



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:06 am BST

PDB ID : 5Y86  
Title : Crystal structure of kinase  
Authors : Kim, K.L.; Cha, J.S.; Cho, Y.S.; Kim, H.Y.; Chang, N.P.; Cho, H.S.  
Deposited on : 2017-08-18  
Resolution : 1.90 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

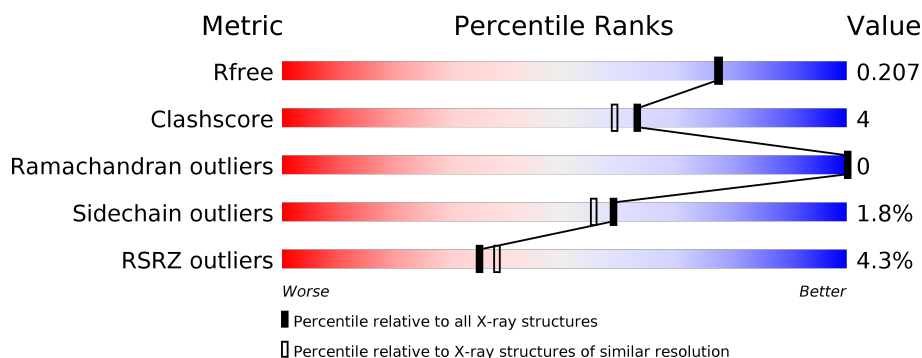
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	588	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	SEP	A	445	-	X	-	-
4	EDO	A	608	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	A	612	-	X	-	-

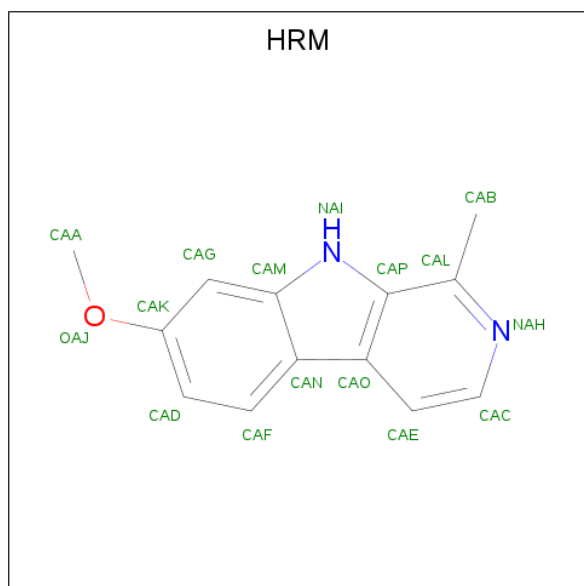


In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Dual specificity tyrosine-phosphorylation-regulated kinase 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	P	S	0	0	0
			3208	2050	570	569	4	15			

- Molecule 2 is 7-METHOXY-1-METHYL-9H-BETA-CARBOLINE (three-letter code: HRM) (formula:  $C_{13}H_{12}N_2O$ ) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			16	13	2	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula:  $\text{O}_4\text{P}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



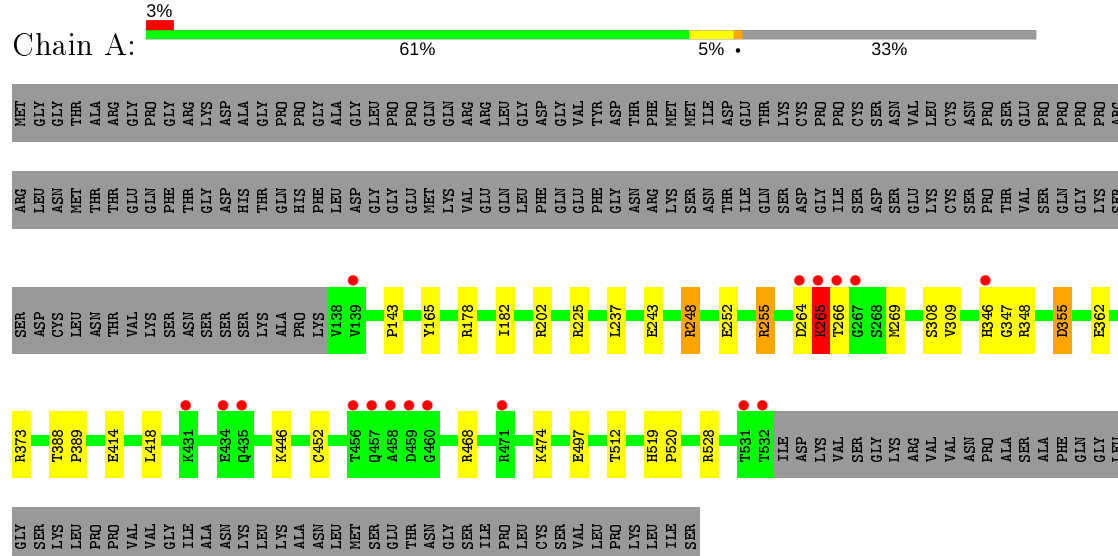
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	350	Total	O	0	0
			350	350		



- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	43.00 Å 76.52 Å 148.47 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 29.88 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-1.90) 99.9 (29.88-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.81 (at 1.91 Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, $R_{free}$	0.167 , 0.196 0.179 , 0.207	Depositor DCC
$R_{free}$ test set	1964 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.8	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 55.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3622	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, SEP, TPO, PO4, EDO, HRM, PTR

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	1.11	3/3237 (0.1%)	1.05	13/4357 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	497	GLU	CD-OE1	7.48	1.33	1.25
1	A	243	GLU	CD-OE1	7.02	1.33	1.25
1	A	202	ARG	CD-NE	-5.84	1.36	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	ARG	NE-CZ-NH2	-18.02	111.29	120.30
1	A	202	ARG	NE-CZ-NH1	10.03	125.31	120.30
1	A	178	ARG	NE-CZ-NH2	-9.43	115.58	120.30
1	A	373	ARG	NE-CZ-NH2	-8.37	116.12	120.30
1	A	178	ARG	NE-CZ-NH1	8.11	124.35	120.30
1	A	265	LYS	N-CA-C	-7.59	90.51	111.00
1	A	225	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	A	269	MET	CG-SD-CE	6.72	110.95	100.20
1	A	266	THR	CB-CA-C	-6.47	94.14	111.60
1	A	225	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	A	355	ASP	N-CA-C	6.05	127.34	111.00
1	A	266	THR	N-CA-C	5.18	124.98	111.00
1	A	255	ARG	NE-CZ-NH1	5.08	122.84	120.30

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	3208	0	3231	26	1
2	A	16	0	12	0	0
3	A	10	0	0	1	0
4	A	32	0	48	9	0
5	A	6	0	8	1	1
6	A	350	0	0	4	0
All	All	3622	0	3299	28	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 4.

All (28) 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:528:ARG:HH21	1:A:528:ARG:HG3	1.47	0.79
1:A:182:ILE:H	5:A:612:GOL:H2	1.57	0.70
1:A:309:VAL:H	4:A:608:EDO:H22	1.57	0.69
1:A:308:SER:HA	4:A:608:EDO:H21	1.76	0.68
1:A:512:TPO:O3P	6:A:701:HOH:O	2.15	0.64
1:A:512:TPO:O2P	1:A:512:TPO:HG21	1.96	0.64
1:A:528:ARG:HG3	1:A:528:ARG:NH2	2.14	0.63
4:A:611:EDO:C1	6:A:707:HOH:O	2.48	0.61
1:A:309:VAL:H	4:A:608:EDO:C2	2.18	0.56
1:A:248:ARG:NE	6:A:703:HOH:O	2.31	0.55
1:A:264:ASP:OD1	1:A:265:LYS:O	2.25	0.54
1:A:452:CYS:O	4:A:610:EDO:H21	2.09	0.53
1:A:355:ASP:O	1:A:355:ASP:CG	2.43	0.53
1:A:519:HIS:CG	1:A:520:PRO:HD2	2.45	0.51
3:A:603:PO4:O3	6:A:702:HOH:O	2.19	0.51
1:A:468:ARG:NH2	1:A:474:LYS:HG3	2.25	0.51
1:A:252:GLU:OE2	1:A:255:ARG:NH1	2.45	0.49
1:A:264:ASP:OD1	1:A:265:LYS:N	2.46	0.49
1:A:248:ARG:HH21	1:A:248:ARG:CG	2.27	0.48
1:A:346:HIS:ND1	1:A:347:GLY:N	2.61	0.47
1:A:308:SER:CA	4:A:608:EDO:H21	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:PRO:HG3	1:A:165:TYR:O	2.15	0.46
1:A:309:VAL:HG12	4:A:608:EDO:H22	2.00	0.43
1:A:248:ARG:CG	1:A:248:ARG:NH2	2.79	0.42
1:A:452:CYS:O	4:A:610:EDO:C2	2.68	0.42
1:A:388:THR:N	1:A:389:PRO:CD	2.83	0.41
1:A:348:ARG:O	4:A:609:EDO:H12	2.21	0.40
1:A:355:ASP:OD1	1:A:355:ASP:C	2.59	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:A:414:GLU:OE1	5:A:612:GOL:O2[3_645]	2.10	0.10

## 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	389/588 (66%)	378 (97%)	11 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	340/505 (67%)	334 (98%)	6 (2%)	59 55

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	237	LEU
1	A	248	ARG
1	A	265	LYS
1	A	362	GLU
1	A	418	LEU
1	A	446	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	SEP	A	445	1	8,9,10	3.19	5 (62%)	8,12,14	5.34	5 (62%)
1	SEP	A	350	1	8,9,10	0.99	0	8,12,14	2.50	3 (37%)
1	PTR	A	369	1	15,16,17	1.24	2 (13%)	19,22,24	1.06	2 (10%)
1	TPO	A	512	1	8,10,11	1.78	1 (12%)	10,14,16	1.86	2 (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
1	SEP	A	445	1	-	3/5/8/10	-
1	SEP	A	350	1	-	0/5/8/10	-
1	PTR	A	369	1	-	3/10/11/13	0/1/1/1
1	TPO	A	512	1	-	3/9/11/13	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	445	SEP	P-OG	5.92	1.79	1.60
1	A	512	TPO	P-OG1	4.56	1.67	1.59
1	A	445	SEP	CB-CA	4.15	1.64	1.52
1	A	445	SEP	OG-CB	3.95	1.60	1.44
1	A	369	PTR	P-OH	-2.84	1.54	1.59
1	A	445	SEP	P-O2P	-2.43	1.45	1.54
1	A	445	SEP	P-O3P	-2.38	1.45	1.54
1	A	369	PTR	CE1-CZ	-2.28	1.34	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	445	SEP	OG-CB-CA	11.05	118.90	108.14
1	A	445	SEP	P-OG-CB	6.11	135.11	118.30
1	A	445	SEP	O2P-P-OG	6.07	122.88	106.73
1	A	445	SEP	OG-P-O1P	-4.81	92.98	106.47
1	A	350	SEP	OG-CB-CA	-4.60	103.67	108.14
1	A	512	TPO	P-OG1-CB	-4.36	110.02	123.21
1	A	350	SEP	OG-P-O1P	-3.65	96.23	106.47
1	A	350	SEP	O3P-P-O2P	2.93	118.83	107.64
1	A	512	TPO	O3P-P-O1P	2.62	120.95	110.68
1	A	369	PTR	O3P-P-O2P	2.05	115.48	107.64
1	A	369	PTR	OH-CZ-CE1	2.00	125.19	119.23
1	A	445	SEP	O2P-P-O1P	2.00	118.51	110.68

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	445	SEP	N-CA-CB-OG
1	A	369	PTR	O-C-CA-CB
1	A	512	TPO	CB-OG1-P-O1P

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Mol	Chain	Res	Type	Atoms
1	A	512	TPO	CB-OG1-P-O3P
1	A	369	PTR	CA-CB-CG-CD1
1	A	369	PTR	CA-CB-CG-CD2
1	A	445	SEP	CB-OG-P-O2P
1	A	445	SEP	CA-CB-OG-P
1	A	512	TPO	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	512	TPO	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

12 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$
4	EDO	A	611	-	3,3,3	0.93	0	2,2,2	0.67	0
4	EDO	A	608	-	3,3,3	0.59	0	2,2,2	2.07	1 (50%)
4	EDO	A	604	-	3,3,3	0.49	0	2,2,2	0.31	0
3	PO4	A	603	-	4,4,4	0.52	0	6,6,6	1.21	0
4	EDO	A	609	-	3,3,3	0.24	0	2,2,2	0.98	0
3	PO4	A	602	-	4,4,4	1.45	2 (50%)	6,6,6	1.89	1 (16%)
2	HRM	A	601	-	18,18,18	2.06	6 (33%)	21,26,26	2.24	8 (38%)
4	EDO	A	605	-	3,3,3	0.59	0	2,2,2	0.19	0
4	EDO	A	610	-	3,3,3	1.06	0	2,2,2	1.19	0
5	GOL	A	612	-	5,5,5	1.18	1 (20%)	5,5,5	1.61	2 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	A	606	-	3,3,3	0.20	0	2,2,2	0.75	0
4	EDO	A	607	-	3,3,3	0.69	0	2,2,2	0.87	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
4	EDO	A	611	-	-	1/1/1/1	-
4	EDO	A	608	-	-	1/1/1/1	-
4	EDO	A	604	-	-	1/1/1/1	-
4	EDO	A	609	-	-	0/1/1/1	-
2	HRM	A	601	-	-	0/2/2/2	0/3/3/3
4	EDO	A	605	-	-	0/1/1/1	-
4	EDO	A	610	-	-	1/1/1/1	-
5	GOL	A	612	-	-	4/4/4/4	-
4	EDO	A	606	-	-	1/1/1/1	-
4	EDO	A	607	-	-	0/1/1/1	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HRM	CAB-CAL	-4.57	1.47	1.50
2	A	601	HRM	CAL-NAH	3.97	1.35	1.32
2	A	601	HRM	CAG-CAM	-3.08	1.37	1.41
2	A	601	HRM	CAE-CAC	2.72	1.40	1.36
2	A	601	HRM	CAE-CAO	-2.22	1.36	1.41
5	A	612	GOL	O2-C2	-2.17	1.36	1.43
2	A	601	HRM	CAL-CAP	2.15	1.46	1.43
3	A	602	PO4	P-O3	-2.04	1.48	1.54
3	A	602	PO4	P-O4	-2.01	1.48	1.54

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	HRM	CAB-CAL-NAH	-5.03	107.88	117.67
2	A	601	HRM	CAB-CAL-CAP	4.97	130.05	121.74
3	A	602	PO4	O3-P-O2	-3.85	95.61	107.97
2	A	601	HRM	OAJ-CAK-CAG	-3.14	115.87	124.43
4	A	608	EDO	O2-C2-C1	2.64	130.90	111.91
2	A	601	HRM	CAO-CAN-CAM	2.63	108.96	106.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	HRM	CAK-CAG-CAM	2.49	121.88	119.27
2	A	601	HRM	CAC-CAE-CAO	-2.36	117.74	119.77
5	A	612	GOL	C3-C2-C1	2.24	120.43	111.70
2	A	601	HRM	CAD-CAK-CAG	-2.22	117.82	120.81
2	A	601	HRM	CAD-CAF-CAN	-2.20	118.46	121.63
5	A	612	GOL	O3-C3-C2	2.20	120.74	110.20

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	612	GOL	O1-C1-C2-O2
5	A	612	GOL	O1-C1-C2-C3
5	A	612	GOL	C1-C2-C3-O3
4	A	604	EDO	O1-C1-C2-O2
5	A	612	GOL	O2-C2-C3-O3
4	A	608	EDO	O1-C1-C2-O2
4	A	606	EDO	O1-C1-C2-O2
4	A	611	EDO	O1-C1-C2-O2
4	A	610	EDO	O1-C1-C2-O2

There are no ring outliers.

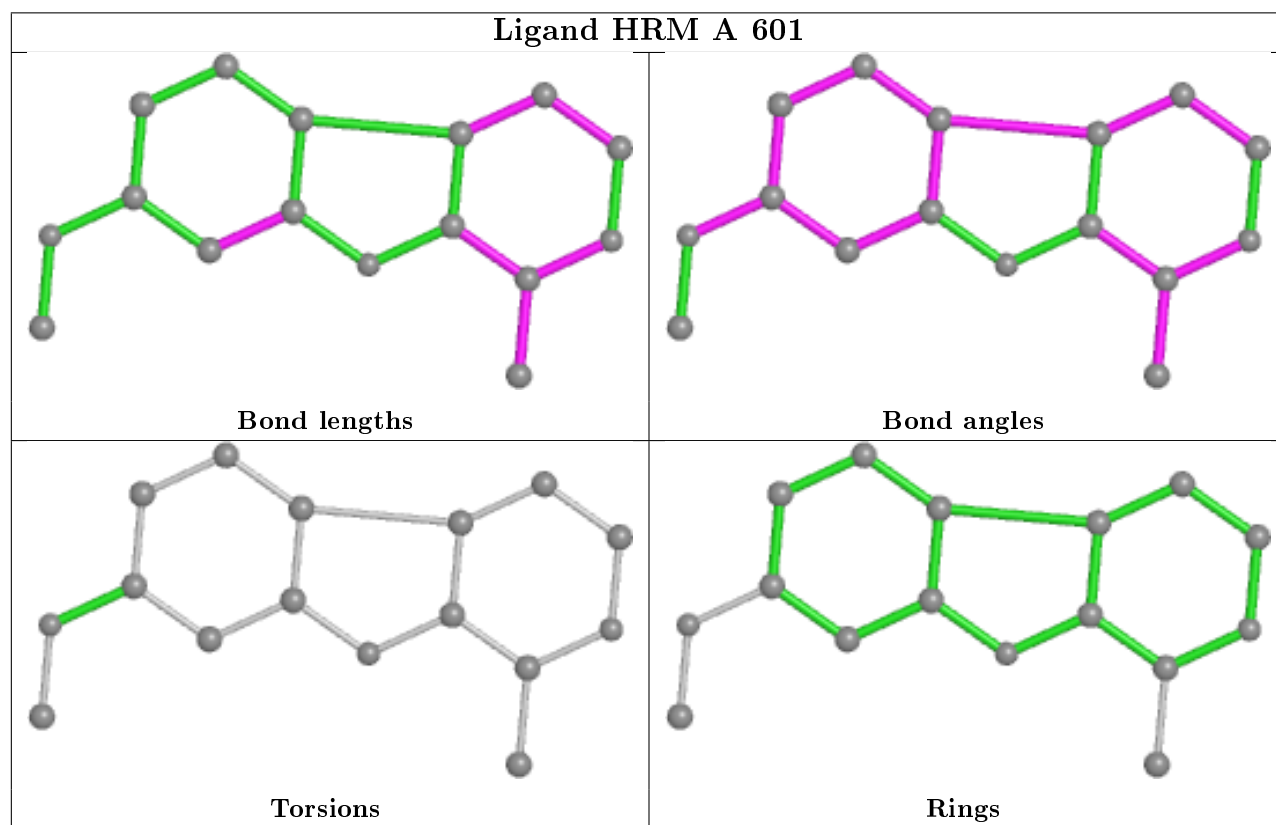
6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	611	EDO	1	0
4	A	608	EDO	5	0
3	A	603	PO4	1	0
4	A	609	EDO	1	0
4	A	610	EDO	2	0
5	A	612	GOL	1	1

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](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	391/588 (66%)	-0.02	17 (4%) 35 38	8, 17, 39, 68	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	266	THR	7.7
1	A	265	LYS	7.5
1	A	458	ALA	6.4
1	A	532	THR	5.2
1	A	267	GLY	4.5
1	A	459	ASP	4.1
1	A	457	GLN	3.1
1	A	434	GLU	2.9
1	A	471	ARG	2.7
1	A	431	LYS	2.6
1	A	456	THR	2.6
1	A	531	THR	2.6
1	A	346	HIS	2.6
1	A	435	GLN	2.3
1	A	460	GLY	2.2
1	A	139	VAL	2.1
1	A	264	ASP	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> 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
1	SEP	A	445	10/11	0.84	0.16	18,27,43,46	0
1	TPO	A	512	11/12	0.87	0.20	12,18,56,59	0
1	SEP	A	350	10/11	0.91	0.14	14,24,52,54	0
1	PTR	A	369	16/17	0.99	0.08	10,10,12,12	0

### 6.3 Carbohydrates [i](#)

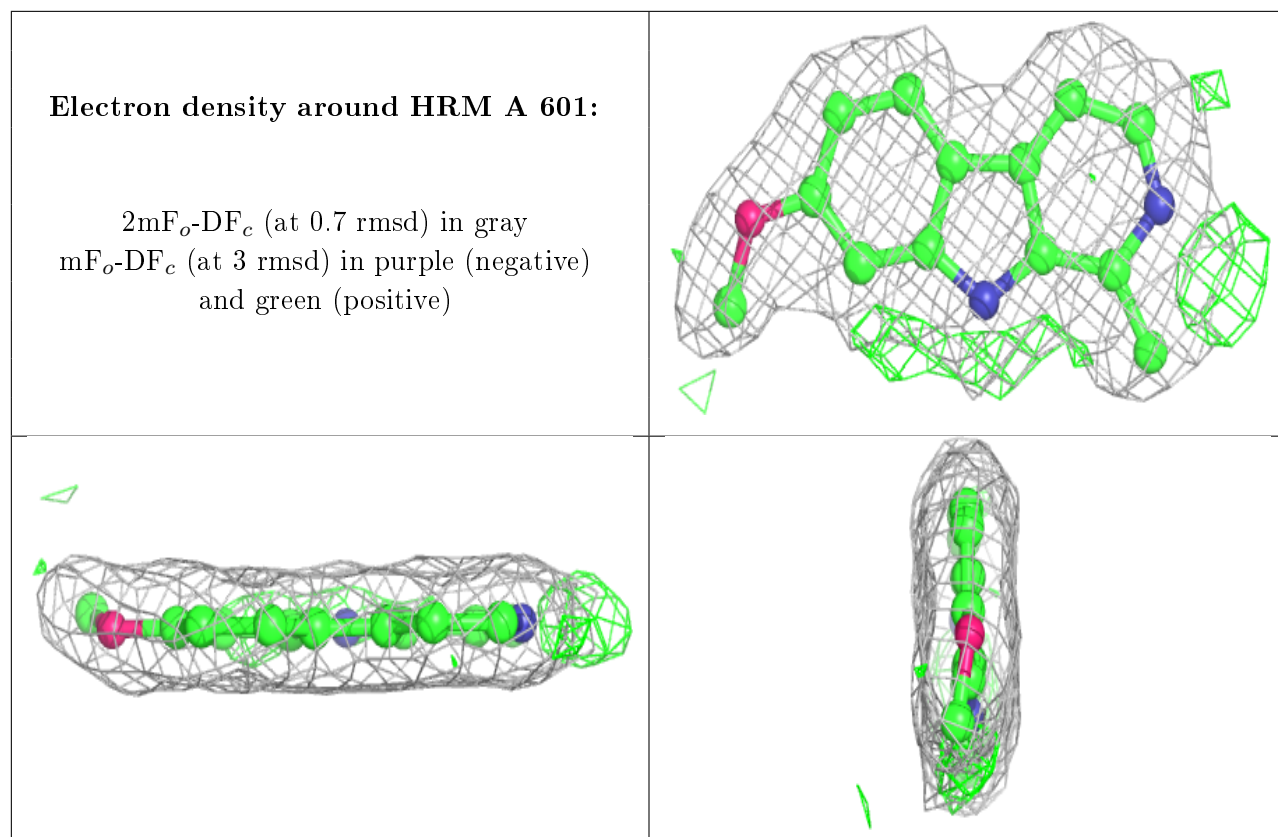
There are no carbohydrates in this entry.

### 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, 95<sup>th</sup> 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	EDO	A	611	4/4	0.73	0.37	41,48,50,50	0
4	EDO	A	610	4/4	0.74	0.28	33,37,41,48	0
4	EDO	A	608	4/4	0.84	0.17	31,32,34,35	0
5	GOL	A	612	6/6	0.86	0.23	27,35,36,40	0
4	EDO	A	604	4/4	0.89	0.09	34,36,39,40	0
4	EDO	A	607	4/4	0.90	0.13	28,29,35,41	0
4	EDO	A	609	4/4	0.92	0.13	35,37,40,45	0
4	EDO	A	606	4/4	0.92	0.11	24,26,29,34	0
3	PO4	A	603	5/5	0.92	0.21	40,42,50,51	0
3	PO4	A	602	5/5	0.95	0.11	31,41,44,47	0
2	HRM	A	601	16/16	0.95	0.14	12,14,23,25	0
4	EDO	A	605	4/4	0.96	0.11	14,18,23,27	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 [i](#)

There are no such residues in this entry.