



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 04:25 PM EDT

PDB ID : 5EFQ / pdb_00005efq
Title : Crystal structure of human Cdk13/Cyclin K in complex with ADP-aluminum fluoride
Authors : Hoenig, D.; Greifenberg, A.K.; Anand, K.; Geyer, M.
Deposited on : 2015-10-24
Resolution : 2.00 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

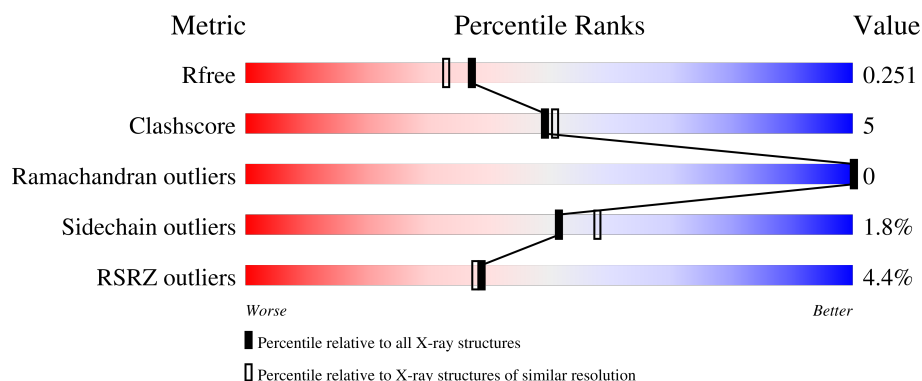
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

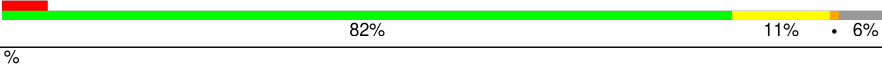
The reported resolution of this entry is 2.00 Å.

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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	347	
1	C	347	
2	B	268	
2	D	268	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9353 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 Cyclin-dependent kinase 13.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	P	S	0	0	0
			2537	1636	424	457	1	19			
1	C	326	Total	C	N	O	P	S	0	0	0
			2563	1651	431	461	1	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	693	GLY	-	expression tag	UNP Q14004
C	693	GLY	-	expression tag	UNP Q14004

- Molecule 2 is a protein called Cyclin-K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	242	Total	C	N	O	S	0	0	0
			1978	1289	328	350	11			
2	D	239	Total	C	N	O	S	0	0	0
			1920	1254	313	341	12			

There are 2 discrepancies between the modelled and reference sequences:

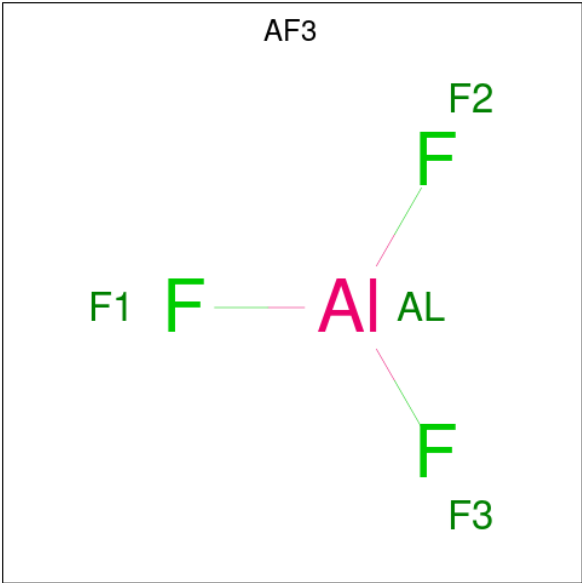
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP O75909
D	0	GLY	-	expression tag	UNP O75909

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 4 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Al	F	0	0
			4	1	3		
4	C	1	Total	Al	F	0	0
			4	1	3		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

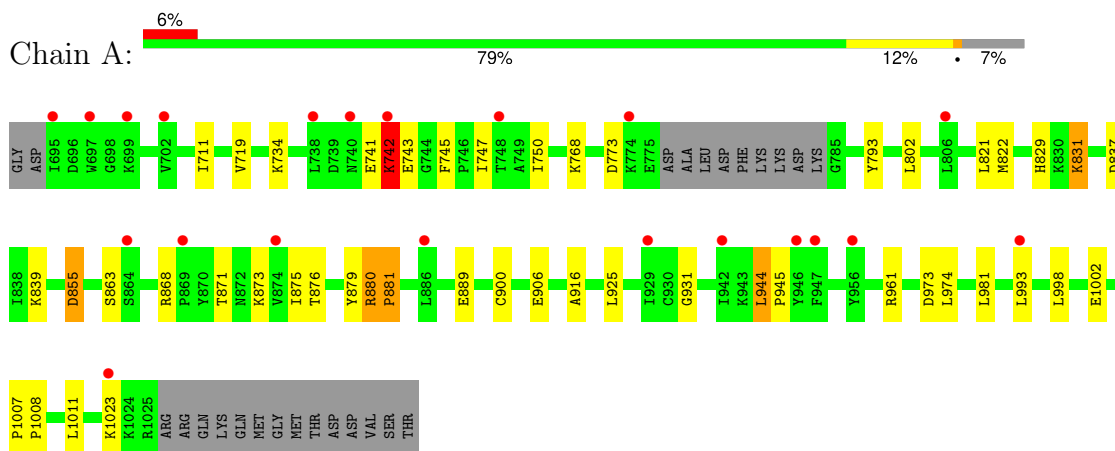
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	79	Total 79	O 79	0	0
6	B	82	Total 82	O 82	0	0
6	C	72	Total 72	O 72	0	0
6	D	56	Total 56	O 56	0	0

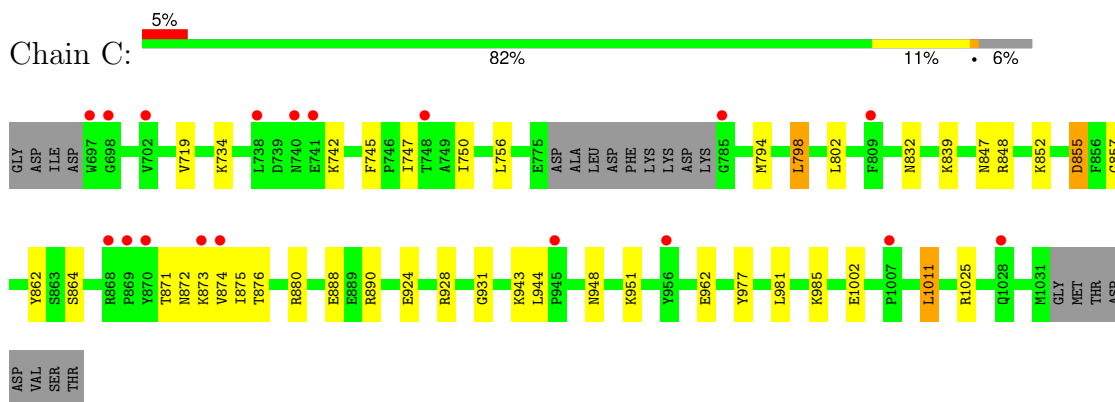
3 Residue-property plots

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.

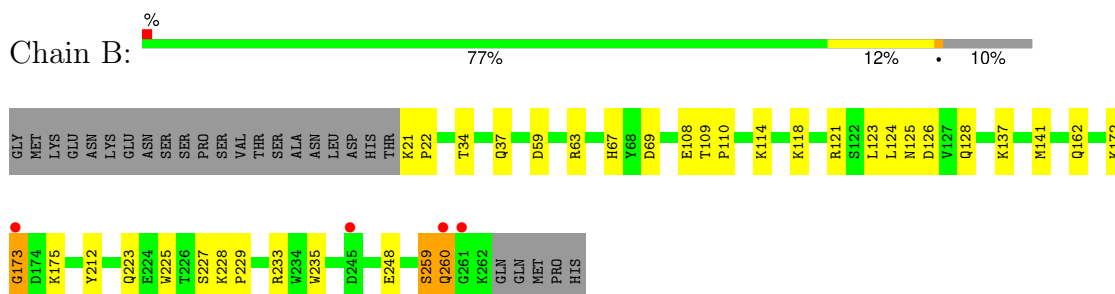
• Molecule 1: Cyclin-dependent kinase 13



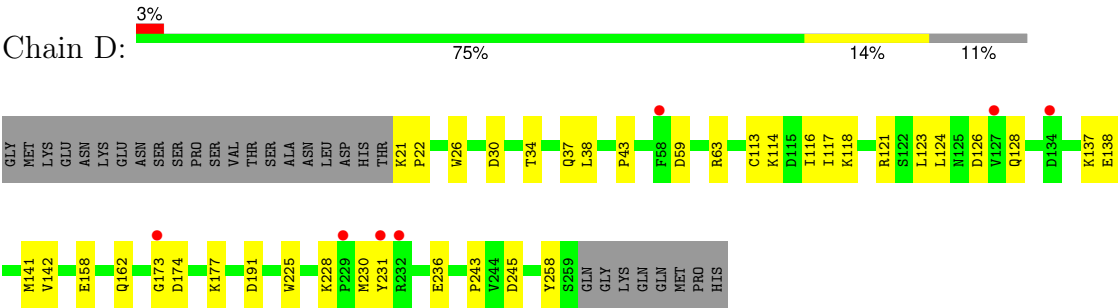
• Molecule 1: Cyclin-dependent kinase 13



• Molecule 2: Cyclin-K



● Molecule 2: Cyclin-K



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	50.78Å 81.82Å 93.14Å 74.08° 84.26° 76.89°	Depositor
Resolution (Å)	46.19 – 2.00 46.19 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.7 (46.19-2.00) 95.1 (46.19-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.194 , 0.247 0.201 , 0.251	Depositor DCC
R_{free} test set	4506 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	41.6	Xtriage
Anisotropy	0.573	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.5	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	0.97	EDS
Total number of atoms	9353	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% 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, TPO, ADP, AF3

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	0.56	1/2587 (0.0%)	1.02	14/3506 (0.4%)
1	C	0.51	0/2613	0.91	11/3543 (0.3%)
2	B	0.58	1/2033 (0.0%)	0.96	9/2759 (0.3%)
2	D	0.50	0/1975	0.83	0/2691
All	All	0.54	2/9208 (0.0%)	0.94	34/12499 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	260	GLN	CA-C	-5.84	1.45	1.52
1	A	881	PRO	CA-C	5.54	1.55	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	831	LYS	N-CA-C	-15.99	84.42	110.17
1	A	880	ARG	CA-C-N	11.85	128.19	119.66
1	A	880	ARG	C-N-CA	11.85	128.19	119.66
2	B	259	SER	N-CA-C	9.86	121.62	111.07
1	A	773	ASP	N-CA-C	-9.45	94.80	109.25
2	B	260	GLN	N-CA-C	-9.25	91.09	110.80
1	C	855	ASP	N-CA-C	9.21	124.72	111.56
1	A	855	ASP	N-CA-C	9.18	124.68	111.56
2	B	172	LYS	N-CA-C	8.45	126.28	113.61
1	C	874	VAL	N-CA-C	7.22	118.18	112.12
1	A	741	GLU	O-C-N	6.73	131.06	123.19
1	A	944	LEU	CA-C-N	6.66	128.17	119.84
1	A	944	LEU	C-N-CA	6.66	128.17	119.84
1	A	1002	GLU	CA-C-N	6.41	126.91	119.47
1	A	1002	GLU	C-N-CA	6.41	126.91	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	742	LYS	N-CA-C	6.36	121.05	113.16
2	B	228	LYS	CA-C-N	6.19	125.81	119.56
2	B	228	LYS	C-N-CA	6.19	125.81	119.56
1	C	745	PHE	CA-C-N	5.86	127.16	119.84
1	C	745	PHE	C-N-CA	5.86	127.16	119.84
2	B	109	THR	CA-C-N	5.77	125.70	119.76
2	B	109	THR	C-N-CA	5.77	125.70	119.76
1	A	745	PHE	CA-C-N	5.75	127.03	119.84
1	A	745	PHE	C-N-CA	5.75	127.03	119.84
1	C	742	LYS	N-CA-C	-5.71	105.09	112.68
1	C	944	LEU	CA-C-N	5.63	126.88	119.84
1	C	944	LEU	C-N-CA	5.63	126.88	119.84
1	C	1002	GLU	CA-C-N	5.52	125.35	119.28
1	C	1002	GLU	C-N-CA	5.52	125.35	119.28
2	B	173	GLY	N-CA-C	5.46	126.11	113.18
1	C	880	ARG	CA-C-N	5.19	125.72	120.38
1	C	880	ARG	C-N-CA	5.19	125.72	120.38
1	A	743	GLU	N-CA-C	-5.12	105.51	112.26
2	B	259	SER	CB-CA-C	-5.02	103.00	110.88

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	2537	0	2463	29	0
1	C	2563	0	2475	18	0
2	B	1978	0	1925	24	0
2	D	1920	0	1823	24	0
3	A	27	0	12	0	0
3	C	27	0	12	1	0
4	A	4	0	0	1	0
4	C	4	0	0	0	0
5	A	2	0	0	0	0
5	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	79	0	0	3	0
6	B	82	0	0	3	0
6	C	72	0	0	2	0
6	D	56	0	0	2	0
All	All	9353	0	8710	96	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 5.

All (96) 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:A:742:LYS:HE2	1:A:742:LYS:HA	1.16	1.11
1:A:742:LYS:HA	1:A:742:LYS:CE	2.01	0.90
1:C:948:ASN:HA	1:C:951:LYS:HE3	1.58	0.85
1:A:974:LEU:HD22	1:A:998:LEU:HD11	1.68	0.76
1:C:875:ILE:N	6:C:1201:HOH:O	2.07	0.74
1:A:875:ILE:N	6:A:1201:HOH:O	2.12	0.71
2:D:121:ARG:NH2	2:D:126:ASP:OD1	2.24	0.70
2:B:114:LYS:NZ	6:B:302:HOH:O	2.27	0.67
1:C:872:ASN:ND2	1:C:888:GLU:O	2.27	0.66
2:B:173:GLY:HA3	2:B:225:TRP:CD1	2.31	0.65
2:D:228:LYS:HG2	2:D:231:TYR:HB2	1.78	0.64
2:D:63:ARG:HD2	2:D:123:LEU:HD11	1.82	0.60
3:C:1101:ADP:O3B	6:C:1202:HOH:O	2.16	0.60
2:B:121:ARG:NH2	2:B:126:ASP:OD1	2.35	0.60
1:C:794:MET:HE3	1:C:852:LYS:HD2	1.87	0.57
2:B:137:LYS:O	2:B:141:MET:HG2	2.06	0.56
1:A:821:LEU:HG	1:A:822:MET:HE2	1.88	0.55
2:D:137:LYS:O	2:D:141:MET:HG2	2.05	0.55
1:A:879:TYR:OH	1:A:906:GLU:OE1	2.25	0.55
1:A:822:MET:HE1	1:A:900:CYS:SG	2.48	0.54
2:D:124:LEU:HD22	2:D:128:GLN:HB3	1.89	0.54
2:D:114:LYS:O	2:D:118:LYS:HG3	2.08	0.54
2:B:162:GLN:NE2	6:B:304:HOH:O	2.41	0.53
1:A:742:LYS:HE2	1:A:742:LYS:CA	2.10	0.53
2:D:138:GLU:O	2:D:142:VAL:HG23	2.09	0.52
1:A:876:THR:HG22	6:A:1208:HOH:O	2.08	0.52
1:C:924:GLU:OE2	1:C:928:ARG:NE	2.34	0.52
1:A:742:LYS:HG2	6:B:376:HOH:O	2.08	0.52
1:A:747:ILE:HA	1:A:750:ILE:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:889:GLU:OE1	6:A:1202:HOH:O	2.20	0.49
1:A:719:VAL:HG22	1:A:734:LYS:HG2	1.94	0.49
2:B:59:ASP:O	2:B:63:ARG:HG3	2.14	0.48
2:B:212:TYR:OH	2:B:248:GLU:OE2	2.22	0.48
2:D:158:GLU:OE2	6:D:301:HOH:O	2.20	0.48
2:B:227:SER:O	2:B:229:PRO:HD3	2.13	0.48
1:C:924:GLU:O	1:C:928:ARG:HG3	2.13	0.48
1:C:848:ARG:O	1:C:848:ARG:HG3	2.13	0.48
1:C:719:VAL:HG22	1:C:734:LYS:HG2	1.96	0.48
2:D:158:GLU:OE1	2:D:162:GLN:NE2	2.40	0.48
1:A:916:ALA:HB2	1:A:925:LEU:HD12	1.96	0.47
2:B:125:ASN:OD1	2:B:125:ASN:C	2.56	0.47
2:B:114:LYS:HA	2:B:114:LYS:HD3	1.69	0.47
2:D:191:ASP:OD2	2:D:258:TYR:OH	2.24	0.47
2:D:117:ILE:HD11	2:D:137:LYS:HA	1.95	0.47
1:A:961:ARG:NH2	1:A:973:ASP:OD1	2.32	0.47
2:B:233:ARG:HG3	2:B:235:TRP:CZ2	2.50	0.47
2:D:230:MET:O	2:D:230:MET:HE3	2.15	0.46
1:A:839:LYS:HD3	1:A:876:THR:HG21	1.96	0.46
2:D:236:GLU:HG2	6:D:307:HOH:O	2.16	0.46
2:B:259:SER:O	2:B:260:GLN:OE1	2.34	0.46
2:B:67:HIS:CE1	2:B:69:ASP:HB2	2.51	0.46
1:C:855:ASP:C	1:C:855:ASP:OD1	2.59	0.45
2:B:67:HIS:ND1	2:B:69:ASP:HB2	2.32	0.45
2:B:233:ARG:HG3	2:B:235:TRP:CH2	2.51	0.45
1:C:832:ASN:HA	1:C:862:TYR:CE1	2.51	0.45
1:C:798:LEU:HD12	1:C:798:LEU:HA	1.77	0.45
2:D:243:PRO:HB2	2:D:245:ASP:OD1	2.16	0.45
1:A:742:LYS:CE	1:A:742:LYS:CA	2.85	0.44
2:B:63:ARG:HH11	2:B:123:LEU:HD21	1.81	0.44
2:B:118:LYS:HA	2:B:118:LYS:HD3	1.86	0.44
1:C:756:LEU:HD23	1:C:756:LEU:HA	1.85	0.44
1:A:837:ASP:OD2	4:A:1102:AF3:F2	2.25	0.43
1:A:855:ASP:OD1	1:A:855:ASP:C	2.61	0.43
1:C:847:ASN:HA	1:C:1011:LEU:HD23	1.99	0.43
1:C:931:GLY:O	1:C:981:LEU:HD11	2.19	0.43
1:A:711:ILE:HD13	1:A:793:TYR:HE1	1.84	0.43
1:A:998:LEU:HD12	1:A:998:LEU:N	2.33	0.42
1:C:747:ILE:HA	1:C:750:ILE:HD12	2.01	0.42
2:D:26:TRP:HB3	2:D:30:ASP:HB2	2.01	0.42
1:A:863:SER:HB3	1:A:868:ARG:NH2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:174:ASP:HB3	2:D:177:LYS:HE2	2.01	0.42
2:B:124:LEU:HD22	2:B:128:GLN:HB3	2.00	0.42
2:B:121:ARG:HA	2:B:121:ARG:HD2	1.76	0.42
2:D:34:THR:OG1	2:D:37:GLN:HG2	2.20	0.42
2:B:21:LYS:HA	2:B:22:PRO:HD3	1.86	0.42
1:A:829:HIS:O	1:A:831:LYS:O	2.37	0.41
2:B:108:GLU:C	2:B:110:PRO:HD3	2.45	0.41
1:A:829:HIS:C	1:A:831:LYS:O	2.63	0.41
1:A:944:LEU:HA	1:A:945:PRO:HD3	1.94	0.41
2:B:114:LYS:O	2:B:118:LYS:HG2	2.20	0.41
1:C:839:LYS:HD3	1:C:876:THR:HG21	2.00	0.41
1:C:855:ASP:C	1:C:857:GLY:H	2.27	0.41
2:B:34:THR:OG1	2:B:37:GLN:HG2	2.20	0.41
2:D:113:CYS:O	2:D:117:ILE:HD12	2.21	0.41
1:A:1007:PRO:HA	1:A:1008:PRO:HD3	1.89	0.41
2:D:37:GLN:HE22	2:D:43:PRO:HA	1.86	0.41
1:A:880:ARG:HA	1:A:881:PRO:HD2	1.66	0.41
1:A:931:GLY:O	1:A:981:LEU:HD11	2.19	0.41
2:D:38:LEU:HD23	2:D:38:LEU:HA	1.83	0.41
2:D:21:LYS:HA	2:D:22:PRO:HD3	1.80	0.41
2:D:113:CYS:HA	2:D:116:ILE:HD12	2.03	0.41
2:B:114:LYS:HE2	2:B:137:LYS:HD2	2.03	0.41
2:D:173:GLY:HA3	2:D:225:TRP:CD1	2.56	0.40
1:C:977:TYR:HE1	1:C:985:LYS:O	2.04	0.40
2:D:59:ASP:O	2:D:63:ARG:HG3	2.21	0.40
1:A:768:LYS:HB3	1:A:768:LYS:HE3	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	317/347 (91%)	310 (98%)	7 (2%)	0	100	100
1	C	321/347 (92%)	314 (98%)	7 (2%)	0	100	100
2	B	240/268 (90%)	236 (98%)	4 (2%)	0	100	100
2	D	237/268 (88%)	232 (98%)	5 (2%)	0	100	100
All	All	1115/1230 (91%)	1092 (98%)	23 (2%)	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	264/310 (85%)	258 (98%)	6 (2%)	44	49
1	C	264/310 (85%)	255 (97%)	9 (3%)	32	33
2	B	208/241 (86%)	206 (99%)	2 (1%)	68	75
2	D	197/241 (82%)	197 (100%)	0	100	100
All	All	933/1102 (85%)	916 (98%)	17 (2%)	51	58

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

Mol	Chain	Res	Type
1	A	742	LYS
1	A	802	LEU
1	A	873	LYS
1	A	993	LEU
1	A	1011	LEU
1	A	1023	LYS
2	B	175	LYS
2	B	223	GLN
1	C	798	LEU
1	C	802	LEU
1	C	864	SER
1	C	873	LYS
1	C	890	ARG

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Mol	Chain	Res	Type
1	C	943	LYS
1	C	962	GLU
1	C	1011	LEU
1	C	1025	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	718	GLN
1	A	832	ASN
1	A	1015	GLN
2	B	200	GLN
2	B	223	GLN
2	B	253	GLN
1	C	1015	GLN
2	D	37	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	TPO	A	871	1	8,10,11	1.35	2 (25%)	10,14,16	1.43	2 (20%)
1	TPO	C	871	1	8,10,11	1.41	2 (25%)	10,14,16	1.21	1 (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
1	TPO	A	871	1	-	1/9/11/13	-
1	TPO	C	871	1	-	1/9/11/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	871	TPO	P-O2P	-2.43	1.45	1.54
1	A	871	TPO	P-O3P	-2.28	1.46	1.54
1	A	871	TPO	P-O2P	-2.24	1.46	1.54
1	C	871	TPO	P-O3P	-2.06	1.47	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	871	TPO	O-C-CA	-2.55	118.22	124.77
1	A	871	TPO	OG1-P-O1P	-2.39	100.81	109.33
1	C	871	TPO	O-C-CA	-2.21	119.08	124.77

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	871	TPO	O-C-CA-CB
1	C	871	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	C	1101	5	28,29,29	1.94	8 (28%)	43,45,45	1.88	11 (25%)
4	AF3	C	1102	-	0,3,3	-	-	-		
4	AF3	A	1102	-	0,3,3	-	-	-		
3	ADP	A	1101	5	28,29,29	1.97	9 (32%)	43,45,45	1.96	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
3	ADP	C	1101	5	-	0/16/32/32	0/3/3/3
3	ADP	A	1101	5	-	1/16/32/32	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1101	ADP	C5-N7	-4.61	1.30	1.39
3	A	1101	ADP	C5-N7	-4.55	1.30	1.39
3	A	1101	ADP	PA-O3A	-4.27	1.54	1.59
3	C	1101	ADP	PA-O3A	-4.04	1.55	1.59
3	C	1101	ADP	C4-N9	-3.65	1.30	1.37
3	A	1101	ADP	C8-N9	-3.65	1.31	1.37
3	C	1101	ADP	C8-N9	-3.30	1.31	1.37
3	A	1101	ADP	C4-N9	-3.07	1.31	1.37
3	A	1101	ADP	C5-C4	2.94	1.44	1.39
3	C	1101	ADP	C5-C4	2.72	1.43	1.39
3	A	1101	ADP	PB-O2B	-2.63	1.45	1.54
3	C	1101	ADP	PB-O2B	-2.35	1.46	1.54
3	C	1101	ADP	PA-O2A	-2.34	1.44	1.55
3	C	1101	ADP	PB-O3B	-2.17	1.46	1.54
3	A	1101	ADP	PA-O2A	-2.14	1.45	1.55
3	A	1101	ADP	PB-O3B	-2.04	1.47	1.54
3	A	1101	ADP	PA-O1A	-2.03	1.43	1.50

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	ADP	C5-C4-N3	-6.52	117.74	126.72
3	C	1101	ADP	C5-C4-N3	-5.53	119.10	126.72
3	A	1101	ADP	N3-C4-N9	4.60	134.99	127.17
3	A	1101	ADP	C4-C5-N7	-4.33	105.63	110.58
3	C	1101	ADP	C2'-C1'-N9	-4.30	102.61	113.30
3	C	1101	ADP	N3-C4-N9	4.15	134.23	127.17
3	C	1101	ADP	C4-C5-N7	-3.73	106.32	110.58
3	A	1101	ADP	C2-N3-C4	3.73	120.94	111.83
3	A	1101	ADP	C2'-C1'-N9	-3.50	104.60	113.30
3	C	1101	ADP	C2-N3-C4	3.37	120.06	111.83
3	A	1101	ADP	C5-N7-C8	3.07	108.27	103.45
3	C	1101	ADP	C5-N7-C8	2.88	107.98	103.45
3	C	1101	ADP	C4-N9-C8	2.56	108.43	105.74
3	C	1101	ADP	N3-C2-N1	-2.50	124.80	128.58
3	A	1101	ADP	N3-C2-N1	-2.48	124.83	128.58
3	C	1101	ADP	N9-C8-N7	-2.35	110.60	113.94
3	A	1101	ADP	C6-C5-N7	2.23	136.38	132.09
3	A	1101	ADP	C3'-C2'-C1'	2.16	105.55	101.46
3	C	1101	ADP	C3'-C2'-C1'	2.12	105.47	101.46
3	C	1101	ADP	C6-C5-N7	2.01	135.97	132.09

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1101	ADP	PA-O3A-PB-O2B

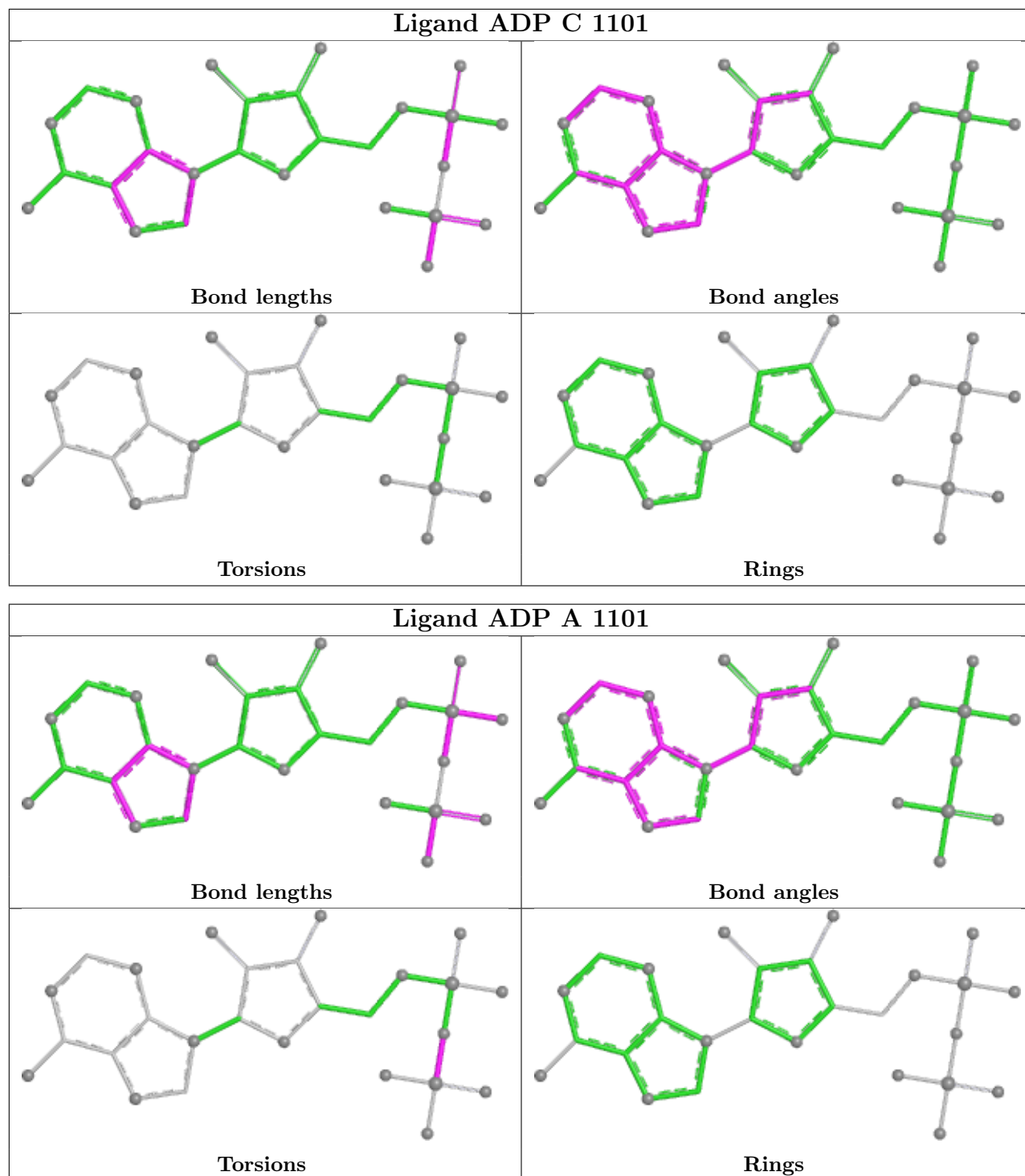
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1101	ADP	1	0
4	A	1102	AF3	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	321/347 (92%)	0.74	21 (6%) 25 23	41, 64, 102, 130	0
1	C	325/347 (93%)	0.63	18 (5%) 30 29	38, 62, 106, 144	0
2	B	242/268 (90%)	0.33	4 (1%) 69 68	33, 51, 88, 125	0
2	D	239/268 (89%)	0.58	7 (2%) 53 52	37, 60, 104, 134	0
All	All	1127/1230 (91%)	0.59	50 (4%) 39 38	33, 60, 102, 144	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	738	LEU	5.3
2	B	173	GLY	4.0
2	D	58	PHE	4.0
1	A	869	PRO	3.8
1	C	869	PRO	3.5
2	D	231	TYR	3.5
1	C	741	GLU	3.5
1	A	695	ILE	3.4
2	D	229	PRO	3.2
1	C	874	VAL	3.2
2	B	261	GLY	3.2
1	A	946	TYR	3.0
1	C	870	TYR	3.0
1	A	864	SER	3.0
1	C	702	VAL	2.8
1	C	698	GLY	2.8
1	A	740	ASN	2.8
1	C	697	TRP	2.8
1	A	738	LEU	2.7
2	D	134	ASP	2.6
2	D	232	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	742	LYS	2.5
1	C	868	ARG	2.5
1	A	993	LEU	2.4
2	B	260	GLN	2.4
1	A	874	VAL	2.4
1	C	945	PRO	2.4
1	A	702	VAL	2.4
1	A	956	TYR	2.3
2	B	245	ASP	2.3
1	A	929	ILE	2.3
1	A	942	ILE	2.3
1	C	785	GLY	2.3
1	A	699	LYS	2.3
1	A	947	PHE	2.3
1	A	774	LYS	2.3
2	D	127	VAL	2.2
2	D	173	GLY	2.2
1	A	886	LEU	2.2
1	A	1023	LYS	2.2
1	A	697	TRP	2.2
1	C	748	THR	2.2
1	C	1007	PRO	2.1
1	C	809	PHE	2.1
1	C	873	LYS	2.1
1	A	748	THR	2.1
1	C	956	TYR	2.1
1	A	806	LEU	2.0
1	C	740	ASN	2.0
1	C	1028	GLN	2.0

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

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(Å ²)	Q<0.9
1	TPO	A	871	11/12	0.92	0.10	48,59,64,73	0
1	TPO	C	871	11/12	0.92	0.10	44,53,62,65	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

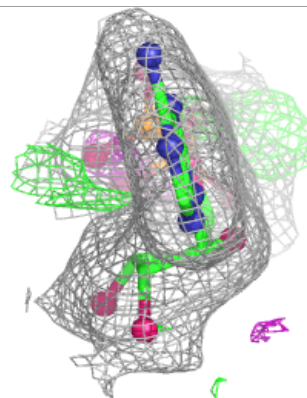
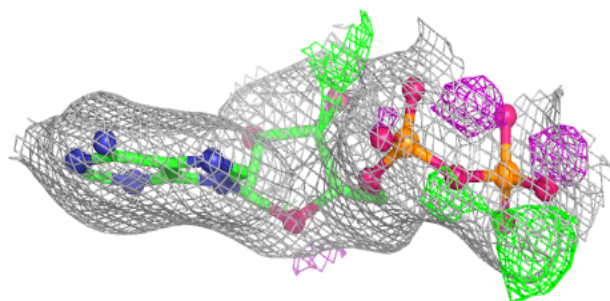
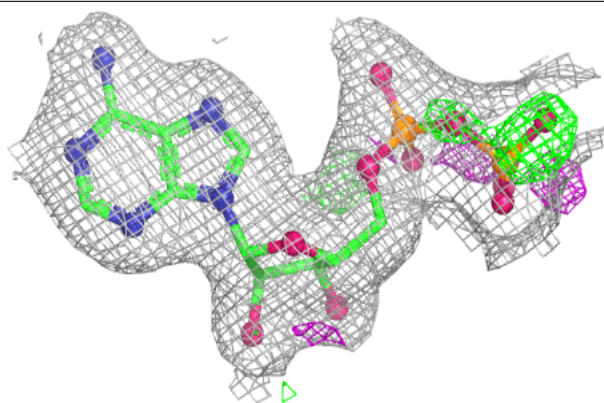
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	AF3	C	1102	4/4	0.84	0.14	50,95,144,160	0
5	MG	A	1104	1/1	0.85	0.11	68,68,68,68	0
5	MG	C	1104	1/1	0.87	0.15	75,75,75,75	0
4	AF3	A	1102	4/4	0.91	0.10	49,80,94,120	0
3	ADP	C	1101	27/27	0.95	0.08	42,48,66,105	0
3	ADP	A	1101	27/27	0.96	0.08	42,49,61,96	0
5	MG	C	1103	1/1	0.98	0.04	44,44,44,44	0
5	MG	A	1103	1/1	0.99	0.04	49,49,49,49	0

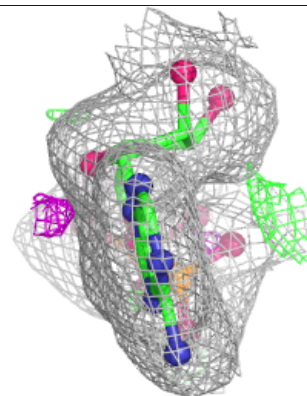
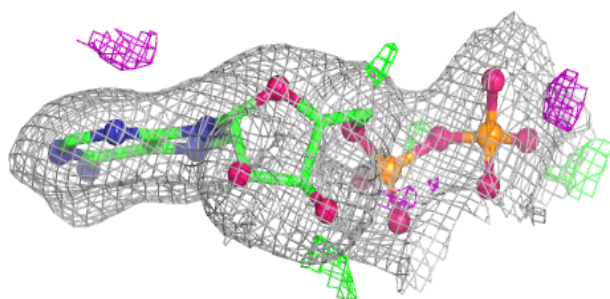
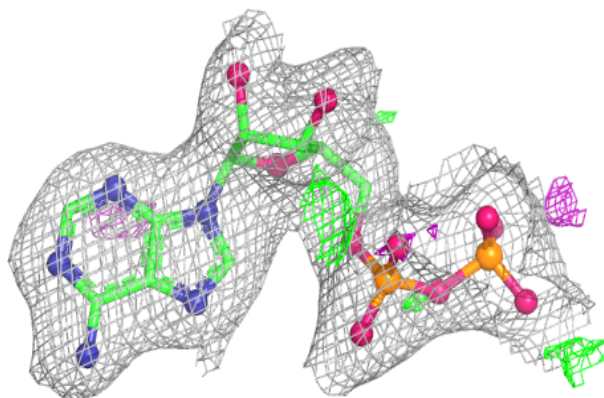
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP C 1101:

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

**Electron density around ADP A 1101:**

$2mF_o-DF_c$ (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.