



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 4, 2026 – 10:13 am BST

PDB ID : 32AW / pdb_000032aw
Title : Crystal structure of human CDK9/cyclin K in complex with NVP-2
Authors : Kaltheuner, I.H.; Anand, K.; Hagelueken, G.; Geyer, M.
Deposited on : 2026-07-01
Resolution : 3.25 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.8.4, CSD as541be (2020)
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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

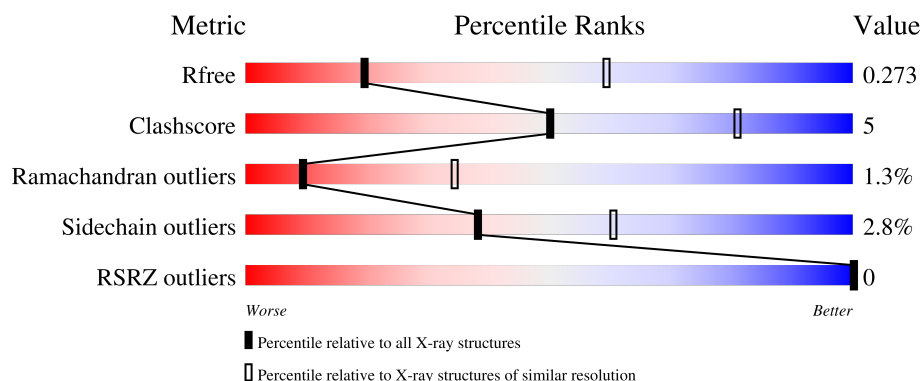
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	374	
1	C	374	
1	E	374	
2	B	268	
2	D	268	

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Mol	Chain	Length	Quality of chain
2	F	268	80% 7% 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13444 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 9.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	P	S	0	0	0
			2636	1692	451	476	1	16			
1	C	306	Total	C	N	O	P	S	0	0	0
			2477	1590	426	446	1	14			
1	E	301	Total	C	N	O	P	S	0	0	0
			2435	1565	415	440	1	14			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A0A096P1Z7
C	-1	GLY	-	expression tag	UNP A0A096P1Z7
E	-1	GLY	-	expression tag	UNP A0A096P1Z7

- Molecule 2 is a protein called Cyclin-K.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	228	Total	C	N	O	S		0	0	0
			1890	1230	314	336	10				
2	D	234	Total	C	N	O	S		0	0	0
			1943	1264	324	344	11				
2	F	235	Total	C	N	O	S		0	0	0
			1955	1273	325	346	11				

There are 3 discrepancies between the modelled and reference sequences:

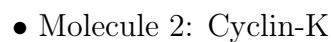
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP O75909
D	0	GLY	-	expression tag	UNP O75909
F	0	GLY	-	expression tag	UNP O75909

- Molecule 3 is 4-[[[6-[5-chloranyl-2-[[4-[[[(2 {R})-1-methoxypropan-2-yl]amino]phenyl]amino

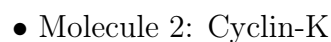
[illegible]

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 36	C 27	Cl 1	N 6	O 2	0	0
3	C	1	Total 36	C 27	Cl 1	N 6	O 2	0	0
3	E	1	Total 36	C 27	Cl 1	N 6	O 2	0	0

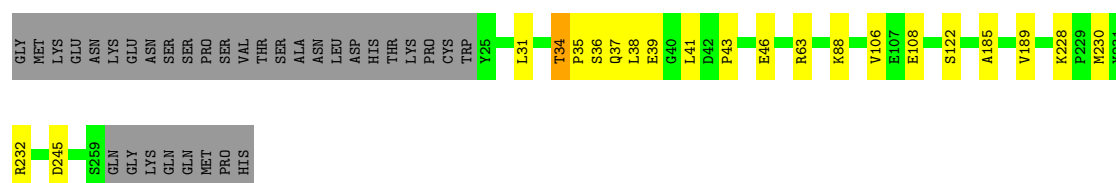
Chain B: 78% 7% 15%



Chain D: 76% 11% 13%



Chain F: 80% 7% 12%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	146.23Å 146.23Å 100.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.86 – 3.25 47.86 – 3.25	Depositor EDS
% Data completeness (in resolution range)	77.7 (47.86-3.25) 77.7 (47.86-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 3.25Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.265 , 0.302 0.239 , 0.273	Depositor DCC
R_{free} test set	27379 reflections (89.48%)	wwPDB-VP
Wilson B-factor (Å ²)	115.8	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 100.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.074 for -h,-k,l 0.388 for h,-h-k,-l 0.076 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13444	wwPDB-VP
Average B, all atoms (Å ²)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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: A1KBG, TPO

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	0.35	0/2680	0.62	0/3620
1	C	0.41	0/2515	0.64	0/3393
1	E	0.35	0/2472	0.59	0/3337
2	B	0.20	0/1938	0.46	0/2621
2	D	0.25	0/1994	0.65	2/2697 (0.1%)
2	F	0.24	0/2007	0.50	0/2715
All	All	0.32	0/13606	0.59	2/18383 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	242	VAL	N-CA-C	5.46	113.44	107.60
2	D	53	GLY	N-CA-C	5.25	119.49	112.77

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	2636	0	2682	46	0
1	C	2477	0	2525	39	0
1	E	2435	0	2474	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1890	0	1877	10	0
2	D	1943	0	1934	19	0
2	F	1955	0	1943	14	0
3	A	36	0	0	4	0
3	C	36	0	0	1	0
3	E	36	0	0	4	0
All	All	13444	0	13435	143	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.

The worst 5 of 143 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:F:37:GLN:HE21	2:F:43:PRO:HD3	1.27	0.99
2:B:233:ARG:HB2	2:B:236:GLU:HG3	1.53	0.87
1:C:172:ARG:HG3	2:D:108:GLU:HG2	1.69	0.75
1:C:245:CYS:HA	1:C:273:ARG:HB3	1.72	0.71
1:E:79:VAL:HG21	3:E:1001:A1KBG:CL14	2.28	0.69

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	321/374 (86%)	288 (90%)	22 (7%)	11 (3%)	3	17
1	C	299/374 (80%)	277 (93%)	17 (6%)	5 (2%)	7	29
1	E	292/374 (78%)	277 (95%)	13 (4%)	2 (1%)	18	48
2	B	224/268 (84%)	219 (98%)	5 (2%)	0	100	100
2	D	232/268 (87%)	226 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	233/268 (87%)	224 (96%)	6 (3%)	3 (1%)	9	34
All	All	1601/1926 (83%)	1511 (94%)	69 (4%)	21 (1%)	9	34

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	PHE
1	A	273	ARG
1	A	334	SER
1	A	339	LEU
1	A	340	ALA

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	289/330 (88%)	275 (95%)	14 (5%)	23	50
1	C	270/330 (82%)	261 (97%)	9 (3%)	33	57
1	E	266/330 (81%)	258 (97%)	8 (3%)	36	59
2	B	204/241 (85%)	200 (98%)	4 (2%)	48	66
2	D	210/241 (87%)	205 (98%)	5 (2%)	43	64
2	F	211/241 (88%)	210 (100%)	1 (0%)	81	82
All	All	1450/1713 (85%)	1409 (97%)	41 (3%)	38	60

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	112	LYS
1	E	106	CYS
2	D	156	GLN
1	E	27	GLN
1	E	156	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	200	GLN
2	D	253	GLN
2	F	253	GLN
2	F	37	GLN
2	F	200	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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	186	1	8,10,11	2.44	1 (12%)	10,14,16	1.17	1 (10%)
1	TPO	C	186	1	8,10,11	2.42	1 (12%)	10,14,16	1.22	1 (10%)
1	TPO	E	186	1	8,10,11	2.46	1 (12%)	10,14,16	1.25	0

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	186	1	-	1/9/11/13	-
1	TPO	C	186	1	-	1/9/11/13	-
1	TPO	E	186	1	-	0/9/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	186	TPO	P-OG1	6.78	1.72	1.59
1	A	186	TPO	P-OG1	6.72	1.72	1.59
1	C	186	TPO	P-OG1	6.66	1.71	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	TPO	OG1-P-O1P	-2.16	101.06	109.39
1	C	186	TPO	P-OG1-CB	-2.05	117.01	123.21

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	186	TPO	CB-OG1-P-O3P
1	C	186	TPO	CB-OG1-P-O1P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	186	TPO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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
3	A1KBG	C	1001	-	38,39,39	2.14	9 (23%)	44,53,53	1.79	8 (18%)
3	A1KBG	A	1001	-	38,39,39	2.15	9 (23%)	44,53,53	2.31	12 (27%)
3	A1KBG	E	1001	-	38,39,39	2.18	9 (23%)	44,53,53	1.71	7 (15%)

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	A1KBG	C	1001	-	-	13/21/34/34	0/4/4/4
3	A1KBG	A	1001	-	-	7/21/34/34	0/4/4/4
3	A1KBG	E	1001	-	-	2/21/34/34	0/4/4/4

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	A1KBG	C17-N21	7.09	1.46	1.36
3	C	1001	A1KBG	C29-C35	6.79	1.60	1.47
3	E	1001	A1KBG	C29-C35	6.78	1.60	1.47
3	C	1001	A1KBG	C17-N21	6.62	1.46	1.36
3	A	1001	A1KBG	C29-C35	6.41	1.60	1.47

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	A1KBG	C15-N16-C17	10.84	126.19	118.06
3	C	1001	A1KBG	C15-N16-C17	6.74	123.12	118.06
3	E	1001	A1KBG	C15-N16-C17	6.43	122.88	118.06
3	A	1001	A1KBG	C29-C28-N21	-4.03	108.60	114.11
3	A	1001	A1KBG	C34-C29-C30	3.87	112.40	108.49

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	A1KBG	C11-C12-C15-C20

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Mol	Chain	Res	Type	Atoms
3	A	1001	A1KBG	C11-C12-C15-N16
3	C	1001	A1KBG	C18-C17-N21-C28
3	C	1001	A1KBG	N16-C17-N21-C28
3	C	1001	A1KBG	C24-C23-C25-O26

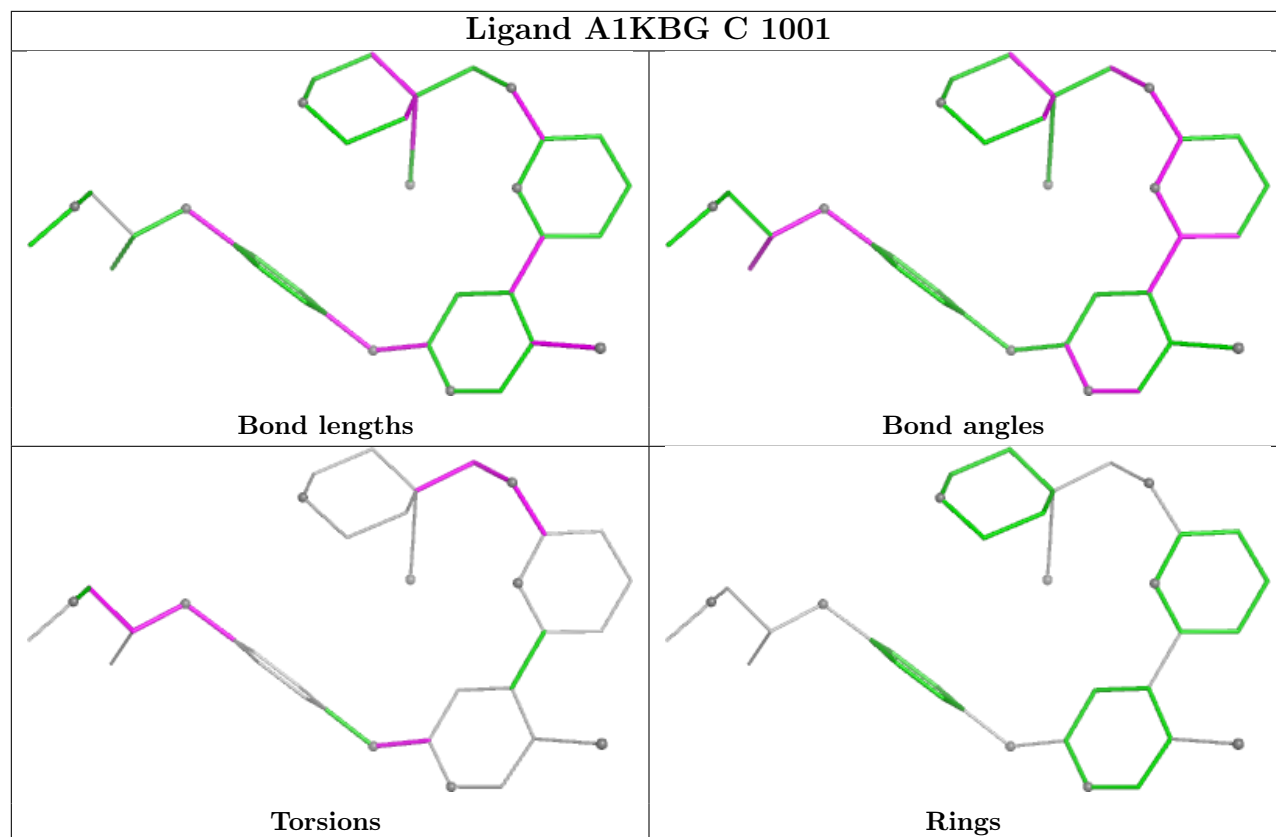
There are no ring outliers.

3 monomers are involved in 9 short contacts:

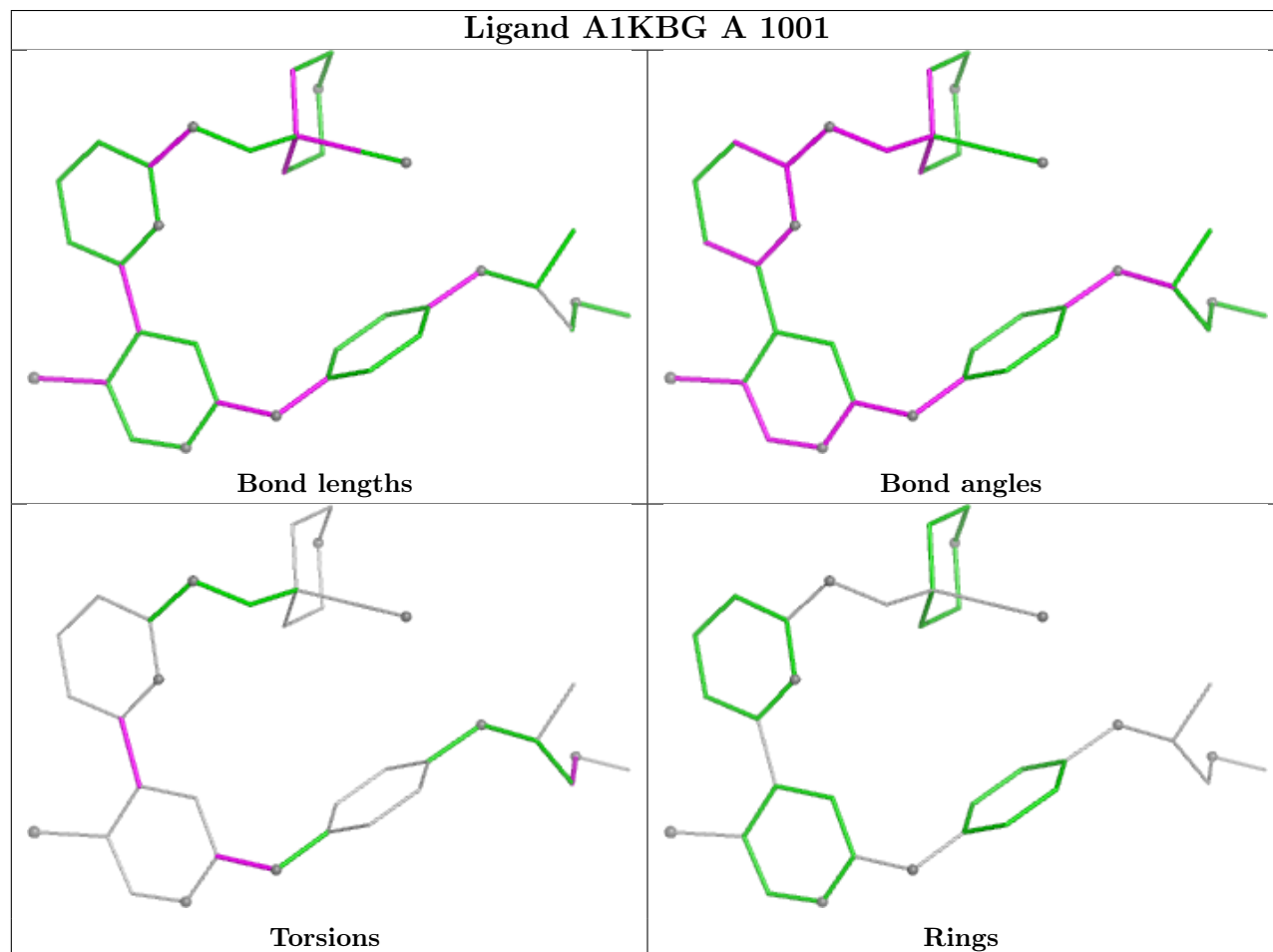
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1001	A1KBG	1	0
3	A	1001	A1KBG	4	0
3	E	1001	A1KBG	4	0

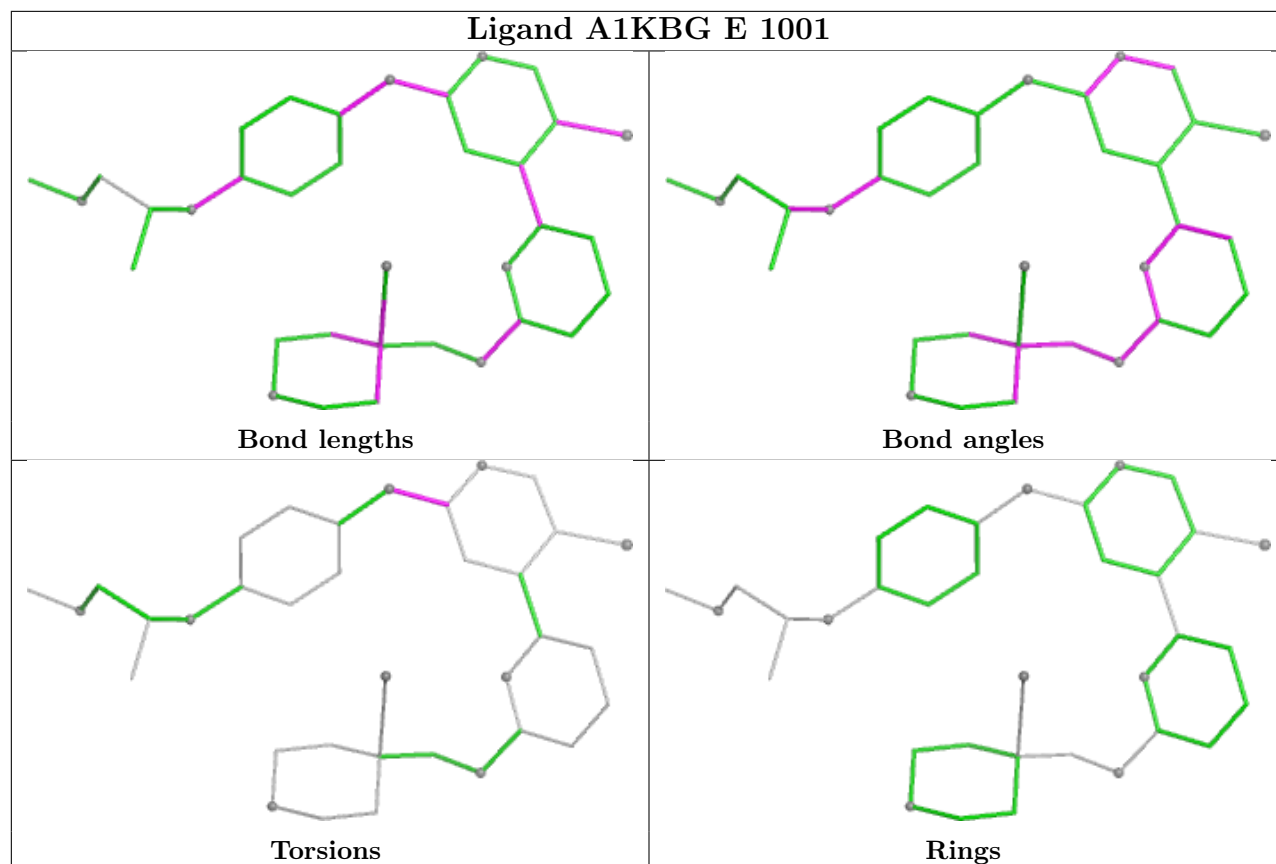
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand A1KBG C 1001



Ligand A1KBG A 1001





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	325/374 (86%)	-1.52	0 100 100	75, 110, 158, 197	0
1	C	305/374 (81%)	-1.45	0 100 100	62, 109, 158, 186	0
1	E	300/374 (80%)	-1.49	0 100 100	64, 100, 148, 200	0
2	B	228/268 (85%)	-1.48	0 100 100	101, 144, 178, 189	0
2	D	234/268 (87%)	-1.15	0 100 100	112, 166, 194, 223	0
2	F	235/268 (87%)	-1.49	0 100 100	83, 127, 167, 212	0
All	All	1627/1926 (84%)	-1.44	0 100 100	62, 122, 178, 223	0

There are no RSRZ outliers to report.

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	C	186	11/12	0.99	0.02	97,119,130,133	0
1	TPO	A	186	11/12	1.00	0.01	84,93,107,112	0
1	TPO	E	186	11/12	1.00	0.03	86,94,104,107	0

6.3 Carbohydrates

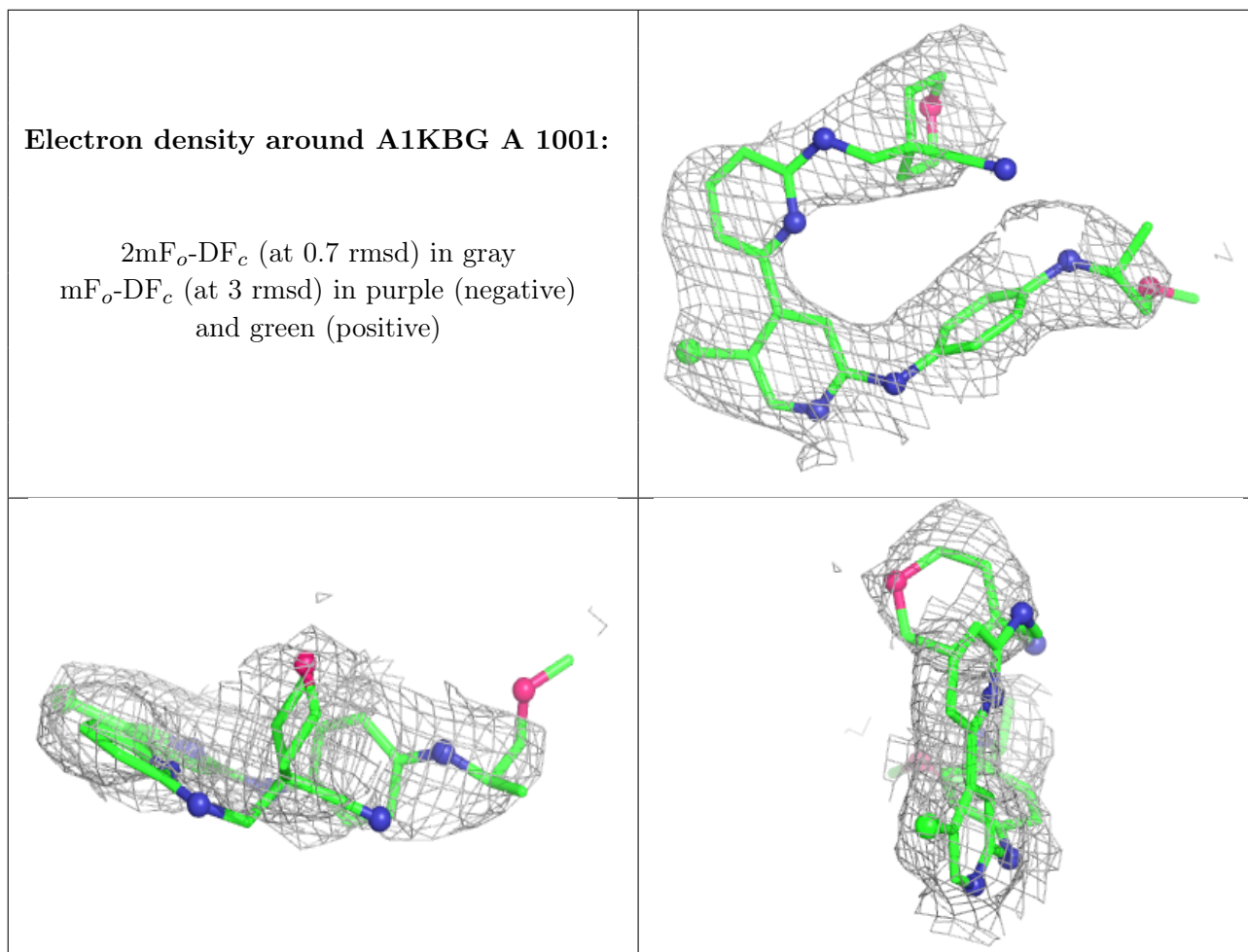
There are no oligosaccharides in this entry.

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.

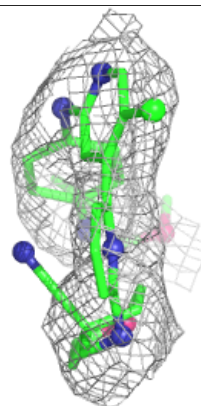
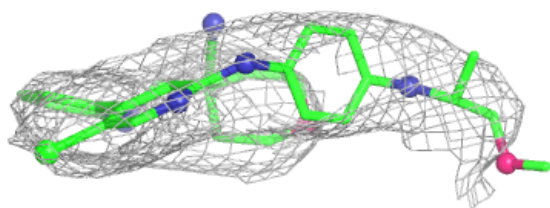
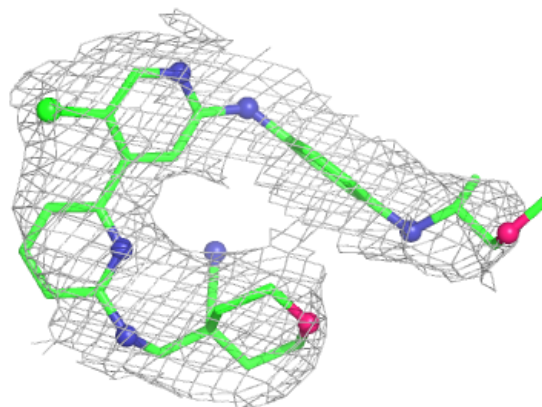
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	A1KBG	A	1001	36/36	0.99	0.04	97,120,141,154	0
3	A1KBG	C	1001	36/36	1.00	0.03	84,98,125,135	0
3	A1KBG	E	1001	36/36	1.00	0.03	91,102,114,117	0

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.

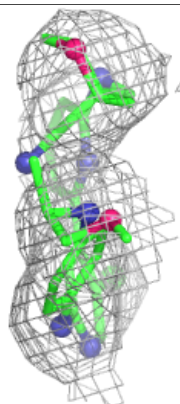
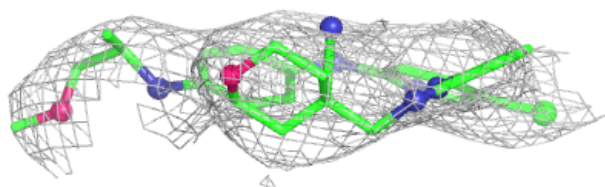
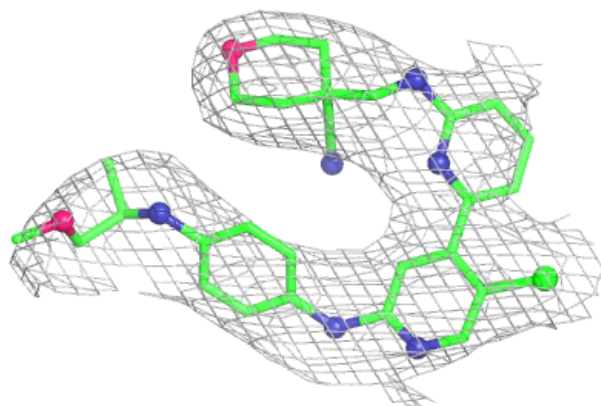


Electron density around A1KBG C 1001:

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

**Electron density around A1KBG E 1001:**

$2mF_o-DF_c$ (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.