

Full wwPDB X-ray Structure Validation Report (i)

Dec 16, 2023 – 11:09 AM EST

PDB ID : 201V

Title: Structure of full length GRP94 with ADP bound

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Deposited on : 2006-11-29

Resolution : 2.45 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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) 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 : 2.36

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)

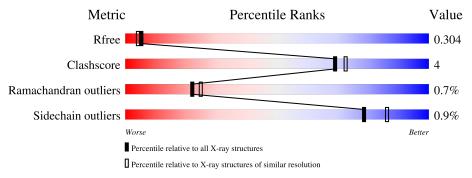
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\ DIFFRACTION$

The reported resolution of this entry is 2.45 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	Similar resolution
11100110	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)

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 >=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%

Mol	Chain	Length	Quality of chain						
1	A	666	78%	8%	13%				
1	В	666	76%	11%	14%				



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9607 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 Endoplasmin.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	578	Total 4666	C 2978	N 785	O 886	S 17	0	13	0
			4000	2910	100	000	11			
1	R	575	Total	С	N	O	$O S \mid O \mid O \mid$	0	0	
1	ע	313	4623	2946	776	885	16			U

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	52	MET	-	expression tag	UNP P41148
A	53	GLY	-	expression tag	UNP P41148
A	54	SER	-	expression tag	UNP P41148
A	55	SER	-	expression tag	UNP P41148
A	56	HIS	-	expression tag	UNP P41148
A	57	HIS	-	expression tag	UNP P41148
A	58	HIS	-	expression tag	UNP P41148
A	59	HIS	-	expression tag	UNP P41148
A	60	HIS	-	expression tag	UNP P41148
A	61	HIS	-	expression tag	UNP P41148
A	62	SER	-	expression tag	UNP P41148
A	63	SER	-	expression tag	UNP P41148
A	64	GLY	-	expression tag	UNP P41148
A	65	LEU	-	expression tag	UNP P41148
A	66	VAL	-	expression tag	UNP P41148
A	67	PRO	-	expression tag	UNP P41148
A	68	ARG	-	expression tag	UNP P41148
A	69	GLY	-	expression tag	UNP P41148
A	70	SER	-	expression tag	UNP P41148
A	71	HIS	-	expression tag	UNP P41148
A	72	MET	-	expression tag	UNP P41148
A	287	GLY	-	see remark 999	UNP P41148
A	288	GLY	-	see remark 999	UNP P41148
A	289	GLY	-	see remark 999	UNP P41148
A	290	GLY	-	see remark 999	UNP P41148

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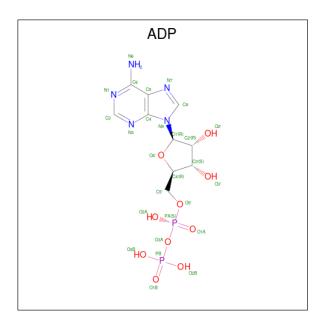
Chain	Residue	Modelled	Actual	Comment	Reference
В	52	MET	-	expression tag	UNP P41148
В	53	GLY	-	expression tag	UNP P41148
В	54	SER	-	expression tag	UNP P41148
В	55	SER	-	expression tag	UNP P41148
В	56	HIS	-	expression tag	UNP P41148
В	57	HIS	-	expression tag	UNP P41148
В	58	HIS	-	expression tag	UNP P41148
В	59	HIS	-	expression tag	UNP P41148
В	60	HIS	-	expression tag	UNP P41148
В	61	HIS	-	expression tag	UNP P41148
В	62	SER	-	expression tag	UNP P41148
В	63	SER	-	expression tag	UNP P41148
В	64	GLY	-	expression tag	UNP P41148
В	65	LEU	_	expression tag	UNP P41148
В	66	VAL	-	expression tag	UNP P41148
В	67	PRO	-	expression tag	UNP P41148
В	68	ARG	-	expression tag	UNP P41148
В	69	GLY	-	expression tag	UNP P41148
В	70	SER	-	expression tag	UNP P41148
В	71	HIS	-	expression tag	UNP P41148
В	72	MET		expression tag	UNP P41148
В	287	GLY	-	see remark 999	UNP P41148
В	288	GLY	-	see remark 999	UNP P41148
В	289	GLY	-	see remark 999	UNP P41148
В	290	GLY	-	see remark 999	UNP P41148

• Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mg 2 2	0	0
2	В	2	Total Mg 2 2	0	0

 \bullet 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	
9	Λ	1	Total	С	N	О	Р	0	0
3	A	1	27	10	5	10	2	U	
9	D	1	Total	С	N	О	Р	0	
3	Б	1	27	10	5	10	2		0

• Molecule 4 is water.

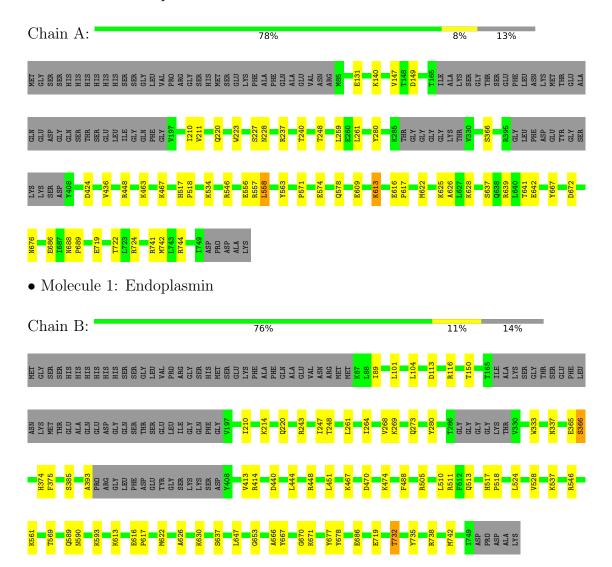
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	135	Total O 135 135	0	0
4	В	125	Total O 125 125	0	0



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. 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. 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: Endoplasmin





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	99.08Å 108.85Å 148.98Å	Donositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 - 2.45	Depositor
Resolution (A)	47.70 - 2.45	EDS
% Data completeness	99.6 (20.00-2.45)	Depositor
(in resolution range)	99.6 (47.70-2.45)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) > 1$	2.15 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
D D.	0.248 , 0.299	Depositor
R, R_{free}	0.264 , 0.304	DCC
R_{free} test set	2972 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	57.8	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.31 , 70.8	EDS
L-test for twinning ²	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9607	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.28% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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, MG

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		nd lengths	Bond angles		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.53	$6/4792 \ (0.1\%)$	0.67	2/6465~(0.0%)	
1	В	0.41	0/4708	0.64	1/6351 (0.0%)	
All	All	0.47	6/9500 (0.1%)	0.66	3/12816 (0.0%)	

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
1	A	131	GLU	CD-OE2	8.02	1.34	1.25
1	A	237	ARG	C-O	7.10	1.36	1.23
1	A	131	GLU	CD-OE1	6.67	1.32	1.25
1	A	147	VAL	C-O	6.33	1.35	1.23
1	A	237	ARG	C-N	6.07	1.44	1.33
1	A	280	TYR	C-O	5.67	1.34	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
1	A	558	LEU	CA-CB-CG	5.71	128.43	115.30
1	В	451	LEU	CA-CB-CG	5.61	128.19	115.30
1	A	546	ARG	NE-CZ-NH1	-5.18	117.71	120.30

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



. 1	, .	• 1	1 (α	α 1 1	1. /	1	1 , 1	1 1
the ass	zmmetric	11n1f	whereas S	Symm-	Clashes	LISTS ST	vmmetri	v-related	clashes
UIIC COD	y IIIIII OUI IO	aiii o,	WITCICOD	\cup y IIIIII	CIUDIICD	110000	y IIIIIIC UI	y iciauca	CIGOTICO.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4666	0	4617	30	0
1	В	4623	0	4571	42	0
2	A	2	0	0	0	0
2	В	2	0	0	0	0
3	A	27	0	12	0	0
3	В	27	0	12	0	0
4	A	135	0	0	2	0
4	В	125	0	0	4	0
All	All	9607	0	9212	68	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 (68) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
1:B:637:SER:HB2	1:B:686:GLU:HB3	1.62	0.82
1:A:724:ARG:HD2	1:B:732:THR:HG23	1.67	0.76
1:A:741[B]:ARG:HH11	1:A:741[B]:ARG:CG	2.03	0.71
1:A:210:ILE:HG13	1:A:248:THR:HB	1.76	0.67
1:A:741[B]:ARG:HH11	1:A:741[B]:ARG:HG2	1.59	0.66
1:A:556:GLU:HB3	1:A:641:THR:HB	1.81	0.63
1:A:625:LYS:HA	1:A:628:LYS:HD2	1.82	0.62
1:B:104:LEU:HD22	1:B:247:ILE:HD13	1.82	0.61
1:A:637:SER:HB2	1:A:686:GLU:HB3	1.82	0.61
1:B:470:ASP:OD2	1:B:505:ARG:NH2	2.35	0.58
1:B:590:ASN:HB3	1:B:593:LYS:HD2	1.87	0.57
1:B:653:GLY:HA2	1:B:678:TYR:HB2	1.88	0.56
1:A:140:LYS:HA	1:A:259:LEU:HD13	1.88	0.56
1:A:741[A]:ARG:HA	1:A:744[A]:ARG:HE	1.72	0.54
1:B:210:ILE:HB	1:B:248:THR:HB	1.90	0.54
1:B:414:ARG:HD2	1:B:444:LEU:HD22	1.89	0.53
1:B:413:VAL:HG23	1:B:444:LEU:HD13	1.91	0.52
1:B:666:ALA:O	1:B:671:LYS:N	2.39	0.52
1:B:474:LYS:HB2	4:B:872:HOH:O	2.10	0.52
1:B:517:HIS:CG	1:B:518:PRO:HD2	2.45	0.51
1:A:571:PRO:HG3	1:B:667:TYR:CE2	2.46	0.50
1:A:563:TYR:O	4:A:775:HOH:O	2.20	0.49
1:B:113:ASP:OD1	1:B:116:ARG:NH2	2.46	0.49
1:B:537:LYS:HD3	1:B:589:GLN:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
1:A:463:LYS:O	1:A:467:LYS:HG2	2.13	0.48
1:B:337:ASN:ND2	4:B:841:HOH:O	2.45	0.48
1:B:513:GLN:OE1	1:B:546:ARG:NH1	2.45	0.48
1:B:261:LEU:HA	1:B:264:ILE:HG22	1.96	0.47
1:B:719:GLU:OE2	1:B:735:TYR:HD1	1.97	0.47
1:A:667:TYR:HE1	1:B:569:THR:O	1.99	0.46
1:A:622:MET:HA	1:A:626:ALA:HB3	1.98	0.46
1:B:393:ALA:HA	1:B:488:PHE:HE2	1.80	0.46
1:B:622:MET:HA	1:B:626:ALA:HB3	1.98	0.46
1:A:220:GLN:HE22	1:A:240:THR:HB	1.81	0.45
1:B:647:LEU:HD23	1:B:647:LEU:HA	1.72	0.45
1:B:719:GLU:OE1	1:B:738:ARG:NH2	2.46	0.45
1:A:534:LYS:HA	1:A:534:LYS:HD2	1.84	0.45
1:A:517:HIS:CG	1:A:518:PRO:HD2	2.51	0.45
1:B:616:GLU:N	1:B:617:PRO:HD2	2.31	0.45
1:B:393:ALA:HA	1:B:488:PHE:CE2	2.51	0.45
1:B:375:PHE:CE1	1:B:467:LYS:HG3	2.51	0.44
1:A:719:GLU:O	1:A:722:THR:HB	2.18	0.44
1:B:524:LEU:O	1:B:528:VAL:HG23	2.16	0.44
1:B:269:LYS:O	1:B:273:GLN:NE2	2.51	0.44
1:A:616:GLU:N	1:A:617:PRO:HD2	2.33	0.44
1:A:574:GLU:HB2	4:A:845:HOH:O	2.18	0.43
1:B:150:THR:O	1:B:243:ARG:NH2	2.48	0.43
1:B:630:LYS:NZ	4:B:828:HOH:O	2.48	0.43
1:B:561:LYS:HD3	1:B:561:LYS:HA	1.82	0.43
1:B:101:LEU:HD21	1:B:268:VAL:HG12	2.00	0.43
1:A:688:ASN:HA	1:A:689:PRO:HD2	1.93	0.42
1:A:211:VAL:HG22	1:A:223:TRP:HB3	2.00	0.42
1:B:613:LYS:HD2	1:B:613:LYS:HA	1.92	0.42
1:A:557:ARG:HB2	1:A:639:ARG:HA	2.00	0.42
1:B:365:GLU:O	1:B:366:SER:HB3	2.19	0.42
1:A:424:ASP:OD1	1:A:424:ASP:N	2.53	0.42
1:A:574:GLU:O	1:A:578:GLN:HB2	2.20	0.42
1:B:505:ARG:HG3	4:B:779:HOH:O	2.19	0.41
1:B:666:ALA:HA	1:B:670:GLY:HA3	2.02	0.41
1:A:742:MET:SD	1:B:742:MET:HB3	2.61	0.41
1:A:641:THR:HG22	1:A:642:GLU:N	2.36	0.41
1:B:214:LYS:HD3	1:B:220:GLN:HB2	2.02	0.41
1:B:510:LEU:O	1:B:511:ARG:HD3	2.20	0.41
1:A:639:ARG:HD2	1:A:686:GLU:OE1	2.21	0.41
1:A:609:GLU:O	1:A:613:LYS:HD2	2.22	0.40

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Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	Clash overlap (Å)
1:B:374:HIS:HA	1:B:385:SER:O	2.22	0.40
1:A:641:THR:HG22	1:A:642:GLU:HG3	2.03	0.40
1:B:280:TYR:HB3	1:B:333:TRP:HB3	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	Perce	entiles
1	A	583/666 (88%)	549 (94%)	29 (5%)	5 (1%)	17	19
1	В	565/666 (85%)	523 (93%)	39 (7%)	3 (0%)	29	34
All	All	1148/1332 (86%)	1072 (93%)	68 (6%)	8 (1%)	22	25

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	SER
1	A	366	SER
1	В	366	SER
1	A	228	ASN
1	В	89	ILE
1	A	676	ASN
1	В	677	TYR
1	A	672	ASP

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	Perce	ntiles
1	A	508/598 (85%)	502 (99%)	6 (1%)	71	81
1	В	504/598 (84%)	501 (99%)	3 (1%)	86	91
All	All	1012/1196 (85%)	1003 (99%)	9 (1%)	78	86

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	ASP
1	A	261	LEU
1	A	436	VAL
1	A	448	ARG
1	A	558	LEU
1	A	613	LYS
1	В	440	ASP
1	В	448	ARG
1	В	732	THR

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

Mol	Chain	Res	Type
1	A	500	HIS
1	A	681	GLN
1	В	337	ASN
1	В	681	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 monosaccharides in this entry.



5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 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	Trino	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Dag	Link	Bo	ond leng	ths	В	ond ang	cles
MIOI	Type	Chain	Res	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2																
3	ADP	A	301	2	24,29,29	1.08	1 (4%)	29,45,45	1.35	2 (6%)																
3	ADP	В	302	2	24,29,29	1.16	2 (8%)	29,45,45	1.49	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	301	2	-	1/12/32/32	0/3/3/3
3	ADP	В	302	2	-	2/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	$Ideal(\AA)$
3	В	302	ADP	O4'-C1'	3.58	1.46	1.41
3	A	301	ADP	O4'-C1'	3.20	1.45	1.41
3	В	302	ADP	PB-O3B	2.19	1.63	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
3	A	301	ADP	N3-C2-N1	-4.65	121.41	128.68
3	В	302	ADP	N3-C2-N1	-4.62	121.46	128.68
3	В	302	ADP	PA-O3A-PB	-4.42	117.67	132.83
3	A	301	ADP	PA-O3A-PB	-2.46	124.39	132.83

There are no chirality outliers.

All (3) torsion outliers are listed below:

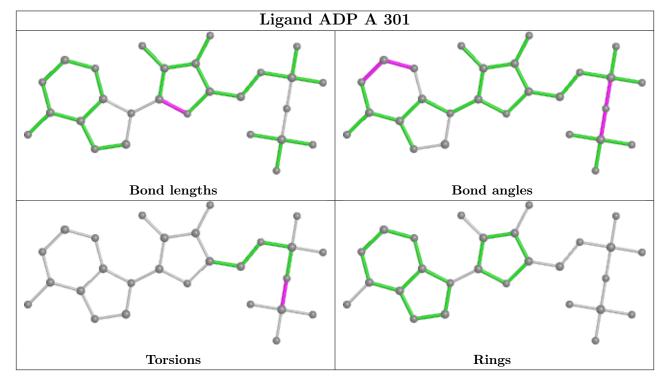


Mol	Chain	Res	Type	Atoms
3	В	302	ADP	O4'-C4'-C5'-O5'
3	В	302	ADP	C3'-C4'-C5'-O5'
3	A	301	ADP	PA-O3A-PB-O2B

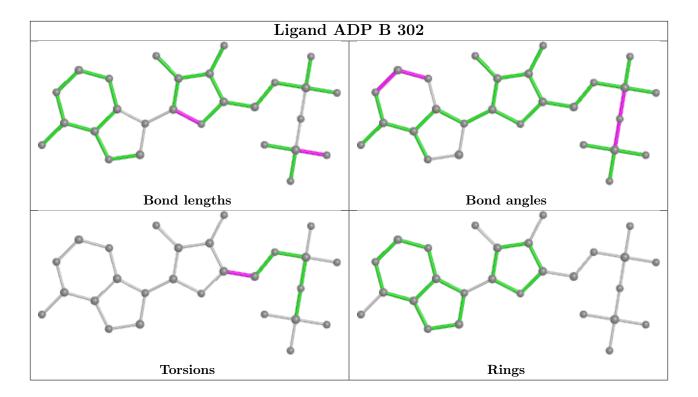
There are no ring outliers.

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.







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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

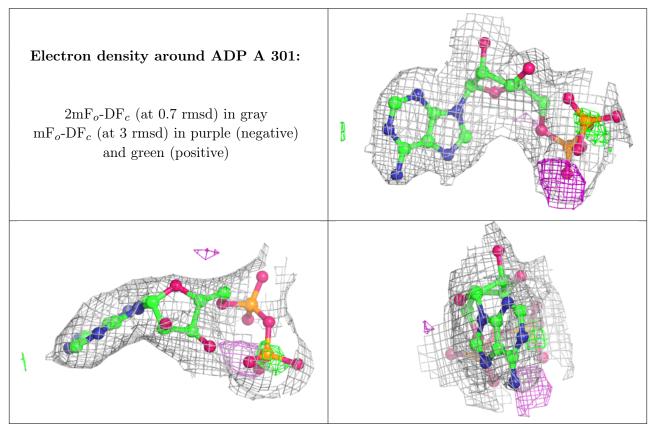
6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

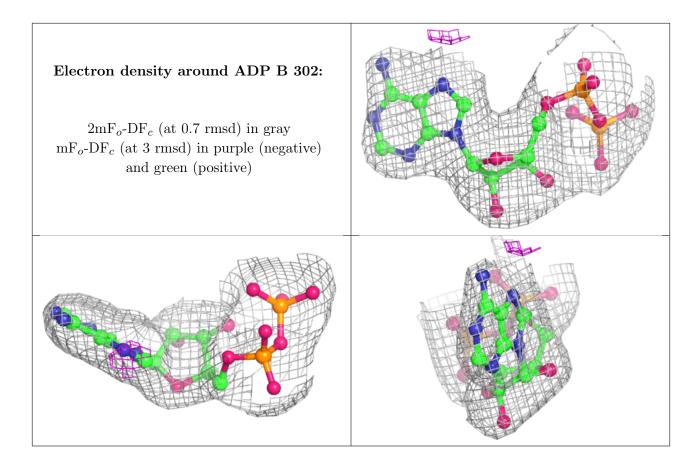
6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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.







6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

