Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 04:51 am BST

PDB ID	:	4WW4
Title	:	Double-heterohexameric rings of full-length Rvb1(ADP)/Rvb2(ADP)
Authors	:	Lakomek, K.; Hopfner, K.-P.
Deposited on	:	2014-11-10
Resolution	:	2.94 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

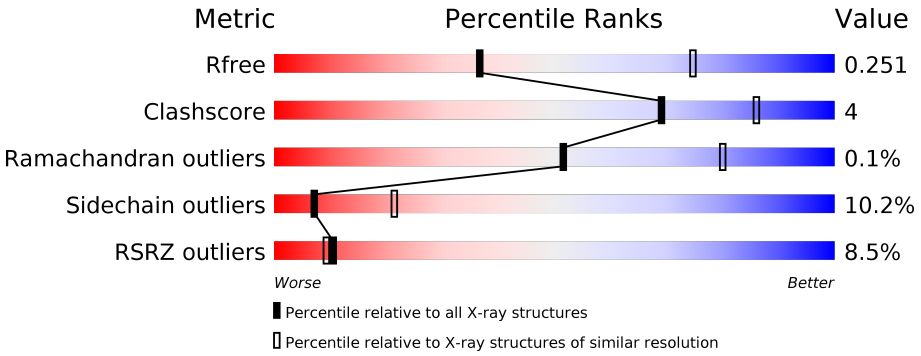
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 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	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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 <=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	462	10% 75% 14% • 10%
2	B	513	5% 71% 13% • 15%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6603 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 RuvB-like 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3190	1999	573	604	14			

- Molecule 2 is a protein called RuvB-like 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	435	Total	C	N	O	S	0	0	0
			3345	2092	592	647	14			

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-24	MET	-	initiating methionine	UNP G0RYC2
B	-23	GLY	-	expression tag	UNP G0RYC2
B	-22	SER	-	expression tag	UNP G0RYC2
B	-21	SER	-	expression tag	UNP G0RYC2
B	-20	HIS	-	expression tag	UNP G0RYC2
B	-19	HIS	-	expression tag	UNP G0RYC2
B	-18	HIS	-	expression tag	UNP G0RYC2
B	-17	HIS	-	expression tag	UNP G0RYC2
B	-16	HIS	-	expression tag	UNP G0RYC2
B	-15	HIS	-	expression tag	UNP G0RYC2
B	-14	HIS	-	expression tag	UNP G0RYC2
B	-13	HIS	-	expression tag	UNP G0RYC2
B	-12	SER	-	expression tag	UNP G0RYC2
B	-11	SER	-	expression tag	UNP G0RYC2
B	-10	GLY	-	expression tag	UNP G0RYC2
B	-9	LEU	-	expression tag	UNP G0RYC2
B	-8	GLU	-	expression tag	UNP G0RYC2
B	-7	VAL	-	expression tag	UNP G0RYC2
B	-6	LEU	-	expression tag	UNP G0RYC2
B	-5	PHE	-	expression tag	UNP G0RYC2

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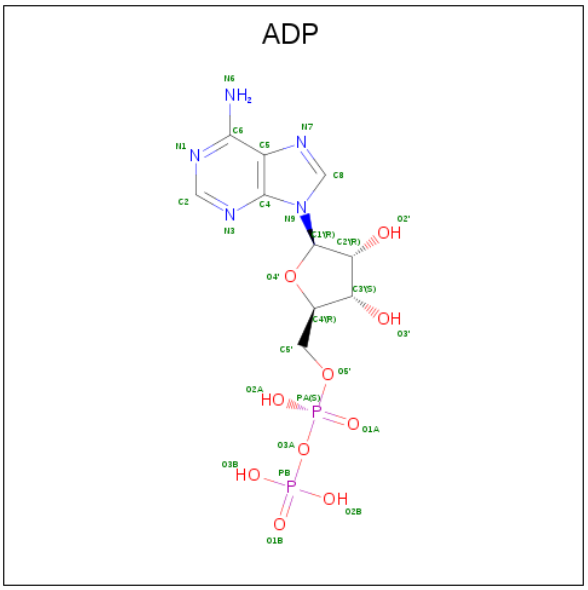
Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLN	-	expression tag	UNP G0RYC2
B	-3	GLY	-	expression tag	UNP G0RYC2
B	-2	PRO	-	expression tag	UNP G0RYC2
B	-1	GLY	-	expression tag	UNP G0RYC2
B	0	SER	-	expression tag	UNP G0RYC2

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 4 is water.

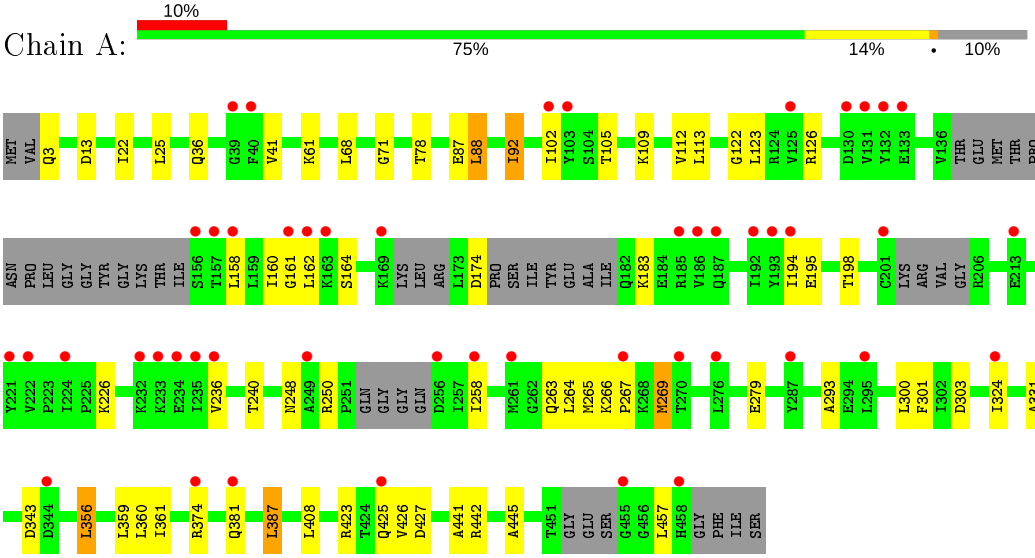
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	O	0	0
			4	4		
4	B	10	Total	O	0	0
			10	10		

3 Residue-property plots (i)

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

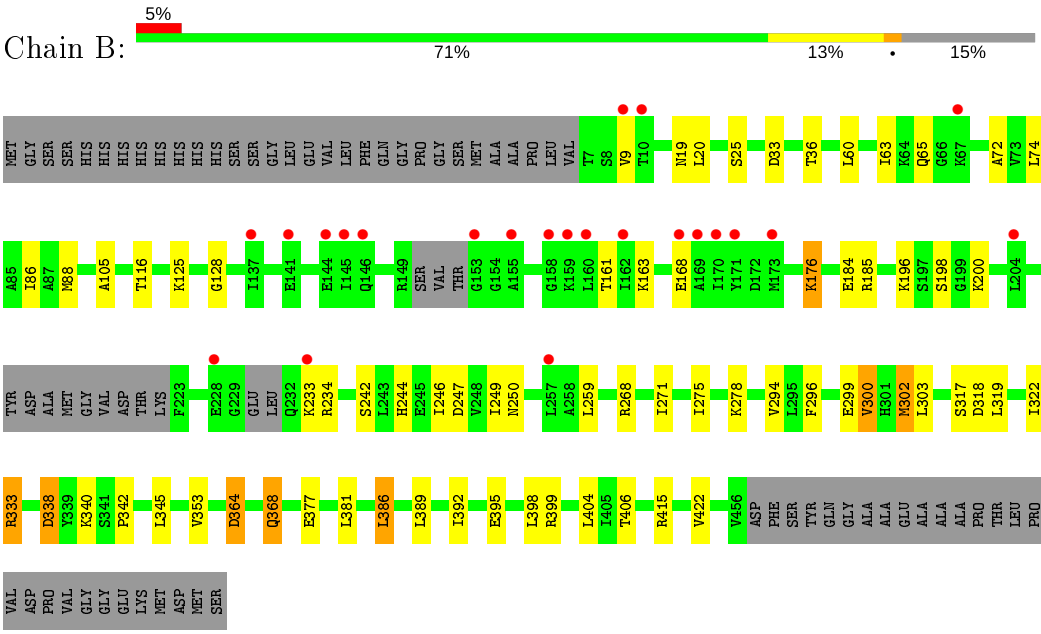
- Molecule 1: RuvB-like 1

Chain A:



- Molecule 2: RuvB-like 2

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	206.85Å 206.85Å 137.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	64.16 – 2.94 64.16 – 2.94	Depositor EDS
% Data completeness (in resolution range)	97.2 (64.16-2.94) 97.2 (64.16-2.94)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 2.96Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, R_{free}	0.198 , 0.223 0.215 , 0.251	Depositor DCC
R_{free} test set	1193 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	77.4	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 76.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6603	wwPDB-VP
Average B, all atoms (Å^2)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 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: 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	0.39	0/3227	0.64	0/4353
2	B	0.38	0/3383	0.62	0/4551
All	All	0.39	0/6610	0.63	0/8904

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	3190	0	3272	22	0
2	B	3345	0	3430	32	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
4	A	4	0	0	0	0
4	B	10	0	0	0	0
All	All	6603	0	6726	49	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 4.

All (49) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:246:ILE:HG22	2:B:275:ILE:HG12	1.79	0.65
1:A:387:LEU:HB3	1:A:426:VAL:HB	1.87	0.57
1:A:122:GLY:HA2	1:A:240:THR:HA	1.87	0.57
1:A:78:THR:HG22	1:A:301:PHE:CE2	2.40	0.56
2:B:294:VAL:HG22	2:B:322:ILE:HB	1.86	0.56
1:A:266:LYS:HG3	1:A:269:MET:H	1.73	0.54
2:B:163:LYS:HG2	2:B:168:GLU:HA	1.90	0.53
1:A:267:PRO:HB3	2:B:116:THR:HG22	1.90	0.53
1:A:340:ARG:HH22	2:B:338:ASP:H	1.57	0.52
2:B:72:ALA:HB3	2:B:353:VAL:HG12	1.91	0.52
2:B:80:SER:HB3	2:B:398:LEU:HB2	1.92	0.51
2:B:60:LEU:HA	2:B:63:ILE:HD12	1.93	0.50
1:A:88:LEU:HB3	1:A:92:ILE:HD13	1.93	0.50
2:B:9:VAL:HG23	2:B:249:ILE:HD11	1.95	0.49
2:B:300:VAL:HG12	2:B:303:LEU:HD12	1.96	0.48
2:B:333:ARG:HD3	2:B:340:LYS:HE3	1.94	0.48
1:A:71:GLY:O	1:A:333:ASN:HA	2.14	0.47
2:B:247:ASP:HA	2:B:275:ILE:HD13	1.96	0.47
1:A:126:ARG:HE	1:A:236:VAL:HG12	1.80	0.46
1:A:36:GLN:HG2	1:A:41:VAL:HG22	1.97	0.45
1:A:68:LEU:HD23	1:A:361:ILE:HG12	1.99	0.45
2:B:128:GLY:HA2	2:B:242:SER:HA	1.98	0.44
1:A:263:GLN:HG3	2:B:319:LEU:HD12	1.99	0.44
2:B:299:GLU:O	2:B:302:MET:HB2	2.18	0.44
2:B:74:LEU:HD23	2:B:325:MET:HG3	1.99	0.44
2:B:381:LEU:HD13	2:B:386:LEU:HG	2.00	0.44
2:B:268:ARG:HB2	2:B:271:ILE:HD12	2.00	0.44
1:A:356:LEU:HA	1:A:359:LEU:HD12	2.00	0.43
2:B:84:THR:HG22	2:B:296:PHE:CE2	2.53	0.43
1:A:78:THR:HG22	1:A:301:PHE:HE2	1.81	0.43
2:B:33:ASP:HB3	2:B:36:THR:O	2.18	0.43
1:A:102:ILE:HG12	1:A:113:LEU:HD13	2.00	0.42
1:A:445:ALA:HB2	2:B:342:PRO:HB3	2.01	0.42
1:A:303:ASP:HA	1:A:331:ALA:HB3	2.01	0.42
2:B:125:LYS:HE2	2:B:244:HIS:CE1	2.54	0.42
2:B:250:ASN:HB2	2:B:275:ILE:HD11	2.01	0.42
2:B:25:SER:HB2	2:B:185:ARG:HH21	1.85	0.42
2:B:300:VAL:HG11	2:B:325:MET:SD	2.60	0.42
2:B:176:LYS:H	2:B:176:LYS:HG3	1.70	0.41
2:B:9:VAL:HG23	2:B:249:ILE:CD1	2.49	0.41
2:B:364:ASP:O	2:B:368:GLN:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:105:ALA:HB1	2:B:303:LEU:HG	2.03	0.41
1:A:102:ILE:HG22	1:A:109:LYS:HG2	2.02	0.41
2:B:296:PHE:HA	2:B:324:ILE:O	2.21	0.41
1:A:3:GLN:HB3	1:A:248:ASN:ND2	2.35	0.40
1:A:441:ALA:HB1	2:B:342:PRO:HG2	2.04	0.40
1:A:123:LEU:HD22	1:A:293:ALA:HB1	2.03	0.40
2:B:392:ILE:HG21	2:B:404:LEU:HD12	2.03	0.40
1:A:25:LEU:HD12	1:A:87:GLU:HG3	2.03	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	402/462 (87%)	381 (95%)	20 (5%)	1 (0%)	47 76
2	B	427/513 (83%)	416 (97%)	11 (3%)	0	100 100
All	All	829/975 (85%)	797 (96%)	31 (4%)	1 (0%)	51 80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	161	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	341/377 (90%)	301 (88%)	40 (12%)	5 15
2	B	363/423 (86%)	331 (91%)	32 (9%)	10 28
All	All	704/800 (88%)	632 (90%)	72 (10%)	7 21

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASP
1	A	22	ILE
1	A	61	LYS
1	A	88	LEU
1	A	92	ILE
1	A	105	THR
1	A	112	VAL
1	A	158	LEU
1	A	160	ILE
1	A	162	LEU
1	A	164	SER
1	A	174	ASP
1	A	183	LYS
1	A	194	ILE
1	A	195	GLU
1	A	198	THR
1	A	216	LEU
1	A	219	GLU
1	A	226	LYS
1	A	250	ARG
1	A	258	ILE
1	A	264	LEU
1	A	265	MET
1	A	269	MET
1	A	279	GLU
1	A	300	LEU
1	A	324	ILE
1	A	340	ARG
1	A	343	ASP
1	A	356	LEU
1	A	360	LEU
1	A	374	ARG
1	A	381	GLN
1	A	387	LEU
1	A	408	LEU

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Mol	Chain	Res	Type
1	A	423	ARG
1	A	425	GLN
1	A	427	ASP
1	A	442	ARG
1	A	457	LEU
2	B	19	ASN
2	B	20	LEU
2	B	65	GLN
2	B	86	ILE
2	B	88	MET
2	B	161	THR
2	B	176	LYS
2	B	184	GLU
2	B	196	LYS
2	B	198	SER
2	B	200	LYS
2	B	233	LYS
2	B	234	ARG
2	B	259	LEU
2	B	278	LYS
2	B	300	VAL
2	B	302	MET
2	B	317	SER
2	B	318	ASP
2	B	333	ARG
2	B	338	ASP
2	B	345	LEU
2	B	364	ASP
2	B	368	GLN
2	B	377	GLU
2	B	386	LEU
2	B	389	LEU
2	B	395	GLU
2	B	399	ARG
2	B	406	THR
2	B	415	ARG
2	B	422	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	263	GLN

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Mol	Chain	Res	Type
2	B	49	GLN
2	B	244	HIS
2	B	394	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

2 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	$\#\|Z\| > 2$
3	ADP	A	501	-	24,29,29	0.65	0	29,45,45	0.86	1 (3%)
3	ADP	B	501	-	24,29,29	0.66	0	29,45,45	0.99	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
3	ADP	A	501	-	-	5/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	B	501	-	-	7/12/32/32	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	501	ADP	O2B-PB-O3A	2.47	112.93	104.64
3	B	501	ADP	C5-C6-N6	2.32	123.88	120.35
3	A	501	ADP	C5-C6-N6	2.27	123.81	120.35

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	ADP	C5'-O5'-PA-O2A
3	B	501	ADP	PA-O3A-PB-O2B
3	B	501	ADP	PA-O3A-PB-O3B
3	B	501	ADP	C5'-O5'-PA-O1A
3	B	501	ADP	C5'-O5'-PA-O2A
3	A	501	ADP	C5'-O5'-PA-O3A
3	B	501	ADP	C5'-O5'-PA-O3A
3	A	501	ADP	C5'-O5'-PA-O1A
3	B	501	ADP	C4'-C5'-O5'-PA
3	A	501	ADP	C4'-C5'-O5'-PA
3	B	501	ADP	PA-O3A-PB-O1B
3	A	501	ADP	PB-O3A-PA-O2A

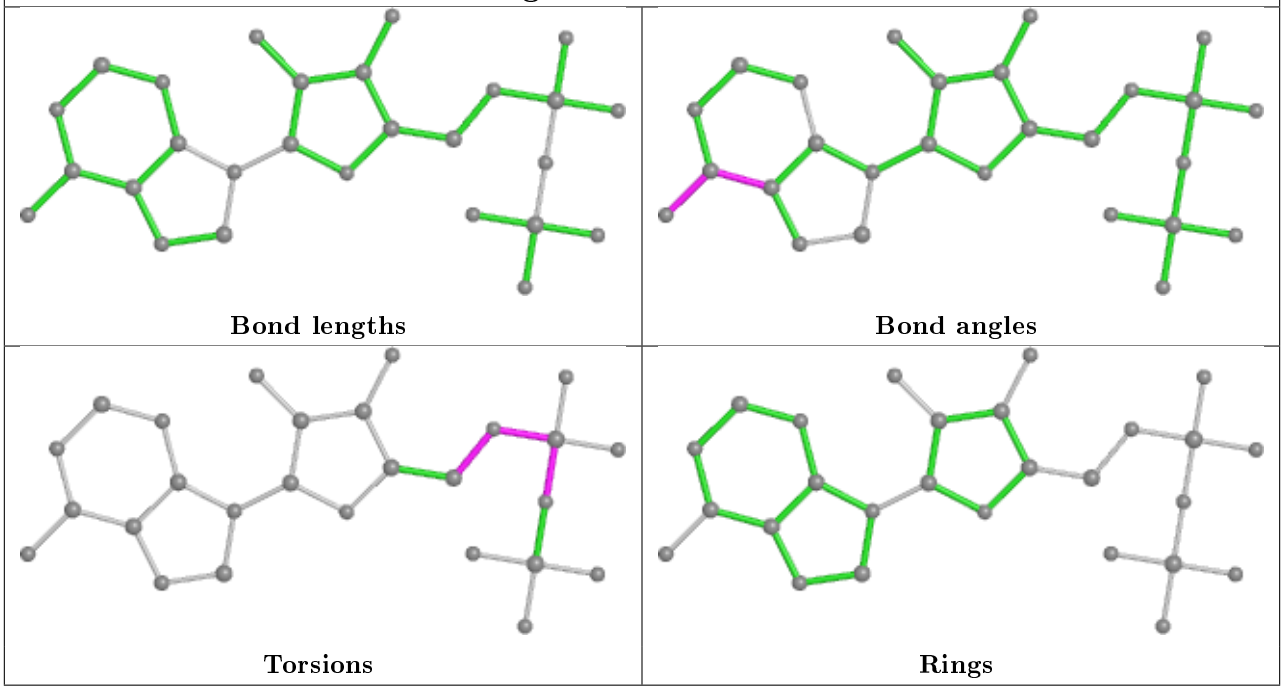
There are no ring outliers.

No monomer is involved in short contacts.

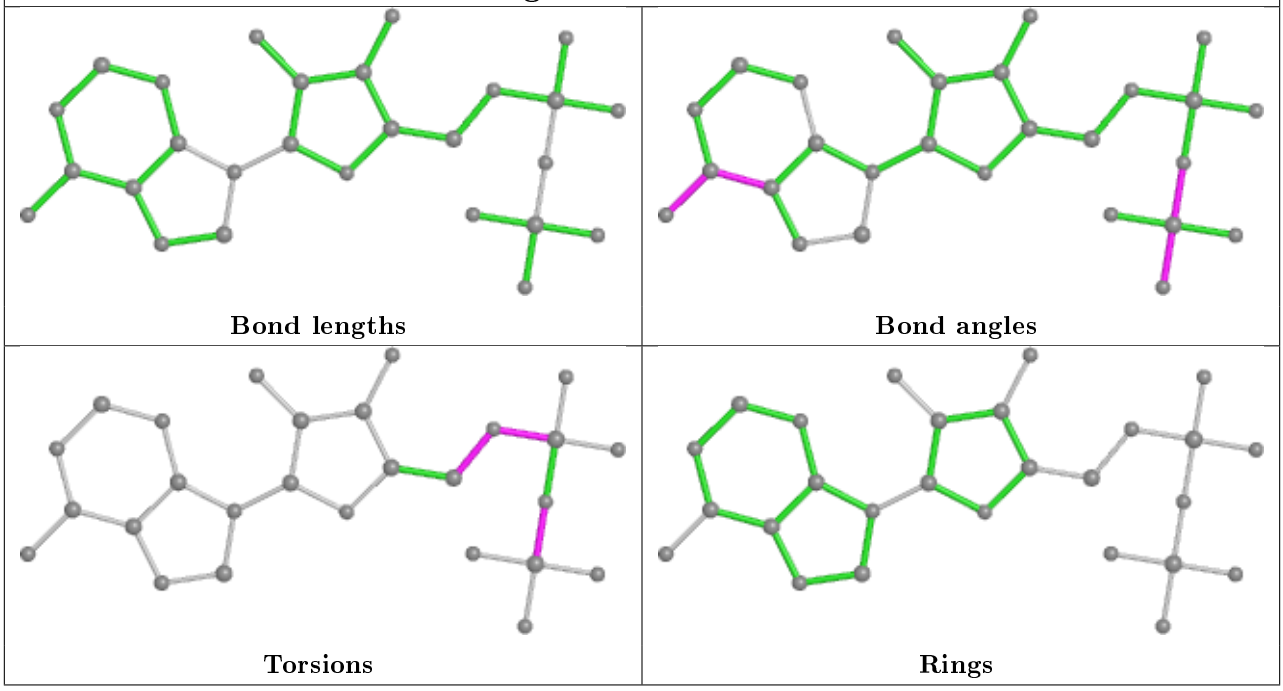
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

Ligand ADP A 501



Ligand ADP B 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	416/462 (90%)	0.77	48 (11%) 4 4	57, 101, 152, 174	0
2	B	435/513 (84%)	0.46	24 (5%) 25 23	55, 94, 128, 180	0
All	All	851/975 (87%)	0.61	72 (8%) 10 9	55, 97, 143, 180	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	194	ILE	7.0
1	A	157	THR	6.9
2	B	158	GLY	6.3
1	A	267	PRO	5.8
1	A	131	VAL	5.5
1	A	458	HIS	5.5
1	A	161	GLY	4.9
2	B	169	ALA	4.7
2	B	171	TYR	4.5
1	A	186	VAL	4.3
1	A	156	SER	3.9
2	B	204	LEU	3.7
2	B	146	GLN	3.7
1	A	287	TYR	3.6
1	A	234	GLU	3.6
1	A	192	ILE	3.6
1	A	193	TYR	3.5
1	A	224	ILE	3.3
1	A	261	MET	3.3
1	A	158	LEU	3.3
2	B	173	MET	3.2
1	A	270	THR	3.2
2	B	9	VAL	3.2
1	A	133	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	207	SER	3.1
2	B	67	LYS	3.1
2	B	144	GLU	3.1
2	B	145	ILE	3.1
2	B	160	LEU	3.1
2	B	170	ILE	3.0
1	A	381	GLN	2.9
1	A	249	ALA	2.9
1	A	103	TYR	2.8
1	A	233	LYS	2.8
2	B	159	LYS	2.8
1	A	187	GLN	2.7
1	A	258	ILE	2.7
1	A	236	VAL	2.7
1	A	201	CYS	2.6
1	A	222	VAL	2.6
1	A	221	TYR	2.6
1	A	102	ILE	2.6
1	A	295	LEU	2.6
1	A	232	LYS	2.5
1	A	162	LEU	2.5
1	A	256	ASP	2.5
1	A	374	ARG	2.5
2	B	257	LEU	2.4
1	A	132	TYR	2.4
1	A	125	VAL	2.4
1	A	455	GLY	2.4
1	A	425	GLN	2.4
1	A	40	PHE	2.3
1	A	235	ILE	2.3
2	B	10	THR	2.3
1	A	276	LEU	2.3
2	B	141	GLU	2.2
2	B	137	ILE	2.2
2	B	228	GLU	2.2
1	A	163	LYS	2.2
2	B	233	LYS	2.2
2	B	168	GLU	2.2
2	B	153	GLY	2.2
1	A	324	ILE	2.1
1	A	185	ARG	2.1
1	A	213	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	39	GLY	2.1
2	B	162	ILE	2.1
2	B	155	ALA	2.1
1	A	344	ASP	2.0
1	A	130	ASP	2.0
1	A	169	LYS	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)

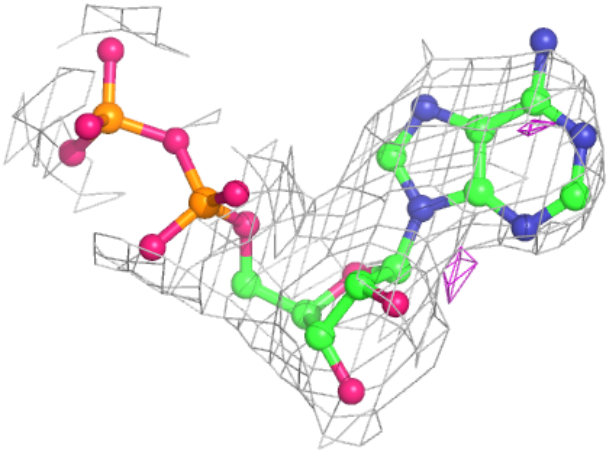
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

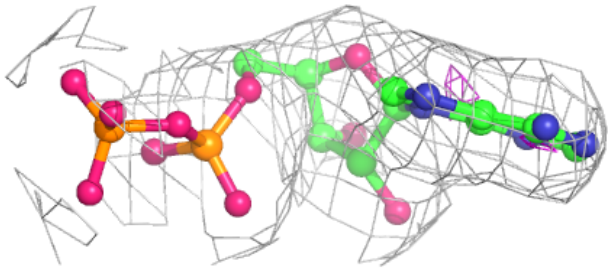
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ADP	A	501	27/27	0.96	0.21	73,82,88,89	0
3	ADP	B	501	27/27	0.96	0.17	67,75,84,85	0

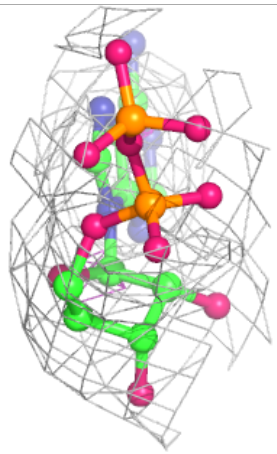
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 501:

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

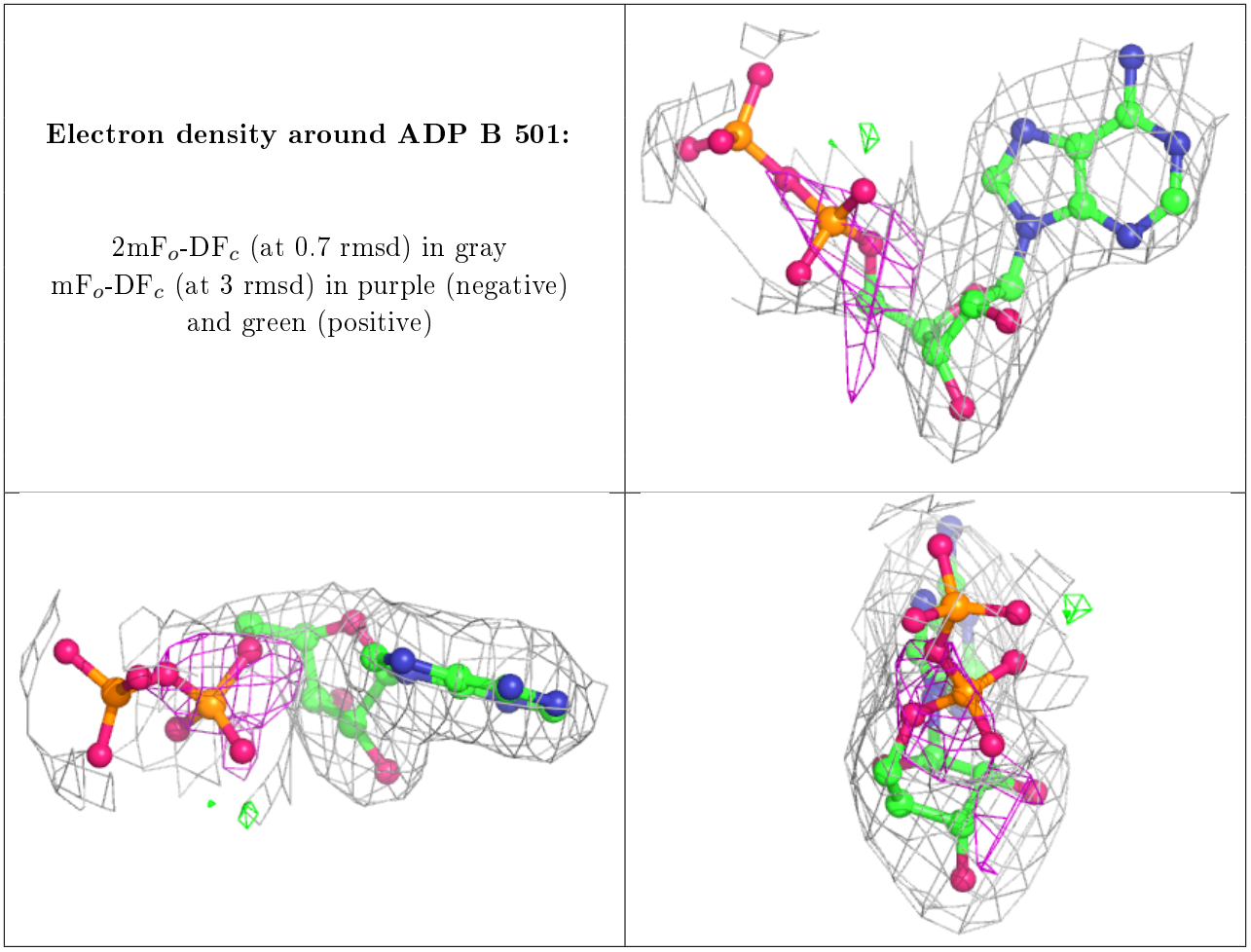






Electron density around ADP B 501:

$2mF_o$-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

There are no such residues in this entry.