



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 29, 2024 – 05:44 PM EDT

PDB ID : 4HND
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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

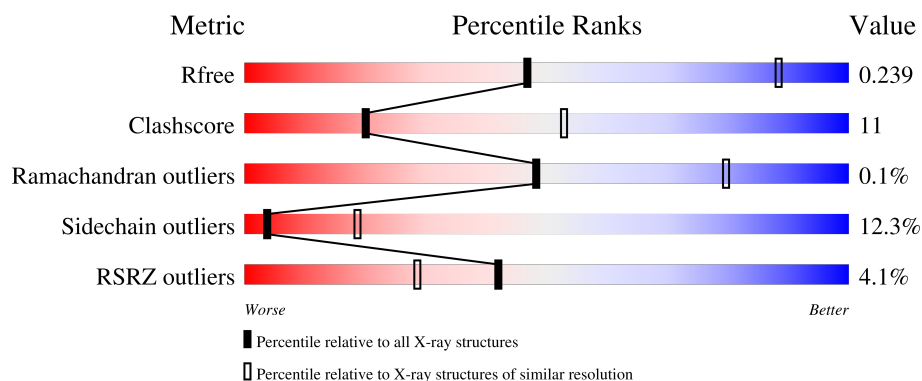
1 Overall quality at a glance

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}	164625	1370 (3.20-3.20)
Clashscore	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)
RSRZ outliers	164620	1371 (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	
1	B	384	

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.

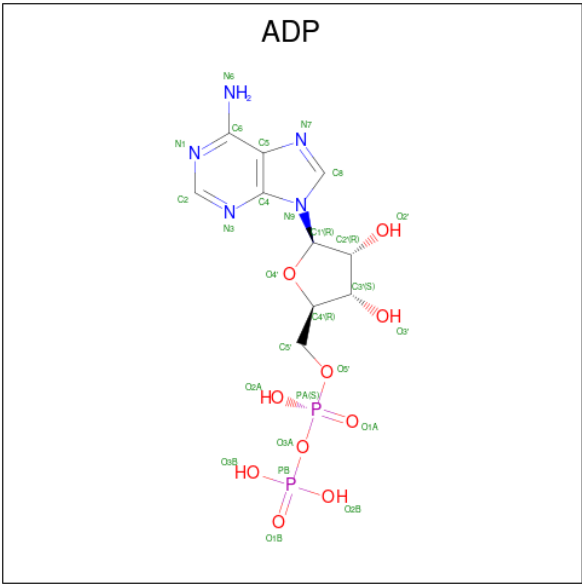
- Molecule 1 is a protein called Phosphatidylinositol 4-kinase type 2-alpha.

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 (three-letter code: 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 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 (5.08%)	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 [i](#)

5.1 Standard geometry [i](#)

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	0.59	5/2941 (0.2%)	0.64	0/3983
1	B	0.53	3/2799 (0.1%)	0.62	0/3796
All	All	0.56	8/5740 (0.1%)	0.63	0/7779

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	366	TRP	CD2-CE2	5.72	1.48	1.41
1	A	359	TRP	CD2-CE2	5.65	1.48	1.41
1	A	314	TRP	CD2-CE2	5.31	1.47	1.41
1	A	366	TRP	CD2-CE2	5.27	1.47	1.41
1	A	169	TRP	CD2-CE2	5.14	1.47	1.41
1	B	166	TRP	CD2-CE2	5.14	1.47	1.41
1	A	166	TRP	CD2-CE2	5.13	1.47	1.41
1	B	169	TRP	CD2-CE2	5.02	1.47	1.41

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	2867	0	2856	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2728	0	2698	65	1
2	A	27	0	12	0	0
2	B	27	0	12	0	0
All	All	5649	0	5578	125	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 11.

All (125) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:A:164:PRO:O	1:A:165:LYS:C	2.39	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:129:ARG:NH2	1:B:135:SER:HB3	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:ARG:HB2	1:B:210:ARG:HH11	1.77	0.49
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:B:99:ARG:HG3	1:B:101:ARG:HG3	1.96	0.48
1:B:306:ASN:HD22	1:B:306:ASN:C	2.16	0.47
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:B:408:ASP:C	1:B:410:GLY:H	2.18	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:B:202:LYS:HZ3	1:B:396:ASP:HB3	1.82	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: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: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
1:A:385:LEU:HD23	1:A:385:LEU:HA	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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%)	37	69
1	B	329/384 (86%)	312 (95%)	17 (5%)	0	100	100
All	All	674/768 (88%)	643 (95%)	30 (4%)	1 (0%)	48	80

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%)	262 (86%)	41 (14%)	3	15
1	B	289/329 (88%)	257 (89%)	32 (11%)	5	22
All	All	592/658 (90%)	519 (88%)	73 (12%)	4	19

All (73) 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	131	TYR
1	A	144	GLN
1	A	155	ASN
1	A	163	ASN
1	A	170	LEU
1	A	203	LEU
1	A	210	ARG
1	A	211	THR
1	A	218	SER
1	A	226	ILE
1	A	228	ARG
1	A	235	ARG
1	A	247	ARG
1	A	248	PHE
1	A	264	VAL
1	A	278	GLU
1	A	280	GLU
1	A	281	PRO
1	A	289	GLN
1	A	290	LEU

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Mol	Chain	Res	Type
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	449	VAL
1	B	99	ARG
1	B	104	PHE
1	B	113	VAL
1	B	119	LEU
1	B	122	GLU
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	203	LEU
1	B	210	ARG
1	B	211	THR
1	B	231	SER
1	B	253	LEU
1	B	280	GLU
1	B	289	GLN
1	B	292	LEU
1	B	306	ASN
1	B	313	ASN
1	B	319	ASP
1	B	338	PRO
1	B	339	VAL

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Mol	Chain	Res	Type
1	B	341	LYS
1	B	347	ASN
1	B	383	LEU
1	B	384	ILE
1	B	413	ARG
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 (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	ASN
1	A	163	ASN
1	A	261	GLN
1	A	313	ASN
1	A	347	ASN
1	A	419	GLN
1	A	426	GLN
1	A	437	ASN
1	A	445	GLN
1	B	96	GLN
1	B	102	ASN
1	B	163	ASN
1	B	206	ASN
1	B	261	GLN
1	B	306	ASN
1	B	347	ASN
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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	A	500	-	24,29,29	0.98	2 (8%)	29,45,45	1.57	6 (20%)
2	ADP	B	500	-	24,29,29	1.13	2 (8%)	29,45,45	1.30	3 (10%)

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	500	-	-	5/12/32/32	0/3/3/3
2	ADP	B	500	-	-	2/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	ADP	PA-O3A	3.45	1.63	1.59
2	A	500	ADP	C2-N3	2.22	1.35	1.32
2	B	500	ADP	C2-N3	2.12	1.35	1.32
2	A	500	ADP	O4'-C1'	2.03	1.43	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	ADP	N3-C2-N1	-3.84	123.46	128.67
2	A	500	ADP	N3-C2-N1	-3.46	123.98	128.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	ADP	C4'-O4'-C1'	3.40	113.03	109.92
2	B	500	ADP	C4-C5-N7	-2.93	106.24	109.34
2	A	500	ADP	O5'-C5'-C4'	2.66	118.05	108.99
2	A	500	ADP	C4-C5-N7	-2.55	106.64	109.34
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.

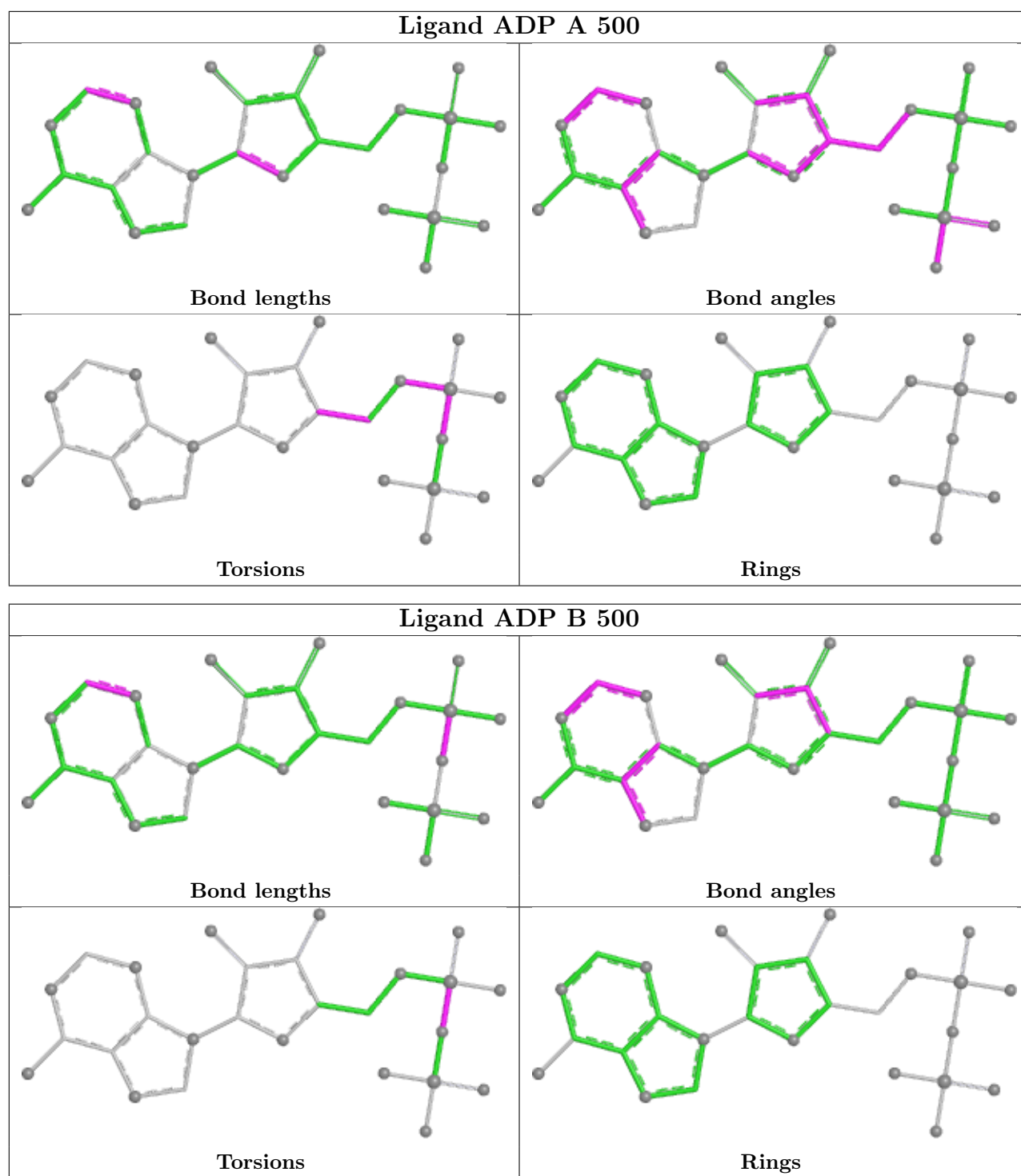
All (7) torsion outliers are listed below:

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%)	-0.36	13 (3%)	45 31	41, 68, 138, 202	1 (0%)
1	B	335/384 (87%)	-0.19	15 (4%)	39 26	41, 76, 151, 226	3 (0%)
All	All	686/768 (89%)	-0.28	28 (4%)	42 28	41, 72, 150, 226	4 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	179	PHE	7.2
1	A	72	LEU	3.8
1	B	97	ALA	3.6
1	A	169	TRP	3.4
1	B	338	PRO	3.3
1	A	164	PRO	3.0
1	A	338	PRO	3.0
1	B	134	SER	2.6
1	B	451	VAL	2.6
1	B	450	ILE	2.6
1	A	167	THR	2.6
1	B	87	GLN	2.5
1	A	71	PRO	2.5
1	A	166	TRP	2.5
1	A	170	LEU	2.5
1	B	170	LEU	2.5
1	B	166	TRP	2.4
1	B	339	VAL	2.4
1	A	321	PRO	2.3
1	B	133	GLY	2.3
1	A	131	TYR	2.2
1	B	165	LYS	2.2
1	B	99	ARG	2.2
1	B	169	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	98	HIS	2.1
1	A	132	GLN	2.1
1	A	227	ASP	2.1
1	B	253	LEU	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](#)

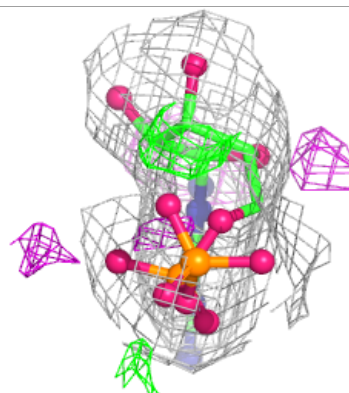
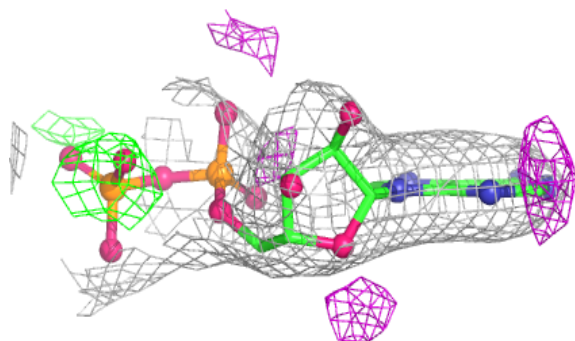
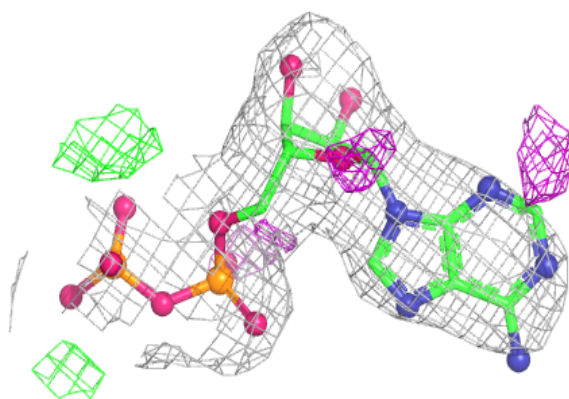
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

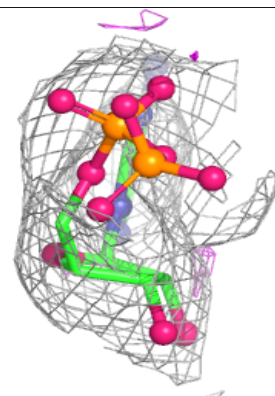
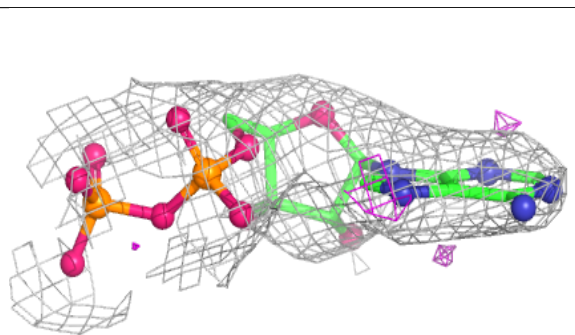
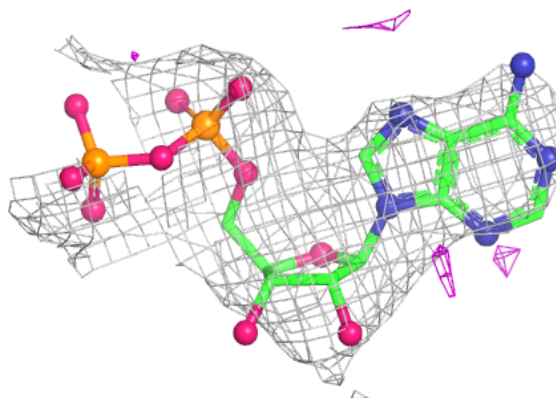
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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