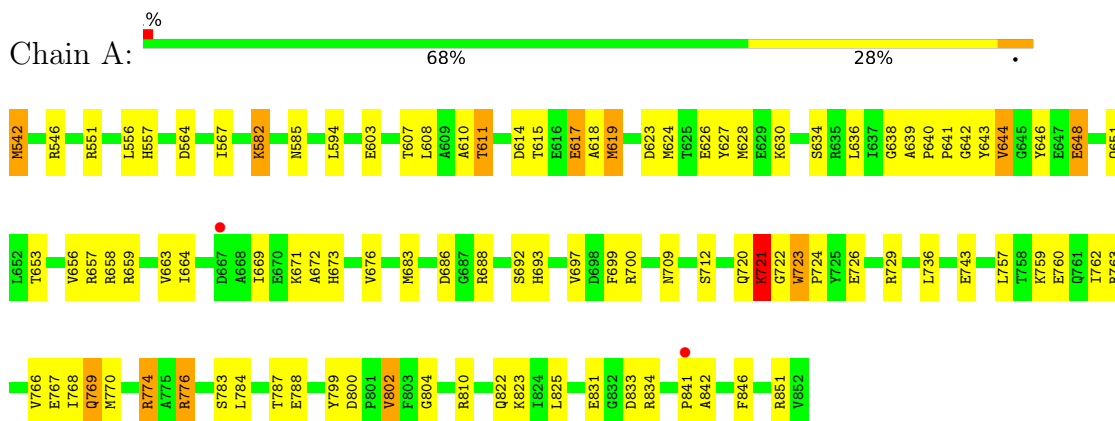


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			
2	A	1	Total	27	10	5	10	2	0	0
2	B	1	Total	27	10	5	10	2	0	0
2	C	1	Total	27	10	5	10	2	0	0

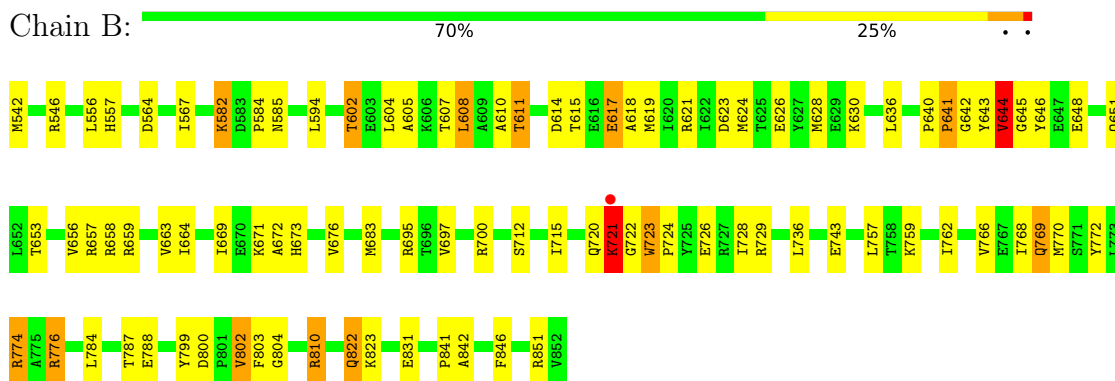
### 3 Residue-property plots i

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

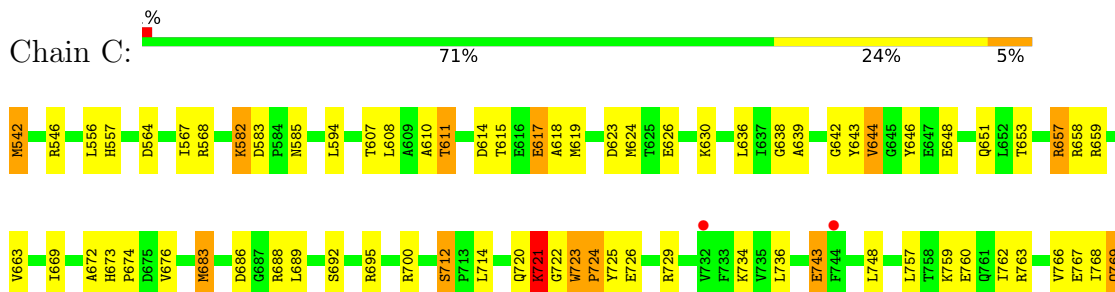
- Molecule 1: Chaperone protein ClpB



- Molecule 1: Chaperone protein ClpB



- Molecule 1: Chaperone protein ClpB





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.15Å 116.81Å 68.94Å 90.00° 119.52° 90.00°	Depositor
Resolution (Å)	41.85 – 3.40 41.85 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.0 (41.85-3.40) 99.0 (41.85-3.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.16 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.233 , 0.261 0.236 , 0.256	Depositor DCC
$R_{free}$ test set	647 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	86.5	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 53.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.049 for -h-l,k,h 0.049 for l,k,-h-l 0.040 for h,-k,-h-l 0.044 for -h-l,-k,l 0.041 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7527	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.57	1/2518 (0.0%)	0.88	2/3388 (0.1%)
1	B	0.61	2/2518 (0.1%)	0.89	3/3388 (0.1%)
1	C	0.60	2/2518 (0.1%)	0.89	2/3388 (0.1%)
All	All	0.59	5/7554 (0.1%)	0.89	7/10164 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	643	TYR	C-N	9.49	1.46	1.33
1	A	641	PRO	C-O	8.61	1.34	1.23
1	C	644	VAL	CA-CB	6.11	1.62	1.54
1	B	643	TYR	C-O	5.34	1.30	1.23
1	C	642	GLY	C-N	5.24	1.41	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	642	GLY	O-C-N	9.16	131.88	122.54
1	C	642	GLY	CA-C-O	6.89	126.43	119.27
1	B	640	PRO	O-C-N	5.93	124.04	121.31
1	B	642	GLY	O-C-N	5.27	129.55	122.70
1	B	715	ILE	N-CA-C	-5.14	106.90	113.22
1	A	833	ASP	N-CA-C	5.08	116.84	110.24
1	C	568	ARG	N-CA-C	-5.04	105.48	110.97

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2482	0	2549	64	0
1	B	2482	0	2549	57	0
1	C	2482	0	2549	57	0
2	A	27	0	12	3	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
All	All	7527	0	7683	170	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 11.

All (170) 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:774:ARG:HH11	1:B:774:ARG:HG3	1.43	0.83
1:A:582:LYS:HE3	1:A:582:LYS:HA	1.61	0.83
1:A:774:ARG:HG3	1:A:774:ARG:HH11	1.43	0.81
1:C:774:ARG:HH11	1:C:774:ARG:HG3	1.47	0.80
1:C:582:LYS:HE3	1:C:582:LYS:HA	1.64	0.80
1:A:653:THR:O	1:A:657:ARG:HB2	1.83	0.79
1:B:582:LYS:HE3	1:B:582:LYS:HA	1.62	0.78
1:C:653:THR:O	1:C:657:ARG:HB2	1.83	0.78
1:B:653:THR:O	1:B:657:ARG:HB2	1.85	0.76
1:B:585:ASN:HA	1:B:700:ARG:HD2	1.69	0.73
1:B:607:THR:O	1:B:611:THR:CG2	2.36	0.73
1:C:607:THR:O	1:C:611:THR:CG2	2.37	0.72
1:A:603:GLU:CG	2:A:901:ADP:H2'	2.22	0.70
1:A:825:LEU:O	1:B:546:ARG:HD3	1.92	0.70
1:C:638:GLY:O	1:C:692:SER:HB2	1.92	0.70
1:C:769:GLN:HE21	1:C:769:GLN:HA	1.58	0.69
1:C:618:ALA:HA	1:C:659:ARG:HD3	1.74	0.67
1:C:607:THR:O	1:C:611:THR:HG22	1.96	0.65
1:B:594:LEU:HD11	1:B:736:LEU:HD11	1.78	0.65
1:B:607:THR:O	1:B:611:THR:HG22	1.96	0.65
1:C:726:GLU:HG2	1:C:729:ARG:HH12	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:638:GLY:O	1:A:692:SER:HB2	1.97	0.65
1:B:726:GLU:HG2	1:B:729:ARG:HH12	1.60	0.64
1:A:624:MSE:HE1	1:A:676:VAL:HG11	1.79	0.64
1:A:585:ASN:HA	1:A:700:ARG:HD2	1.79	0.64
1:B:823:LYS:HE2	1:B:846:PHE:HB2	1.80	0.64
1:A:603:GLU:HG2	2:A:901:ADP:H2'	1.80	0.64
1:A:594:LEU:HD11	1:A:736:LEU:HD11	1.78	0.63
1:A:607:THR:O	1:A:611:THR:CG2	2.46	0.62
1:B:607:THR:O	1:B:611:THR:HG23	1.98	0.62
1:A:823:LYS:HE2	1:A:846:PHE:HB2	1.82	0.62
1:A:726:GLU:HG2	1:A:729:ARG:HH12	1.64	0.61
1:C:823:LYS:HE2	1:C:846:PHE:HB2	1.82	0.60
1:B:723:TRP:N	1:B:723:TRP:CD1	2.70	0.60
1:C:723:TRP:N	1:C:723:TRP:CD1	2.69	0.60
1:C:607:THR:O	1:C:611:THR:HG23	2.00	0.60
1:A:723:TRP:CD1	1:A:723:TRP:N	2.70	0.60
1:B:774:ARG:HG3	1:B:774:ARG:NH1	2.16	0.59
1:A:721:LYS:O	1:A:723:TRP:N	2.36	0.59
1:A:636:LEU:HA	1:A:651:GLN:HE22	1.69	0.58
1:A:774:ARG:HG3	1:A:774:ARG:NH1	2.17	0.58
1:C:624:MSE:CE	1:C:672:ALA:HB2	2.33	0.58
1:B:803:PHE:HZ	1:C:734:LYS:HG2	1.69	0.58
1:B:721:LYS:O	1:B:723:TRP:N	2.37	0.58
1:C:594:LEU:HD11	1:C:736:LEU:HD11	1.86	0.57
1:A:776:ARG:HH21	1:B:584:PRO:HD3	1.69	0.57
1:A:556:LEU:HD23	1:A:611:THR:HG21	1.87	0.57
1:A:769:GLN:HE21	1:A:769:GLN:HA	1.70	0.56
1:C:762:ILE:O	1:C:766:VAL:HG23	2.06	0.56
1:C:721:LYS:O	1:C:723:TRP:N	2.39	0.56
1:A:542:MSE:SE	1:A:546:ARG:HG2	2.56	0.56
1:A:825:LEU:O	1:B:546:ARG:CD	2.53	0.56
1:B:624:MSE:CE	1:B:672:ALA:HB2	2.36	0.56
1:B:757:LEU:HD12	1:B:799:TYR:HE1	1.70	0.56
1:B:621:ARG:HD2	1:C:743:GLU:OE2	2.06	0.56
1:C:624:MSE:HE1	1:C:676:VAL:HG11	1.88	0.55
1:A:607:THR:O	1:A:611:THR:HG22	2.06	0.55
1:A:757:LEU:HD12	1:A:799:TYR:HE1	1.72	0.55
1:A:607:THR:O	1:A:611:THR:HG23	2.06	0.55
1:B:624:MSE:HE1	1:B:676:VAL:HG11	1.89	0.55
1:A:766:VAL:O	1:A:770:MSE:HG2	2.06	0.55
1:A:800:ASP:OD2	1:A:802:VAL:HG22	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:624:MSE:HE2	1:C:672:ALA:CB	2.37	0.54
1:B:766:VAL:O	1:B:770:MSE:HG2	2.07	0.54
1:A:762:ILE:O	1:A:766:VAL:HG23	2.07	0.54
1:B:762:ILE:O	1:B:766:VAL:HG23	2.08	0.54
1:B:556:LEU:HD23	1:B:611:THR:HG21	1.88	0.54
1:C:800:ASP:OD2	1:C:802:VAL:HG22	2.09	0.53
1:C:624:MSE:HE2	1:C:672:ALA:HB2	1.90	0.53
1:B:769:GLN:HE21	1:B:769:GLN:HA	1.74	0.53
1:C:624:MSE:CE	1:C:672:ALA:CB	2.87	0.52
1:C:585:ASN:HA	1:C:700:ARG:HD2	1.92	0.52
1:C:766:VAL:O	1:C:770:MSE:HG2	2.10	0.52
1:B:624:MSE:HE2	1:B:672:ALA:HB2	1.92	0.52
1:C:639:ALA:O	1:C:646:TYR:HD2	1.93	0.52
1:C:774:ARG:HG3	1:C:774:ARG:NH1	2.19	0.52
1:B:624:MSE:HE2	1:B:672:ALA:CB	2.40	0.52
1:A:841:PRO:HD2	1:A:842:ALA:H	1.76	0.51
1:B:636:LEU:HA	1:B:651:GLN:HE22	1.74	0.51
1:C:618:ALA:HA	1:C:659:ARG:HH11	1.76	0.51
1:C:556:LEU:HD23	1:C:611:THR:HG21	1.93	0.50
1:A:634:SER:HB2	1:A:639:ALA:HA	1.93	0.50
1:A:646:TYR:CZ	1:A:693:HIS:CE1	3.00	0.50
1:B:624:MSE:CE	1:B:672:ALA:CB	2.90	0.50
1:B:800:ASP:OD2	1:B:802:VAL:HG22	2.10	0.50
1:B:557:HIS:CE1	1:B:567:ILE:HD12	2.47	0.49
1:B:803:PHE:CZ	1:C:734:LYS:HG2	2.47	0.49
1:C:757:LEU:HD12	1:C:799:TYR:HE1	1.78	0.48
1:A:628:MSE:HG2	1:A:671:LYS:O	2.13	0.48
1:A:618:ALA:HA	1:A:659:ARG:HD3	1.95	0.47
1:B:623:ASP:O	1:B:626:GLU:HG2	2.15	0.47
1:B:602:THR:O	1:B:605:ALA:HB3	2.15	0.47
1:B:618:ALA:HA	1:B:659:ARG:HD3	1.97	0.47
1:A:618:ALA:HA	1:A:659:ARG:HH11	1.80	0.47
1:A:603:GLU:HG3	2:A:901:ADP:H2'	1.96	0.47
1:A:630:LYS:HE2	1:A:673:HIS:HE2	1.79	0.46
1:A:624:MSE:CE	1:A:672:ALA:HB2	2.45	0.46
1:A:557:HIS:CE1	1:A:567:ILE:HD12	2.51	0.46
1:A:623:ASP:O	1:A:626:GLU:HG2	2.15	0.46
1:B:628:MSE:HG2	1:B:671:LYS:O	2.15	0.46
1:B:636:LEU:HD22	1:B:676:VAL:HG13	1.98	0.46
1:C:760:GLU:HA	1:C:763:ARG:HH11	1.81	0.45
1:C:619:MSE:HA	1:C:663:VAL:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:619:MSE:HA	1:B:663:VAL:O	2.17	0.45
1:C:623:ASP:O	1:C:626:GLU:HG2	2.17	0.45
1:A:776:ARG:HD2	1:A:776:ARG:HA	1.57	0.45
1:A:841:PRO:CD	1:A:842:ALA:H	2.29	0.45
1:C:557:HIS:CE1	1:C:567:ILE:HD12	2.51	0.45
1:B:787:THR:HG22	1:B:788:GLU:N	2.32	0.44
1:A:648:GLU:H	1:A:648:GLU:CD	2.26	0.44
1:B:656:VAL:HG22	1:B:664:ILE:HD11	1.99	0.44
1:C:624:MSE:HG3	1:C:669:ILE:HA	1.99	0.44
1:C:776:ARG:HA	1:C:776:ARG:HD2	1.60	0.43
1:A:624:MSE:HG3	1:A:669:ILE:HA	2.00	0.43
1:A:760:GLU:HA	1:A:763:ARG:HH11	1.84	0.43
1:B:610:ALA:O	1:B:614:ASP:HA	2.18	0.43
1:B:776:ARG:HD2	1:B:776:ARG:HA	1.60	0.43
1:C:610:ALA:O	1:C:614:ASP:HA	2.17	0.43
1:C:615:THR:OG1	1:C:617:GLU:HG2	2.18	0.43
1:A:686:ASP:C	1:A:688:ARG:N	2.74	0.43
1:A:624:MSE:HE2	1:A:672:ALA:CB	2.47	0.43
1:B:822:GLN:HE21	1:B:822:GLN:HB2	1.61	0.43
1:C:787:THR:HG22	1:C:788:GLU:N	2.34	0.43
1:A:640:PRO:O	1:A:643:TYR:HB2	2.18	0.43
1:B:641:PRO:HA	1:B:646:TYR:CZ	2.54	0.43
1:C:800:ASP:O	1:C:804:GLY:N	2.52	0.43
1:B:800:ASP:O	1:B:804:GLY:N	2.52	0.43
1:A:624:MSE:CE	1:A:672:ALA:CB	2.96	0.42
1:B:841:PRO:HD2	1:B:842:ALA:H	1.84	0.42
1:C:686:ASP:C	1:C:688:ARG:N	2.74	0.42
1:C:724:PRO:HB2	1:C:725:TYR:H	1.65	0.42
1:A:551:ARG:HE	1:A:551:ARG:HB3	1.65	0.42
1:B:615:THR:OG1	1:B:617:GLU:HG2	2.19	0.42
1:C:542:MSE:SE	1:C:546:ARG:HG2	2.69	0.42
1:B:615:THR:HG23	1:B:618:ALA:HB2	2.01	0.42
1:A:774:ARG:HH11	1:A:774:ARG:CG	2.23	0.42
1:B:624:MSE:HG3	1:B:669:ILE:HA	2.00	0.42
1:B:644:VAL:HG23	1:B:645:GLY:H	1.84	0.42
1:C:689:LEU:HD12	1:C:689:LEU:HA	1.87	0.42
1:B:810:ARG:NH2	1:C:748:LEU:O	2.53	0.42
1:C:636:LEU:HD22	1:C:676:VAL:HG13	2.01	0.42
1:B:657:ARG:NH2	1:B:695:ARG:HD2	2.35	0.41
1:A:615:THR:OG1	1:A:617:GLU:HG2	2.20	0.41
1:A:643:TYR:O	1:A:644:VAL:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:653:THR:HB	1:A:697:VAL:HG21	2.02	0.41
1:A:783:SER:HB2	1:A:834:ARG:HA	2.02	0.41
1:C:638:GLY:C	1:C:692:SER:HB2	2.44	0.41
1:C:763:ARG:HD2	1:C:792:ASP:OD2	2.20	0.41
1:A:619:MSE:HA	1:A:663:VAL:O	2.21	0.41
1:A:639:ALA:O	1:A:646:TYR:HD2	2.04	0.41
1:A:656:VAL:HG22	1:A:664:ILE:HD11	2.03	0.41
1:B:653:THR:HB	1:B:697:VAL:HG21	2.03	0.41
1:C:636:LEU:HA	1:C:651:GLN:HE22	1.86	0.41
1:A:610:ALA:O	1:A:614:ASP:HA	2.21	0.41
1:C:630:LYS:HE2	1:C:673:HIS:HE2	1.85	0.41
1:A:787:THR:HG22	1:A:788:GLU:N	2.36	0.41
1:B:630:LYS:HE2	1:B:673:HIS:HE2	1.84	0.41
1:B:772:TYR:OH	1:C:583:ASP:HA	2.21	0.41
1:C:657:ARG:NH2	1:C:695:ARG:HD2	2.35	0.41
1:A:800:ASP:O	1:A:804:GLY:N	2.54	0.41
1:C:712:SER:C	1:C:714:LEU:H	2.29	0.41
1:A:624:MSE:HE2	1:A:672:ALA:HB2	2.02	0.40
1:B:618:ALA:HA	1:B:659:ARG:HH11	1.85	0.40
1:C:695:ARG:HE	1:C:695:ARG:HB2	1.74	0.40
1:C:683:MSE:HB2	1:C:689:LEU:HD13	2.02	0.40
1:A:626:GLU:HG3	1:A:627:TYR:CE1	2.57	0.40
1:A:709:ASN:OD1	1:A:709:ASN:N	2.52	0.40
1:B:604:LEU:O	1:B:608:LEU:HB2	2.22	0.40
1:C:673:HIS:HA	1:C:674:PRO:HD3	1.93	0.40
1:A:656:VAL:HG21	1:A:699:PHE:CE2	2.56	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	309/311 (99%)	281 (91%)	22 (7%)	6 (2%)	6	26
1	B	309/311 (99%)	280 (91%)	22 (7%)	7 (2%)	5	23
1	C	309/311 (99%)	281 (91%)	22 (7%)	6 (2%)	6	26
All	All	927/933 (99%)	842 (91%)	66 (7%)	19 (2%)	6	25

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	721	LYS
1	B	644	VAL
1	B	721	LYS
1	C	644	VAL
1	C	721	LYS
1	A	720	GLN
1	A	722	GLY
1	B	641	PRO
1	B	720	GLN
1	B	722	GLY
1	C	720	GLN
1	C	722	GLY
1	A	724	PRO
1	B	724	PRO
1	C	724	PRO
1	A	712	SER
1	B	712	SER
1	C	712	SER
1	A	644	VAL

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	262/255 (103%)	237 (90%)	25 (10%)	8	29
1	B	262/255 (103%)	236 (90%)	26 (10%)	7	26
1	C	262/255 (103%)	236 (90%)	26 (10%)	7	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	786/765 (103%)	709 (90%)	77 (10%)	7 27

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	542	MSE
1	A	564	ASP
1	A	582	LYS
1	A	608	LEU
1	A	611	THR
1	A	617	GLU
1	A	619	MSE
1	A	648	GLU
1	A	658	ARG
1	A	683	MSE
1	A	721	LYS
1	A	723	TRP
1	A	743	GLU
1	A	759	LYS
1	A	767	GLU
1	A	768	ILE
1	A	769	GLN
1	A	774	ARG
1	A	776	ARG
1	A	784	LEU
1	A	802	VAL
1	A	810	ARG
1	A	822	GLN
1	A	831	GLU
1	A	851	ARG
1	B	542	MSE
1	B	564	ASP
1	B	582	LYS
1	B	602	THR
1	B	608	LEU
1	B	611	THR
1	B	617	GLU
1	B	644	VAL
1	B	648	GLU
1	B	658	ARG
1	B	683	MSE
1	B	721	LYS

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Mol	Chain	Res	Type
1	B	723	TRP
1	B	728	ILE
1	B	743	GLU
1	B	759	LYS
1	B	768	ILE
1	B	769	GLN
1	B	774	ARG
1	B	776	ARG
1	B	784	LEU
1	B	802	VAL
1	B	810	ARG
1	B	822	GLN
1	B	831	GLU
1	B	851	ARG
1	C	542	MSE
1	C	564	ASP
1	C	582	LYS
1	C	608	LEU
1	C	611	THR
1	C	617	GLU
1	C	643	TYR
1	C	648	GLU
1	C	657	ARG
1	C	658	ARG
1	C	683	MSE
1	C	721	LYS
1	C	723	TRP
1	C	743	GLU
1	C	759	LYS
1	C	767	GLU
1	C	768	ILE
1	C	769	GLN
1	C	774	ARG
1	C	776	ARG
1	C	784	LEU
1	C	802	VAL
1	C	810	ARG
1	C	822	GLN
1	C	831	GLU
1	C	851	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	651	GLN
1	A	746	ASN
1	A	769	GLN
1	A	822	GLN
1	B	651	GLN
1	B	764	GLN
1	B	769	GLN
1	B	822	GLN
1	C	651	GLN
1	C	769	GLN
1	C	822	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

3 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	ADP	A	901	-	28,29,29	1.42	5 (17%)	43,45,45	1.95	9 (20%)
2	ADP	B	901	-	28,29,29	1.40	4 (14%)	43,45,45	1.96	8 (18%)
2	ADP	C	901	-	28,29,29	1.43	4 (14%)	43,45,45	1.79	8 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	901	-	-	4/16/32/32	0/3/3/3
2	ADP	B	901	-	-	6/16/32/32	0/3/3/3
2	ADP	C	901	-	-	4/16/32/32	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	ADP	C5-C4	4.77	1.47	1.39
2	C	901	ADP	C5-C4	4.54	1.47	1.39
2	A	901	ADP	C5-C4	4.29	1.46	1.39
2	A	901	ADP	C5-N7	-2.99	1.33	1.39
2	C	901	ADP	C5-N7	-2.98	1.33	1.39
2	B	901	ADP	C5-C6	2.49	1.47	1.41
2	B	901	ADP	C5-N7	-2.46	1.34	1.39
2	A	901	ADP	C5-C6	2.37	1.47	1.41
2	C	901	ADP	C8-N7	2.18	1.35	1.31
2	A	901	ADP	C8-N7	2.17	1.35	1.31
2	B	901	ADP	C8-N7	2.17	1.35	1.31
2	A	901	ADP	PB-O3B	2.07	1.62	1.54
2	C	901	ADP	C5-C6	2.04	1.46	1.41

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	ADP	C5-C4-N3	-6.74	117.44	126.72
2	A	901	ADP	C5-C4-N3	-6.43	117.87	126.72
2	B	901	ADP	N3-C4-N9	5.33	136.23	127.17
2	C	901	ADP	C5-C4-N3	-5.29	119.43	126.72
2	A	901	ADP	N3-C4-N9	5.09	135.82	127.17
2	C	901	ADP	N3-C4-N9	4.55	134.90	127.17
2	B	901	ADP	C2-N3-C4	4.15	121.96	111.83
2	A	901	ADP	C2-N3-C4	3.98	121.55	111.83
2	B	901	ADP	N3-C2-N1	-3.51	123.27	128.58
2	A	901	ADP	N3-C2-N1	-3.46	123.34	128.58
2	A	901	ADP	C4-C5-N7	-3.33	106.78	110.58
2	C	901	ADP	C2-N3-C4	3.23	119.73	111.83
2	C	901	ADP	N3-C2-N1	-3.08	123.92	128.58
2	B	901	ADP	C4-C5-N7	-2.89	107.28	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	ADP	O2B-PB-O1B	2.68	121.29	110.83
2	A	901	ADP	C5-N7-C8	2.66	107.63	103.45
2	C	901	ADP	C4-C5-N7	-2.62	107.59	110.58
2	C	901	ADP	C4-N9-C8	2.56	108.43	105.74
2	C	901	ADP	O2B-PB-O1B	2.51	120.62	110.83
2	A	901	ADP	O2B-PB-O1B	2.41	120.23	110.83
2	C	901	ADP	C5-N7-C8	2.31	107.08	103.45
2	A	901	ADP	C3'-C2'-C1'	2.23	105.69	101.46
2	A	901	ADP	C4-N9-C8	2.23	108.08	105.74
2	B	901	ADP	C5-N7-C8	2.11	106.76	103.45
2	B	901	ADP	O3A-PA-O1A	-2.05	104.53	110.70

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	ADP	C5'-O5'-PA-O1A
2	A	901	ADP	C5'-O5'-PA-O3A
2	A	901	ADP	O4'-C4'-C5'-O5'
2	B	901	ADP	C5'-O5'-PA-O1A
2	B	901	ADP	C5'-O5'-PA-O2A
2	B	901	ADP	C5'-O5'-PA-O3A
2	C	901	ADP	C5'-O5'-PA-O1A
2	C	901	ADP	O4'-C4'-C5'-O5'
2	A	901	ADP	C3'-C4'-C5'-O5'
2	C	901	ADP	C3'-C4'-C5'-O5'
2	B	901	ADP	C4'-C5'-O5'-PA
2	B	901	ADP	PB-O3A-PA-O1A
2	B	901	ADP	PB-O3A-PA-O2A
2	C	901	ADP	PB-O3A-PA-O1A

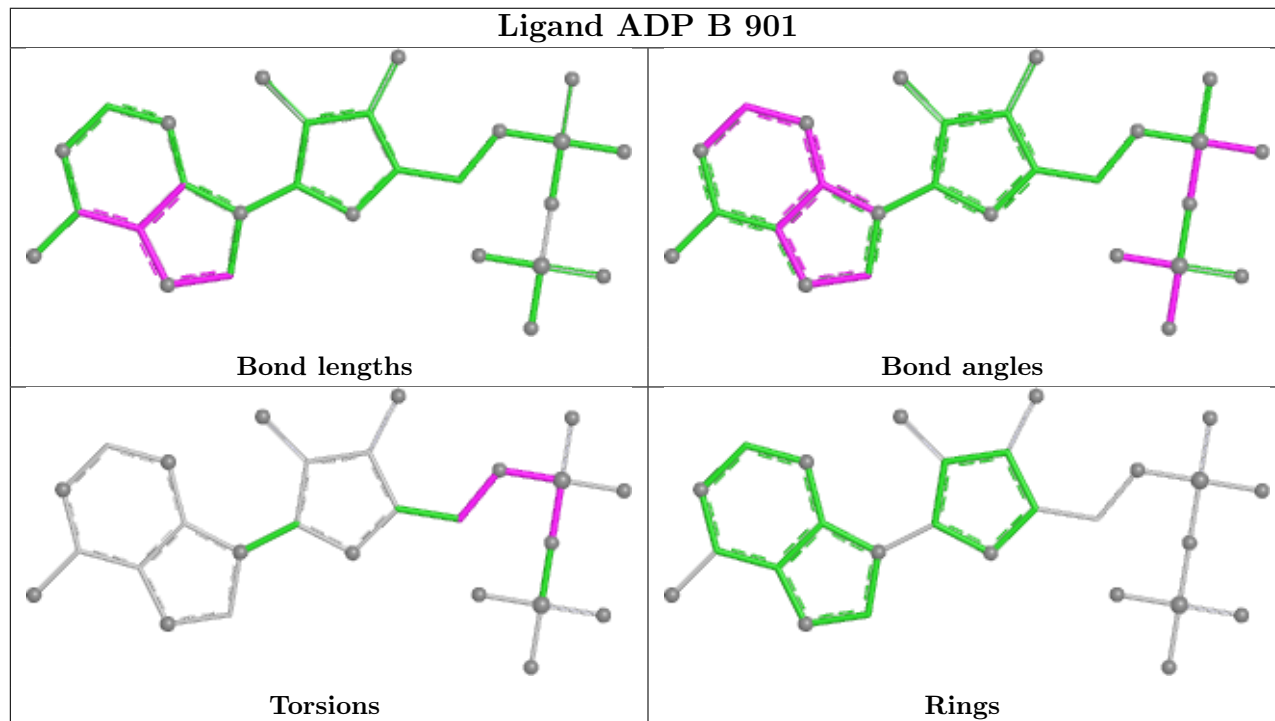
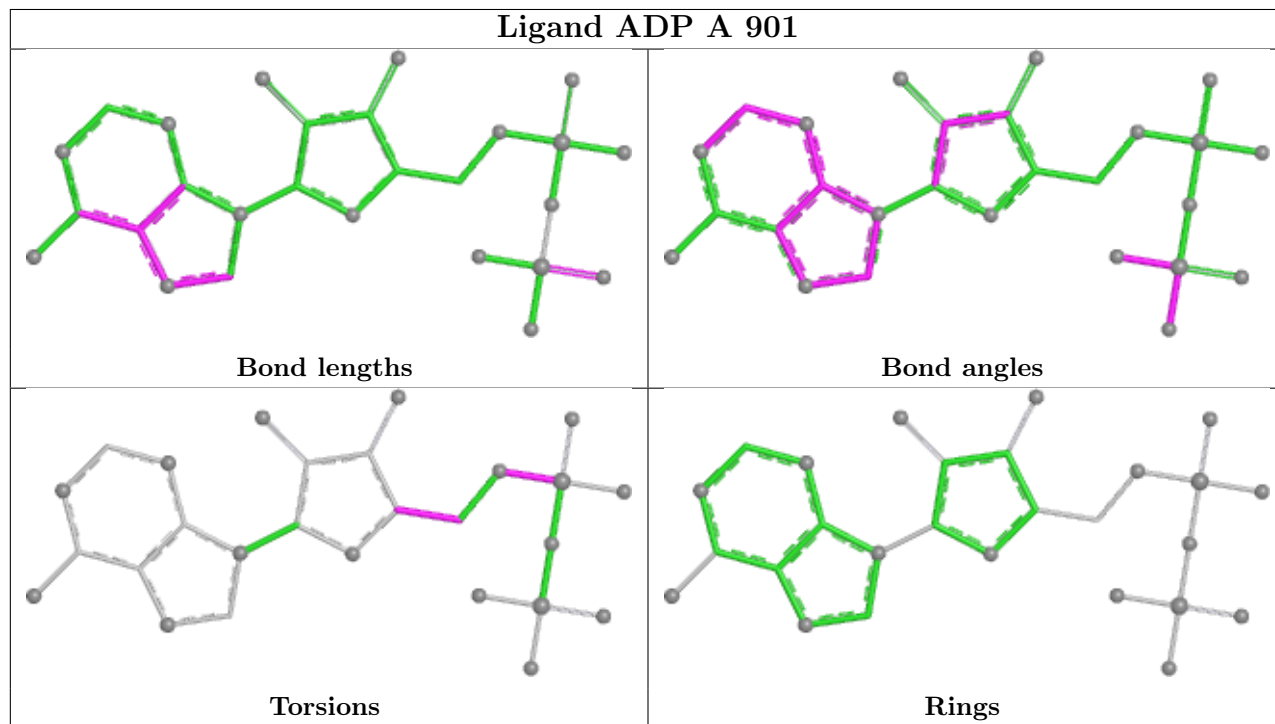
There are no ring outliers.

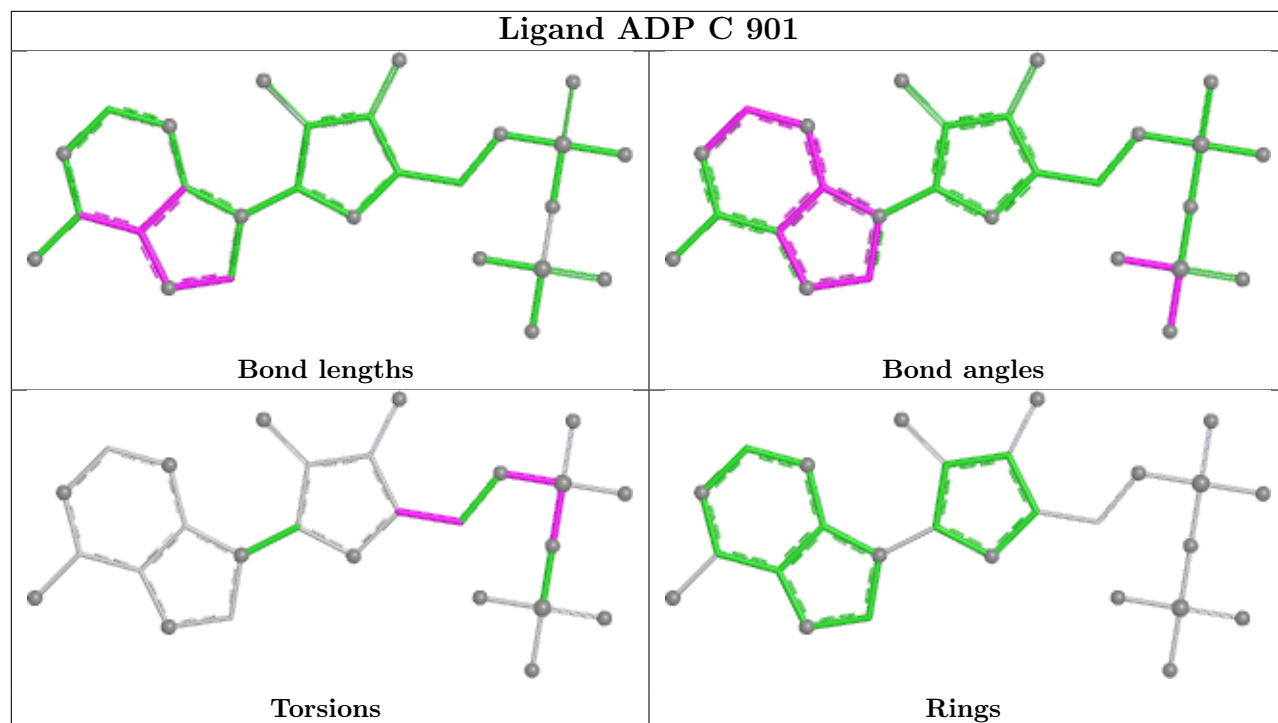
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	ADP	3	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	304/311 (97%)	-0.17	2 (0%) 84 73	69, 105, 172, 193	0
1	B	304/311 (97%)	-0.22	1 (0%) 90 84	58, 97, 155, 177	0
1	C	304/311 (97%)	-0.03	2 (0%) 84 73	62, 102, 169, 211	0
All	All	912/933 (97%)	-0.14	5 (0%) 87 78	58, 102, 167, 211	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	667	ASP	2.5
1	A	841	PRO	2.4
1	C	744	PHE	2.2
1	B	721	LYS	2.0
1	C	732	VAL	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](#)

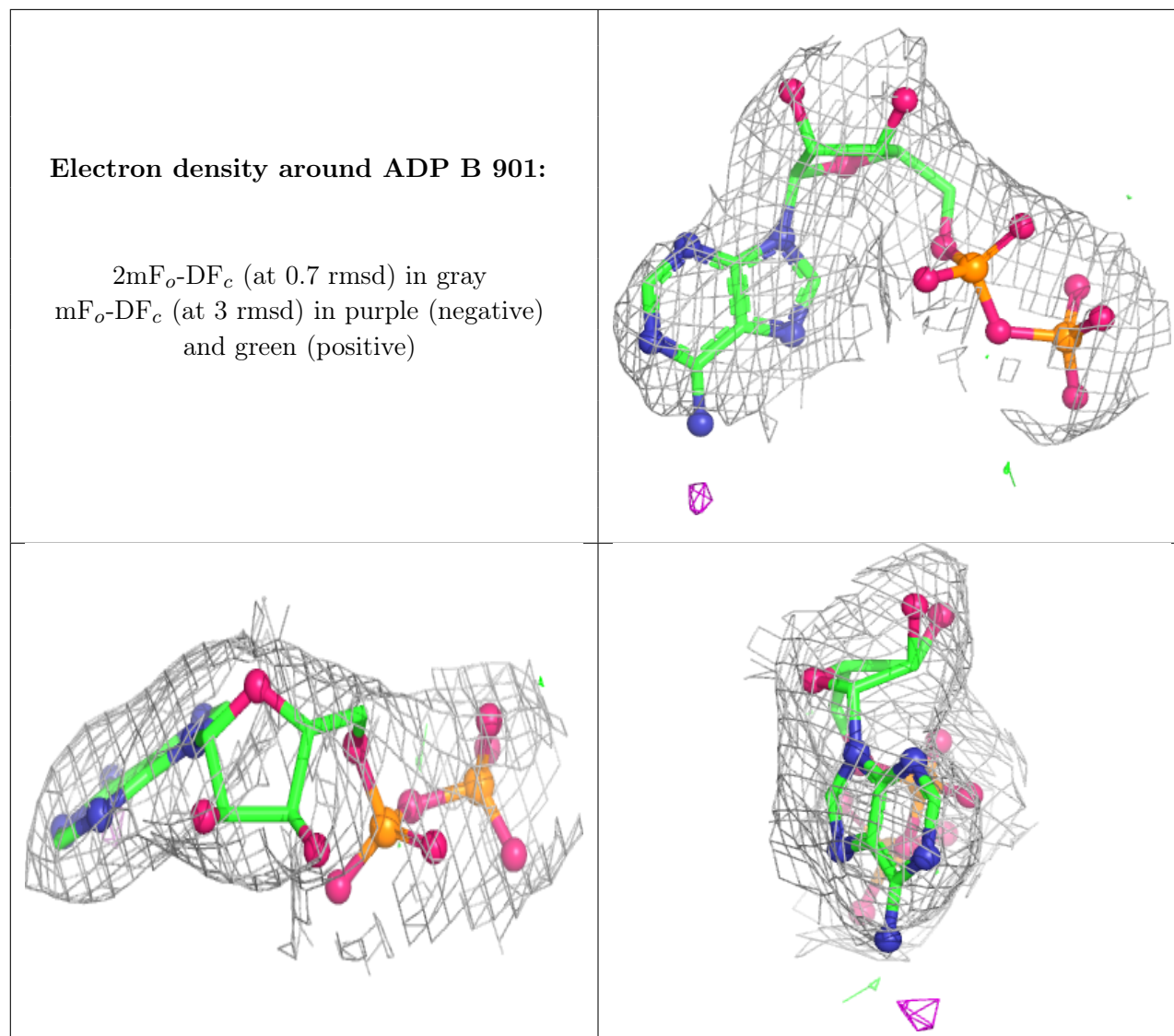
There are no oligosaccharides in this entry.

### 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.

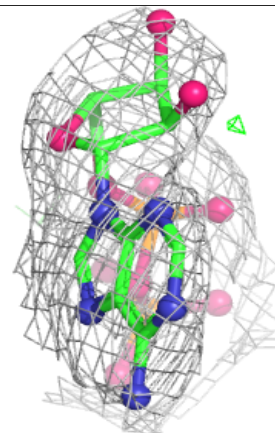
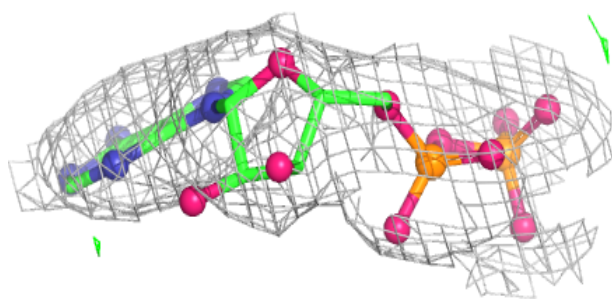
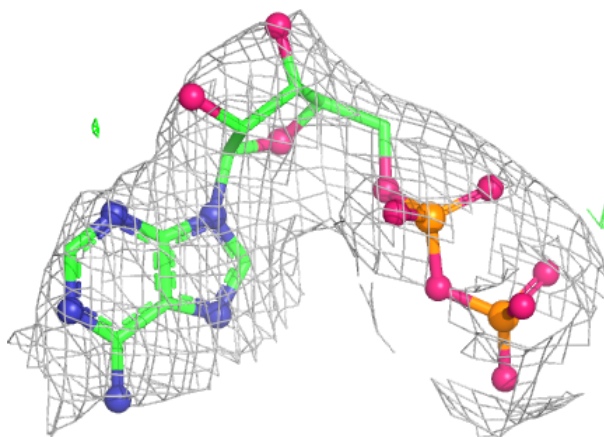
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ADP	B	901	27/27	0.94	0.08	63,66,76,76	0
2	ADP	C	901	27/27	0.94	0.07	69,75,81,81	0
2	ADP	A	901	27/27	0.95	0.06	66,73,92,93	0

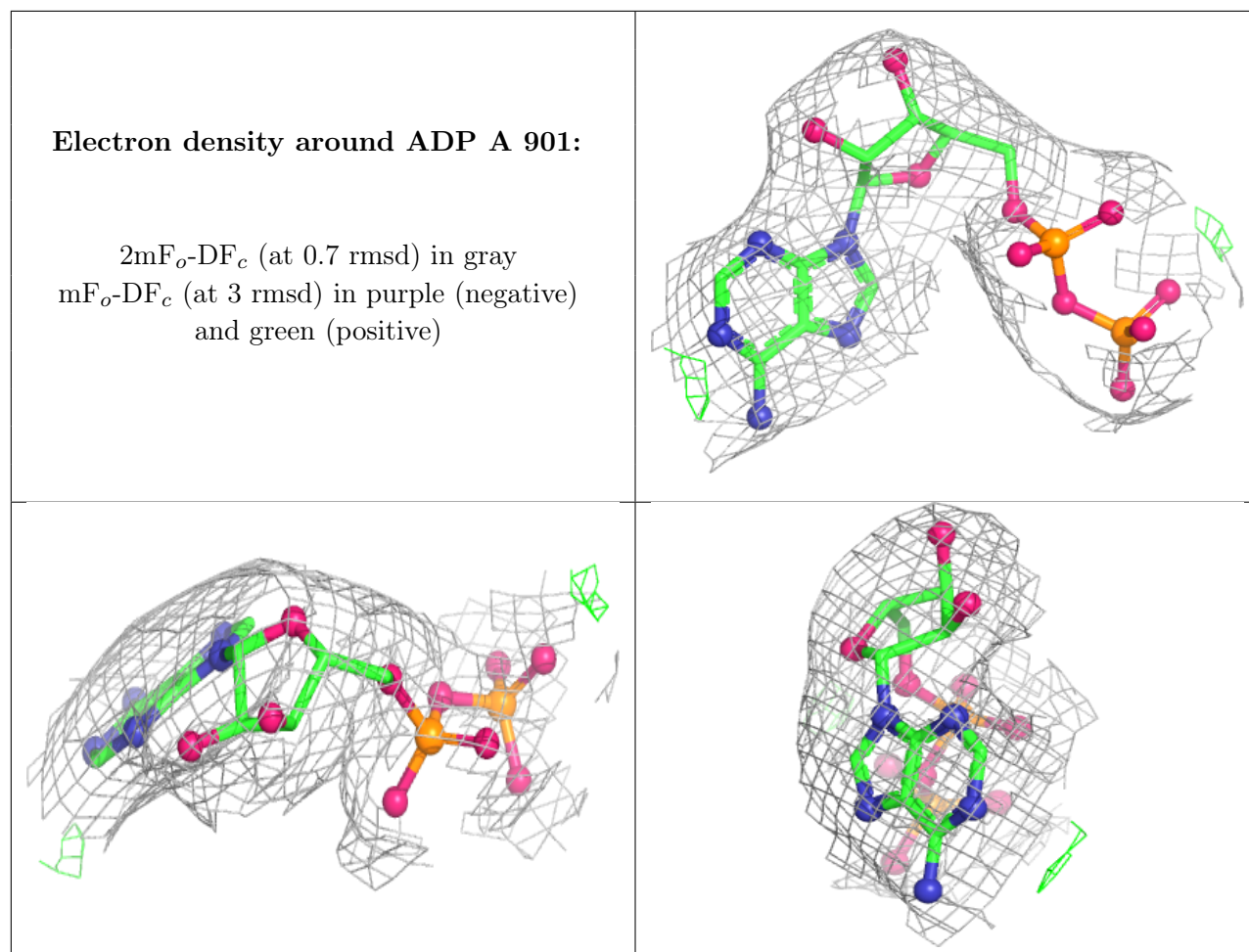
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



**Electron density around ADP C 901:**

$2mF_o-DF_c$  (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.