



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:18 PM UTC

PDB ID : 3EHH / pdb_00003ehh
Title : Crystal structure of DesKC-H188V in complex with ADP
Authors : Albanesi, D.; Alzari, P.M.; Buschiazzi, A.
Deposited on : 2008-09-12
Resolution : 2.10 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

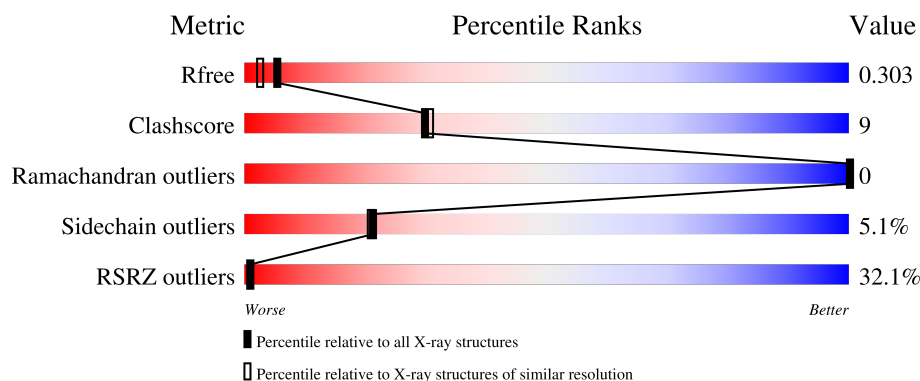
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	218	34% 73% 14% • 12%
1	B	218	21% 74% 13% • 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3227 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.

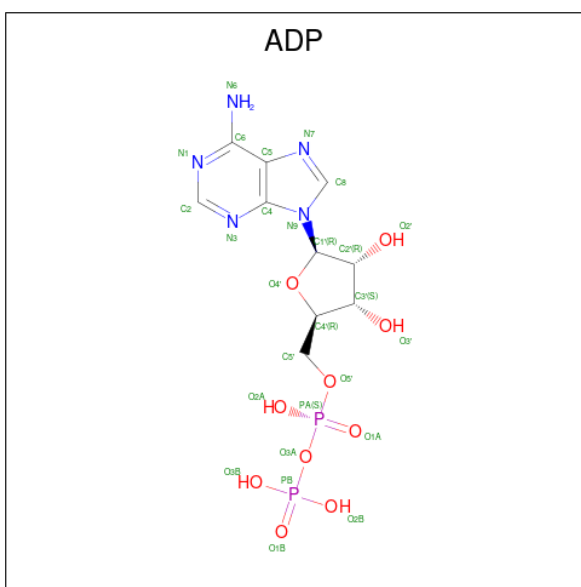
- Molecule 1 is a protein called Sensor kinase (YocF protein).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	192	Total	C	N	O	S	Se	0	4	0
			1532	958	269	293	2	10			
1	B	193	Total	C	N	O	S	Se	0	3	0
			1536	960	272	293	2	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	GLY	-	expression tag	UNP O34757
A	183	MSE	ILE	engineered mutation	UNP O34757
A	188	VAL	HIS	engineered mutation	UNP O34757
A	198	MSE	ILE	engineered mutation	UNP O34757
B	153	GLY	-	expression tag	UNP O34757
B	183	MSE	ILE	engineered mutation	UNP O34757
B	188	VAL	HIS	engineered mutation	UNP O34757
B	198	MSE	ILE	engineered mutation	UNP O34757

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		

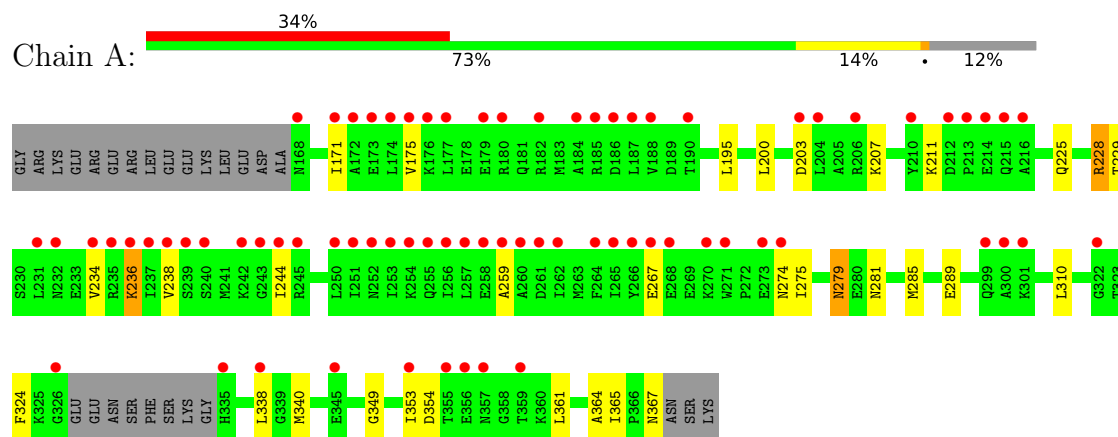
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	52	Total	O	0	0
			52	52		
4	B	51	Total	O	0	0
			51	51		

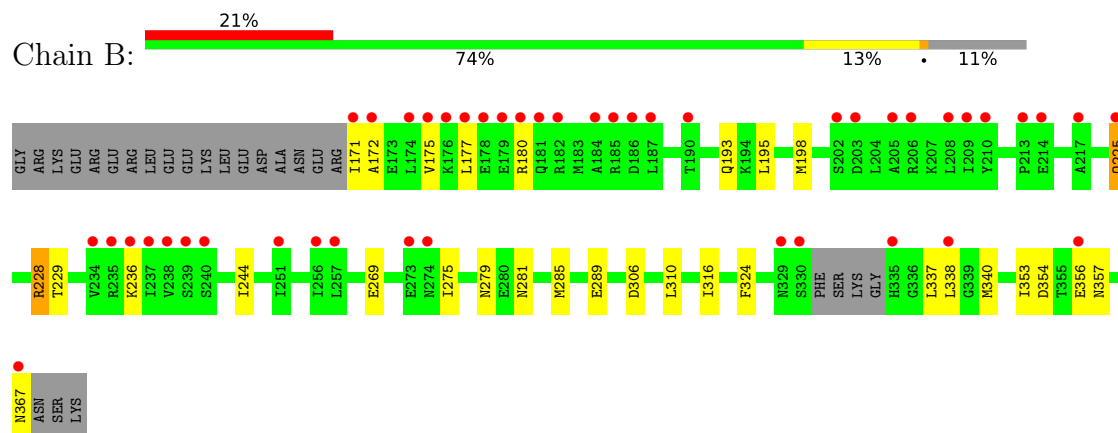
3 Residue-property plots

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: Sensor kinase (YocF protein)



• Molecule 1: Sensor kinase (YocF protein)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	34.74Å 124.05Å 138.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 30.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.7 (30.00-2.10) 97.6 (30.00-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.82 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.193 , 0.232 0.276 , 0.303	Depositor DCC
R_{free} test set	1756 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3227	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.49% 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, CA

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	1.01	2/1543 (0.1%)	0.98	0/2056
1	B	0.98	0/1548	0.95	0/2063
All	All	1.00	2/3091 (0.1%)	0.96	0/4119

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	259	ALA	C-O	-5.81	1.17	1.24
1	A	279	ASN	C-O	-5.35	1.17	1.24

There are no bond angle outliers.

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 the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1532	0	1583	30	0
1	B	1536	0	1584	33	0
2	A	27	0	12	1	0
2	B	27	0	12	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	52	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	51	0	0	5	0
All	All	3227	0	3191	54	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 9.

All (54) 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:172:ALA:O	1:B:175:VAL:HG12	1.68	0.93
1:A:195:LEU:HD11	1:B:198:MSE:SE	2.23	0.88
1:A:244:ILE:H	1:A:281:ASN:HD22	1.29	0.81
1:A:195:LEU:CD1	1:B:198:MSE:SE	2.79	0.80
1:B:244:ILE:H	1:B:281:ASN:HD22	1.28	0.79
1:B:225:GLN:O	1:B:229:THR:HG23	1.84	0.78
1:B:337:LEU:HD23	1:B:340:MSE:HE3	1.67	0.77
1:A:195:LEU:CD1	1:B:195:LEU:HD12	2.16	0.75
1:A:171:ILE:HD12	1:B:171:ILE:CB	2.16	0.75
1:A:195:LEU:HD13	1:B:195:LEU:HD12	1.69	0.74
1:B:275:ILE:HA	1:B:367:ASN:HD21	1.59	0.68
1:A:340[A]:MSE:HE1	1:A:361:LEU:HD23	1.78	0.65
1:B:337:LEU:HD23	1:B:340:MSE:CE	2.26	0.64
1:A:195:LEU:HD13	1:B:195:LEU:CD1	2.28	0.63
1:B:275:ILE:HA	1:B:367:ASN:ND2	2.15	0.62
1:A:228:ARG:NH1	1:A:229:THR:HG22	2.15	0.61
1:A:285[B]:MSE:HE1	4:A:88:HOH:O	2.01	0.59
1:B:337:LEU:HA	1:B:340:MSE:HE3	1.86	0.58
1:B:275:ILE:CA	1:B:367:ASN:HD21	2.18	0.57
1:B:177:LEU:HD13	1:B:180:ARG:HH21	1.70	0.56
1:B:236:LYS:CG	4:B:29:HOH:O	2.53	0.56
1:B:177:LEU:HD13	1:B:180:ARG:NH2	2.20	0.55
1:A:244:ILE:H	1:A:281:ASN:ND2	2.01	0.54
1:A:195:LEU:HD12	1:B:195:LEU:HD12	1.88	0.54
1:A:171:ILE:O	1:A:175:VAL:HG23	2.08	0.53
1:A:195:LEU:HD12	1:B:198:MSE:SE	2.57	0.52
1:B:236:LYS:HG3	4:B:29:HOH:O	2.10	0.52
1:A:234:VAL:O	1:A:238:VAL:HG23	2.11	0.51
1:B:275:ILE:HD11	1:B:279:ASN:HB3	1.92	0.51
1:A:275:ILE:HG22	4:A:96:HOH:O	2.12	0.50
1:B:244:ILE:H	1:B:281:ASN:ND2	2.05	0.48
1:B:285[B]:MSE:HE2	4:B:34:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ILE:HD11	1:A:279:ASN:HB3	1.96	0.48
1:A:349:GLY:HA3	1:A:364:ALA:O	2.14	0.47
1:A:354:ASP:OD1	1:A:354:ASP:C	2.58	0.47
1:A:275:ILE:HA	1:A:367:ASN:ND2	2.30	0.47
1:A:203:ASP:OD2	1:A:207:LYS:NZ	2.48	0.46
1:A:324:PHE:HA	2:A:2500:ADP:C2	2.51	0.45
1:B:225:GLN:OE1	1:B:228:ARG:NH1	2.50	0.45
1:A:228:ARG:HH11	1:A:228:ARG:HG2	1.80	0.45
1:B:354:ASP:OD2	1:B:354:ASP:C	2.60	0.44
1:A:274:ASN:O	1:A:367:ASN:ND2	2.40	0.44
1:B:324:PHE:HA	2:B:3500:ADP:C2	2.53	0.44
1:B:236:LYS:CB	4:B:29:HOH:O	2.66	0.44
1:B:279:ASN:HD22	1:B:279:ASN:HA	1.48	0.43
1:B:306:ASP:O	1:B:316:ILE:HA	2.19	0.43
1:A:225:GLN:O	1:A:229:THR:HG23	2.19	0.43
1:B:289:GLU:HG3	1:B:340:MSE:HE2	2.00	0.43
1:B:269:GLU:OE2	4:B:101:HOH:O	2.21	0.42
1:A:289:GLU:HB3	1:A:340[B]:MSE:HE2	2.01	0.42
1:A:275:ILE:HA	1:A:367:ASN:HD21	1.85	0.42
1:A:171:ILE:CD1	1:B:171:ILE:CB	2.95	0.42
1:A:228:ARG:NH1	1:A:228:ARG:HG2	2.35	0.42
1:A:236:LYS:H	1:A:236:LYS:HG2	1.51	0.41

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	192/218 (88%)	188 (98%)	4 (2%)	0	100	100
1	B	192/218 (88%)	184 (96%)	8 (4%)	0	100	100
All	All	384/436 (88%)	372 (97%)	12 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	171/187 (91%)	162 (95%)	9 (5%)	20	19
1	B	170/187 (91%)	162 (95%)	8 (5%)	23	24
All	All	341/374 (91%)	324 (95%)	17 (5%)	21	22

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	200	LEU
1	A	211	LYS
1	A	228	ARG
1	A	236	LYS
1	A	267	GLU
1	A	310	LEU
1	A	338	LEU
1	A	353	ILE
1	A	365	ILE
1	B	193	GLN
1	B	225	GLN
1	B	228	ARG
1	B	310	LEU
1	B	338	LEU
1	B	353	ILE
1	B	356	GLU
1	B	357	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	224	GLN
1	A	279	ASN

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Mol	Chain	Res	Type
1	A	281	ASN
1	A	357	ASN
1	B	193	GLN
1	B	224	GLN
1	B	279	ASN
1	B	281	ASN
1	B	367	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 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	$\# Z > 2$
2	ADP	A	2500	3	28,29,29	1.46	5 (17%)	43,45,45	1.90	12 (27%)
2	ADP	B	3500	3	28,29,29	1.76	5 (17%)	43,45,45	1.98	12 (27%)

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
2	ADP	A	2500	3	-	2/16/32/32	0/3/3/3
2	ADP	B	3500	3	-	4/16/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3500	ADP	C5-C4	5.72	1.49	1.39
2	A	2500	ADP	C5-C4	4.60	1.47	1.39
2	B	3500	ADP	PA-O3A	3.39	1.63	1.59
2	B	3500	ADP	C5-C6	2.80	1.48	1.41
2	B	3500	ADP	C5-N7	-2.74	1.34	1.39
2	A	2500	ADP	C5-C6	2.68	1.48	1.41
2	A	2500	ADP	C5-N7	-2.66	1.34	1.39
2	A	2500	ADP	C4-N9	-2.43	1.32	1.37
2	B	3500	ADP	C8-N7	2.42	1.36	1.31
2	A	2500	ADP	C8-N7	2.31	1.36	1.31

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3500	ADP	C5-C4-N3	-6.04	118.41	126.72
2	A	2500	ADP	C5-C4-N3	-5.73	118.83	126.72
2	B	3500	ADP	N3-C4-N9	4.83	135.38	127.17
2	A	2500	ADP	C4-C5-N7	-4.23	105.75	110.58
2	A	2500	ADP	N3-C4-N9	4.06	134.07	127.17
2	B	3500	ADP	C2-N3-C4	3.75	120.99	111.83
2	A	2500	ADP	C2-N3-C4	3.68	120.81	111.83
2	B	3500	ADP	N3-C2-N1	-3.19	123.76	128.58
2	B	3500	ADP	O3A-PB-O1B	-3.13	94.55	111.04
2	B	3500	ADP	C4-C5-N7	-3.12	107.01	110.58
2	B	3500	ADP	O2B-PB-O1B	2.94	122.29	110.83
2	A	2500	ADP	C5-N7-C8	2.93	108.06	103.45
2	A	2500	ADP	N3-C2-N1	-2.84	124.29	128.58
2	B	3500	ADP	O3B-PB-O3A	2.72	113.74	104.64
2	B	3500	ADP	O5'-PA-O1A	-2.67	98.34	108.94
2	A	2500	ADP	C6-C5-N7	2.67	137.24	132.09
2	A	2500	ADP	O3A-PB-O1B	-2.59	97.40	111.04
2	A	2500	ADP	C4-N9-C8	2.52	108.38	105.74
2	B	3500	ADP	O2A-PA-O1A	2.29	123.11	112.44
2	A	2500	ADP	N9-C8-N7	-2.27	110.71	113.94
2	A	2500	ADP	O2B-PB-O1B	2.24	119.56	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3500	ADP	C5-N7-C8	2.17	106.86	103.45
2	A	2500	ADP	O4'-C1'-N9	2.16	112.24	108.09
2	B	3500	ADP	O4'-C1'-N9	2.02	111.97	108.09

There are no chirality outliers.

All (6) torsion outliers are listed below:

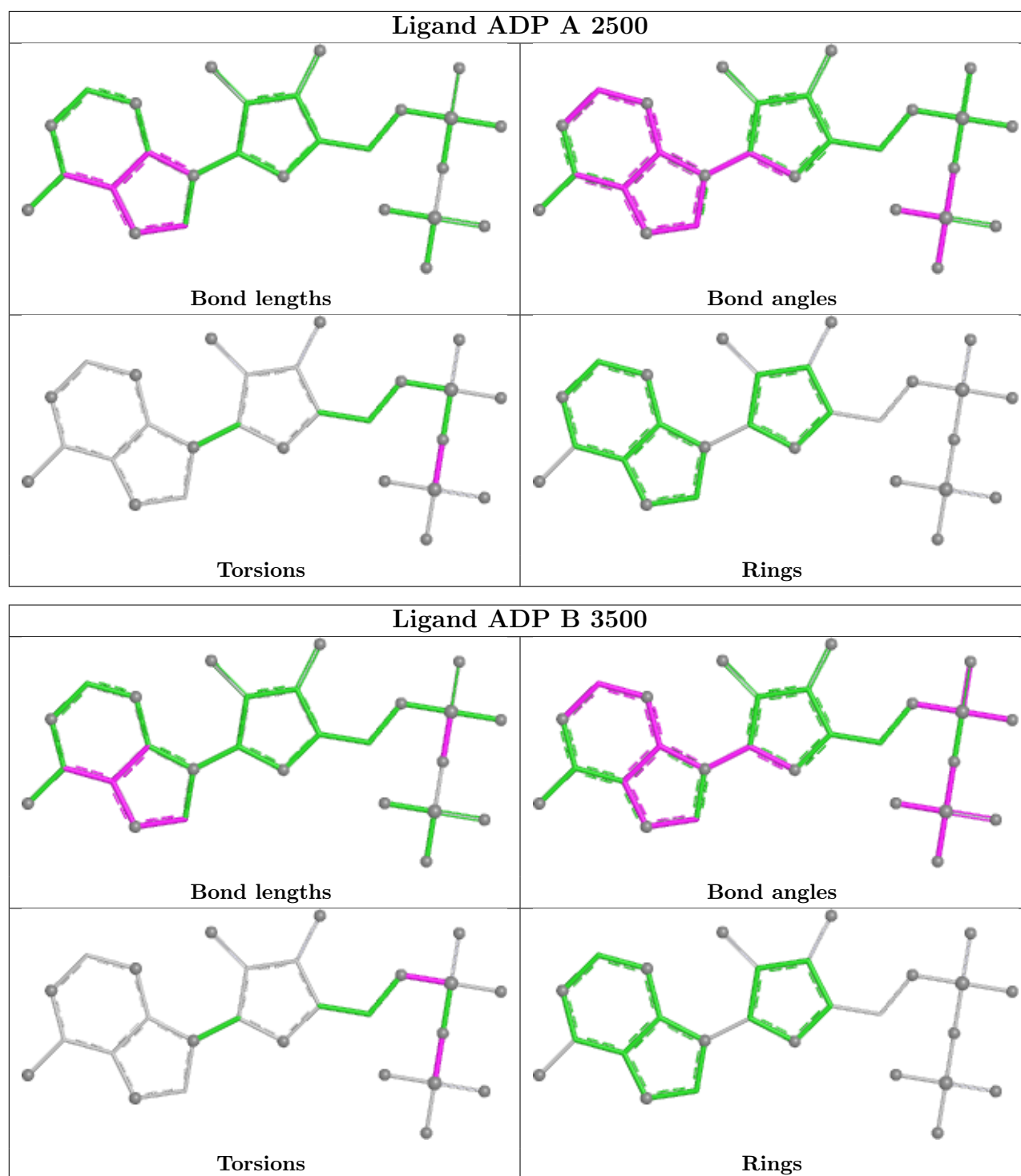
Mol	Chain	Res	Type	Atoms
2	A	2500	ADP	PA-O3A-PB-O2B
2	B	3500	ADP	PA-O3A-PB-O3B
2	A	2500	ADP	PA-O3A-PB-O3B
2	B	3500	ADP	C5'-O5'-PA-O1A
2	B	3500	ADP	PA-O3A-PB-O1B
2	B	3500	ADP	PA-O3A-PB-O2B

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2500	ADP	1	0
2	B	3500	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 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 ⓘ

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	185/218 (84%)	1.82	74 (40%)  	26, 46, 82, 140	1 (0%)
1	B	186/218 (85%)	1.37	45 (24%)  	22, 40, 86, 136	1 (0%)
All	All	371/436 (85%)	1.59	119 (32%)  	22, 42, 86, 140	2 (0%)

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	174	LEU	6.6
1	A	177	LEU	5.7
1	B	174	LEU	5.3
1	A	260	ALA	5.3
1	B	185[A]	ARG	5.2
1	B	175	VAL	5.2
1	B	330	SER	5.2
1	B	177	LEU	5.0
1	B	329	ASN	4.8
1	B	205	ALA	4.8
1	B	234	VAL	4.7
1	A	176	LYS	4.6
1	B	172	ALA	4.5
1	B	274	ASN	4.5
1	A	338	LEU	4.5
1	B	238	VAL	4.4
1	A	213	PRO	4.3
1	B	182	ARG	4.2
1	A	240	SER	4.2
1	A	234	VAL	4.2
1	A	259	ALA	4.1
1	A	175	VAL	4.1
1	A	301	LYS	4.1
1	A	255	GLN	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	256	ILE	4.0
1	A	251	ILE	3.9
1	A	214	GLU	3.9
1	B	171	ILE	3.9
1	A	238	VAL	3.9
1	A	265	ILE	3.8
1	A	216	ALA	3.7
1	A	171	ILE	3.6
1	B	210	TYR	3.6
1	A	258	GLU	3.6
1	B	184	ALA	3.6
1	A	168	ASN	3.6
1	A	172	ALA	3.5
1	B	181	GLN	3.5
1	B	208	LEU	3.5
1	A	239	SER	3.4
1	A	270	LYS	3.4
1	A	257	LEU	3.4
1	A	236	LYS	3.2
1	B	176	LYS	3.2
1	B	214	GLU	3.2
1	B	338	LEU	3.1
1	B	367	ASN	3.0
1	B	335	HIS	3.0
1	B	239	SER	3.0
1	B	179	GLU	3.0
1	A	179	GLU	3.0
1	A	335	HIS	2.9
1	A	184	ALA	2.9
1	B	186	ASP	2.9
1	B	213	PRO	2.9
1	B	236	LYS	2.9
1	A	185	ARG	2.9
1	B	209	ILE	2.9
1	A	242	LYS	2.9
1	A	252[A]	ASN	2.8
1	A	262	ILE	2.8
1	A	253	ILE	2.8
1	B	180	ARG	2.8
1	B	202	SER	2.8
1	A	322	GLY	2.8
1	A	180	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	203	ASP	2.7
1	B	240	SER	2.7
1	A	355	THR	2.7
1	A	268	GLU	2.7
1	A	237	ILE	2.7
1	A	264	PHE	2.6
1	A	182	ARG	2.6
1	A	266	TYR	2.6
1	A	215	GLN	2.6
1	A	299	GLN	2.6
1	B	251	ILE	2.6
1	A	326	GLY	2.6
1	A	243	GLY	2.5
1	B	206	ARG	2.5
1	A	261	ASP	2.5
1	A	187	LEU	2.5
1	B	187	LEU	2.4
1	B	225	GLN	2.4
1	A	353	ILE	2.4
1	A	210	TYR	2.4
1	A	254	LYS	2.4
1	A	173	GLU	2.3
1	B	203	ASP	2.3
1	A	235	ARG	2.3
1	B	237	ILE	2.3
1	B	257	LEU	2.3
1	A	186	ASP	2.3
1	A	356	GLU	2.3
1	A	359	THR	2.3
1	A	232	ASN	2.3
1	A	300	ALA	2.3
1	B	217	ALA	2.3
1	A	250	LEU	2.3
1	B	178	GLU	2.2
1	B	273	GLU	2.2
1	A	273	GLU	2.2
1	A	267	GLU	2.2
1	A	244	ILE	2.1
1	B	256	ILE	2.1
1	A	274	ASN	2.1
1	B	356	GLU	2.1
1	A	190	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	271	TRP	2.1
1	A	204	LEU	2.1
1	A	357	ASN	2.1
1	A	345	GLU	2.1
1	A	206	ARG	2.0
1	A	245	ARG	2.0
1	B	235	ARG	2.0
1	B	190	THR	2.0
1	A	188	VAL	2.0
1	A	231	LEU	2.0
1	A	212	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

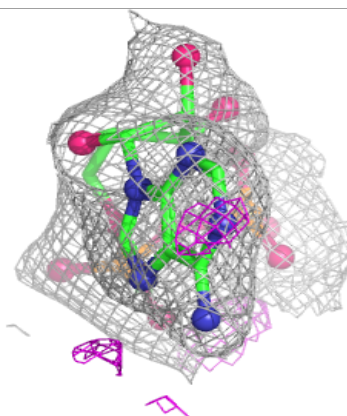
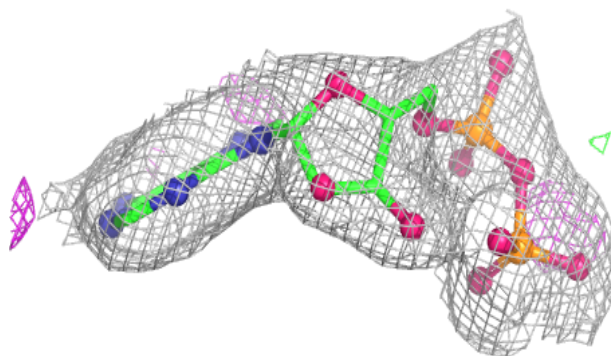
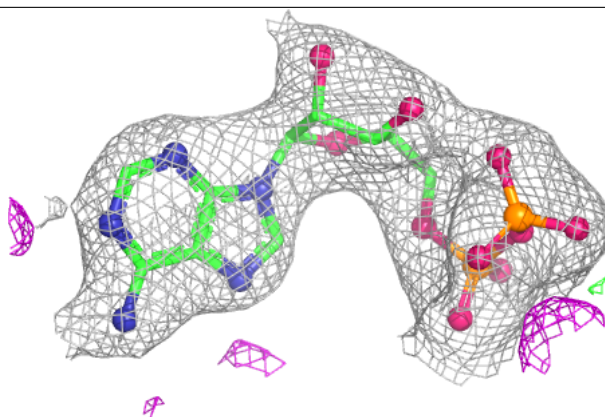
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ADP	A	2500	27/27	0.94	0.09	37,48,58,69	0
2	ADP	B	3500	27/27	0.95	0.10	27,46,58,75	0
3	CA	B	2	1/1	0.96	0.05	38,38,38,38	0
3	CA	A	1	1/1	0.97	0.04	37,37,37,37	0

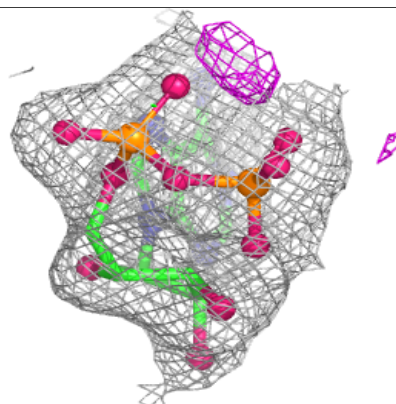
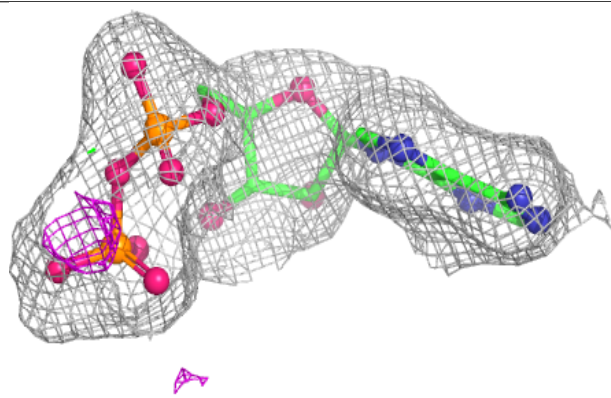
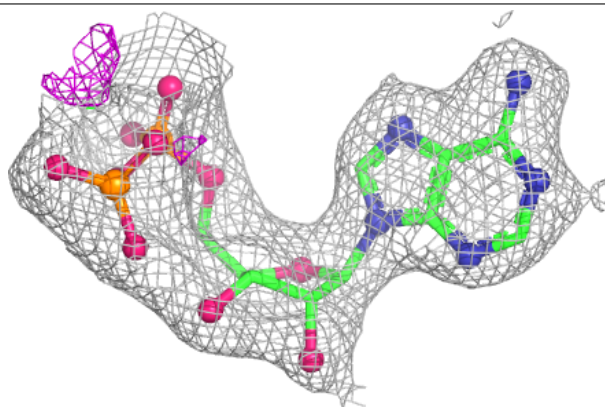
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 2500:

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

**Electron density around ADP B 3500:**

$2mF_o-DF_c$ (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.