Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2023 – 01:18 pm GMT

PDB ID	:	2BKK
Title	:	Crystal structure of Aminoglycoside Phosphotransferase APH(3')-IIIa in complex with the inhibitor AR_3a
Authors	:	Kohl, A.; Amstutz, P.; Parizek, P.; Binz, H.K.; Briand, C.; Capitani, G.; Forrer, P.; Pluckthun, A.; Grutter, M.G.
Deposited on	:	2005-02-16
Resolution	:	2.15 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:

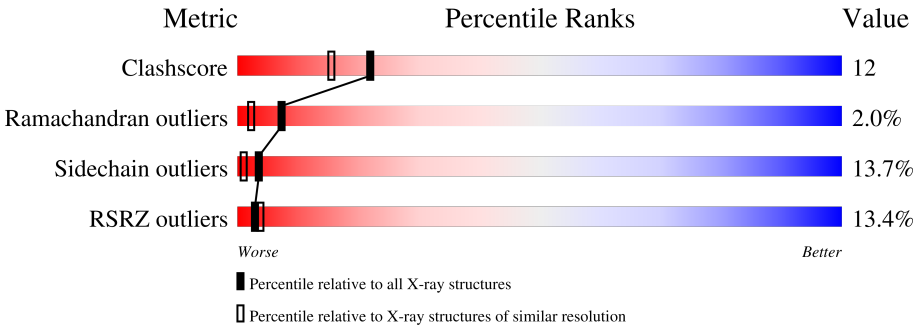
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 2.15 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))
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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% 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	264	5% 69% 20% • 6%
1	C	264	9% 72% 20% 5% • •
2	B	169	20% 61% 28% • 8%
2	D	169	22% 53% 30% 8% • 7%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7000 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 AMINOGLYCOSIDE 3'-PHOSPHOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	0	0	0
			2038	1304	326	398	10			
1	C	262	Total	C	N	O	S	0	0	0
			2165	1382	343	430	10			

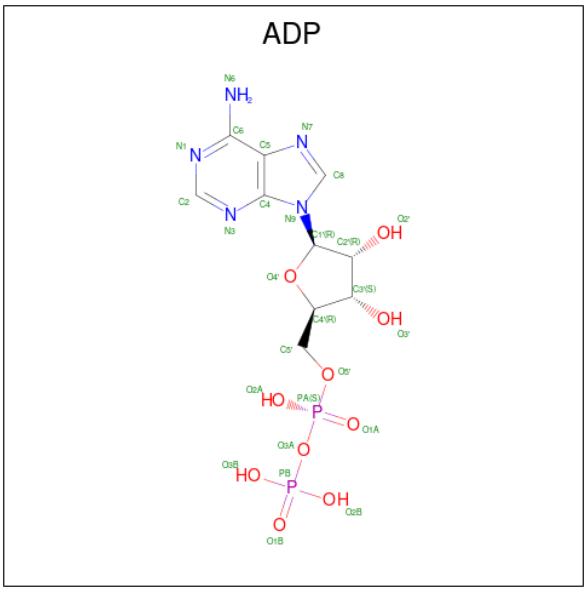
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	SER	CYS	engineered mutation	UNP P00554
C	19	SER	CYS	engineered mutation	UNP P00554

- Molecule 2 is a protein called DESIGNED ANKYRIN REPEAT INHIBITOR AR_3A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	156	Total	C	N	O	S	0	0	1
			1194	756	201	235	2			
2	D	157	Total	C	N	O	S	0	0	1
			1198	758	202	236	2			

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Mg 2 2	0	0
4	C	2	Total Mg 2 2	0	0

- Molecule 5 is water.

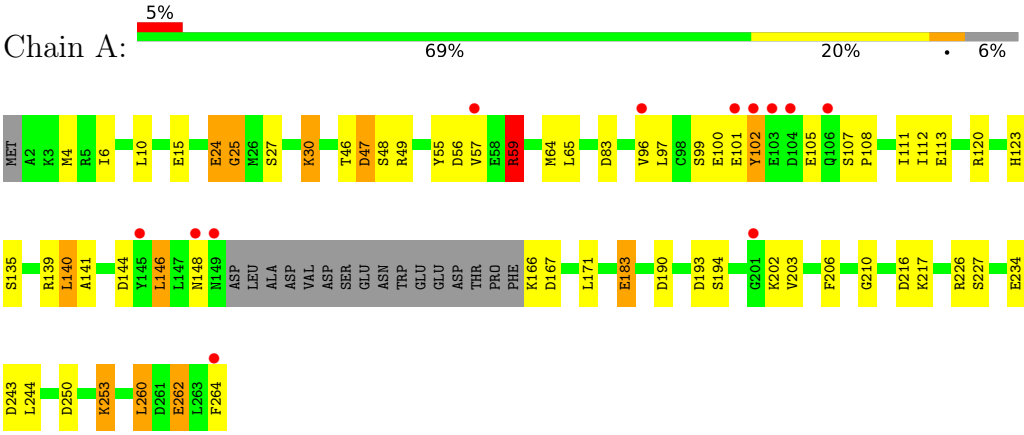
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	115	Total O 115 115	0	0
5	B	53	Total O 53 53	0	0
5	C	130	Total O 130 130	0	0
5	D	49	Total O 49 49	0	0

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.

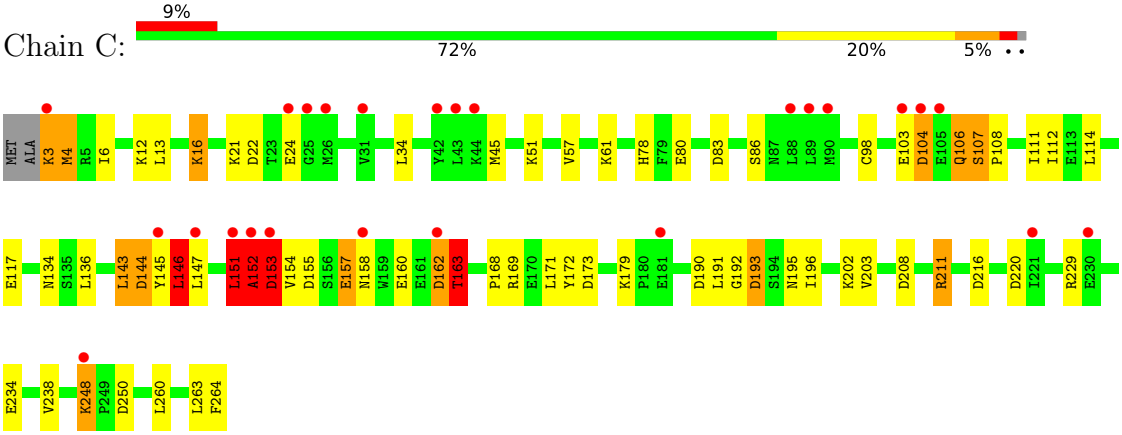
• Molecule 1: AMINOGLYCOSIDE 3'-PHOSPHOTRANSFERASE

Chain A:



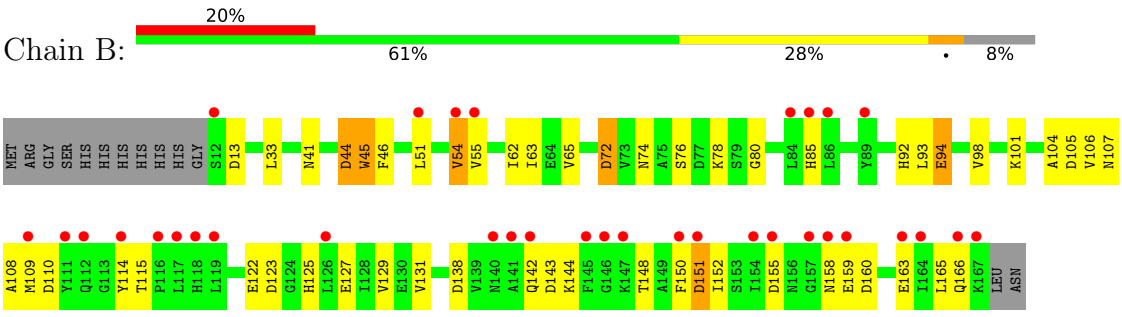
• Molecule 1: AMINOGLYCOSIDE 3'-PHOSPHOTRANSFERASE

Chain C:



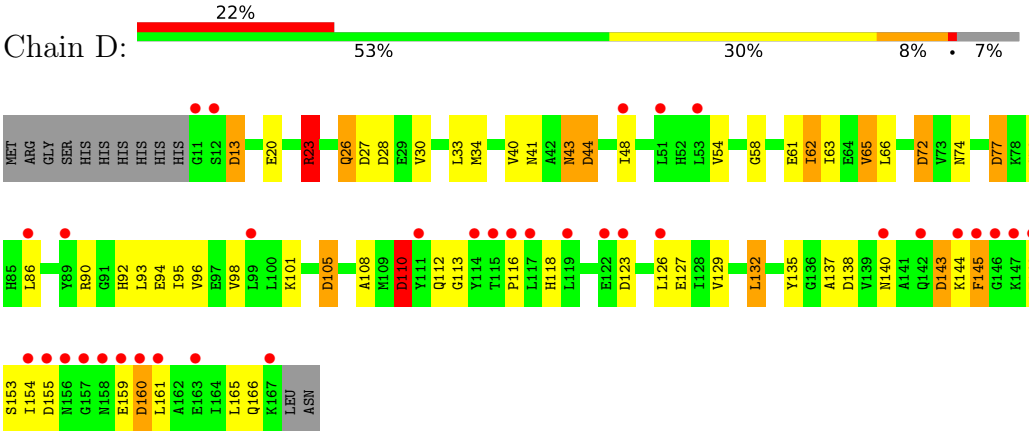
• Molecule 2: DESIGNED ANKYRIN REPEAT INHIBITOR AR_3A

Chain B:



• Molecule 2: DESIGNED ANKYRIN REPEAT INHIBITOR AR_3A

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.67Å 98.08Å 81.30Å 90.00° 110.01° 90.00°	Depositor
Resolution (Å)	20.00 – 2.15 19.90 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.7 (20.00-2.15) 96.6 (19.90-2.15)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 2.15Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.199 , 0.260 0.206 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	44.5	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 57.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7000	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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: MG, 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	0.71	1/2081 (0.0%)	0.95	11/2800 (0.4%)
1	C	0.73	0/2213	0.95	9/2984 (0.3%)
2	B	0.63	0/1215	0.89	8/1652 (0.5%)
2	D	0.66	0/1219	0.98	13/1657 (0.8%)
All	All	0.70	1/6728 (0.0%)	0.94	41/9093 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	MET	SD-CE	-5.62	1.46	1.77

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	216	ASP	CB-CG-OD2	9.11	126.50	118.30
1	C	220	ASP	CB-CG-OD2	8.04	125.54	118.30
1	A	59	ARG	NE-CZ-NH2	-7.85	116.37	120.30
1	A	56	ASP	CB-CG-OD2	7.73	125.25	118.30
2	D	72	ASP	CB-CG-OD2	7.49	125.04	118.30
1	C	83	ASP	CB-CG-OD2	7.18	124.77	118.30
1	A	47	ASP	CB-CG-OD2	6.72	124.35	118.30
1	A	59	ARG	NE-CZ-NH1	6.61	123.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	28	ASP	CB-CG-OD2	6.55	124.20	118.30
2	B	110	ASP	CB-CG-OD2	6.37	124.03	118.30
2	D	155	ASP	CB-CG-OD2	6.34	124.00	118.30
1	A	167	ASP	CB-CG-OD2	6.18	123.86	118.30
2	D	110	ASP	CB-CG-OD2	6.16	123.84	118.30
2	B	72	ASP	CB-CG-OD2	6.14	123.82	118.30
2	B	13	ASP	CB-CG-OD2	6.09	123.78	118.30
2	B	143	ASP	CB-CG-OD2	6.07	123.77	118.30
2	D	151	ASP	CB-CG-OD2	6.07	123.76	118.30
1	C	250	ASP	CB-CG-OD2	5.97	123.68	118.30
2	D	105	ASP	CB-CG-OD2	5.92	123.63	118.30
2	D	123	ASP	CB-CG-OD2	5.87	123.58	118.30
1	A	126	ASP	CB-CG-OD2	5.81	123.53	118.30
2	D	13	ASP	CB-CG-OD2	5.69	123.42	118.30
1	C	162	ASP	CB-CG-OD2	5.67	123.40	118.30
2	D	27	ASP	CB-CG-OD2	5.64	123.38	118.30
1	A	190	ASP	CB-CG-OD2	5.64	123.38	118.30
1	C	193	ASP	CB-CG-OD2	5.61	123.35	118.30
1	C	216	ASP	CB-CG-OD2	5.59	123.33	118.30
2	D	23	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	A	83	ASP	CB-CG-OD2	5.48	123.23	118.30
1	C	144	ASP	CB-CG-OD2	5.44	123.19	118.30
2	B	44	ASP	CB-CG-OD2	5.43	123.18	118.30
1	A	243	ASP	CB-CG-OD2	5.29	123.06	118.30
2	D	77	ASP	CB-CG-OD2	5.24	123.02	118.30
2	B	160	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	193	ASP	CB-CG-OD2	5.19	122.97	118.30
1	C	208	ASP	CB-CG-OD2	5.17	122.96	118.30
2	D	44	ASP	CB-CG-OD2	5.14	122.93	118.30
2	B	155	ASP	CB-CG-OD2	5.13	122.92	118.30
1	C	153	ASP	CB-CG-OD2	5.13	122.91	118.30
2	B	151	ASP	CB-CG-OD2	5.09	122.88	118.30
2	D	160	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	152	ALA	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2038	0	1992	39	0
1	C	2165	0	2091	39	0
2	B	1194	0	1162	35	0
2	D	1198	0	1165	45	0
3	A	27	0	12	1	0
3	C	27	0	12	0	0
4	A	2	0	0	0	0
4	C	2	0	0	0	0
5	A	115	0	0	12	1
5	B	53	0	0	11	0
5	C	130	0	0	8	1
5	D	49	0	0	13	0
All	All	7000	0	6434	154	1

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 12.

All (154) 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:C:146:LEU:HA	5:C:2081:HOH:O	1.34	1.23
2:D:82:THR:OG1	5:D:2030:HOH:O	1.74	1.04
2:D:116:PRO:HD3	5:D:2039:HOH:O	1.59	1.02
2:D:41:ASN:HD21	2:D:72:ASP:H	1.12	0.96
2:B:44:ASP:O	5:B:2025:HOH:O	1.84	0.93
2:D:43:ASN:HA	5:D:2019:HOH:O	1.69	0.90
2:D:132:LEU:O	5:D:2041:HOH:O	1.89	0.89
2:D:101:LYS:NZ	2:D:135:TYR:OH	2.07	0.87
2:B:74:ASN:HD21	2:B:105:ASP:H	1.23	0.86
2:D:108:ALA:O	5:D:2039:HOH:O	1.94	0.85
2:B:45:TRP:N	5:B:2026:HOH:O	2.05	0.81
2:D:74:ASN:HD21	2:D:105:ASP:H	1.27	0.79
1:A:47:ASP:OD1	5:A:2031:HOH:O	2.05	0.74
2:B:127:GLU:O	5:B:2045:HOH:O	2.04	0.73
2:D:48:ILE:O	5:D:2019:HOH:O	2.07	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:LEU:N	5:C:2082:HOH:O	2.22	0.72
1:C:190:ASP:O	1:C:195:ASN:ND2	2.21	0.72
1:A:141:ALA:HB2	5:B:2003:HOH:O	1.91	0.71
1:A:65:LEU:O	5:A:2037:HOH:O	2.10	0.70
2:B:106:VAL:O	5:B:2043:HOH:O	2.09	0.70
1:C:104:ASP:HB2	1:C:106:GLN:HE21	1.56	0.70
2:B:62:ILE:HD12	2:B:65:VAL:HG11	1.75	0.68
2:B:123:ASP:HB3	2:B:125:HIS:ND1	2.07	0.68
1:C:143:LEU:O	1:C:146:LEU:HB3	1.93	0.68
1:A:141:ALA:CB	5:B:2003:HOH:O	2.40	0.67
2:D:41:ASN:ND2	2:D:72:ASP:H	1.90	0.67
1:A:194:SER:OG	5:A:2085:HOH:O	2.12	0.66
2:B:108:ALA:O	2:B:115:THR:HA	1.95	0.66
2:D:110:ASP:OD1	2:D:110:ASP:C	2.33	0.66
1:A:97:LEU:HD21	5:A:2113:HOH:O	1.95	0.65
1:A:59:ARG:HD2	1:A:210:GLY:O	1.96	0.65
2:B:107:ASN:HD21	2:B:138:ASP:H	1.45	0.65
2:D:74:ASN:ND2	2:D:105:ASP:H	1.94	0.64
2:D:137:ALA:N	5:D:2041:HOH:O	2.32	0.63
2:D:43:ASN:HB2	5:D:2017:HOH:O	1.99	0.63
1:C:143:LEU:CD1	1:C:264:PHE:HB3	2.29	0.63
1:C:248:LYS:H	1:C:248:LYS:NZ	1.97	0.62
1:A:46:THR:HG23	1:A:57:VAL:HG13	1.81	0.62
1:C:191:LEU:HD12	1:C:196:ILE:HD11	1.80	0.62
1:A:46:THR:HG21	1:A:55:TYR:O	2.00	0.62
2:B:74:ASN:ND2	2:B:105:ASP:H	1.94	0.61
1:C:152:ALA:O	1:C:153:ASP:O	2.18	0.61
2:B:62:ILE:O	2:B:65:VAL:HG12	2.01	0.60
1:A:97:LEU:CD2	5:A:2113:HOH:O	2.49	0.60
2:B:62:ILE:HA	2:B:65:VAL:HG12	1.83	0.60
2:D:41:ASN:HD21	2:D:72:ASP:N	1.94	0.60
2:D:126:LEU:O	2:D:129:VAL:HG12	2.01	0.60
1:C:144:ASP:O	1:C:147:LEU:HG	2.04	0.58
1:C:3:LYS:O	1:C:4:MET:O	2.21	0.58
1:A:140:LEU:HB3	2:B:45:TRP:CG	2.38	0.58
1:C:155:ASP:OD2	1:C:157:GLU:O	2.22	0.57
2:D:40:VAL:HG23	2:D:66:LEU:HD22	1.86	0.57
1:A:120:ARG:NH1	5:A:2064:HOH:O	2.38	0.56
1:C:98:CYS:SG	5:C:2066:HOH:O	1.96	0.55
2:D:62:ILE:HA	2:D:65:VAL:HG13	1.86	0.55
2:D:127:GLU:H	2:D:127:GLU:CD	2.09	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:GLN:OE1	1:C:107:SER:OG	2.24	0.55
2:D:149:ALA:N	5:D:2046:HOH:O	2.39	0.55
2:B:123:ASP:HB3	2:B:125:HIS:CE1	2.42	0.54
1:C:104:ASP:HB2	1:C:106:GLN:NE2	2.22	0.54
1:C:108:PRO:O	1:C:112:ILE:HG12	2.07	0.54
1:C:172:TYR:OH	2:D:48:ILE:HD12	2.09	0.53
2:D:74:ASN:HD21	2:D:105:ASP:N	2.02	0.53
1:C:248:LYS:H	1:C:248:LYS:HZ3	1.58	0.52
2:B:62:ILE:O	2:B:65:VAL:CG1	2.57	0.52
1:A:6:ILE:CD1	1:A:10:LEU:HD23	2.41	0.51
1:A:97:LEU:HD11	1:A:194:SER:C	2.30	0.51
1:A:105:GLU:O	1:A:105:GLU:HG3	2.11	0.51
2:B:131:VAL:HG23	5:B:2045:HOH:O	2.10	0.51
1:A:135:SER:O	1:A:139:ARG:HG3	2.10	0.51
1:C:146:LEU:CA	5:C:2082:HOH:O	2.59	0.51
2:B:127:GLU:C	5:B:2045:HOH:O	2.46	0.50
1:A:226:ARG:NE	5:A:2094:HOH:O	2.31	0.50
1:C:106:GLN:NE2	1:C:106:GLN:H	2.09	0.50
2:D:93:LEU:O	2:D:96:VAL:HG12	2.12	0.50
1:C:151:LEU:HB2	1:C:153:ASP:HA	1.94	0.50
1:C:146:LEU:HG	1:C:146:LEU:O	2.11	0.49
1:A:6:ILE:HD12	1:A:10:LEU:HD23	1.94	0.49
2:B:54:VAL:CG1	2:B:63:ILE:HG13	2.43	0.49
1:C:134:ASN:ND2	1:C:211:ARG:O	2.44	0.48
2:B:109:MET:HA	2:B:114:TYR:O	2.13	0.48
1:A:108:PRO:O	1:A:112:ILE:HG12	2.13	0.48
1:C:168:PRO:HG3	2:D:79:SER:HB3	1.96	0.48
2:D:20:GLU:OE2	2:D:23:ARG:NH1	2.47	0.48
2:D:92:HIS:HB2	5:D:2032:HOH:O	2.13	0.48
1:A:97:LEU:HD21	1:A:194:SER:HA	1.94	0.48
2:B:74:ASN:HD21	2:B:105:ASP:N	2.01	0.48
1:C:162:ASP:O	1:C:163:THR:O	2.31	0.48
2:B:62:ILE:CD1	2:B:65:VAL:HG11	2.43	0.48
2:D:160:ASP:HA	5:D:2048:HOH:O	2.13	0.48
1:A:250:ASP:CG	1:A:253:LYS:HD3	2.33	0.48
2:B:144:LYS:NZ	5:B:2049:HOH:O	2.47	0.47
2:D:77:ASP:C	2:D:77:ASP:OD1	2.52	0.47
1:C:117:GLU:CD	1:C:203:VAL:HG12	2.35	0.47
2:B:44:ASP:CA	5:B:2026:HOH:O	2.62	0.47
2:B:51:LEU:O	2:B:55:VAL:HG23	2.15	0.47
1:A:226:ARG:NH1	5:A:2094:HOH:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:82:THR:HB	2:D:83:PRO:HD2	1.97	0.47
1:C:211:ARG:HB3	5:C:2105:HOH:O	2.16	0.46
1:A:59:ARG:CD	1:A:210:GLY:O	2.64	0.46
1:C:16:LYS:H	1:C:16:LYS:CD	2.28	0.46
2:D:93:LEU:HA	2:D:96:VAL:HG12	1.97	0.46
1:A:141:ALA:O	1:A:144:ASP:HB3	2.14	0.46
1:A:30:LYS:N	1:A:30:LYS:HD2	2.30	0.46
1:A:96:VAL:HG11	1:A:101:GLU:OE2	2.16	0.46
1:C:192:GLY:O	1:C:196:ILE:HD12	2.16	0.46
2:D:26:GLN:O	2:D:30:VAL:HG23	2.16	0.46
2:B:76:SER:OG	2:B:80:GLY:HA2	2.16	0.45
1:C:143:LEU:HD13	1:C:264:PHE:HB3	1.97	0.45
2:B:41:ASN:HD21	2:B:72:ASP:H	1.65	0.45
2:D:118:HIS:NE2	2:D:148:THR:O	2.49	0.45
2:B:45:TRP:HB2	2:B:46:PHE:CD1	2.52	0.45
2:D:30:VAL:O	2:D:34:MET:HG2	2.17	0.45
1:A:144:ASP:HB2	2:B:45:TRP:HA	1.99	0.45
2:B:85:HIS:HE1	2:B:108:ALA:HB3	1.82	0.45
1:C:264:PHE:O	5:C:2126:HOH:O	2.21	0.45
2:D:54:VAL:HG12	2:D:63:ILE:CG1	2.47	0.44
1:A:24:GLU:O	1:A:25:GLY:O	2.35	0.44
1:A:203:VAL:HG11	1:A:206:PHE:CE1	2.52	0.44
1:A:183:GLU:HG3	5:A:2080:HOH:O	2.18	0.43
1:A:250:ASP:OD2	1:A:253:LYS:HD3	2.18	0.43
2:D:143:ASP:OD1	5:D:2044:HOH:O	2.21	0.43
1:C:229:ARG:HD2	1:C:238:VAL:HG21	2.01	0.43
2:D:113:GLY:HA2	5:D:2040:HOH:O	2.17	0.43
1:A:27:SER:OG	3:A:1265:ADP:O2B	2.27	0.43
2:D:101:LYS:CE	2:D:135:TYR:OH	2.67	0.43
2:D:138:ASP:OD1	2:D:138:ASP:C	2.57	0.42
1:C:45:MET:HB3	1:C:45:MET:HE2	1.98	0.42
2:B:46:PHE:HA	2:B:78:LYS:HD2	2.01	0.42
1:C:45:MET:HA	1:C:86:SER:O	2.19	0.42
1:C:146:LEU:HA	5:C:2082:HOH:O	2.17	0.42
2:D:145:PHE:N	2:D:145:PHE:CD2	2.87	0.42
1:A:203:VAL:HG11	1:A:206:PHE:CZ	2.53	0.42
2:D:58:GLY:O	2:D:95:ILE:HD11	2.19	0.42
2:B:159:GLU:C	2:B:163:GLU:HG2	2.40	0.42
2:D:54:VAL:HG12	2:D:63:ILE:HG13	2.01	0.42
1:A:99:SER:HB3	5:A:2084:HOH:O	2.20	0.42
1:C:78:HIS:HE1	1:C:80:GLU:OE2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ARG:HG2	1:A:132:TYR:CE1	2.55	0.41
1:A:262:GLU:HA	1:A:264:PHE:CE2	2.55	0.41
1:A:15:GLU:HA	5:A:2008:HOH:O	2.20	0.41
2:B:74:ASN:HD21	2:B:104:ALA:HA	1.86	0.41
2:D:40:VAL:HG22	2:D:40:VAL:O	2.21	0.41
2:D:145:PHE:N	2:D:145:PHE:HD2	2.19	0.41
1:A:55:TYR:CE1	1:A:146:LEU:HD11	2.56	0.41
2:B:94:GLU:O	2:B:98:VAL:HG23	2.20	0.41
1:C:104:ASP:CB	1:C:106:GLN:HE21	2.28	0.40
2:D:86:LEU:HD23	2:D:86:LEU:O	2.21	0.40
1:C:21:LYS:HB3	5:C:2015:HOH:O	2.20	0.40
1:A:260:LEU:O	5:A:2108:HOH:O	2.22	0.40
2:B:92:HIS:HB2	5:B:2039:HOH:O	2.22	0.40
2:B:152:ILE:HG22	2:B:152:ILE:O	2.21	0.40
1:C:169:ARG:O	1:C:173:ASP:OD1	2.38	0.40
2:D:48:ILE:N	2:D:48:ILE:HD13	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2109:HOH:O	5:C:2056:HOH:O[2_545]	1.89	0.31

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	243/264 (92%)	229 (94%)	12 (5%)	2 (1%)	19 12
1	C	260/264 (98%)	241 (93%)	10 (4%)	9 (4%)	3 0
2	B	154/169 (91%)	141 (92%)	11 (7%)	2 (1%)	12 6
2	D	155/169 (92%)	130 (84%)	22 (14%)	3 (2%)	8 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	812/866 (94%)	741 (91%)	55 (7%)	16 (2%)	7 2

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	GLY
1	C	4	MET
1	C	153	ASP
1	C	163	THR
1	C	193	ASP
1	A	102	TYR
2	B	148	THR
1	C	146	LEU
1	C	152	ALA
2	D	143	ASP
2	D	149	ALA
2	B	45	TRP
1	C	145	TYR
1	C	151	LEU
1	C	22	ASP
2	D	145	PHE

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	226/242 (93%)	199 (88%)	27 (12%)	5 2
1	C	241/242 (100%)	207 (86%)	34 (14%)	3 1
2	B	123/135 (91%)	110 (89%)	13 (11%)	6 3
2	D	123/135 (91%)	99 (80%)	24 (20%)	1 0
All	All	713/754 (95%)	615 (86%)	98 (14%)	3 1

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	MET
1	A	24	GLU
1	A	30	LYS
1	A	48	SER
1	A	49	ARG
1	A	59	ARG
1	A	100	GLU
1	A	102	TYR
1	A	107	SER
1	A	111	ILE
1	A	113	GLU
1	A	123	HIS
1	A	140	LEU
1	A	146	LEU
1	A	148	ASN
1	A	166	LYS
1	A	171	LEU
1	A	183	GLU
1	A	202	LYS
1	A	217	LYS
1	A	227	SER
1	A	234	GLU
1	A	239	GLU
1	A	244	LEU
1	A	253	LYS
1	A	260	LEU
1	A	262	GLU
2	B	33	LEU
2	B	54	VAL
2	B	93	LEU
2	B	94	GLU
2	B	101	LYS
2	B	122	GLU
2	B	129	VAL
2	B	142	GLN
2	B	150	PHE
2	B	151	ASP
2	B	158	ASN
2	B	165	LEU
2	B	166	GLN
1	C	3	LYS
1	C	6	ILE
1	C	12	LYS

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Mol	Chain	Res	Type
1	C	13	LEU
1	C	16	LYS
1	C	24	GLU
1	C	34	LEU
1	C	51	LYS
1	C	57	VAL
1	C	61	LYS
1	C	103	GLU
1	C	104	ASP
1	C	106	GLN
1	C	107	SER
1	C	111	ILE
1	C	114	LEU
1	C	136	LEU
1	C	143	LEU
1	C	146	LEU
1	C	151	LEU
1	C	153	ASP
1	C	154	VAL
1	C	157	GLU
1	C	158	ASN
1	C	160	GLU
1	C	163	THR
1	C	171	LEU
1	C	179	LYS
1	C	202	LYS
1	C	211	ARG
1	C	234	GLU
1	C	248	LYS
1	C	260	LEU
1	C	263	LEU
2	D	13	ASP
2	D	23	ARG
2	D	26	GLN
2	D	33	LEU
2	D	43	ASN
2	D	44	ASP
2	D	61	GLU
2	D	62	ILE
2	D	65	VAL
2	D	90	ARG
2	D	94	GLU

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Mol	Chain	Res	Type
2	D	98	VAL
2	D	110	ASP
2	D	112	GLN
2	D	132	LEU
2	D	140	ASN
2	D	144	LYS
2	D	152	ILE
2	D	153	SER
2	D	154	ILE
2	D	159	GLU
2	D	161	LEU
2	D	165	LEU
2	D	166	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	HIS
1	A	148	ASN
2	B	26	GLN
2	B	41	ASN
2	B	59	HIS
2	B	74	ASN
2	B	107	ASN
2	B	118	HIS
1	C	78	HIS
1	C	82	HIS
1	C	106	GLN
2	D	36	ASN
2	D	41	ASN
2	D	56	ASN
2	D	74	ASN
2	D	140	ASN

5.3.3 RNA

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	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ADP	A	1265	4	24,29,29	1.48	4 (16%)	29,45,45	1.34	2 (6%)
3	ADP	C	1265	4	24,29,29	1.18	3 (12%)	29,45,45	1.90	4 (13%)

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	1265	4	-	4/12/32/32	0/3/3/3
3	ADP	C	1265	4	-	0/12/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1265	ADP	C2-N3	4.11	1.38	1.32
3	A	1265	ADP	C2-N1	3.53	1.40	1.33
3	C	1265	ADP	C2-N1	2.77	1.39	1.33
3	C	1265	ADP	C2-N3	2.70	1.36	1.32
3	A	1265	ADP	O4'-C1'	2.53	1.44	1.41
3	C	1265	ADP	O4'-C1'	2.05	1.43	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1265	ADP	PB-O1B	2.03	1.57	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1265	ADP	N3-C2-N1	-7.75	116.56	128.68
3	A	1265	ADP	N3-C2-N1	-4.73	121.28	128.68
3	C	1265	ADP	C2-N1-C6	3.62	124.94	118.75
3	C	1265	ADP	PA-O3A-PB	-2.68	123.63	132.83
3	C	1265	ADP	O2B-PB-O3A	2.13	111.79	104.64
3	A	1265	ADP	C3'-C2'-C1'	2.13	104.18	100.98

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1265	ADP	PB-O3A-PA-O2A
3	A	1265	ADP	O4'-C4'-C5'-O5'
3	A	1265	ADP	PB-O3A-PA-O1A
3	A	1265	ADP	C3'-C4'-C5'-O5'

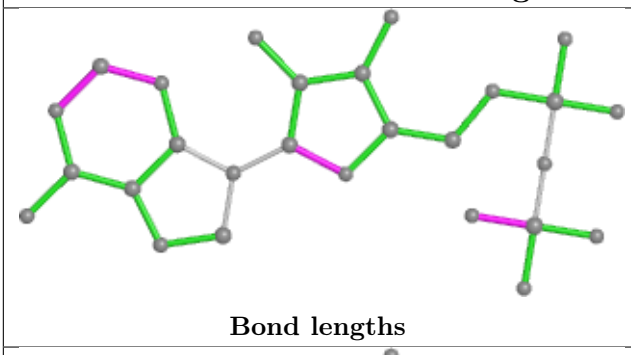
There are no ring outliers.

1 monomer is involved in 1 short contact:

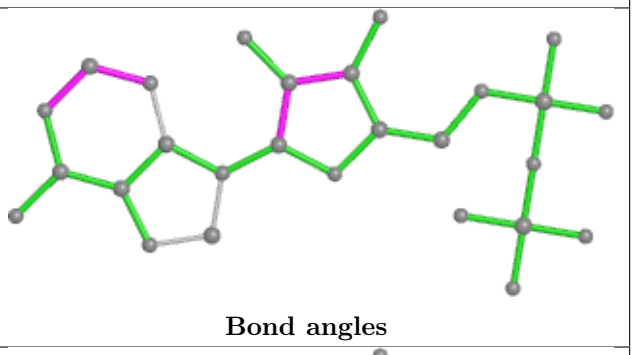
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1265	ADP	1	0

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

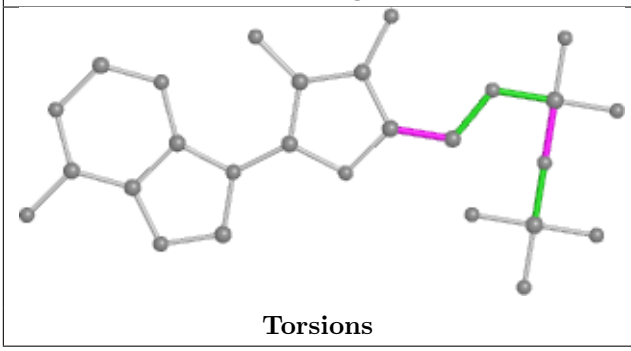
Ligand ADP A 1265



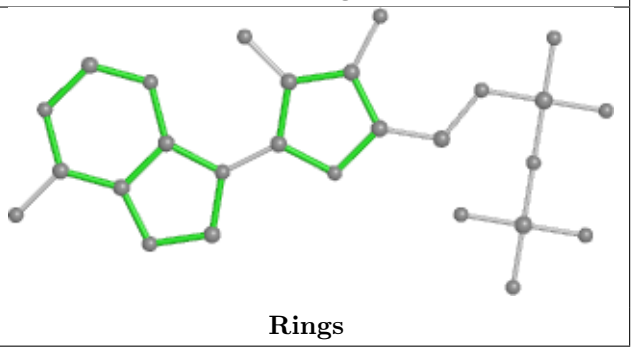
Bond lengths



Bond angles

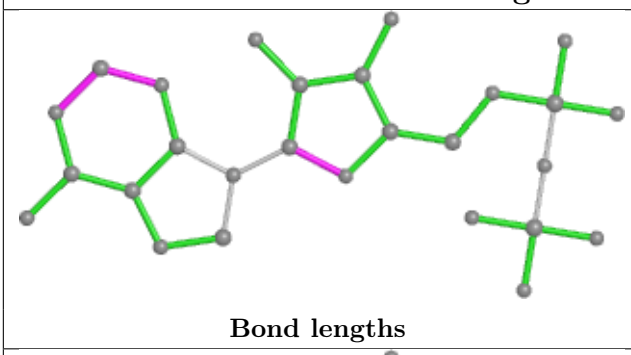


Torsions

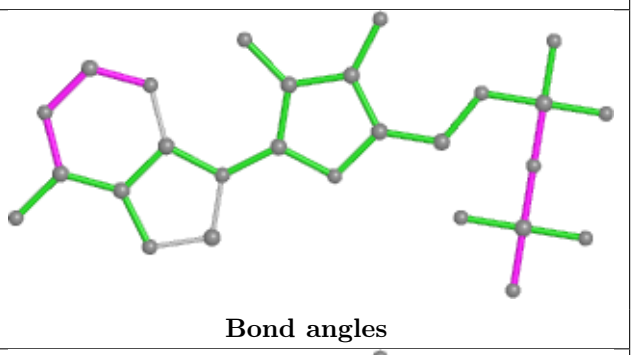


Rings

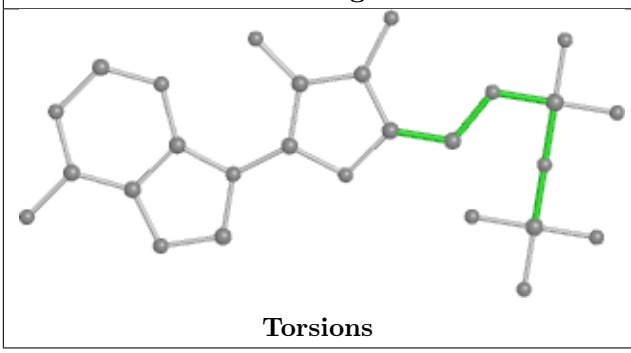
Ligand ADP C 1265



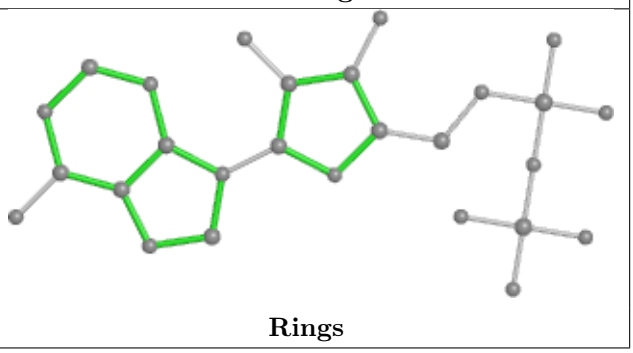
Bond lengths



Bond angles



Torsions



Rings

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, 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	247/264 (93%)	0.38	13 (5%) 26 35	29, 50, 87, 115	0
1	C	262/264 (99%)	0.49	25 (9%) 8 12	30, 47, 83, 112	1 (0%)
2	B	156/169 (92%)	1.10	34 (21%) 0 0	34, 59, 117, 123	0
2	D	157/169 (92%)	1.19	38 (24%) 0 0	31, 59, 117, 128	0
All	All	822/866 (94%)	0.70	110 (13%) 3 4	29, 52, 105, 128	1 (0%)

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	167	LYS	15.6
1	C	152	ALA	9.3
1	A	264	PHE	8.2
1	C	26	MET	6.8
2	B	145	PHE	6.3
2	B	111	TYR	6.2
2	B	150	PHE	6.0
2	D	159	GLU	5.9
1	C	43	LEU	5.7
1	A	149	ASN	5.4
2	B	154	ILE	5.4
2	B	159	GLU	5.3
2	D	154	ILE	5.3
2	D	150	PHE	4.9
2	D	161	LEU	4.8
2	D	167	LYS	4.5
2	B	155	ASP	4.5
2	D	145	PHE	4.4
2	D	111	TYR	4.4
2	D	114	TYR	4.3
1	C	24	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
2	B	147	LYS	4.3
2	B	157	GLY	4.1
2	D	117	LEU	4.1
1	C	158	ASN	4.1
2	B	12	SER	4.0
2	B	166	GLN	4.0
2	D	160	ASP	3.9
2	D	126	LEU	3.9
2	B	89	TYR	3.8
2	B	51	LEU	3.7
1	A	102	TYR	3.7
2	D	144	LYS	3.7
2	B	118	HIS	3.5
2	D	142	GLN	3.5
2	D	86	LEU	3.5
2	B	55	VAL	3.5
2	D	148	THR	3.4
2	B	151	ASP	3.4
2	B	117	LEU	3.3
2	B	146	GLY	3.3
1	C	88	LEU	3.3
2	D	51	LEU	3.3
1	C	162	ASP	3.2
2	D	163	GLU	3.2
2	B	140	ASN	3.1
2	B	142	GLN	3.1
1	C	103	GLU	3.1
2	D	146	GLY	3.0
1	C	153	ASP	3.0
1	C	3	LYS	3.0
2	B	163	GLU	2.9
1	C	104	ASP	2.9
2	B	119	LEU	2.9
2	B	164	ILE	2.8
2	D	156	ASN	2.8
1	A	148	ASN	2.8
2	B	158	ASN	2.8
1	A	96	VAL	2.8
1	C	25	GLY	2.8
1	C	42	TYR	2.8
2	D	147	LYS	2.8
2	D	151	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	109	MET	2.7
2	D	89	TYR	2.7
2	D	123	ASP	2.7
2	B	116	PRO	2.6
1	C	89	LEU	2.6
2	D	99	LEU	2.6
2	B	86	LEU	2.5
2	B	114	TYR	2.5
1	A	201	GLY	2.5
1	A	104	ASP	2.5
1	C	90	MET	2.5
2	B	84	LEU	2.5
2	B	112	GLN	2.5
2	B	54	VAL	2.5
1	A	106	GLN	2.5
1	A	103	GLU	2.5
2	D	157	GLY	2.5
1	C	31	VAL	2.4
2	D	53	LEU	2.4
2	B	85	HIS	2.4
2	D	12	SER	2.4
1	A	145	TYR	2.4
1	C	44	LYS	2.3
1	C	151	LEU	2.3
1	C	105	GLU	2.3
1	C	181	GLU	2.3
1	A	236	GLN	2.3
2	D	158	ASN	2.3
2	D	155	ASP	2.3
1	C	147	LEU	2.2
2	D	122	GLU	2.2
1	A	57	VAL	2.2
2	D	152	ILE	2.2
2	D	119	LEU	2.2
2	B	141	ALA	2.2
2	D	115	THR	2.2
2	D	116	PRO	2.2
2	D	11	GLY	2.1
1	C	230	GLU	2.1
1	C	221	ILE	2.1
1	C	248	LYS	2.1
2	B	126	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	84	LEU	2.0
1	C	145	TYR	2.0
1	A	101	GLU	2.0
2	D	140	ASN	2.0
2	D	48	ILE	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)

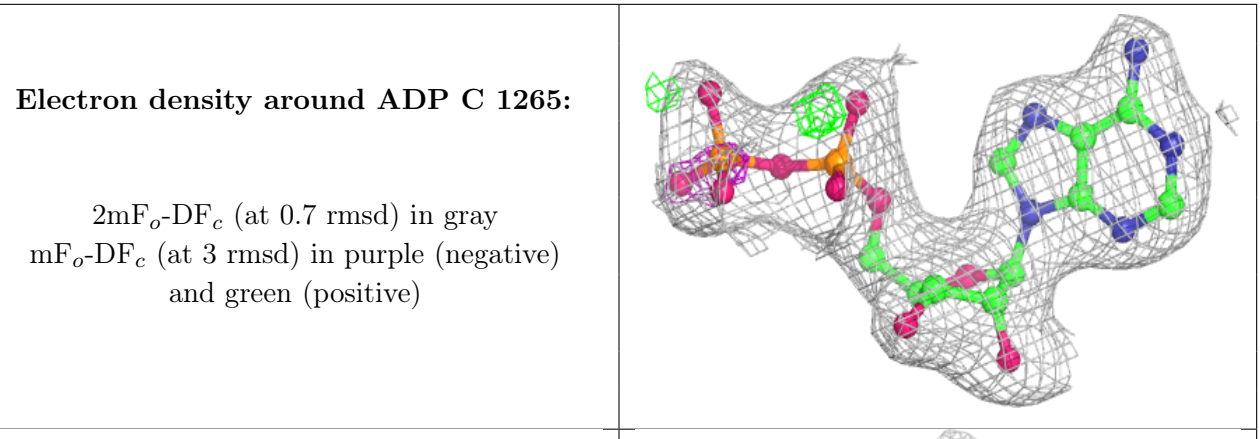
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	MG	C	1267	1/1	0.52	0.33	91,91,91,91	0
4	MG	C	1266	1/1	0.88	0.08	64,64,64,64	0
3	ADP	C	1265	27/27	0.90	0.13	26,42,71,74	0
4	MG	A	1267	1/1	0.92	0.12	60,60,60,60	0
4	MG	A	1266	1/1	0.94	0.03	50,50,50,50	0
3	ADP	A	1265	27/27	0.95	0.08	30,38,48,53	0

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

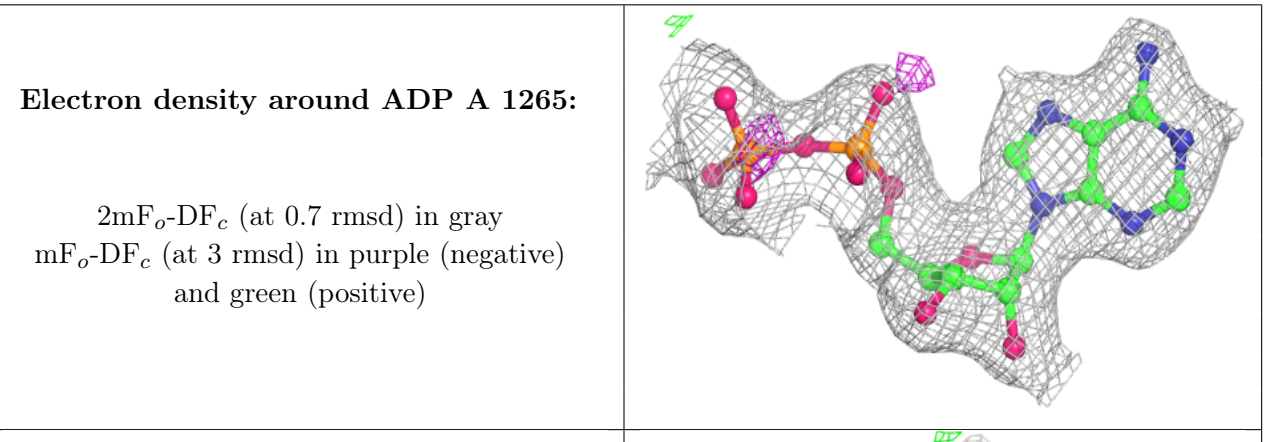
Electron density around ADP C 1265:

$2mF_o$-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 1265:

$2mF_o$-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.