



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:17 AM UTC

PDB ID : 5MO6 / pdb_00005mo6
Title : Crystal Structure of CK2alpha with N-(3-(((2-chloro-[1,1'-biphenyl]-4-yl)met
hyl)amino)propyl)methanesulfonamide bound
Authors : Brear, P.; De Fusco, C.; Georgiou, K.; Iegre, J.; Sore, H.; Hyvonen, M.; Spring,
D.
Deposited on : 2016-12-13
Resolution : 1.82 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

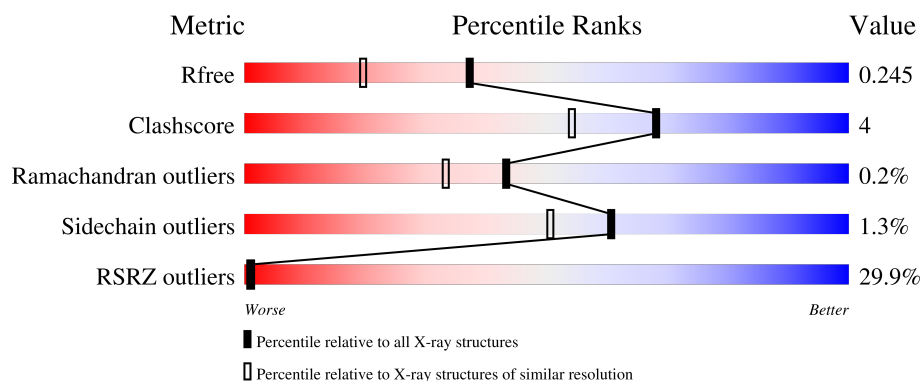
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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	352	10% 82% 10% 8%
1	B	352	45% 82% 9% 8%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5809 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 Casein kinase II subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	324	Total	C	N	O	S	0	4	0
			2770	1775	487	497	11			
1	A	325	Total	C	N	O	S	0	2	0
			2756	1766	482	497	11			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	GLY	-	expression tag	UNP P68400
B	-21	SER	-	expression tag	UNP P68400
B	-20	MET	-	expression tag	UNP P68400
B	-19	ASP	-	expression tag	UNP P68400
B	-18	ILE	-	expression tag	UNP P68400
B	-17	GLU	-	expression tag	UNP P68400
B	-16	PHE	-	expression tag	UNP P68400
B	-15	ASP	-	expression tag	UNP P68400
B	-14	ASP	-	expression tag	UNP P68400
B	-13	ASP	-	expression tag	UNP P68400
B	-12	ALA	-	expression tag	UNP P68400
B	-11	ASP	-	expression tag	UNP P68400
B	-10	ASP	-	expression tag	UNP P68400
B	-9	ASP	-	expression tag	UNP P68400
B	-8	GLY	-	expression tag	UNP P68400
B	-7	SER	-	expression tag	UNP P68400
B	-6	GLY	-	expression tag	UNP P68400
B	-5	SER	-	expression tag	UNP P68400
B	-4	GLY	-	expression tag	UNP P68400
B	-3	SER	-	expression tag	UNP P68400
B	-2	GLY	-	expression tag	UNP P68400
B	-1	SER	-	expression tag	UNP P68400
B	0	GLY	-	expression tag	UNP P68400
B	1	SER	-	expression tag	UNP P68400
B	21	SER	ARG	engineered mutation	UNP P68400

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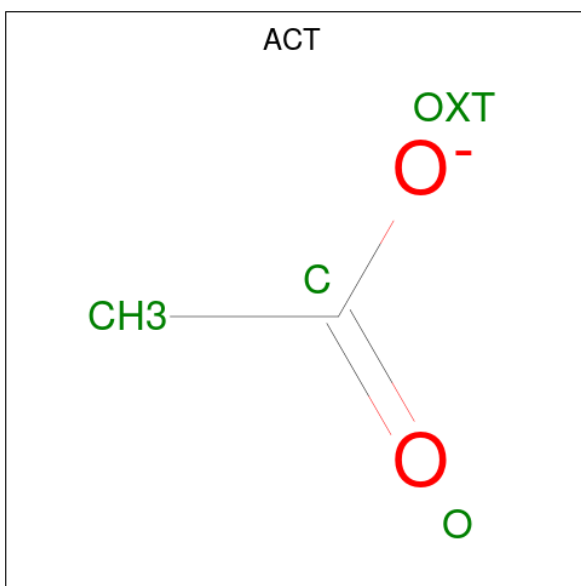
Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	GLY	-	expression tag	UNP P68400
A	-21	SER	-	expression tag	UNP P68400
A	-20	MET	-	expression tag	UNP P68400
A	-19	ASP	-	expression tag	UNP P68400
A	-18	ILE	-	expression tag	UNP P68400
A	-17	GLU	-	expression tag	UNP P68400
A	-16	PHE	-	expression tag	UNP P68400
A	-15	ASP	-	expression tag	UNP P68400
A	-14	ASP	-	expression tag	UNP P68400
A	-13	ASP	-	expression tag	UNP P68400
A	-12	ALA	-	expression tag	UNP P68400
A	-11	ASP	-	expression tag	UNP P68400
A	-10	ASP	-	expression tag	UNP P68400
A	-9	ASP	-	expression tag	UNP P68400
A	-8	GLY	-	expression tag	UNP P68400
A	-7	SER	-	expression tag	UNP P68400
A	-6	GLY	-	expression tag	UNP P68400
A	-5	SER	-	expression tag	UNP P68400
A	-4	GLY	-	expression tag	UNP P68400
A	-3	SER	-	expression tag	UNP P68400
A	-2	GLY	-	expression tag	UNP P68400
A	-1	SER	-	expression tag	UNP P68400
A	0	GLY	-	expression tag	UNP P68400
A	1	SER	-	expression tag	UNP P68400
A	21	SER	ARG	engineered mutation	UNP P68400

- Molecule 2 is 3-[3-[(3-chloranyl-4-phenyl-phenyl)methylamino]propylamino]-3-oxidanylidene-propanoic acid (CCD ID: KXZ) (formula: C₁₉H₂₁ClN₂O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			25	19	1	2	3		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



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

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).

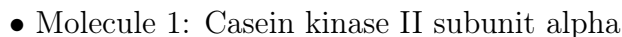


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	49	Total	O	0	0
			49	49		
5	A	191	Total	O	0	0
			191	191		

- Molecule 1: Casein kinase II subunit alpha



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	64.51Å 68.69Å 334.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	167.08 – 1.82 167.08 – 1.82	Depositor EDS
% Data completeness (in resolution range)	98.2 (167.08-1.82) 99.7 (167.08-1.82)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 1.82Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.213 , 0.231 0.226 , 0.245	Depositor DCC
R_{free} test set	3345 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	29.7	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5809	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% 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: KXZ, PO4, ACT

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	1.32	2/2831 (0.1%)	1.18	10/3830 (0.3%)
1	B	0.79	0/2849	1.15	3/3854 (0.1%)
All	All	1.09	2/5680 (0.0%)	1.17	13/7684 (0.2%)

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
1	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	20	PRO	C-N	-47.02	0.67	1.33
1	A	21	SER	C-N	-19.04	1.07	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	GLN	CB-CA-C	12.60	135.50	110.42
1	A	20	PRO	CA-C-N	12.44	145.31	121.54
1	A	20	PRO	C-N-CA	12.44	145.31	121.54
1	A	237	ASP	CA-CB-CG	8.95	121.55	112.60
1	A	126	GLN	N-CA-C	-7.75	94.29	110.80
1	A	314	THR	N-CA-C	-6.60	102.01	110.53
1	B	314	THR	N-CA-C	-6.45	102.22	110.53
1	B	175	ASP	N-CA-C	6.38	119.00	111.02
1	A	72	PRO	CA-C-N	5.76	130.28	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	PRO	C-N-CA	5.76	130.28	122.90
1	A	197	PHE	CA-CB-CG	-5.72	108.08	113.80
1	A	34	GLY	N-CA-C	-5.34	105.25	112.57
1	B	117	ASN	CA-CB-CG	5.15	117.75	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	19[A]	ARG	Sidechain

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	2756	0	2689	24	0
1	B	2770	0	2709	19	1
2	A	25	0	0	1	0
3	A	8	0	6	0	0
4	A	10	0	0	0	0
5	A	191	0	0	2	1
5	B	49	0	0	0	1
All	All	5809	0	5404	40	2

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 (40) 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:20:PRO:C	1:A:21:SER:CA	2.05	1.28
1:A:20:PRO:CA	1:A:21:SER:N	1.96	1.27
1:A:20:PRO:O	1:A:21:SER:N	1.67	1.22
1:A:20:PRO:C	1:A:21:SER:N	0.67	0.77
1:A:225:MET:HG3	2:A:401:KXZ:C15	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:SER:HB3	1:B:230:GLU:HG2	1.74	0.69
1:A:124:LEU:HD23	1:A:128:LEU:HD21	1.80	0.63
1:A:33:TRP:CE3	1:A:100:ILE:HG22	2.34	0.62
1:B:105:VAL:HG11	1:A:20:PRO:HD2	1.84	0.59
1:B:107:ARG:HH22	1:A:89:ARG:HH11	1.51	0.57
1:B:124:LEU:O	1:B:128:LEU:HG	2.07	0.54
1:B:118:ASN:HD22	1:B:164:ILE:H	1.54	0.54
1:A:33:TRP:CZ3	1:A:100:ILE:HG22	2.42	0.54
1:B:50:TYR:CD1	1:B:73:VAL:HG21	2.44	0.52
1:A:118:ASN:HD22	1:A:164:ILE:H	1.57	0.51
1:B:124:LEU:HD22	1:B:128:LEU:HD21	1.92	0.51
1:A:20:PRO:C	1:A:21:SER:C	2.77	0.51
1:A:288:GLU:HG3	5:A:557:HOH:O	2.13	0.48
1:B:5:VAL:HB	1:B:261:TYR:HA	1.94	0.48
1:A:124:LEU:CD2	1:A:128:LEU:HD21	2.42	0.47
1:A:5:VAL:HB	1:A:261:TYR:HA	1.96	0.46
1:A:47:ARG:HG3	1:A:52:GLU:HG3	1.96	0.46
1:B:103:ASP:HB3	1:B:106:SER:OG	2.16	0.46
1:A:163:MET:HE2	1:A:174:ILE:HD13	1.98	0.45
1:B:36:GLN:HG3	1:B:101:VAL:HG21	1.98	0.44
1:B:47:ARG:HG3	1:B:52:GLU:HG3	1.99	0.44
1:B:255:TYR:HA	1:B:258:ILE:HG12	1.98	0.44
1:A:137:MET:HE1	1:A:218:LEU:HG	1.99	0.44
1:B:255:TYR:CD1	1:B:258:ILE:HD11	2.52	0.43
1:B:163:MET:HE2	1:B:174:ILE:HD13	2.00	0.43
1:A:103:ASP:HB3	1:A:106:SER:OG	2.19	0.43
1:B:125:TYR:HA	1:B:128:LEU:HD12	2.01	0.42
1:B:14:ASP:HB3	1:B:17:THR:OG1	2.19	0.42
1:A:244:ARG:HD3	5:A:610:HOH:O	2.19	0.42
1:B:31:VAL:HG13	1:B:100:ILE:HD12	2.01	0.42
1:A:70:LEU:HD13	1:A:78:ILE:HG12	2.02	0.41
1:A:20:PRO:HA	1:A:21:SER:N	2.19	0.41
1:A:50:TYR:HB3	1:A:71:LYS:HB2	2.03	0.41
1:B:33:TRP:CD1	1:A:90:GLY:HA3	2.56	0.40
1:B:50:TYR:HB3	1:B:71:LYS:HB2	2.03	0.40

All (2) 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)
5:A:662:HOH:O	5:A:662:HOH:O[4_597]	1.08	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:LYS:CE	5:B:427:HOH:O[5_545]	2.04	0.16

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	325/352 (92%)	311 (96%)	13 (4%)	1 (0%)	36	26
1	B	326/352 (93%)	314 (96%)	12 (4%)	0	100	100
All	All	651/704 (92%)	625 (96%)	25 (4%)	1 (0%)	43	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	SER

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	301/319 (94%)	298 (99%)	3 (1%)	68	60
1	B	303/319 (95%)	298 (98%)	5 (2%)	53	41
All	All	604/638 (95%)	596 (99%)	8 (1%)	61	50

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	100	ILE
1	B	105	VAL
1	B	170	LYS
1	B	230	GLU
1	B	288	GLU
1	A	105	VAL
1	A	170	LYS
1	A	180	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	62	ASN
1	B	118	ASN
1	B	186	GLN
1	B	262	ASN
1	B	270	ASN
1	A	118	ASN
1	A	168	HIS
1	A	186	GLN
1	A	262	ASN
1	A	270	ASN

5.3.3 RNA [i](#)

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](#)

5 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	PO4	A	404	-	4,4,4	2.65	2 (50%)	6,6,6	0.76	0
3	ACT	A	402	-	3,3,3	1.32	0	3,3,3	0.94	0
4	PO4	A	405	-	4,4,4	2.58	2 (50%)	6,6,6	0.71	0
3	ACT	A	403	-	3,3,3	1.39	0	3,3,3	0.91	0
2	KXZ	A	401	-	26,26,26	0.18	0	33,33,33	0.33	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
2	KXZ	A	401	-	-	4/17/17/17	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	404	PO4	P-O1	4.45	1.60	1.50
4	A	405	PO4	P-O1	4.29	1.60	1.50
4	A	404	PO4	P-O3	2.08	1.60	1.54
4	A	405	PO4	P-O2	2.04	1.60	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

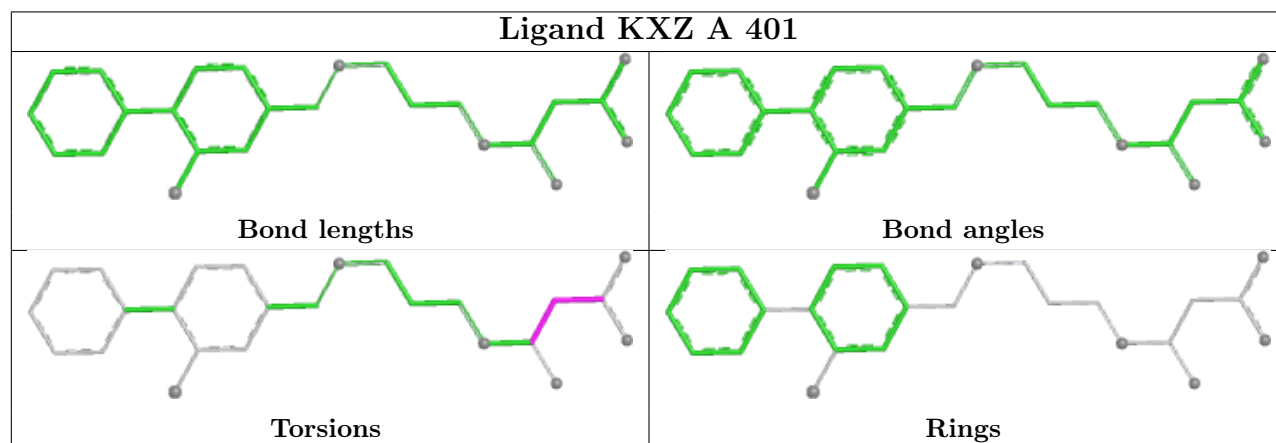
Mol	Chain	Res	Type	Atoms
2	A	401	KXZ	O-C-C1-C2
2	A	401	KXZ	O1-C-C1-C2
2	A	401	KXZ	C-C1-C2-O2
2	A	401	KXZ	C-C1-C2-N

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	KXZ	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 [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
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	21:SER	C	22:GLU	N	1.07
1	A	20:PRO	C	21:SER	N	0.67

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	325/352 (92%)	0.53	34 (10%)	11 12	9, 27, 58, 103	2 (0%)
1	B	324/352 (92%)	2.03	160 (49%)	0 0	19, 62, 107, 124	4 (1%)
All	All	649/704 (92%)	1.28	194 (29%)	1 1	9, 43, 99, 124	6 (0%)

All (194) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	124	LEU	8.9
1	A	125	TYR	8.2
1	A	121	PHE	7.7
1	B	121	PHE	6.4
1	B	327	VAL	6.3
1	B	33	TRP	5.8
1	B	265	LEU	5.3
1	B	269	PHE	5.3
1	B	281	TRP	5.2
1	B	124	LEU	5.1
1	B	105	VAL	5.1
1	B	206	TYR	5.0
1	B	258	ILE	4.9
1	B	128	LEU	4.9
1	B	263	ILE	4.8
1	A	33	TRP	4.8
1	B	35	ASN	4.7
1	B	50	TYR	4.6
1	B	257	TYR	4.6
1	B	119	THR	4.5
1	B	284	PHE	4.5
1	B	272	ILE	4.5
1	B	125	TYR	4.4
1	B	254	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	5	VAL	4.4
1	B	285	VAL	4.4
1	B	251	THR	4.3
1	B	103	ASP	4.3
1	B	248	VAL	4.3
1	A	50	TYR	4.3
1	B	292	LEU	4.2
1	A	107	ARG	4.2
1	B	45	LEU	4.2
1	B	226	ILE	4.2
1	A	105	VAL	4.1
1	B	48	GLY	4.1
1	B	255	TYR	3.9
1	A	73	VAL	3.9
1	B	247	LYS	3.9
1	B	36	GLN	3.9
1	B	249	LEU	3.9
1	B	46	GLY	3.9
1	B	100	ILE	3.9
1	B	300	PHE	3.8
1	B	305	LEU	3.7
1	B	227	PHE	3.7
1	B	34	GLY	3.7
1	A	120	ASP	3.7
1	B	19[A]	ARG	3.7
1	B	282	GLU	3.7
1	B	116	VAL	3.7
1	B	267	PRO	3.7
1	A	119	THR	3.6
1	B	261	TYR	3.6
1	B	102	LYS	3.6
1	A	327	VAL	3.6
1	B	307	TYR	3.6
1	A	104	PRO	3.5
1	B	30	VAL	3.5
1	A	128	LEU	3.5
1	B	297	ALA	3.5
1	B	182	TYR	3.4
1	B	273	LEU	3.4
1	B	104	PRO	3.4
1	B	59	ILE	3.4
1	B	73	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	106	SER	3.4
1	B	298	LEU	3.4
1	B	225	MET	3.4
1	B	17	THR	3.3
1	B	184	PRO	3.3
1	A	122	LYS	3.3
1	B	250	GLY	3.3
1	A	123	GLN	3.2
1	B	266	ASP	3.2
1	B	31	VAL	3.2
1	B	127	THR	3.2
1	B	72	PRO	3.2
1	B	301	LEU	3.2
1	B	57	ILE	3.2
1	B	107	ARG	3.1
1	B	279	LYS	3.1
1	B	117	ASN	3.1
1	B	286	HIS	3.1
1	B	53	VAL	3.1
1	A	288	GLU	3.1
1	B	253	ASP	3.1
1	B	293	VAL	3.1
1	B	49	LYS	3.1
1	B	211	TYR	3.0
1	B	303	LYS	3.0
1	B	304	LEU	3.0
1	B	233	PHE	3.0
1	B	130	ASP	3.0
1	B	122	LYS	3.0
1	B	60	THR	3.0
1	A	74	LYS	3.0
1	B	278	ARG	3.0
1	B	204	VAL	2.9
1	B	64	LYS	2.9
1	B	308	ASP	2.9
1	B	51	SER	2.9
1	B	71	LYS	2.9
1	A	49	LYS	2.9
1	B	185	GLY	2.9
1	B	239	TYR	2.9
1	B	61	ASN	2.9
1	B	270	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	123	GLN	2.8
1	B	41	LEU	2.8
1	B	276	HIS	2.8
1	B	135	PHE	2.8
1	B	232	PHE	2.8
1	A	36	GLN	2.8
1	B	43	ARG	2.8
1	B	166	HIS	2.8
1	B	245	ILE	2.8
1	B	295	PRO	2.8
1	B	283	ARG	2.7
1	A	71	LYS	2.7
1	B	62	ASN	2.7
1	B	129	THR	2.7
1	A	103	ASP	2.7
1	B	44	LYS	2.7
1	A	35	ASN	2.7
1	B	18	HIS	2.7
1	B	216	TRP	2.6
1	B	186	GLN	2.6
1	B	326	THR	2.6
1	B	268	ARG	2.6
1	A	126	GLN	2.6
1	B	131	TYR	2.6
1	B	4	PRO	2.6
1	B	47	ARG	2.6
1	B	222	LEU	2.6
1	B	9	ALA	2.6
1	B	311[A]	SER	2.6
1	A	127	THR	2.6
1	B	54	PHE	2.5
1	B	290	GLN	2.5
1	B	302	ASP	2.5
1	A	265	LEU	2.5
1	B	63	GLU	2.5
1	B	324	PHE	2.5
1	B	274	GLY	2.5
1	A	72	PRO	2.5
1	B	205	ASP	2.5
1	B	76	LYS	2.5
1	B	22	GLU	2.5
1	B	101	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	75	LYS	2.5
1	B	120	ASP	2.4
1	A	205	ASP	2.4
1	B	277	SER	2.4
1	B	323	TYR	2.4
1	A	41	LEU	2.4
1	B	70	LEU	2.4
1	B	325	TYR	2.4
1	B	8	ARG	2.3
1	B	40	GLN	2.3
1	A	34	GLY	2.3
1	B	316	ARG	2.3
1	B	138	TYR	2.3
1	B	259	ASP	2.3
1	B	6	PRO	2.3
1	B	74	LYS	2.3
1	B	313	LEU	2.3
1	B	321	HIS	2.2
1	B	108	THR	2.2
1	B	24	TRP	2.2
1	A	47	ARG	2.2
1	A	59	ILE	2.2
1	B	11	VAL	2.2
1	A	31	VAL	2.2
1	B	37	ASP	2.1
1	B	42	VAL	2.1
1	B	190	VAL	2.1
1	B	29	HIS	2.1
1	B	296	GLU	2.1
1	B	26	TYR	2.1
1	B	133	ILE	2.1
1	B	271	ASP	2.1
1	B	275	ARG	2.1
1	B	291	HIS	2.1
1	B	280	ARG	2.1
1	B	170	LYS	2.1
1	B	287	SER	2.0
1	B	163	MET	2.0
1	B	56	ALA	2.0
1	B	169	ARG	2.0
1	A	63	GLU	2.0
1	A	57	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	262	ASN	2.0
1	B	312	ARG	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](#)

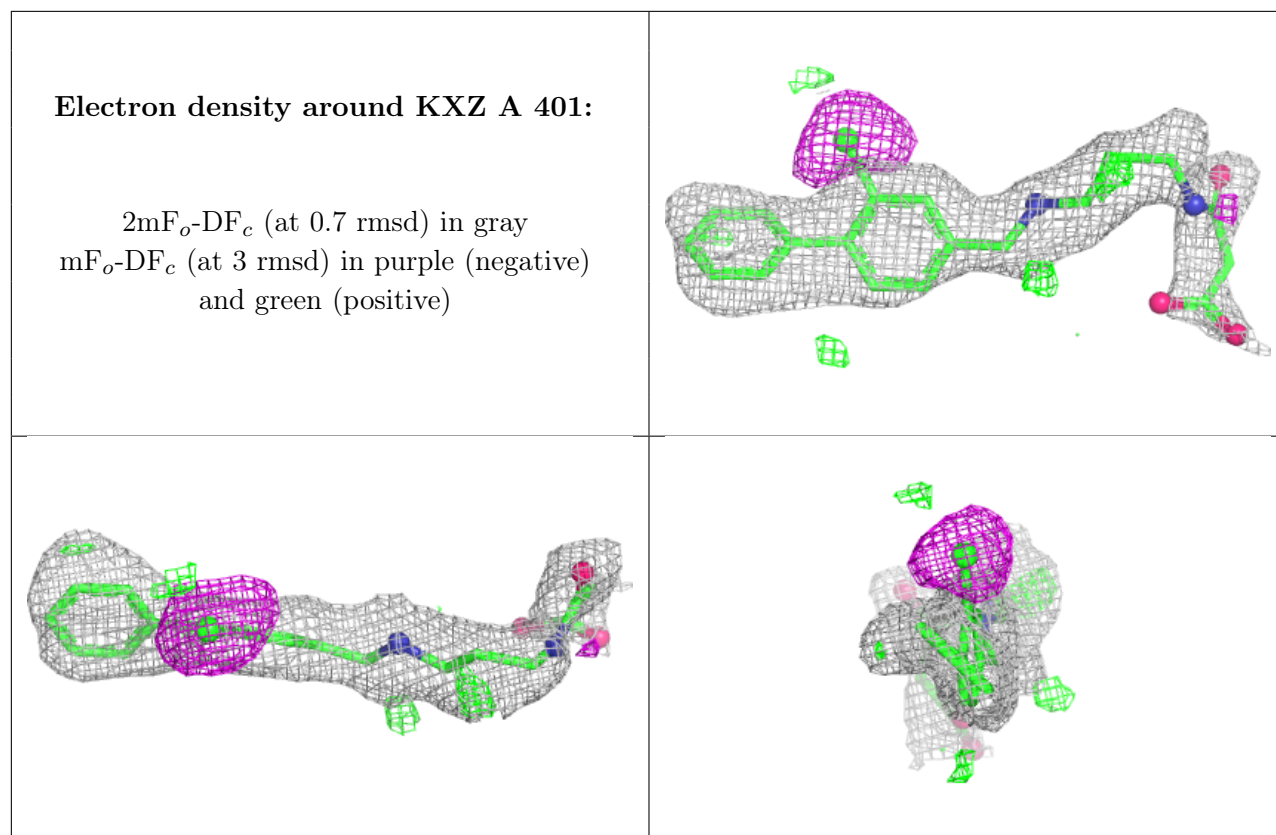
There are no oligosaccharides in this entry.

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
2	KXZ	A	401	25/25	0.67	0.19	41,53,74,75	0
3	ACT	A	402	4/4	0.79	0.14	31,32,34,37	0
4	PO4	A	405	5/5	0.84	0.10	55,57,60,64	0
4	PO4	A	404	5/5	0.85	0.12	50,51,54,56	0
3	ACT	A	403	4/4	0.97	0.06	28,32,35,40	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.