



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:59 AM UTC

PDB ID : 1Y8O / pdb_00001y8o
Title : Crystal structure of the PDK3-L2 complex
Authors : Kato, M.; Chuang, J.L.; Wynn, R.M.; Chuang, D.T.
Deposited on : 2004-12-13
Resolution : 2.48 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

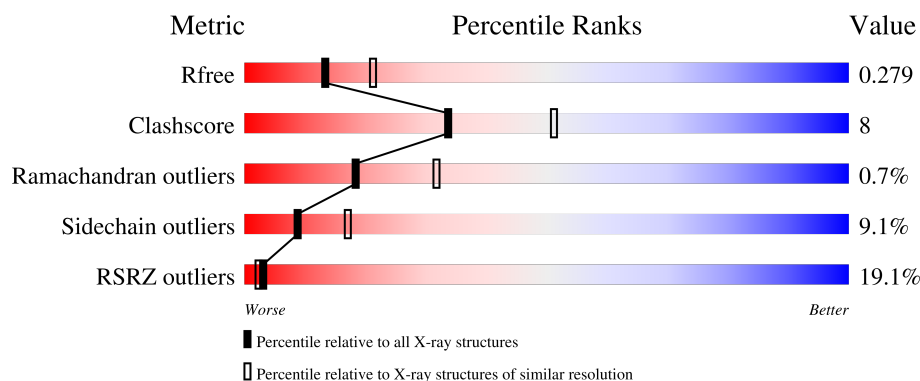
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	419	15% 68% 18% • 11%
2	B	128	22% 54% 19% • 24%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3910 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 [Pyruvate dehydrogenase [lipoamide]] kinase isozyme 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	1	0
			3066	1977	510	566	13			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	GLY	-	cloning artifact	UNP Q15120
A	-11	GLY	-	cloning artifact	UNP Q15120
A	-10	SER	-	cloning artifact	UNP Q15120
A	-9	HIS	-	expression tag	UNP Q15120
A	-8	HIS	-	expression tag	UNP Q15120
A	-7	HIS	-	expression tag	UNP Q15120
A	-6	HIS	-	expression tag	UNP Q15120
A	-5	HIS	-	expression tag	UNP Q15120
A	-4	HIS	-	expression tag	UNP Q15120
A	-3	GLY	-	cloning artifact	UNP Q15120
A	-2	MET	-	cloning artifact	UNP Q15120
A	-1	ALA	-	cloning artifact	UNP Q15120
A	0	ARG	-	cloning artifact	UNP Q15120
A	1	LEU	-	cloning artifact	UNP Q15120
A	2	GLU	-	cloning artifact	UNP Q15120
A	3	ASN	-	cloning artifact	UNP Q15120
A	4	LEU	-	cloning artifact	UNP Q15120
A	5	TYR	-	cloning artifact	UNP Q15120
A	6	PHE	-	cloning artifact	UNP Q15120
A	7	GLN	-	cloning artifact	UNP Q15120
A	8	GLY	-	cloning artifact	UNP Q15120

- Molecule 2 is a protein called Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	97	Total	C	N	O	S	0	0	0
			736	471	115	146	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	106	GLY	-	cloning artifact	UNP P10515
B	107	GLY	-	cloning artifact	UNP P10515
B	108	SER	-	cloning artifact	UNP P10515
B	109	HIS	-	expression tag	UNP P10515
B	110	HIS	-	expression tag	UNP P10515
B	111	HIS	-	expression tag	UNP P10515
B	112	HIS	-	expression tag	UNP P10515
B	113	HIS	-	expression tag	UNP P10515
B	114	HIS	-	expression tag	UNP P10515
B	115	GLY	-	cloning artifact	UNP P10515
B	116	MET	-	cloning artifact	UNP P10515
B	117	ALA	-	cloning artifact	UNP P10515
B	118	ARG	-	cloning artifact	UNP P10515
B	119	LEU	-	cloning artifact	UNP P10515
B	120	GLU	-	cloning artifact	UNP P10515
B	121	ASN	-	cloning artifact	UNP P10515
B	122	LEU	-	cloning artifact	UNP P10515
B	123	TYR	-	cloning artifact	UNP P10515
B	124	PHE	-	cloning artifact	UNP P10515
B	125	GLN	-	cloning artifact	UNP P10515

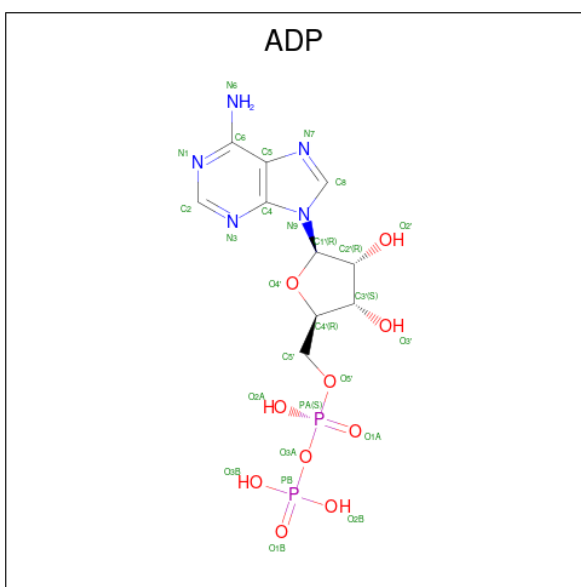
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

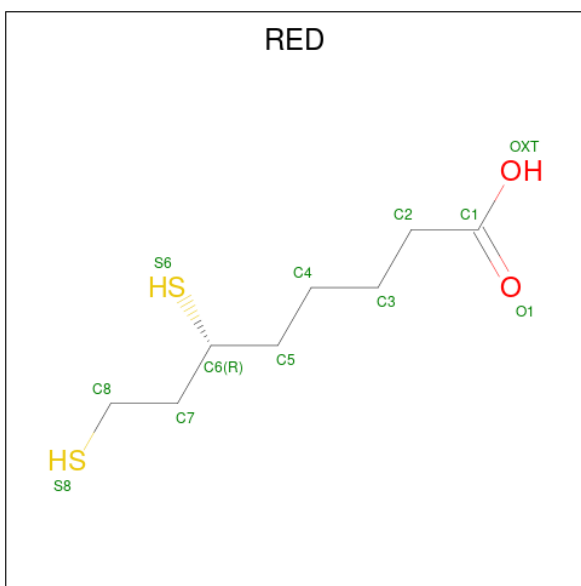
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	K	0	0
			2	2		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 6 is DIHYDROLIPOIC ACID (CCD ID: RED) (formula: $\text{C}_8\text{H}_{16}\text{O}_2\text{S}_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	O	S	0	0
			11	8	1	2		

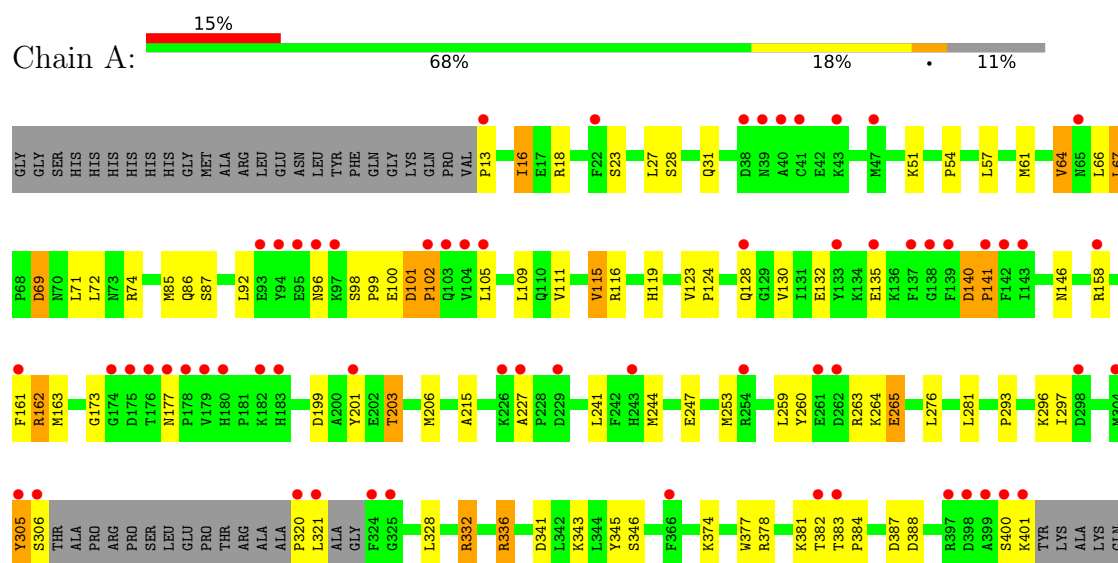
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	63	Total 63	O 63	0	0
7	B	4	Total 4	O 4	0	0

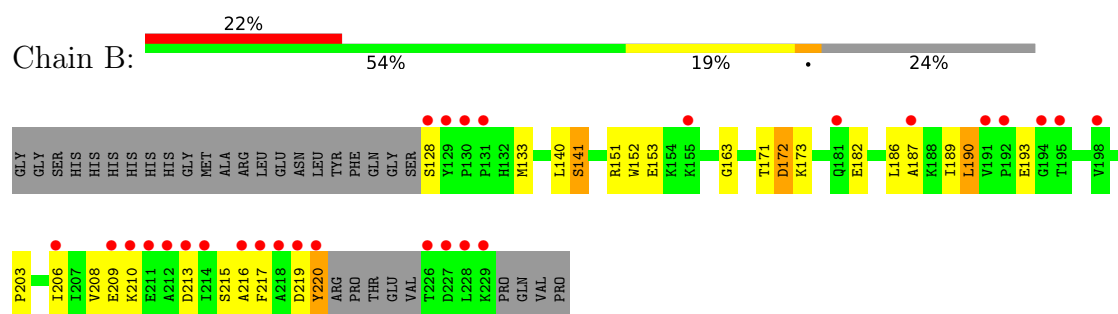
3 Residue-property plots

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: [Pyruvate dehydrogenase [lipoamide]] kinase isozyme 3



- Molecule 2: Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	120.75Å 120.75Å 239.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.48 50.00 – 2.48	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.48) 99.7 (50.00-2.48)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.210 , 0.234 0.261 , 0.279	Depositor DCC
R_{free} test set	1494 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å ²)	64.3	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 33.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3910	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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: MG, RED, K, 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	0.95	5/3145 (0.2%)	1.05	11/4257 (0.3%)
2	B	1.54	7/749 (0.9%)	1.07	5/1017 (0.5%)
All	All	1.09	12/3894 (0.3%)	1.05	16/5274 (0.3%)

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
2	B	0	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	216	ALA	C-N	21.41	1.66	1.33
2	B	216	ALA	C-O	-16.18	1.03	1.24
2	B	220	TYR	C-O	10.50	1.44	1.23
2	B	215	SER	CB-OG	8.71	1.59	1.42
1	A	102	PRO	C-O	6.99	1.33	1.24
2	B	189	ILE	C-O	6.35	1.31	1.24
2	B	216	ALA	CA-C	6.35	1.61	1.52
1	A	101	ASP	CG-OD1	6.24	1.37	1.25
1	A	18	ARG	CZ-NH1	6.04	1.41	1.32
1	A	101	ASP	CG-OD2	5.89	1.36	1.25
2	B	216	ALA	N-CA	5.12	1.52	1.46
1	A	96	ASN	CG-ND2	5.08	1.44	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	388	ASP	N-CA-CB	-7.47	97.86	110.49
1	A	387	ASP	CA-C-N	7.21	135.30	121.54
1	A	387	ASP	C-N-CA	7.21	135.30	121.54
1	A	140	ASP	CA-C-N	7.13	128.76	119.84
1	A	140	ASP	C-N-CA	7.13	128.76	119.84
2	B	172	ASP	N-CA-CB	-5.67	100.91	110.49
2	B	141	SER	N-CA-C	-5.66	101.68	108.25
1	A	215	ALA	CA-C-N	-5.62	114.46	120.03
1	A	215	ALA	C-N-CA	-5.62	114.46	120.03
1	A	227	ALA	CA-C-N	5.54	126.76	119.84
1	A	227	ALA	C-N-CA	5.54	126.76	119.84
2	B	215	SER	N-CA-C	5.26	117.69	111.33
2	B	216	ALA	O-C-N	5.23	129.55	122.59
1	A	96	ASN	OD1-CG-ND2	5.14	127.74	122.60
1	A	305	TYR	N-CA-C	-5.14	105.57	111.07
2	B	215	SER	O-C-N	5.14	127.56	122.12

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	171	THR	Peptide

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	3066	0	3029	43	0
2	B	736	0	727	17	0
3	A	1	0	0	0	0
4	A	2	0	0	0	0
5	A	27	0	12	0	0
6	B	11	0	15	4	0
7	A	63	0	0	3	0
7	B	4	0	0	0	0
All	All	3910	0	3783	59	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 8.

All (59) 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)
2:B:173:LYS:HZ3	6:B:373:RED:C1	1.18	1.53
2:B:173:LYS:NZ	6:B:373:RED:C1	1.78	1.43
1:A:247:GLU:HG3	7:A:560:HOH:O	1.35	1.21
2:B:173:LYS:HZ2	6:B:373:RED:C1	1.77	0.92
1:A:28:SER:H	1:A:31:GLN:HE21	1.26	0.82
2:B:208:VAL:HG11	2:B:213:ASP:HB2	1.65	0.76
1:A:201:TYR:CZ	1:A:253:MET:HE3	2.25	0.71
2:B:187:ALA:HB2	2:B:208:VAL:HG23	1.74	0.69
1:A:199:ASP:O	1:A:203:THR:HG23	1.95	0.66
1:A:332:ARG:HD2	7:A:540:HOH:O	1.97	0.64
1:A:99:PRO:C	1:A:101:ASP:H	2.08	0.61
1:A:320:PRO:O	1:A:321:LEU:HB2	2.03	0.58
2:B:208:VAL:HG11	2:B:213:ASP:CB	2.34	0.57
1:A:276:LEU:HD13	1:A:281:LEU:HD23	1.86	0.57
1:A:69:ASP:OD2	1:A:69:ASP:N	2.32	0.57
1:A:57:LEU:O	1:A:61:MET:HG3	2.06	0.56
2:B:206:ILE:HD11	2:B:220:TYR:CE2	2.41	0.55
1:A:67:LEU:HG	1:A:71:LEU:HD23	1.88	0.54
1:A:378:ARG:O	1:A:382:THR:HG23	2.09	0.53
1:A:332:ARG:O	1:A:336:ARG:HG2	2.09	0.52
1:A:87:SER:OG	1:A:119:HIS:HE1	1.93	0.52
1:A:158:ARG:HH12	1:A:162:ARG:NH1	2.08	0.51
1:A:374:LYS:HG3	2:B:163:GLY:HA3	1.93	0.51
2:B:217:PHE:C	2:B:219:ASP:H	2.17	0.51
1:A:158:ARG:HH22	1:A:162:ARG:NH1	2.09	0.51
1:A:123:VAL:HB	1:A:124:PRO:HD3	1.92	0.50
1:A:293:PRO:HG2	1:A:296:LYS:HD3	1.94	0.50
2:B:151:ARG:HD3	2:B:153:GLU:OE2	2.11	0.50
1:A:74:ARG:HD3	1:A:132:GLU:HB3	1.95	0.49
1:A:16:ILE:HD11	1:A:85:MET:SD	2.55	0.47
1:A:57:LEU:HG	1:A:161:PHE:CE2	2.51	0.46
1:A:64:VAL:HA	1:A:67:LEU:HD22	1.98	0.46
1:A:260:TYR:HA	1:A:263:ARG:HG3	1.97	0.46
2:B:173:LYS:NZ	6:B:373:RED:O1	2.37	0.46
1:A:51:LYS:O	1:A:54:PRO:HD2	2.16	0.46
1:A:98:SER:HA	1:A:99:PRO:HD2	1.84	0.45
1:A:343:LYS:HD3	1:A:345[A]:TYR:OH	2.17	0.45
1:A:163:MET:HE2	7:A:538:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:LEU:HD21	1:A:173:GLY:HA2	1.98	0.44
2:B:208:VAL:HG12	2:B:209:GLU:N	2.33	0.44
1:A:263:ARG:HB3	1:A:265:GLU:HG2	1.99	0.44
1:A:87:SER:OG	1:A:119:HIS:CE1	2.71	0.44
2:B:209:GLU:OE1	2:B:210:LYS:HE3	2.18	0.44
1:A:140:ASP:HA	1:A:141:PRO:HD2	1.64	0.43
1:A:241:LEU:HA	1:A:244:MET:HE3	2.00	0.43
1:A:99:PRO:C	1:A:101:ASP:N	2.76	0.43
1:A:140:ASP:OD2	1:A:140:ASP:C	2.61	0.42
2:B:173:LYS:HB3	2:B:173:LYS:HE3	1.77	0.42
2:B:152:TRP:HD1	2:B:193:GLU:HG3	1.83	0.42
1:A:101:ASP:HA	1:A:102:PRO:HD2	1.96	0.42
1:A:61:MET:HA	1:A:64:VAL:HG13	2.02	0.41
1:A:336:ARG:HD3	1:A:341:ASP:OD1	2.20	0.41
1:A:259:LEU:HD23	1:A:260:TYR:CE2	2.55	0.41
1:A:383:THR:OG1	1:A:384:PRO:HD2	2.21	0.41
1:A:111:VAL:O	1:A:115:VAL:HG13	2.21	0.40
1:A:305:TYR:O	1:A:306:SER:HB2	2.20	0.40
1:A:377:TRP:CZ2	1:A:381:LYS:HG3	2.56	0.40
2:B:190:LEU:HD23	2:B:203:PRO:HB2	2.04	0.40
2:B:217:PHE:C	2:B:219:ASP:N	2.79	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	369/419 (88%)	361 (98%)	6 (2%)	2 (0%)	24	40
2	B	93/128 (73%)	91 (98%)	1 (1%)	1 (1%)	11	20
All	All	462/547 (84%)	452 (98%)	7 (2%)	3 (1%)	18	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	172	ASP
1	A	100	GLU
1	A	141	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	341/374 (91%)	310 (91%)	31 (9%)	9	17
2	B	79/109 (72%)	72 (91%)	7 (9%)	9	18
All	All	420/483 (87%)	382 (91%)	38 (9%)	9	17

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	PRO
1	A	16	ILE
1	A	23	SER
1	A	27	LEU
1	A	64	VAL
1	A	66	LEU
1	A	67	LEU
1	A	69	ASP
1	A	72	LEU
1	A	86	GLN
1	A	92	LEU
1	A	105	LEU
1	A	115	VAL
1	A	116	ARG
1	A	128	GLN
1	A	130	VAL
1	A	135	GLU
1	A	146	ASN
1	A	162	ARG
1	A	177	ASN

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Mol	Chain	Res	Type
1	A	203	THR
1	A	206	MET
1	A	264	LYS
1	A	265	GLU
1	A	297	ILE
1	A	328	LEU
1	A	332	ARG
1	A	336	ARG
1	A	346	SER
1	A	400	SER
1	A	401	LYS
2	B	128	SER
2	B	133	MET
2	B	140	LEU
2	B	141	SER
2	B	182	GLU
2	B	186	LEU
2	B	190	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	39	ASN
1	A	70	ASN
1	A	73	ASN
1	A	86	GLN
1	A	119	HIS
1	A	128	GLN
1	A	177	ASN
1	A	240	HIS
1	A	302	ASN
2	B	181	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 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$
5	ADP	A	504	3,4	28,29,29	1.65	4 (14%)	43,45,45	1.79	10 (23%)
6	RED	B	373	-	8,10,11	0.55	0	5,10,12	4.73	1 (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
5	ADP	A	504	3,4	-	2/16/32/32	0/3/3/3
6	RED	B	373	-	-	4/8/9/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	504	ADP	C5-C4	5.43	1.48	1.39
5	A	504	ADP	PA-O3A	3.44	1.63	1.59
5	A	504	ADP	C5-C6	2.92	1.49	1.41
5	A	504	ADP	C5-N7	-2.16	1.35	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	373	RED	C7-C8-S8	-10.33	102.98	113.74
5	A	504	ADP	C5-C4-N3	-5.22	119.52	126.72
5	A	504	ADP	N3-C4-N9	4.58	134.96	127.17
5	A	504	ADP	C4-C5-N7	-3.11	107.03	110.58
5	A	504	ADP	N3-C2-N1	-3.04	123.98	128.58
5	A	504	ADP	C2-N3-C4	3.03	119.24	111.83
5	A	504	ADP	C4-N9-C8	2.61	108.48	105.74
5	A	504	ADP	C2-N1-C6	2.60	123.00	118.73
5	A	504	ADP	C5-N7-C8	2.32	107.10	103.45
5	A	504	ADP	O3A-PA-O1A	-2.18	104.15	110.70
5	A	504	ADP	O2A-PA-O1A	2.01	121.81	112.44

There are no chirality outliers.

All (6) torsion outliers are listed below:

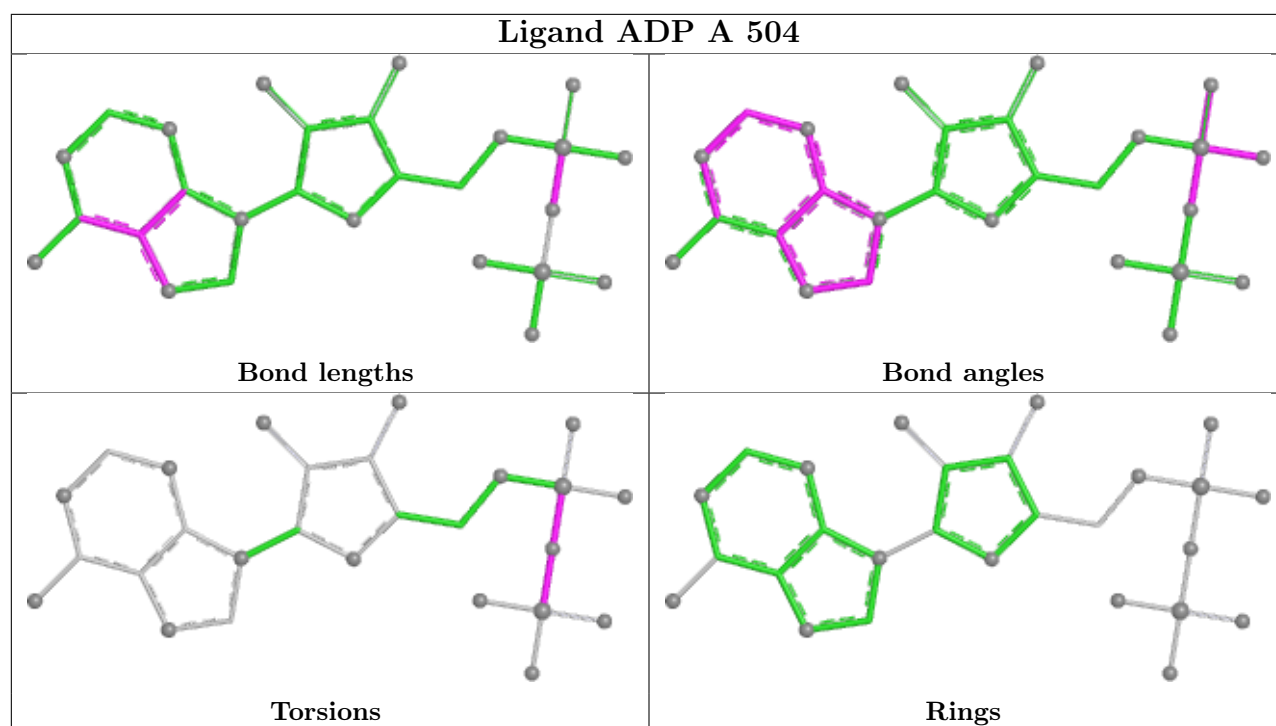
Mol	Chain	Res	Type	Atoms
6	B	373	RED	C6-C7-C8-S8
6	B	373	RED	C3-C4-C5-C6
5	A	504	ADP	PB-O3A-PA-O5'
5	A	504	ADP	PA-O3A-PB-O2B
6	B	373	RED	C4-C5-C6-C7
6	B	373	RED	C4-C5-C6-S6

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	373	RED	4	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	216:ALA	C	217:PHE	N	1.66

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	374/419 (89%)	1.31	62 (16%) 4 3	27, 62, 81, 121	1 (0%)
2	B	97/128 (75%)	1.86	28 (28%) 1 1	53, 63, 86, 121	0
All	All	471/547 (86%)	1.42	90 (19%) 3 2	27, 62, 82, 121	1 (0%)

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	226	THR	9.0
2	B	228	LEU	9.0
1	A	176	THR	7.5
1	A	139	PHE	7.2
1	A	321	LEU	7.1
1	A	142	PHE	7.1
1	A	320	PRO	7.1
2	B	229	LYS	6.8
1	A	324	PHE	6.8
1	A	306	SER	6.6
2	B	220	TYR	6.3
1	A	304	MET	6.1
1	A	179	VAL	6.0
1	A	399	ALA	5.9
2	B	227	ASP	5.8
1	A	305	TYR	5.6
1	A	13	PRO	5.6
1	A	400	SER	5.1
1	A	401	LYS	5.1
1	A	161	PHE	4.8
2	B	129	TYR	4.7
2	B	218	ALA	4.5
2	B	216	ALA	4.3
1	A	38	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	383	THR	4.1
2	B	128	SER	4.0
1	A	174	GLY	3.9
2	B	209	GLU	3.9
1	A	177	ASN	3.7
1	A	227	ALA	3.6
1	A	158	ARG	3.6
1	A	201	TYR	3.6
1	A	40	ALA	3.5
1	A	178	PRO	3.4
2	B	217	PHE	3.3
2	B	219	ASP	3.3
1	A	182	LYS	3.2
1	A	65	ASN	3.2
2	B	212	ALA	3.2
1	A	141	PRO	3.2
1	A	398	ASP	3.2
1	A	175	ASP	3.1
1	A	180	HIS	3.1
1	A	102	PRO	3.1
2	B	130	PRO	3.1
1	A	397	ARG	3.0
1	A	382	THR	2.9
2	B	210	LYS	2.9
1	A	138	GLY	2.9
1	A	47	MET	2.7
2	B	213	ASP	2.7
1	A	262	ASP	2.6
1	A	254	ARG	2.6
1	A	43	LYS	2.6
2	B	187	ALA	2.6
1	A	226	LYS	2.6
1	A	39	ASN	2.5
1	A	97	LYS	2.5
1	A	261	GLU	2.5
1	A	298	ASP	2.5
1	A	41	CYS	2.5
1	A	93	GLU	2.5
1	A	103	GLN	2.5
2	B	192	PRO	2.4
1	A	135	GLU	2.4
2	B	211	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	105	LEU	2.4
1	A	128	GLN	2.4
2	B	181	GLN	2.4
1	A	137	PHE	2.4
1	A	325	GLY	2.4
1	A	229	ASP	2.3
2	B	131	PRO	2.3
1	A	183	HIS	2.3
1	A	94	TYR	2.3
1	A	133	TYR	2.3
2	B	214	ILE	2.3
1	A	104	VAL	2.2
2	B	198	VAL	2.1
2	B	195	THR	2.1
1	A	366	PHE	2.1
1	A	243	HIS	2.1
1	A	95	GLU	2.1
2	B	155	LYS	2.1
2	B	191	VAL	2.1
1	A	22	PHE	2.0
1	A	96	ASN	2.0
1	A	143	ILE	2.0
2	B	194	GLY	2.0
2	B	206	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](#)

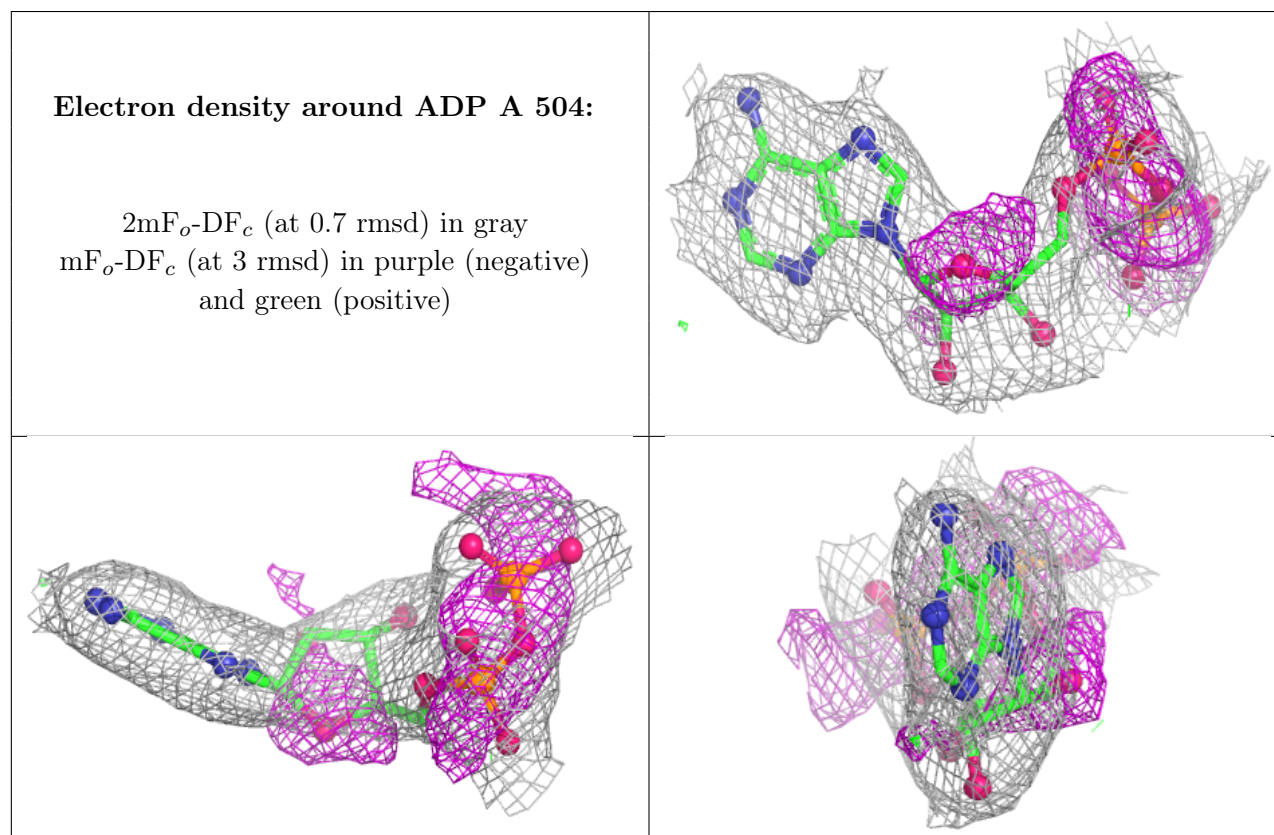
There are no oligosaccharides in this entry.

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
3	MG	A	501	1/1	0.84	0.17	96,96,96,96	0
5	ADP	A	504	27/27	0.85	0.14	59,76,84,85	0
4	K	A	502	1/1	0.89	0.14	88,88,88,88	0
4	K	A	503	1/1	0.92	0.11	65,65,65,65	0
6	RED	B	373	11/12	0.92	0.14	46,50,57,62	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.