



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 08:16 AM EDT

PDB ID : 1Z5C
Title : Topoisomerase VI-B, ADP Pi bound dimer form
Authors : Corbett, K.D.; Berger, J.M.
Deposited on : 2005-03-17
Resolution : 2.20 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

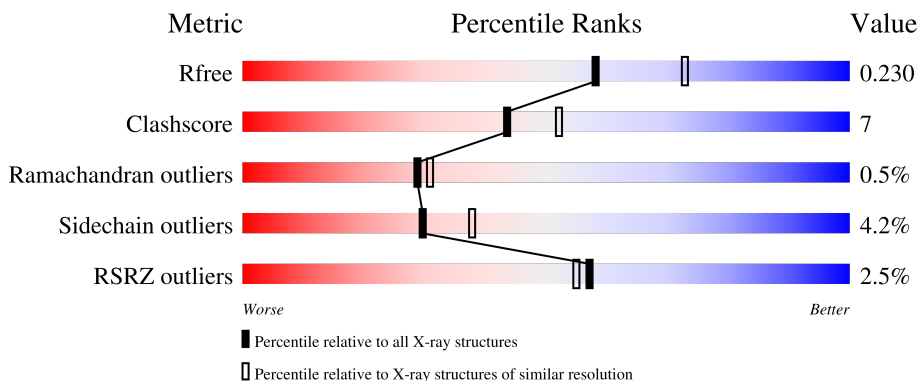
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	469	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 15px; background-color: red; margin-bottom: 2px;"></div> <div style="width: 100%; height: 15px; background-color: green; margin-bottom: 2px;"></div> <div style="width: 100%; height: 15px; background-color: yellow; margin-bottom: 2px;"></div> <div style="width: 100%; height: 15px; background-color: grey; margin-bottom: 2px;"></div> </div> <p style="margin-top: 0;">84% 14% ..</p>
1	B	469	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 15px; background-color: red; margin-bottom: 2px;"></div> <div style="width: 100%; height: 15px; background-color: green; margin-bottom: 2px;"></div> <div style="width: 100%; height: 15px; background-color: yellow; margin-bottom: 2px;"></div> <div style="width: 100%; height: 15px; background-color: grey; margin-bottom: 2px;"></div> </div> <p style="margin-top: 0;">4% 79% 17% ..</p>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7699 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 Type II DNA topoisomerase VI subunit B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	466	3745	2410	627	702	1	5	0	0	0
1	B	460	3676	2368	611	691	1	5	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	MSE	MET	modified residue	UNP O05207
A	121	MSE	MET	modified residue	UNP O05207
A	303	TYR	ASP	SEE REMARK 999	UNP O05207
A	409	MSE	MET	modified residue	UNP O05207
A	412	MSE	MET	modified residue	UNP O05207
A	435	ASP	ASN	SEE REMARK 999	UNP O05207
A	445	MSE	MET	modified residue	UNP O05207
B	107	MSE	MET	modified residue	UNP O05207
B	121	MSE	MET	modified residue	UNP O05207
B	303	TYR	ASP	SEE REMARK 999	UNP O05207
B	409	MSE	MET	modified residue	UNP O05207
B	412	MSE	MET	modified residue	UNP O05207
B	435	ASP	ASN	SEE REMARK 999	UNP O05207
B	445	MSE	MET	modified residue	UNP O05207

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

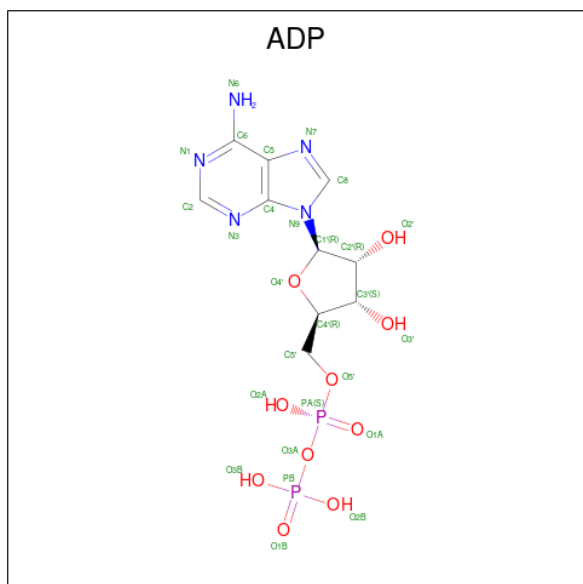
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

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

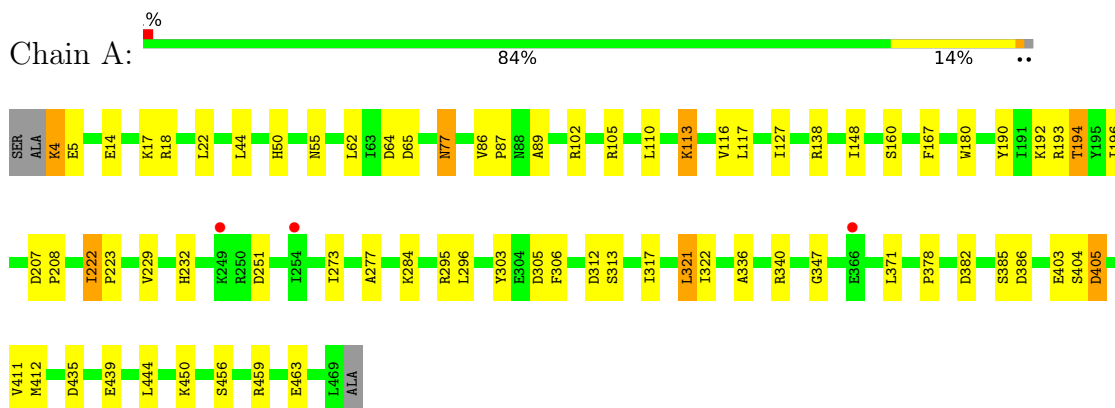
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	98	Total 98	O 98	0	0
5	B	114	Total 114	O 114	0	0

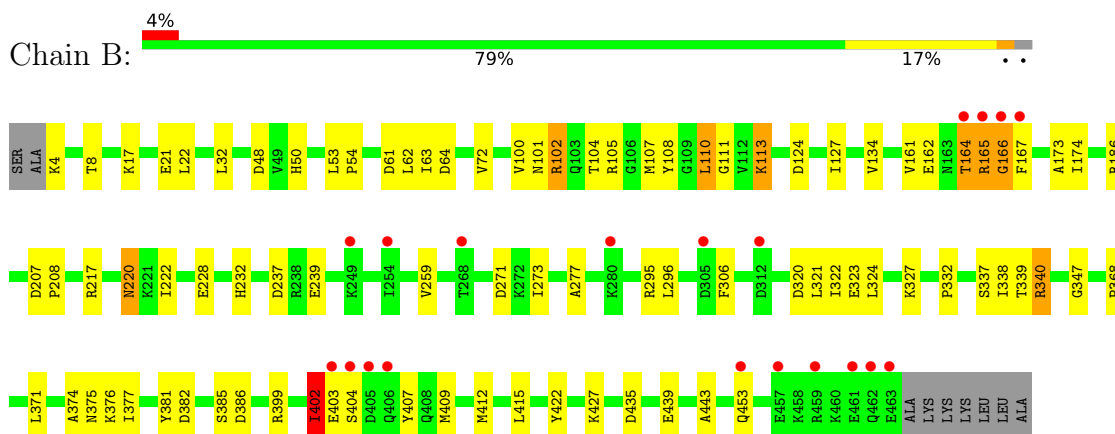
3 Residue-property plots [i](#)

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: Type II DNA topoisomerase VI subunit B



- Molecule 1: Type II DNA topoisomerase VI subunit B



4 Data and refinement statistics i

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α , β , γ	74.50Å 74.50Å 346.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.20 19.94 – 2.01	Depositor EDS
% Data completeness (in resolution range)	94.2 (20.00-2.20) 94.9 (19.94-2.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.01Å)	Xtrriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.194 , 0.232 0.195 , 0.230	Depositor DCC
R_{free} test set	3554 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	30.9	Xtrriage
Anisotropy	0.073	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.055 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7699	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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: ADP, PO4, 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	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.66	0/3821	0.74	7/5160 (0.1%)
1	B	0.68	0/3752	0.76	11/5073 (0.2%)
All	All	0.67	0/7573	0.75	18/10233 (0.2%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	61	ASP	CB-CG-OD2	6.57	124.21	118.30
1	A	64	ASP	CB-CG-OD2	6.11	123.80	118.30
1	B	320	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	435	ASP	CB-CG-OD2	5.99	123.69	118.30
1	B	435	ASP	CB-CG-OD2	5.84	123.56	118.30
1	B	124	ASP	CB-CG-OD2	5.82	123.54	118.30
1	A	386	ASP	CB-CG-OD2	5.68	123.41	118.30
1	A	382	ASP	CB-CG-OD2	5.57	123.32	118.30
1	B	382	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	312	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	217	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	B	340	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	271	ASP	CB-CG-OD2	5.17	122.96	118.30
1	A	65	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	405	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	386	ASP	CB-CG-OD2	5.08	122.87	118.30
1	B	64	ASP	CB-CG-OD2	5.05	122.85	118.30
1	B	237	ASP	CB-CG-OD2	5.04	122.83	118.30

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	3745	0	3812	53	0
1	B	3676	0	3719	60	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
5	A	98	0	0	2	0
5	B	114	0	0	2	0
All	All	7699	0	7555	101	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 7.

All (101) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ILE:HG23	1:A:412:MSE:CE	1.67	1.24
1:B:322:ILE:HG23	1:B:412:MSE:CE	1.73	1.16
1:A:4:LYS:HE3	1:B:102:ARG:HH21	0.99	1.07
1:A:322:ILE:HG23	1:A:412:MSE:HE1	1.19	1.06
1:B:322:ILE:HG23	1:B:412:MSE:HE2	1.38	1.06
1:A:4:LYS:HE3	1:B:102:ARG:NH2	1.77	0.99
1:A:77:ASN:H	1:A:77:ASN:HD22	1.18	0.89
1:B:322:ILE:HG23	1:B:412:MSE:HE1	1.54	0.87
1:A:4:LYS:CE	1:B:102:ARG:HH21	1.87	0.87
1:A:322:ILE:CG2	1:A:412:MSE:CE	2.54	0.85
1:A:322:ILE:CG2	1:A:412:MSE:HE1	2.07	0.83
1:A:322:ILE:HG23	1:A:412:MSE:HE2	1.58	0.83
1:A:102:ARG:HH11	1:B:4:LYS:HE3	1.43	0.80
1:B:403:GLU:HG2	1:B:404:SER:H	1.51	0.76
1:B:368:PRO:HG3	1:B:409:MSE:HE3	1.71	0.72
1:B:322:ILE:CG2	1:B:412:MSE:CE	2.64	0.69
1:B:340:ARG:HD3	1:B:439:GLU:OE2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:ARG:HD3	1:B:104:THR:HG23	1.74	0.68
1:A:50:HIS:CE1	1:B:4:LYS:HG2	2.30	0.67
1:A:336:ALA:HB1	1:A:450:LYS:HD2	1.77	0.67
1:A:50:HIS:HE1	1:B:4:LYS:HG2	1.61	0.66
1:A:340:ARG:HD3	1:A:439:GLU:OE2	1.97	0.65
1:A:116:VAL:HG22	1:A:127:ILE:HG21	1.79	0.64
1:A:4:LYS:HG2	1:B:50:HIS:HE1	1.63	0.63
1:A:193:ARG:NH1	5:A:3053:HOH:O	2.28	0.61
1:A:273:ILE:HD11	1:A:306:PHE:CE1	2.36	0.60
1:B:102:ARG:HD3	1:B:104:THR:CG2	2.32	0.60
1:B:322:ILE:CG2	1:B:412:MSE:HE2	2.22	0.58
1:B:165:ARG:O	1:B:167:PHE:N	2.37	0.57
1:A:102:ARG:NH1	1:B:4:LYS:HE3	2.17	0.57
1:A:251:ASP:OD1	1:A:284:LYS:HD3	2.05	0.56
1:A:385:SER:HB3	1:B:385:SER:HB3	1.86	0.56
1:A:5:GLU:OE2	1:B:50:HIS:NE2	2.36	0.55
1:B:402:ILE:HG22	1:B:402:ILE:O	2.06	0.55
1:B:407:TYR:CE1	1:B:409:MSE:HE2	2.42	0.55
1:A:192:LYS:O	1:A:196:ILE:HG12	2.09	0.53
1:B:399:ARG:O	1:B:399:ARG:HG2	2.09	0.53
1:A:55:ASN:H	1:A:77:ASN:ND2	2.08	0.52
1:B:232:HIS:O	1:B:347:GLY:HA2	2.10	0.52
1:A:190:TYR:O	1:A:194:THR:HG23	2.10	0.52
1:A:207:ASP:HB2	1:A:208:PRO:CD	2.40	0.52
1:A:321:LEU:HD22	5:A:3051:HOH:O	2.09	0.52
1:B:375:ASN:O	1:B:376:LYS:HB2	2.09	0.51
1:B:164:THR:O	1:B:166:GLY:N	2.42	0.50
1:B:17:LYS:HD3	1:B:17:LYS:C	2.32	0.50
1:B:340:ARG:HD2	1:B:443:ALA:HB2	1.94	0.50
1:B:403:GLU:HG2	1:B:404:SER:N	2.25	0.50
1:B:186:ARG:HD3	1:B:381:TYR:CZ	2.47	0.50
1:A:322:ILE:CG2	1:A:412:MSE:HE2	2.34	0.49
1:B:207:ASP:HB2	1:B:208:PRO:CD	2.42	0.49
1:B:110:LEU:HD22	1:B:110:LEU:O	2.13	0.49
1:B:324:LEU:C	1:B:324:LEU:HD23	2.33	0.49
1:A:77:ASN:HD22	1:A:77:ASN:N	1.92	0.48
1:A:89:ALA:O	1:A:113:LYS:CE	2.60	0.48
1:A:303:TYR:CZ	1:A:305:ASP:HB2	2.48	0.48
1:B:161:VAL:HG12	1:B:162:GLU:O	2.12	0.48
1:A:273:ILE:HD11	1:A:306:PHE:CZ	2.49	0.48
1:B:323:GLU:HG3	1:B:337:SER:OG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:GLU:OE1	5:B:3059:HOH:O	2.20	0.48
1:B:134:VAL:HB	5:B:3106:HOH:O	2.14	0.47
1:A:55:ASN:H	1:A:77:ASN:HD21	1.62	0.47
1:B:327:LYS:HA	1:B:332:PRO:HD3	1.96	0.47
1:B:127:ILE:HG13	1:B:174:ILE:HG12	1.97	0.46
1:B:207:ASP:HB2	1:B:208:PRO:HD2	1.97	0.46
1:B:273:ILE:HD11	1:B:306:PHE:CE1	2.50	0.46
1:B:422:TYR:CE2	1:B:427:LYS:HD2	2.51	0.46
1:B:48:ASP:HA	1:B:222:ILE:HD11	1.97	0.46
1:B:277:ALA:O	1:B:295:ARG:NH1	2.48	0.46
1:A:77:ASN:H	1:A:77:ASN:ND2	1.99	0.46
1:A:4:LYS:HG2	1:B:50:HIS:CE1	2.49	0.46
1:A:89:ALA:O	1:A:113:LYS:HE3	2.16	0.45
1:A:232:HIS:O	1:A:347:GLY:HA2	2.17	0.45
1:B:100:VAL:CG2	1:B:228:GLU:CD	2.85	0.45
1:A:44:LEU:HB3	1:A:105:ARG:CZ	2.47	0.45
1:A:117:LEU:CD2	1:A:148:ILE:CD1	2.94	0.45
1:B:105:ARG:HB3	1:B:377:ILE:HD11	1.99	0.45
1:A:222:ILE:HG13	1:A:223:PRO:HD2	1.98	0.44
1:A:317:ILE:HG23	1:A:321:LEU:HD13	2.00	0.43
1:A:411:VAL:CG1	1:A:444:LEU:HD21	2.48	0.43
1:B:324:LEU:HD23	1:B:324:LEU:O	2.18	0.43
1:B:164:THR:OG1	1:B:165:ARG:N	2.51	0.43
1:B:403:GLU:H	1:B:403:GLU:CD	2.21	0.43
1:A:277:ALA:O	1:A:295:ARG:HD2	2.18	0.43
1:A:180:TRP:CE2	1:A:208:PRO:HD2	2.54	0.43
1:A:194:THR:HG22	1:A:378:PRO:CG	2.49	0.43
1:B:273:ILE:HD11	1:B:306:PHE:HE1	1.84	0.43
1:B:374:ALA:HA	1:B:415:LEU:O	2.18	0.42
1:A:77:ASN:ND2	1:A:77:ASN:N	2.64	0.41
1:B:107:MSE:HE2	1:B:108:TYR:CE1	2.55	0.41
1:A:14:GLU:O	1:A:18:ARG:HG3	2.21	0.41
1:A:86:VAL:HB	1:A:87:PRO:HD3	2.03	0.41
1:B:72:VAL:O	1:B:173:ALA:HA	2.21	0.41
1:A:4:LYS:O	1:A:4:LYS:HG3	2.19	0.41
1:B:113:LYS:HD3	1:B:113:LYS:H	1.86	0.41
1:B:53:LEU:HA	1:B:54:PRO:HD3	1.82	0.41
1:A:17:LYS:HE2	1:B:239:GLU:HB2	2.03	0.40
1:A:148:ILE:HG23	1:A:148:ILE:HD12	1.80	0.40
1:A:138:ARG:HD3	1:A:160:SER:OG	2.22	0.40
1:B:338:ILE:HG13	1:B:339:THR:N	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:VAL:HG22	1:A:313:SER:HB3	2.04	0.40
1:B:220:ASN:H	1:B:220:ASN:HD22	1.69	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	464/469 (99%)	458 (99%)	6 (1%)	0	100	100
1	B	458/469 (98%)	444 (97%)	9 (2%)	5 (1%)	14	12
All	All	922/938 (98%)	902 (98%)	15 (2%)	5 (0%)	29	31

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	166	GLY
1	B	101	ASN
1	B	165	ARG
1	B	111	GLY
1	B	402	ILE

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	412/411 (100%)	394 (96%)	18 (4%)	28	35
1	B	403/411 (98%)	387 (96%)	16 (4%)	31	40
All	All	815/822 (99%)	781 (96%)	34 (4%)	30	38

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	22	LEU
1	A	62	LEU
1	A	77	ASN
1	A	110	LEU
1	A	113	LYS
1	A	167	PHE
1	A	194	THR
1	A	222	ILE
1	A	296	LEU
1	A	321	LEU
1	A	371	LEU
1	A	403	GLU
1	A	404	SER
1	A	405	ASP
1	A	456	SER
1	A	459	ARG
1	A	463	GLU
1	B	8	THR
1	B	22	LEU
1	B	32	LEU
1	B	62	LEU
1	B	63	ILE
1	B	102	ARG
1	B	110	LEU
1	B	113	LYS
1	B	164	THR
1	B	220	ASN
1	B	259	VAL
1	B	296	LEU
1	B	321	LEU
1	B	371	LEU
1	B	402	ILE
1	B	453	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	77	ASN
1	A	247	ASN
1	B	220	ASN
1	B	247	ASN

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, 2 are monoatomic - leaving 4 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	ADP	A	1001	2	24,29,29	1.33	1 (4%)	29,45,45	1.24	1 (3%)
3	PO4	B	3002	2	4,4,4	1.17	0	6,6,6	1.41	1 (16%)
4	ADP	B	1002	2	24,29,29	1.00	2 (8%)	29,45,45	1.34	1 (3%)
3	PO4	A	3001	2	4,4,4	1.07	0	6,6,6	1.61	2 (33%)

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
4	ADP	A	1001	2	-	1/12/32/32	0/3/3/3
4	ADP	B	1002	2	-	1/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	ADP	C2-N3	5.01	1.40	1.32
4	B	1002	ADP	C2-N3	3.01	1.36	1.32
4	B	1002	ADP	C2-N1	2.21	1.38	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1002	ADP	N3-C2-N1	-5.34	120.33	128.68
4	A	1001	ADP	N3-C2-N1	-4.84	121.11	128.68
3	A	3001	PO4	O4-P-O1	-2.56	101.52	110.89
3	B	3002	PO4	O4-P-O2	-2.15	101.08	107.97
3	A	3001	PO4	O4-P-O3	2.14	114.84	107.97

There are no chirality outliers.

All (2) torsion outliers are listed below:

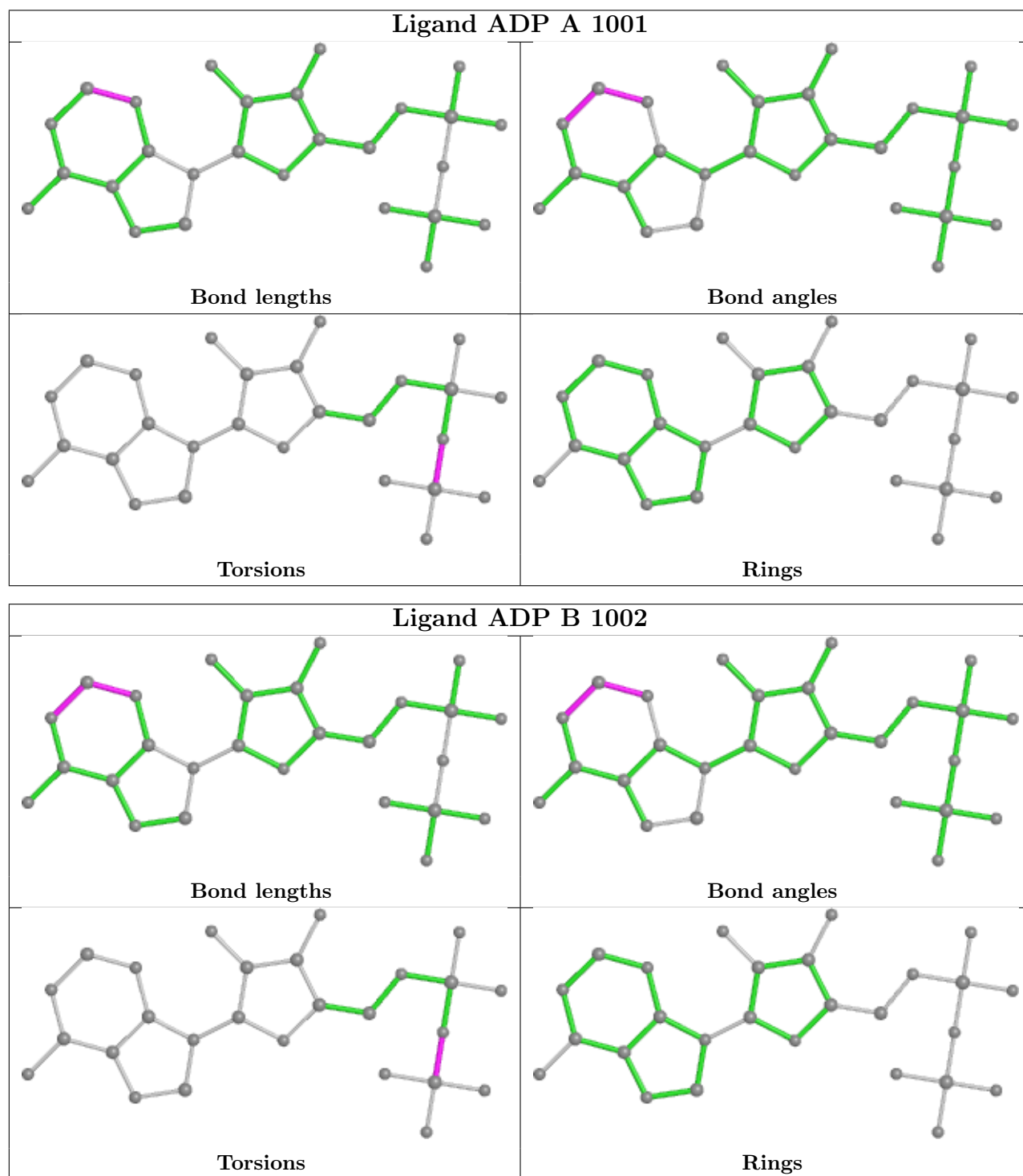
Mol	Chain	Res	Type	Atoms
4	B	1002	ADP	PA-O3A-PB-O2B
4	A	1001	ADP	PA-O3A-PB-O2B

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 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

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	461/469 (98%)	-0.37	3 (0%) 87 86	15, 27, 47, 58	0
1	B	455/469 (97%)	-0.19	20 (4%) 34 32	13, 27, 56, 94	0
All	All	916/938 (97%)	-0.28	23 (2%) 57 55	13, 27, 52, 94	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	406	GLN	3.9
1	B	403	GLU	3.9
1	B	166	GLY	3.9
1	B	459	ARG	3.5
1	B	254	ILE	3.2
1	B	463	GLU	3.2
1	B	461	GLU	3.1
1	B	453	GLN	2.9
1	B	404	SER	2.9
1	B	165	ARG	2.7
1	B	305	ASP	2.6
1	B	280	LYS	2.6
1	B	457	GLU	2.5
1	B	167	PHE	2.5
1	B	462	GLN	2.4
1	B	164	THR	2.3
1	B	405	ASP	2.2
1	A	254	ILE	2.2
1	B	268	THR	2.2
1	A	366	GLU	2.2
1	A	249	LYS	2.0
1	B	249	LYS	2.0
1	B	312	ASP	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](#)

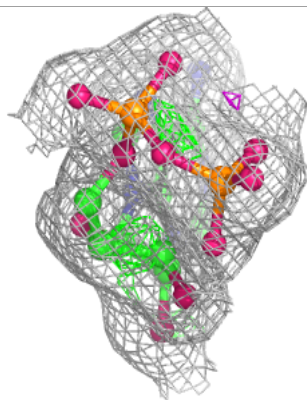
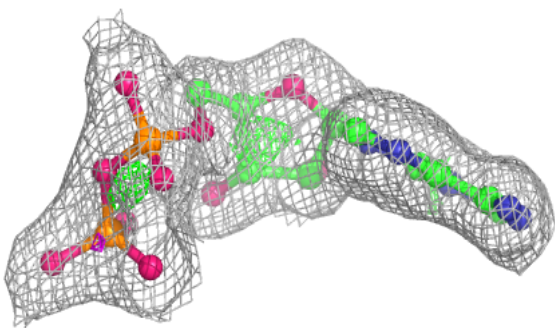
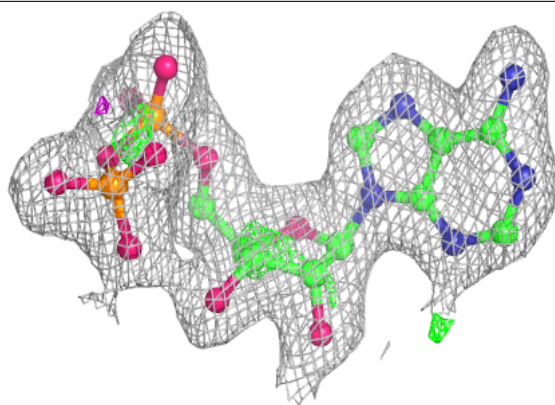
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	B	2002	1/1	0.91	0.15	37,37,37,37	0
3	PO4	A	3001	5/5	0.93	0.12	51,54,59,60	0
3	PO4	B	3002	5/5	0.96	0.14	47,53,55,57	0
2	MG	A	2001	1/1	0.97	0.06	37,37,37,37	0
4	ADP	A	1001	27/27	0.98	0.12	30,33,38,39	0
4	ADP	B	1002	27/27	0.98	0.13	28,30,33,34	0

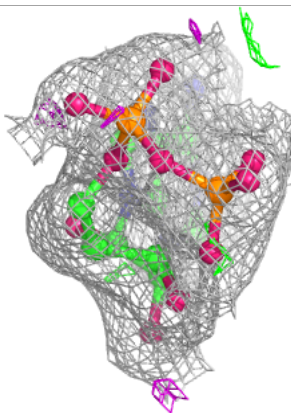
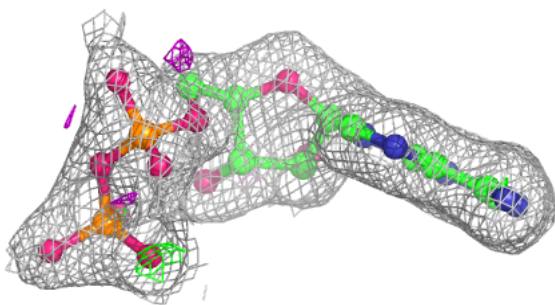
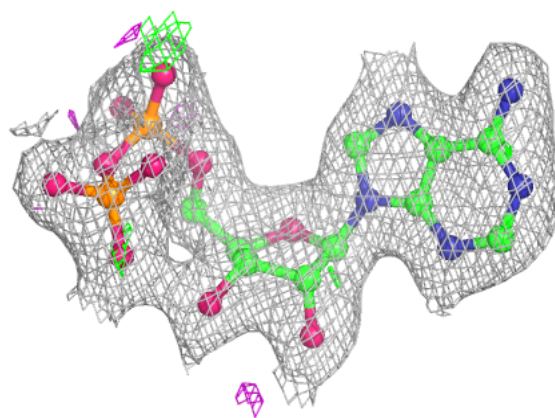
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 1001:

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

**Electron density around ADP B 1002:**

$2mF_o-DF_c$ (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.