



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:47 PM UTC

PDB ID : 4HND / pdb_00004hnd
Title : Crystal structure of the catalytic domain of Selenomethionine substituted human PI4KIIalpha in complex with ADP
Authors : Zhou, Q.; Zhai, Y.; Zhang, K.; Chen, C.; Sun, F.
Deposited on : 2012-10-19
Resolution : 3.20 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	:	4-5-2 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

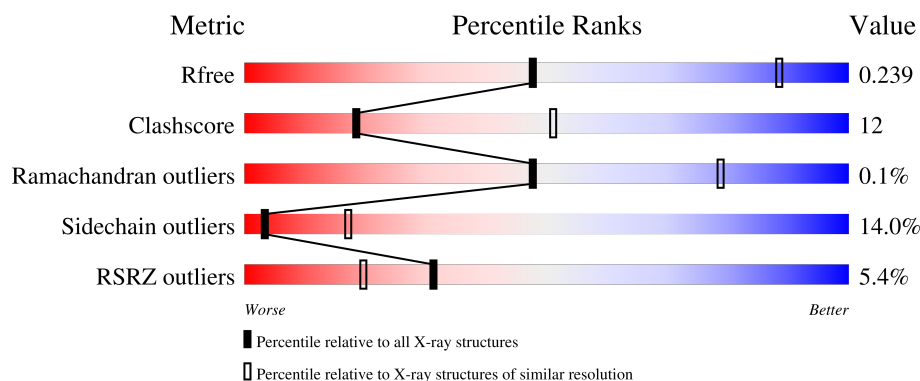
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	384	5% 64% 23% • 8%
1	B	384	5% 62% 23% • 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5649 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.

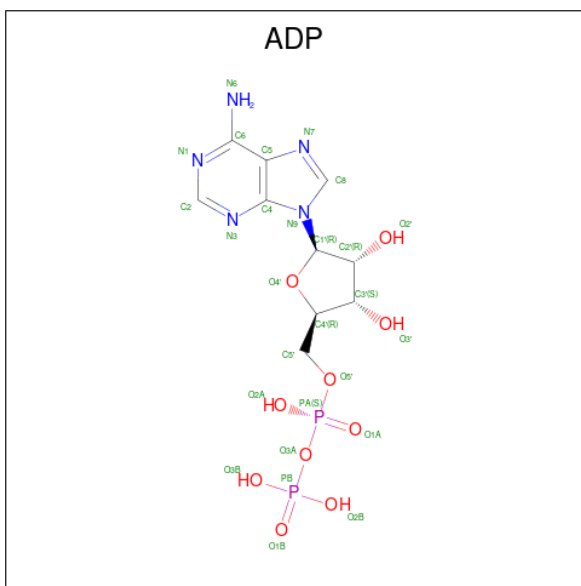
- Molecule 1 is a protein called Phosphatidylinositol 4-kinase type 2-alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	353	Total	C	N	O	S	Se	4	0	0
			2867	1853	498	511	3	2			
1	B	337	Total	C	N	O	S	Se	12	0	0
			2728	1763	467	493	3	2			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	70	GLY	-	expression tag	UNP Q9BTU6
A	71	PRO	-	expression tag	UNP Q9BTU6
A	72	LEU	-	expression tag	UNP Q9BTU6
A	73	GLY	-	expression tag	UNP Q9BTU6
A	74	SER	-	expression tag	UNP Q9BTU6
A	75	PRO	-	expression tag	UNP Q9BTU6
A	76	GLU	-	expression tag	UNP Q9BTU6
A	77	PHE	-	expression tag	UNP Q9BTU6
A	174	SER	CYS	engineered mutation	UNP Q9BTU6
A	175	SER	CYS	engineered mutation	UNP Q9BTU6
A	177	SER	CYS	engineered mutation	UNP Q9BTU6
A	178	SER	CYS	engineered mutation	UNP Q9BTU6
B	70	GLY	-	expression tag	UNP Q9BTU6
B	71	PRO	-	expression tag	UNP Q9BTU6
B	72	LEU	-	expression tag	UNP Q9BTU6
B	73	GLY	-	expression tag	UNP Q9BTU6
B	74	SER	-	expression tag	UNP Q9BTU6
B	75	PRO	-	expression tag	UNP Q9BTU6
B	76	GLU	-	expression tag	UNP Q9BTU6
B	77	PHE	-	expression tag	UNP Q9BTU6
B	174	SER	CYS	engineered mutation	UNP Q9BTU6
B	175	SER	CYS	engineered mutation	UNP Q9BTU6
B	177	SER	CYS	engineered mutation	UNP Q9BTU6
B	178	SER	CYS	engineered mutation	UNP Q9BTU6

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

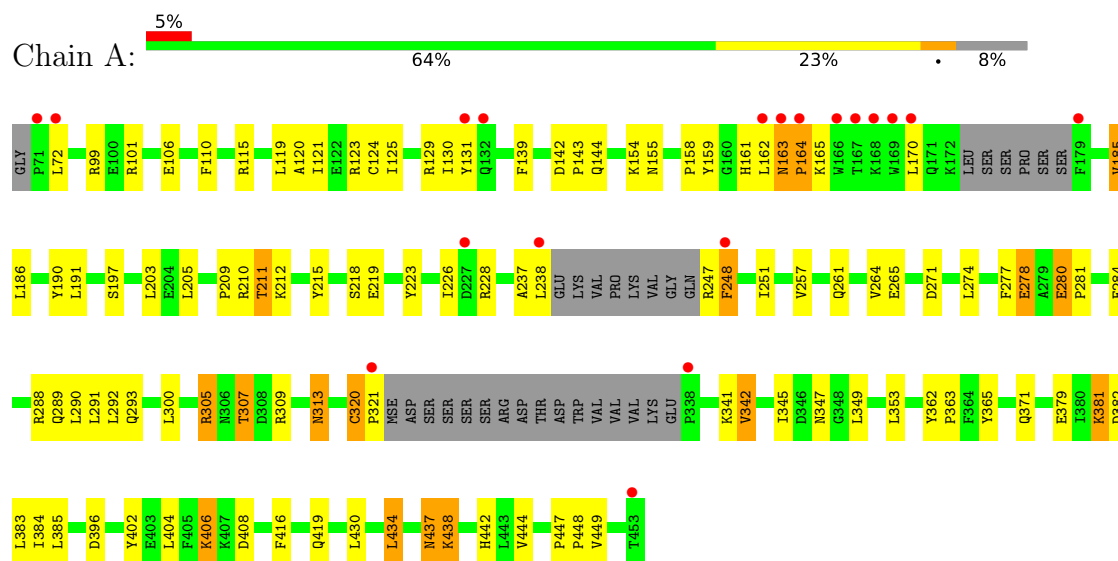


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

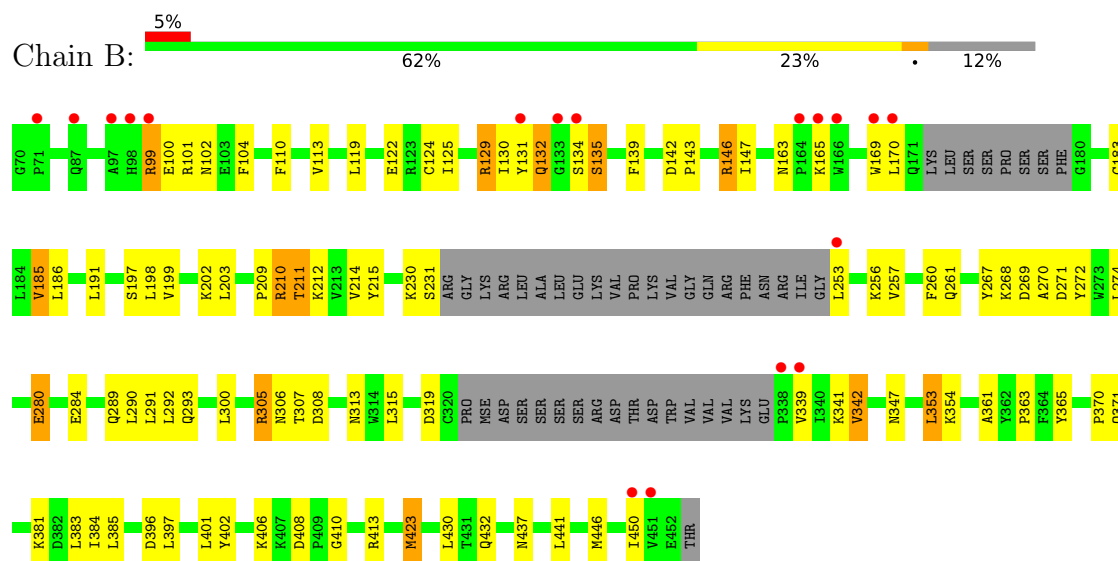
3 Residue-property plots

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: Phosphatidylinositol 4-kinase type 2-alpha



- Molecule 1: Phosphatidylinositol 4-kinase type 2-alpha



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	192.95Å 192.95Å 157.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	136.44 – 3.20 136.44 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (136.44-3.20) 99.8 (136.44-3.20)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.193 , 0.238 0.195 , 0.239	Depositor DCC
R_{free} test set	1256 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	74.6	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5649	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.76	0/2941	0.95	3/3983 (0.1%)
1	B	0.67	0/2799	0.92	2/3796 (0.1%)
All	All	0.72	0/5740	0.94	5/7779 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	186	LEU	N-CA-C	8.02	119.71	110.97
1	A	186	LEU	N-CA-C	6.94	118.54	110.97
1	A	345	ILE	N-CA-C	6.28	119.68	113.53
1	B	280	GLU	CB-CA-C	5.74	116.19	110.33
1	A	345	ILE	CB-CA-C	-5.04	105.71	110.65

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	2867	0	2856	65	0
1	B	2728	0	2698	70	1
2	A	27	0	12	0	0
2	B	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5649	0	5578	134	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 (134) 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:129:ARG:HD2	1:B:134:SER:O	1.42	1.19
1:A:280:GLU:HG2	1:A:280:GLU:O	1.48	1.08
1:B:130:ILE:CD1	1:B:139:PHE:CE2	2.42	1.02
1:A:402:TYR:O	1:A:406:LYS:HG2	1.64	0.95
1:B:130:ILE:CD1	1:B:139:PHE:CZ	2.51	0.93
1:A:278:GLU:HA	1:A:278:GLU:OE1	1.69	0.90
1:A:307:THR:HB	1:A:349:LEU:O	1.73	0.89
1:B:130:ILE:HD13	1:B:139:PHE:CD2	2.09	0.88
1:B:130:ILE:HD11	1:B:139:PHE:CE1	2.10	0.86
1:A:320:CYS:HB2	1:A:321:PRO:HD3	1.57	0.85
1:B:130:ILE:HD12	1:B:139:PHE:CZ	2.13	0.83
1:A:402:TYR:O	1:A:406:LYS:CG	2.28	0.81
1:B:129:ARG:HG2	1:B:131:TYR:O	1.80	0.81
1:A:278:GLU:OE1	1:A:278:GLU:CA	2.29	0.81
1:A:438:LYS:NZ	1:A:442:HIS:HB3	1.97	0.80
1:B:129:ARG:CD	1:B:134:SER:O	2.30	0.79
1:B:130:ILE:CD1	1:B:139:PHE:CD2	2.66	0.78
1:B:130:ILE:HD13	1:B:139:PHE:CE2	2.15	0.77
1:B:130:ILE:HD11	1:B:139:PHE:CD1	2.18	0.77
1:B:185:VAL:HG23	1:B:353:LEU:HD23	1.67	0.77
1:B:129:ARG:HH21	1:B:135:SER:CB	1.97	0.76
1:B:102:ASN:HD21	1:B:215:TYR:H	1.31	0.76
1:A:305:ARG:O	1:A:305:ARG:HG3	1.86	0.75
1:A:197:SER:HB2	1:A:211:THR:HG23	1.70	0.73
1:B:110:PHE:CE2	1:B:212:LYS:HB2	2.25	0.71
1:B:306:ASN:HD22	1:B:307:THR:N	1.89	0.71
1:B:130:ILE:HD12	1:B:139:PHE:CE2	2.24	0.70
1:B:306:ASN:ND2	1:B:308:ASP:H	1.90	0.69
1:A:293:GLN:HB3	1:A:342:VAL:HG13	1.74	0.69
1:B:130:ILE:HD11	1:B:139:PHE:CZ	2.26	0.68
1:A:438:LYS:HZ3	1:A:442:HIS:HB3	1.59	0.68
1:B:211:THR:HG22	1:B:261:GLN:HG3	1.76	0.68
1:A:402:TYR:CE2	1:A:406:LYS:HD2	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:LYS:O	1:A:385:LEU:HB2	1.97	0.65
1:B:129:ARG:NH2	1:B:135:SER:OG	2.30	0.65
1:B:271:ASP:HA	1:B:274:LEU:HB2	1.80	0.64
1:A:164:PRO:O	1:A:165:LYS:C	2.39	0.64
1:B:146:ARG:HD3	1:B:146:ARG:H	1.63	0.63
1:A:211:THR:HB	1:A:261:GLN:HA	1.81	0.62
1:B:110:PHE:HE2	1:B:212:LYS:HB2	1.64	0.62
1:A:280:GLU:O	1:A:280:GLU:CG	2.30	0.61
1:A:185:VAL:HG12	1:A:353:LEU:HD23	1.83	0.60
1:A:209:PRO:O	1:A:211:THR:HG22	2.02	0.59
1:B:305:ARG:O	1:B:305:ARG:HG3	2.02	0.59
1:B:401:LEU:HD11	1:B:423:MSE:HE1	1.84	0.59
1:B:129:ARG:HH21	1:B:135:SER:HB3	1.66	0.59
1:A:284:GLU:OE2	1:B:284:GLU:OE1	2.21	0.59
1:B:432:GLN:HB3	1:B:446:MSE:HE1	1.86	0.56
1:A:211:THR:HG21	1:A:261:GLN:HE21	1.69	0.56
1:A:438:LYS:HZ2	1:A:442:HIS:HB3	1.70	0.56
1:B:129:ARG:NH2	1:B:135:SER:CB	2.67	0.56
1:A:309:ARG:HH12	1:A:347:ASN:ND2	2.04	0.56
1:A:381:LYS:NZ	1:A:437:ASN:HD22	2.05	0.55
1:B:130:ILE:HD11	1:B:139:PHE:CG	2.41	0.55
1:A:416:PHE:HA	1:A:419:GLN:HE21	1.71	0.55
1:B:268:LYS:HD2	1:B:272:TYR:CE2	2.42	0.54
1:A:219:GLU:O	1:A:228:ARG:NH2	2.41	0.54
1:B:130:ILE:HG22	1:B:131:TYR:CD1	2.43	0.54
1:B:402:TYR:CE2	1:B:406:LYS:HD3	2.43	0.53
1:A:72:LEU:HD12	1:A:72:LEU:H	1.75	0.52
1:B:199:VAL:HG22	1:B:397:LEU:HD11	1.91	0.52
1:A:191:LEU:HD11	1:A:408:ASP:HB2	1.90	0.52
1:B:110:PHE:CD2	1:B:212:LYS:HD2	2.45	0.52
1:B:306:ASN:HD22	1:B:306:ASN:C	2.16	0.52
1:B:129:ARG:NH2	1:B:135:SER:HB3	2.24	0.51
1:B:408:ASP:C	1:B:410:GLY:H	2.18	0.51
1:A:158:PRO:HB2	1:A:159:TYR:CD2	2.45	0.51
1:A:363:PRO:HG2	1:A:365:TYR:CE1	2.45	0.51
1:A:278:GLU:OE1	1:A:278:GLU:O	2.29	0.51
1:B:129:ARG:HD3	1:B:135:SER:HA	1.93	0.50
1:A:305:ARG:NH2	1:A:362:TYR:O	2.44	0.50
1:A:320:CYS:HB2	1:A:321:PRO:CD	2.36	0.50
1:B:210:ARG:HB2	1:B:210:ARG:NH1	2.27	0.50
1:B:210:ARG:HB2	1:B:210:ARG:HH11	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:LYS:HD2	1:B:437:ASN:OD1	2.13	0.48
1:B:130:ILE:CD1	1:B:139:PHE:CG	2.96	0.48
1:A:237:ALA:HB2	1:A:251:ILE:HD11	1.96	0.48
1:B:191:LEU:HD11	1:B:408:ASP:HB2	1.96	0.48
1:A:190:TYR:OH	1:A:408:ASP:OD1	2.27	0.48
1:B:99:ARG:HG3	1:B:101:ARG:HG3	1.96	0.48
1:A:163:ASN:HB3	1:A:164:PRO:HD3	1.96	0.47
1:A:309:ARG:HH12	1:A:347:ASN:HD21	1.61	0.47
1:B:183:CYS:HB2	1:B:354:LYS:HG3	1.96	0.47
1:A:215:TYR:CE2	1:A:257:VAL:HB	2.50	0.46
1:B:211:THR:HG21	1:B:261:GLN:HE21	1.81	0.46
1:B:197:SER:HB2	1:B:211:THR:HG23	1.97	0.46
1:B:402:TYR:CZ	1:B:406:LYS:HD3	2.50	0.46
1:A:142:ASP:HB2	1:A:143:PRO:CD	2.46	0.46
1:A:120:ALA:HB1	1:A:125:ILE:HB	1.98	0.46
1:B:230:LYS:HG2	1:B:230:LYS:O	2.16	0.46
1:A:406:LYS:HB2	1:A:406:LYS:HE2	1.53	0.45
1:A:123:ARG:O	1:A:124:CYS:HB2	2.17	0.45
1:B:209:PRO:O	1:B:211:THR:HG22	2.17	0.45
1:B:202:LYS:NZ	1:B:396:ASP:HB3	2.32	0.45
1:A:154:LYS:HD2	1:A:190:TYR:CE1	2.53	0.44
1:A:277:PHE:O	1:A:280:GLU:O	2.35	0.44
1:A:320:CYS:CB	1:A:321:PRO:HD3	2.39	0.44
1:A:434:LEU:HD12	1:A:434:LEU:HA	1.80	0.44
1:B:363:PRO:HG2	1:B:365:TYR:CE1	2.53	0.44
1:A:161:HIS:CD2	1:A:162:LEU:HG	2.53	0.44
1:A:278:GLU:OE1	1:A:278:GLU:C	2.60	0.43
1:B:198:LEU:C	1:B:198:LEU:HD23	2.43	0.43
1:B:202:LYS:HZ3	1:B:396:ASP:HB3	1.82	0.43
1:A:163:ASN:C	1:A:163:ASN:HD22	2.26	0.43
1:B:163:ASN:HD22	1:B:165:LYS:HB2	1.83	0.43
1:A:271:ASP:HA	1:A:274:LEU:HB2	2.00	0.43
1:B:269:ASP:O	1:B:270:ALA:C	2.61	0.43
1:A:110:PHE:CD2	1:A:212:LYS:HD2	2.54	0.42
1:A:218:SER:O	1:A:223:TYR:HE2	2.01	0.42
1:A:291:LEU:HD21	1:A:371:GLN:HG3	2.01	0.42
1:B:147:ILE:H	1:B:147:ILE:HD12	1.84	0.42
1:B:122:GLU:C	1:B:124:CYS:H	2.28	0.42
1:B:211:THR:HA	1:B:260:PHE:O	2.19	0.42
1:A:248:PHE:HD1	1:A:248:PHE:HA	1.69	0.42
1:A:130:ILE:HG12	1:A:139:PHE:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:LEU:HD23	1:A:385:LEU:HA	1.85	0.41
1:B:99:ARG:O	1:B:100:GLU:C	2.63	0.41
1:A:205:LEU:HD21	1:A:384:ILE:HD11	2.02	0.41
1:A:130:ILE:HG12	1:A:139:PHE:CE2	2.56	0.41
1:A:291:LEU:HA	1:A:291:LEU:HD23	1.83	0.41
1:B:142:ASP:OD1	1:B:143:PRO:HD2	2.20	0.41
1:A:313:ASN:HD22	1:A:313:ASN:HA	1.46	0.41
1:A:447:PRO:HA	1:A:448:PRO:HD3	1.80	0.41
1:B:131:TYR:O	1:B:132:GLN:C	2.62	0.41
1:A:101:ARG:O	1:A:115:ARG:NH1	2.53	0.41
1:B:370:PRO:HG2	1:B:371:GLN:OE1	2.21	0.41
1:A:288:ARG:NH2	1:A:379:GLU:OE2	2.54	0.41
1:B:284:GLU:HA	1:B:284:GLU:OE2	2.21	0.40
1:A:238:LEU:HD13	1:A:248:PHE:CE1	2.56	0.40
1:B:293:GLN:HB3	1:B:342:VAL:HG13	2.04	0.40
1:A:99:ARG:C	1:A:101:ARG:H	2.29	0.40
1:B:215:TYR:CE2	1:B:257:VAL:HB	2.56	0.40
1:B:267:TYR:HB3	1:B:315:LEU:HB3	2.03	0.40
1:B:385:LEU:HA	1:B:385:LEU:HD23	1.81	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)
1:B:361:ALA:O	1:B:361:ALA:O[8_555]	1.86	0.34

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	345/384 (90%)	331 (96%)	13 (4%)	1 (0%)	36 68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	329/384 (86%)	312 (95%)	17 (5%)	0	100	100
All	All	674/768 (88%)	643 (95%)	30 (4%)	1 (0%)	48	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	164	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	303/329 (92%)	260 (86%)	43 (14%)	3	17
1	B	289/329 (88%)	249 (86%)	40 (14%)	3	18
All	All	592/658 (90%)	509 (86%)	83 (14%)	3	17

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	GLU
1	A	119	LEU
1	A	121	ILE
1	A	129	ARG
1	A	131	TYR
1	A	144	GLN
1	A	155	ASN
1	A	163	ASN
1	A	170	LEU
1	A	185	VAL
1	A	203	LEU
1	A	210	ARG
1	A	211	THR
1	A	226	ILE
1	A	247	ARG

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Mol	Chain	Res	Type
1	A	248	PHE
1	A	264	VAL
1	A	265	GLU
1	A	278	GLU
1	A	280	GLU
1	A	281	PRO
1	A	289	GLN
1	A	290	LEU
1	A	292	LEU
1	A	300	LEU
1	A	305	ARG
1	A	307	THR
1	A	313	ASN
1	A	320	CYS
1	A	341	LYS
1	A	342	VAL
1	A	381	LYS
1	A	382	ASP
1	A	383	LEU
1	A	396	ASP
1	A	404	LEU
1	A	406	LYS
1	A	430	LEU
1	A	434	LEU
1	A	437	ASN
1	A	438	LYS
1	A	444	VAL
1	A	449	VAL
1	B	99	ARG
1	B	104	PHE
1	B	113	VAL
1	B	119	LEU
1	B	125	ILE
1	B	129	ARG
1	B	132	GLN
1	B	135	SER
1	B	146	ARG
1	B	169	TRP
1	B	170	LEU
1	B	185	VAL
1	B	203	LEU
1	B	210	ARG

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Mol	Chain	Res	Type
1	B	211	THR
1	B	214	VAL
1	B	231	SER
1	B	253	LEU
1	B	256	LYS
1	B	280	GLU
1	B	289	GLN
1	B	290	LEU
1	B	291	LEU
1	B	292	LEU
1	B	300	LEU
1	B	305	ARG
1	B	313	ASN
1	B	319	ASP
1	B	339	VAL
1	B	341	LYS
1	B	342	VAL
1	B	347	ASN
1	B	353	LEU
1	B	383	LEU
1	B	384	ILE
1	B	413	ARG
1	B	423	MSE
1	B	430	LEU
1	B	441	LEU
1	B	450	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	ASN
1	A	163	ASN
1	A	187	ASN
1	A	261	GLN
1	A	287	ASN
1	A	313	ASN
1	A	347	ASN
1	A	378	GLN
1	A	419	GLN
1	A	426	GLN
1	A	437	ASN
1	A	442	HIS

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Mol	Chain	Res	Type
1	A	445	GLN
1	B	96	GLN
1	B	102	ASN
1	B	187	ASN
1	B	261	GLN
1	B	306	ASN
1	B	417	HIS
1	B	419	GLN
1	B	429	ASN
1	B	445	GLN

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 ⓘ

2 ligands are modelled in this entry.

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	B	500	-	28,29,29	1.58	5 (17%)	43,45,45	1.86	10 (23%)
2	ADP	A	500	-	28,29,29	1.49	4 (14%)	43,45,45	1.86	9 (20%)

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	B	500	-	-	2/16/32/32	0/3/3/3
2	ADP	A	500	-	-	5/16/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	ADP	C5-C4	5.07	1.48	1.39
2	B	500	ADP	C5-C4	4.98	1.48	1.39
2	B	500	ADP	PA-O3A	3.45	1.63	1.59
2	B	500	ADP	C5-C6	3.18	1.49	1.41
2	A	500	ADP	C5-C6	2.83	1.48	1.41
2	A	500	ADP	C5-N7	-2.39	1.34	1.39
2	B	500	ADP	C8-N7	2.37	1.36	1.31
2	A	500	ADP	C8-N7	2.35	1.36	1.31
2	B	500	ADP	C5-N7	-2.08	1.35	1.39

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	ADP	C5-C4-N3	-5.90	118.59	126.72
2	A	500	ADP	C5-C4-N3	-5.87	118.63	126.72
2	A	500	ADP	N3-C4-N9	4.43	134.70	127.17
2	B	500	ADP	N3-C4-N9	4.41	134.67	127.17
2	B	500	ADP	C2-N3-C4	3.87	121.29	111.83
2	B	500	ADP	C4-C5-N7	-3.80	106.24	110.58
2	A	500	ADP	C2-N3-C4	3.59	120.59	111.83
2	A	500	ADP	C4-C5-N7	-3.45	106.64	110.58
2	B	500	ADP	N3-C2-N1	-3.38	123.46	128.58
2	A	500	ADP	N3-C2-N1	-3.04	123.98	128.58
2	A	500	ADP	O5'-C5'-C4'	2.66	118.05	108.99
2	B	500	ADP	C5-N7-C8	2.54	107.44	103.45
2	B	500	ADP	C6-C5-N7	2.48	136.87	132.09
2	A	500	ADP	C5-N7-C8	2.26	107.00	103.45
2	B	500	ADP	C4-N9-C8	2.18	108.03	105.74
2	B	500	ADP	C3'-C2'-C1'	2.09	105.42	101.46
2	A	500	ADP	O3B-PB-O2B	2.07	115.55	107.80
2	A	500	ADP	C2'-C3'-C4'	2.06	106.58	102.61
2	B	500	ADP	C2'-C3'-C4'	2.06	106.58	102.61

There are no chirality outliers.

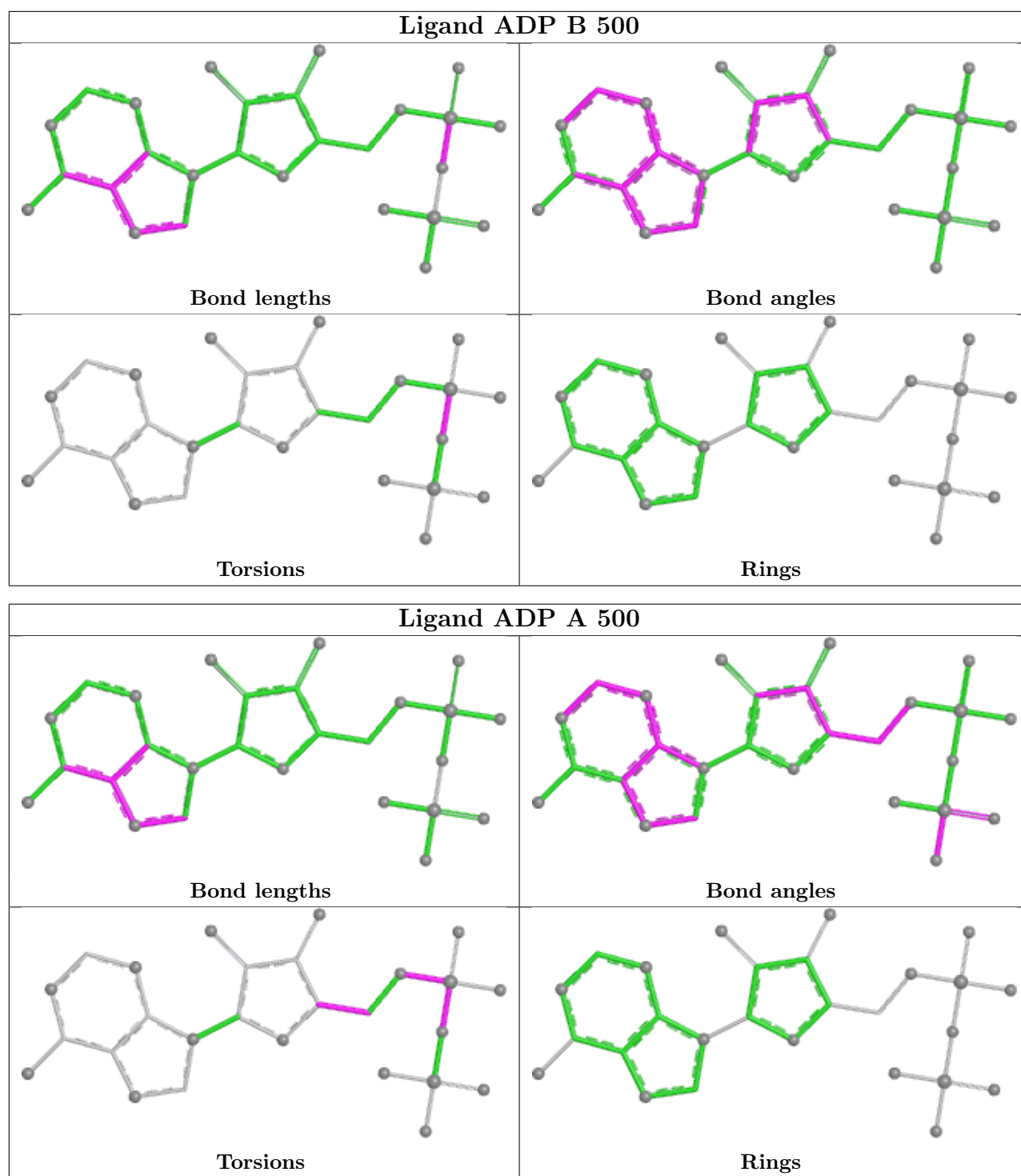
All (7) torsion outliers are listed below:

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

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 ⓘ

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	351/384 (91%)	-0.22	19 (5%)	31 20	41, 68, 138, 202	1 (0%)
1	B	335/384 (87%)	-0.05	18 (5%)	31 20	41, 76, 151, 226	3 (0%)
All	All	686/768 (89%)	-0.13	37 (5%)	31 20	41, 72, 150, 226	4 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	179	PHE	7.4
1	A	72	LEU	4.0
1	B	97	ALA	3.7
1	A	169	TRP	3.6
1	B	338	PRO	3.5
1	A	164	PRO	3.2
1	A	338	PRO	3.2
1	B	134	SER	2.8
1	B	451	VAL	2.7
1	A	166	TRP	2.7
1	A	71	PRO	2.7
1	B	450	ILE	2.7
1	A	167	THR	2.7
1	B	87	GLN	2.7
1	A	170	LEU	2.7
1	B	166	TRP	2.6
1	B	170	LEU	2.6
1	B	339	VAL	2.5
1	A	321	PRO	2.5
1	B	133	GLY	2.4
1	A	131	TYR	2.4
1	B	169	TRP	2.4
1	B	165	LYS	2.3
1	B	98	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	99	ARG	2.3
1	A	132	GLN	2.3
1	A	227	ASP	2.3
1	B	253	LEU	2.2
1	A	248	PHE	2.1
1	A	162	LEU	2.1
1	A	453	THR	2.1
1	A	163	ASN	2.1
1	A	238	LEU	2.1
1	B	164	PRO	2.1
1	B	71	PRO	2.0
1	B	131	TYR	2.0
1	A	168	LYS	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](#)

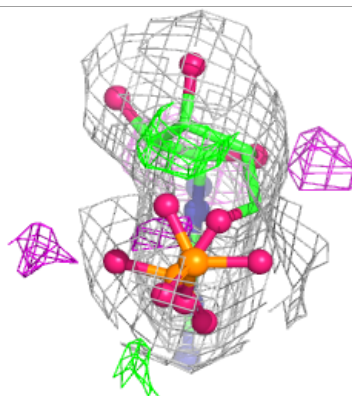
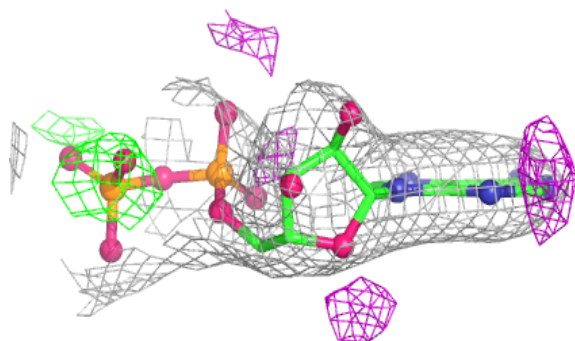
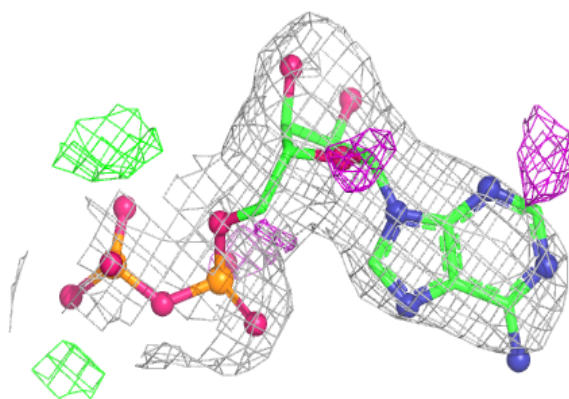
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	500	27/27	0.91	0.11	72,79,140,146	0
2	ADP	B	500	27/27	0.92	0.11	104,109,138,149	0

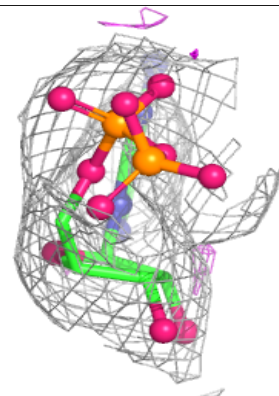
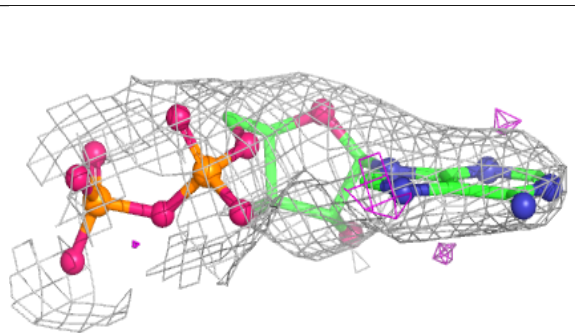
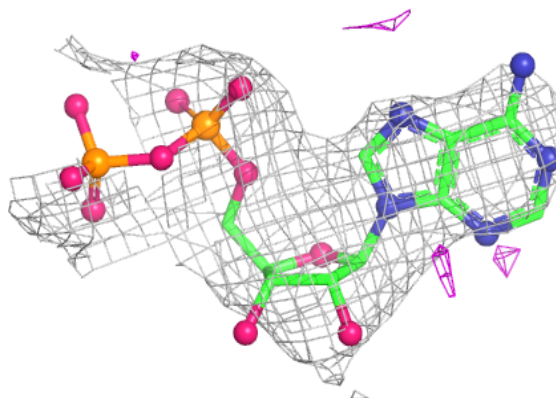
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 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 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.