



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 6, 2022 – 05:05 pm BST

PDB ID : 7PMM
Title : DEAD-box helicase DbpA in the active conformation bound to a ss/dsRNA junction and ADP/BeF3
Authors : Wurm, J.P.
Deposited on : 2021-09-02
Resolution : 3.00 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 types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.30
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

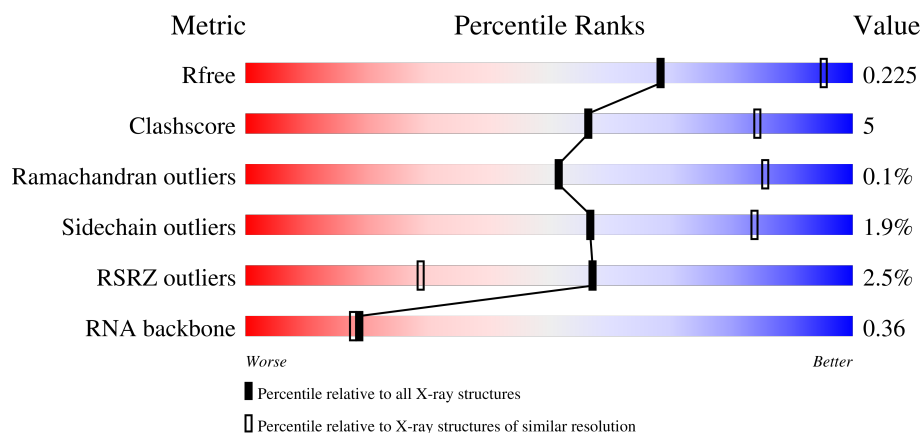
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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 $\leq 5\%$. 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	459	<div> <div>91%</div> <div>9%</div> </div>
1	B	459	<div> <div>5%</div> <div>82%</div> <div>12%</div> <div>•</div> </div>
2	C	44	<div> <div>2%</div> <div>32%</div> <div>39%</div> <div>25%</div> <div>5%</div> </div>
2	D	44	<div> <div>2%</div> <div>50%</div> <div>32%</div> <div>16%</div> <div>•</div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8687 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 ATP-dependent RNA helicase DbpA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	0	0
			3451	2167	621	645	18			
1	B	439	Total	C	N	O	S	0	0	0
			3328	2091	598	621	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P21693
A	0	GLY	-	expression tag	UNP P21693
B	-1	GLY	-	expression tag	UNP P21693
B	0	GLY	-	expression tag	UNP P21693

- Molecule 2 is a RNA chain called RNA (45mer) containing HP92 of the 23S rRNA.

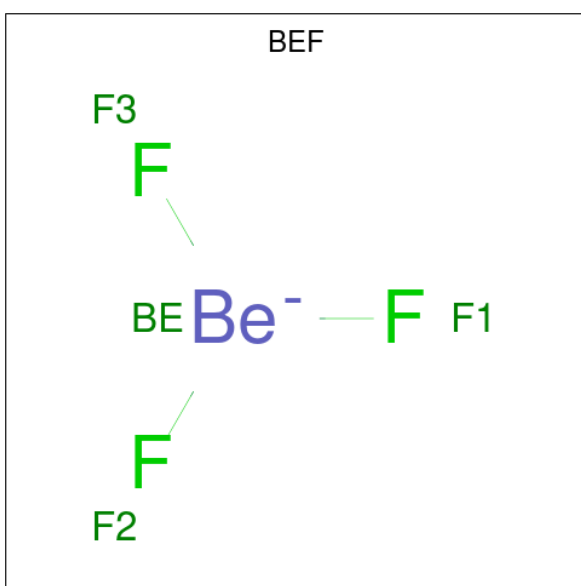
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	42	Total	C	N	O	P	0	0	0
			887	395	155	295	42			
2	D	44	Total	C	N	O	P	0	0	0
			935	417	162	312	44			

- 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 27	C 10	N 5	O 10	P 2	0	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 4 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).

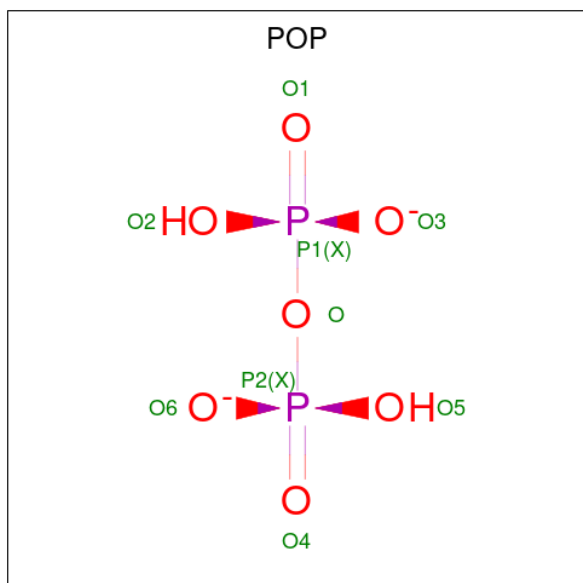


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 4	Be 1	F 3	0	0
4	B	1	Total 4	Be 1	F 3	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $\text{H}_2\text{O}_7\text{P}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	P	0	0
			9	7	2		

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



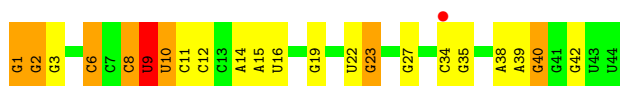
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 8 is water.

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

- Molecule 1: ATP-dependent RNA helicase DbpA





4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	169.69Å 169.69Å 111.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.39 – 3.00 48.39 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.39-3.00) 100.0 (48.39-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.85 (at 3.01Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874+SVN	Depositor
R, R_{free}	0.197 , 0.225 0.197 , 0.225	Depositor DCC
R_{free} test set	1665 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	95.1	Xtrriage
Anisotropy	0.257	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8687	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: BEF, MG, ADP, PO4, POP

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	0.26	0/3506	0.46	0/4756
1	B	0.25	0/3379	0.46	0/4583
2	C	0.35	0/988	1.02	3/1533 (0.2%)
2	D	0.42	0/1043	1.04	10/1623 (0.6%)
All	All	0.29	0/8916	0.65	13/12495 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	G	OP1-P-OP2	-7.97	107.64	119.60
2	D	1	G	O5'-P-OP1	-7.93	98.56	105.70
2	D	40	G	N3-C4-N9	5.97	129.58	126.00
2	D	11	C	P-O3'-C3'	5.97	126.86	119.70
2	C	29	C	C2-N1-C1'	5.85	125.23	118.80
2	D	9	U	C2-N1-C1'	5.69	124.53	117.70
2	D	40	G	C6-C5-N7	-5.52	127.09	130.40
2	C	12	C	C2-N1-C1'	5.48	124.83	118.80
2	C	9	U	C2-N1-C1'	5.44	124.23	117.70
2	D	40	G	N9-C4-C5	-5.18	103.33	105.40
2	D	40	G	C4-C5-N7	5.17	112.87	110.80
2	D	6	C	C2-N1-C1'	5.14	124.46	118.80
2	D	40	G	C5-C6-O6	-5.14	125.52	128.60

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	3451	0	3538	24	0
1	B	3328	0	3405	34	0
2	C	887	0	450	17	0
2	D	935	0	473	10	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	C	9	0	0	0	0
7	D	5	0	0	0	0
8	A	4	0	0	0	0
8	B	4	0	0	0	0
All	All	8687	0	7890	80	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 5.

All (80) 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:168:ASP:OD1	1:B:197:ARG:NH1	2.23	0.72
1:B:397:PRO:O	1:B:401:LEU:HD12	1.99	0.63
1:B:111:PRO:HG2	1:B:114:MET:HG2	1.80	0.63
1:A:234:ARG:HE	1:A:373:SER:HB3	1.65	0.60
2:C:37:G:H2'	2:C:38:A:O4'	2.03	0.59
1:A:401:LEU:HD22	2:D:23:G:H1'	1.86	0.58
1:A:408:ILE:HG13	1:A:440:GLN:HG2	1.86	0.57
1:B:79:PRO:HD2	1:B:83:LEU:HD23	1.87	0.57
1:B:314:VAL:HA	1:B:342:ILE:O	2.04	0.57
1:B:415:ILE:HD12	2:C:23:G:H21	1.71	0.56
1:B:157:ARG:HH22	2:D:3:G:H1'	1.71	0.55
1:A:408:ILE:HG13	1:A:440:GLN:HB3	1.89	0.55
2:D:1:G:H3'	2:D:2:G:H8	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:ILE:O	1:B:171:ILE:HG12	2.08	0.54
1:A:156:ASP:HA	1:A:191:ILE:HG21	1.90	0.54
1:B:230:PRO:O	1:B:234:ARG:HG3	2.08	0.54
2:C:22:U:O2'	2:C:23:G:H5'	2.07	0.54
2:D:14:A:O2'	2:D:15:A:H5'	2.08	0.54
1:B:415:ILE:HD12	2:C:23:G:N2	2.25	0.52
2:C:7:C:H2'	2:C:8:C:H6	1.76	0.51
1:A:400:VAL:HG21	1:A:425:VAL:HG11	1.92	0.51
2:C:30:A:H2'	2:C:31:U:C6	2.47	0.49
1:A:105:THR:HA	1:A:127:VAL:O	2.11	0.49
1:A:57:PHE:HB3	1:A:183:PHE:CE1	2.48	0.49
1:A:379:GLU:OE1	1:A:379:GLU:N	2.45	0.49
1:B:43:VAL:HG22	1:B:181:LEU:HD22	1.95	0.48
1:A:234:ARG:HH21	1:A:373:SER:HB3	1.78	0.48
1:B:105:THR:HA	1:B:127:VAL:O	2.14	0.48
1:A:228:LYS:NZ	1:A:349:GLU:OE2	2.42	0.48
2:C:33:U:O2'	2:C:35:G:OP1	2.31	0.48
1:B:400:VAL:HG21	1:B:425:VAL:HG11	1.95	0.48
1:B:46:GLN:HA	1:B:184:SER:O	2.13	0.47
1:B:177:SER:O	1:B:177:SER:OG	2.31	0.47
2:C:6:C:H2'	2:C:7:C:C6	2.49	0.47
1:B:306:ASP:OD2	1:B:308:LYS:NZ	2.48	0.47
2:C:38:A:H2'	2:C:39:A:C8	2.49	0.47
1:B:103:ILE:HG12	1:B:125:ILE:HB	1.96	0.47
1:A:396:ARG:HG2	1:A:399:ASP:OD2	2.15	0.46
1:A:404:LEU:HA	1:A:408:ILE:CG2	2.46	0.46
1:B:191:ILE:HA	1:B:194:ILE:HG12	1.98	0.46
1:A:220:PHE:CE1	1:A:364:LEU:HD22	2.51	0.46
1:B:250:THR:HG22	1:B:252:LYS:H	1.80	0.46
1:B:251:LYS:HG2	1:B:272:HIS:HB2	1.97	0.45
1:B:441:LEU:HB3	1:B:453:VAL:HG21	1.98	0.45
2:C:39:A:H2'	2:C:40:G:H8	1.82	0.45
1:A:79:PRO:HD2	1:A:83:LEU:HD23	1.99	0.45
2:D:1:G:H3'	2:D:2:G:C8	2.52	0.44
2:D:38:A:H2'	2:D:39:A:C8	2.53	0.44
1:B:349:GLU:H	1:B:349:GLU:HG2	1.60	0.44
1:B:396:ARG:H	1:B:396:ARG:HG2	1.60	0.44
2:D:9:U:C4	2:D:10:U:C4	3.06	0.44
1:B:38:LEU:HD22	1:B:63:GLN:HG2	1.99	0.44
2:C:6:C:H2'	2:C:7:C:H6	1.82	0.44
1:A:152:MET:HB3	1:A:152:MET:HE2	1.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:ALA:O	1:B:194:ILE:HG23	2.18	0.43
1:B:385:LEU:HD11	1:B:427:VAL:HB	1.99	0.43
1:A:268:ALA:HA	1:A:294:VAL:O	2.18	0.43
1:A:97:PHE:O	1:A:99:PRO:HD3	2.18	0.43
1:B:234:ARG:HD3	1:B:371:ALA:O	2.19	0.43
1:B:246:VAL:HG22	1:B:314:VAL:HG22	2.01	0.43
1:A:4:PHE:CE1	1:A:26:MET:HG2	2.54	0.43
2:C:15:A:O2'	2:C:17:A:OP1	2.33	0.43
1:A:322:PRO:HB2	1:A:359:MET:SD	2.59	0.43
1:A:404:LEU:HD13	1:A:415:ILE:HG12	2.00	0.43
2:C:33:U:C2	2:C:35:G:C8	3.07	0.43
1:B:74:ALA:HB3	1:B:125:ILE:HG12	2.00	0.42
2:C:32:U:O2'	2:C:33:U:H5'	2.20	0.42
1:B:88:ALA:O	1:B:92:ARG:HG3	2.20	0.42
2:C:33:U:O2'	2:C:35:G:H5''	2.19	0.41
1:A:449:LYS:NZ	1:A:450:THR:O	2.48	0.41
2:C:36:G:H2'	2:C:37:G:H5'	2.03	0.41
1:A:79:PRO:O	2:C:4:A:H5'	2.20	0.41
2:D:8:C:H5''	2:D:8:C:H6	1.85	0.41
2:D:38:A:C6	2:D:39:A:C6	3.09	0.41
1:B:169:ASP:O	1:B:172:ARG:HG2	2.21	0.41
2:D:22:U:O2'	2:D:23:G:H5''	2.21	0.41
1:B:441:LEU:HD12	1:B:441:LEU:HA	1.83	0.41
1:A:214:PRO:O	1:A:216:ILE:N	2.53	0.40
1:B:303:ARG:O	1:B:305:LEU:HD12	2.21	0.40
1:B:346:ALA:HB1	1:B:347:PRO:HD2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	455/459 (99%)	445 (98%)	10 (2%)	0	100	100
1	B	431/459 (94%)	420 (97%)	10 (2%)	1 (0%)	47	82
All	All	886/918 (96%)	865 (98%)	20 (2%)	1 (0%)	51	85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	370	PRO

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	368/368 (100%)	363 (99%)	5 (1%)	67	88
1	B	357/368 (97%)	348 (98%)	9 (2%)	47	79
All	All	725/736 (98%)	711 (98%)	14 (2%)	57	84

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	ARG
1	A	172	ARG
1	A	279	ASP
1	A	440	GLN
1	A	457	LYS
1	B	90	GLU
1	B	177	SER
1	B	349	GLU
1	B	363	LYS
1	B	372	ASN
1	B	392	LYS
1	B	415	ILE
1	B	441	LEU
1	B	452	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	39/44 (88%)	17 (43%)	2 (5%)
2	D	43/44 (97%)	14 (32%)	0
All	All	82/88 (93%)	31 (37%)	2 (2%)

All (31) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	9	U
2	C	10	U
2	C	12	C
2	C	19	G
2	C	22	U
2	C	23	G
2	C	24	U
2	C	27	G
2	C	29	C
2	C	33	U
2	C	36	G
2	C	37	G
2	C	38	A
2	C	39	A
2	C	40	G
2	C	41	G
2	C	43	U
2	D	2	G
2	D	6	C
2	D	8	C
2	D	9	U
2	D	10	U
2	D	12	C
2	D	16	U
2	D	19	G
2	D	23	G
2	D	27	G
2	D	34	C
2	D	35	G
2	D	40	G
2	D	42	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	28	C
2	C	39	A

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 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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
4	BEF	A	501	3	0,3,3	-	-	-		
4	BEF	B	501	3	0,3,3	-	-	-		
3	ADP	A	500	4,5	24,29,29	1.48	4 (16%)	29,45,45	1.63	3 (10%)
7	PO4	D	101	2	4,4,4	0.77	0	6,6,6	0.57	0
3	ADP	B	500	4,5	24,29,29	1.20	2 (8%)	29,45,45	1.57	5 (17%)
6	POP	C	101	2	6,8,8	0.65	0	13,13,13	0.95	0

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	B	500	4,5	-	6/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	POP	C	101	2	-	0/6/6/6	-
3	ADP	A	500	4,5	-	4/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	500	ADP	O4'-C1'	3.26	1.45	1.41
3	A	500	ADP	PB-O1B	3.25	1.61	1.50
3	A	500	ADP	O4'-C1'	3.01	1.45	1.41
3	A	500	ADP	PA-O1A	2.84	1.61	1.50
3	A	500	ADP	C8-N7	-2.51	1.30	1.34
3	B	500	ADP	C8-N7	-2.36	1.30	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	ADP	PA-O3A-PB	-5.84	112.79	132.83
3	B	500	ADP	PA-O3A-PB	-4.79	116.40	132.83
3	A	500	ADP	N3-C2-N1	-4.00	122.43	128.68
3	B	500	ADP	N3-C2-N1	-3.99	122.44	128.68
3	B	500	ADP	O3B-PB-O3A	2.77	113.94	104.64
3	A	500	ADP	O3B-PB-O3A	2.75	113.87	104.64
3	B	500	ADP	PA-O5'-C5'	-2.45	107.31	121.68
3	B	500	ADP	C4-C5-N7	-2.31	106.99	109.40

There are no chirality outliers.

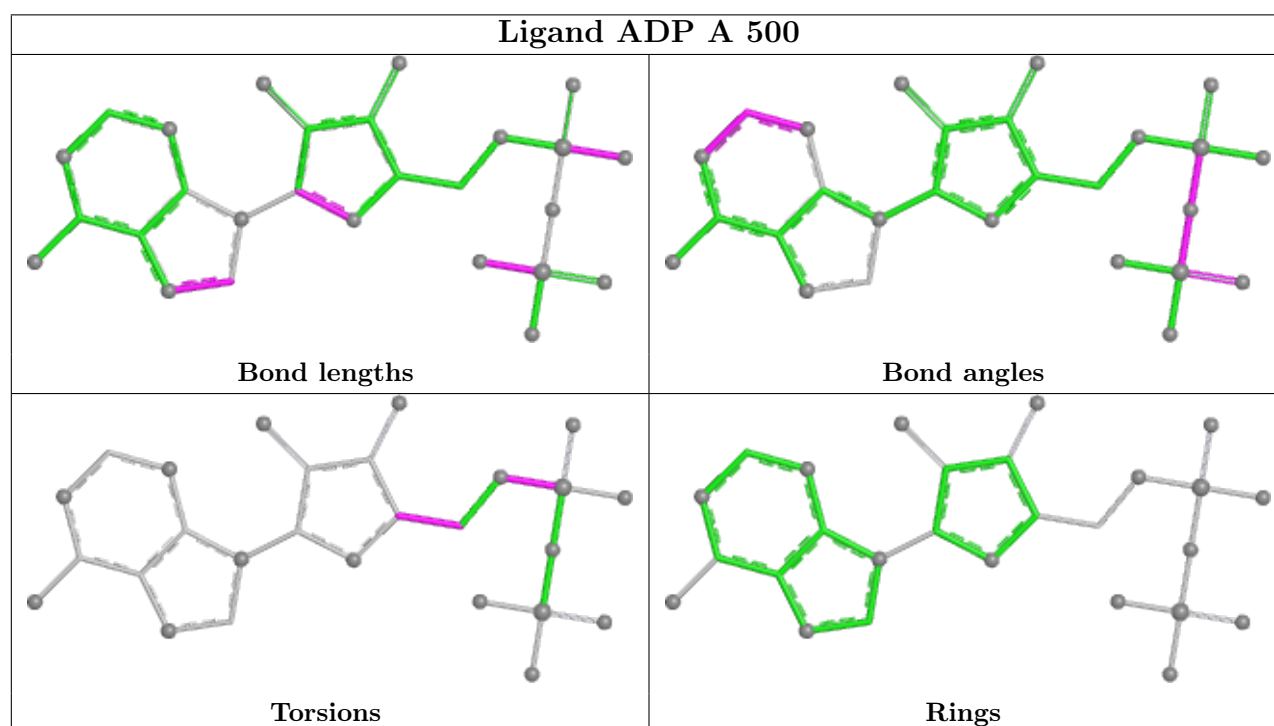
All (10) torsion outliers are listed below:

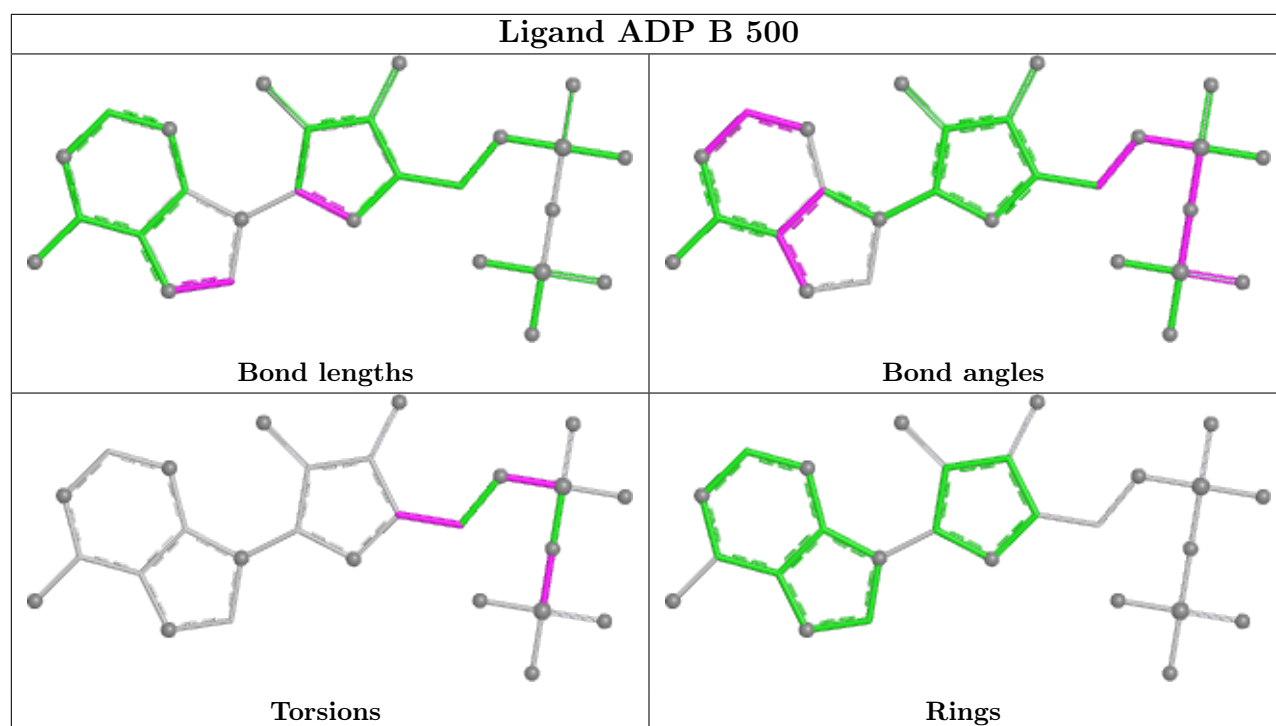
Mol	Chain	Res	Type	Atoms
3	A	500	ADP	C5'-O5'-PA-O3A
3	B	500	ADP	PA-O3A-PB-O2B
3	B	500	ADP	PA-O3A-PB-O3B
3	B	500	ADP	C5'-O5'-PA-O1A
3	A	500	ADP	O4'-C4'-C5'-O5'
3	B	500	ADP	O4'-C4'-C5'-O5'
3	B	500	ADP	C3'-C4'-C5'-O5'
3	A	500	ADP	C5'-O5'-PA-O2A
3	A	500	ADP	C3'-C4'-C5'-O5'
3	B	500	ADP	PA-O3A-PB-O1B

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 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, 95th 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	457/459 (99%)	-0.08	1 (0%) 95 87	56, 81, 132, 180	0
1	B	439/459 (95%)	0.17	22 (5%) 28 10	67, 111, 180, 221	0
2	C	42/44 (95%)	0.23	1 (2%) 59 30	91, 180, 241, 249	0
2	D	44/44 (100%)	0.08	1 (2%) 60 31	104, 147, 210, 218	0
All	All	982/1006 (97%)	0.05	25 (2%) 57 29	56, 100, 183, 249	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	401	LEU	4.2
1	B	375	ILE	4.0
1	B	400	VAL	3.7
1	B	451	CYS	3.6
1	B	387	ILE	3.4
1	B	386	CYS	3.4
1	B	454	ARG	3.4
1	B	448	GLY	3.3
1	B	374	SER	3.2
1	B	415	ILE	3.1
1	B	414	ASP	3.0
1	B	453	VAL	3.0
1	B	413	ALA	2.9
1	B	441	LEU	2.8
1	B	446	ILE	2.8
2	C	40	G	2.7
2	D	34	C	2.5
1	A	445	LYS	2.5
1	B	263	GLU	2.5
1	B	452	ARG	2.4
1	B	385	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	412	GLY	2.2
1	B	363	LYS	2.1
1	B	345	CYS	2.0
1	B	113	GLY	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 monosaccharides in this entry.

6.4 Ligands [i](#)

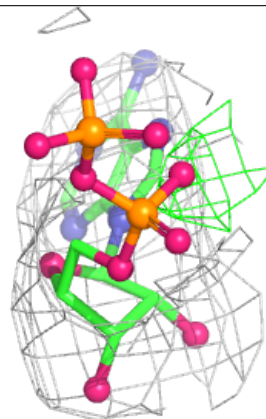
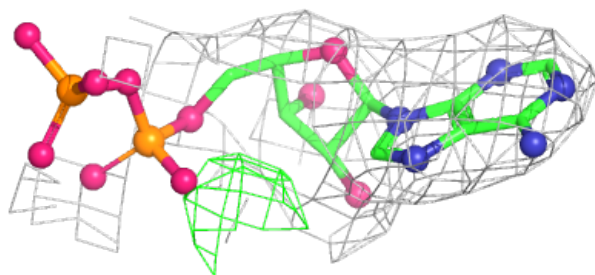
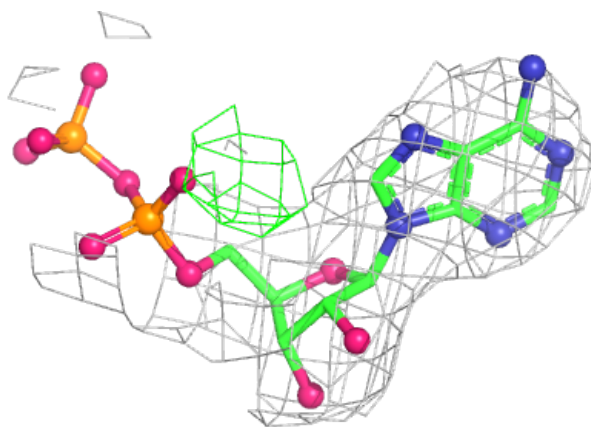
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	PO4	D	101	5/5	0.86	0.20	206,207,216,219	0
6	POP	C	101	9/9	0.89	0.11	164,170,201,206	0
3	ADP	B	500	27/27	0.93	0.21	85,96,102,103	0
4	BEF	B	501	4/4	0.94	0.30	92,92,93,95	0
5	MG	A	502	1/1	0.95	0.19	63,63,63,63	0
4	BEF	A	501	4/4	0.96	0.24	63,63,65,66	0
3	ADP	A	500	27/27	0.97	0.18	63,66,73,84	0
5	MG	B	502	1/1	0.97	0.22	90,90,90,90	0

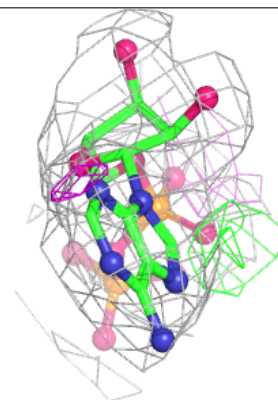
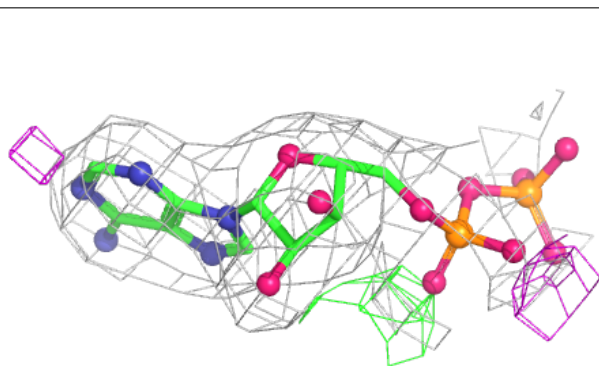
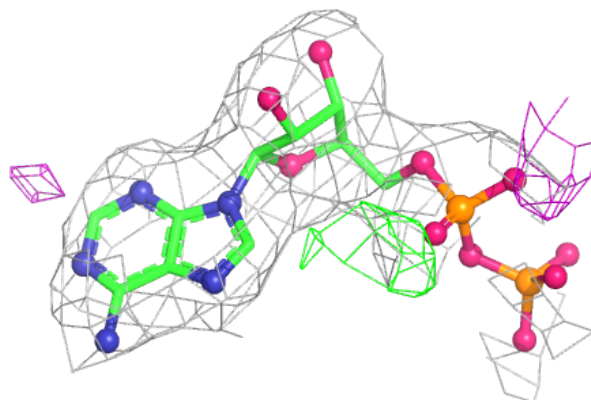
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP B 500:

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

**Electron density around ADP A 500:**

$2mF_o-DF_c$ (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.