



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:17 AM UTC

PDB ID : 5XP5 / pdb_00005xp5
Title : C-Src in complex with ATP-Chf
Authors : Duan, Y.; Guo, M.; Dai, S.; Chen, L.; Chen, Y.
Deposited on : 2017-06-01
Resolution : 2.10 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

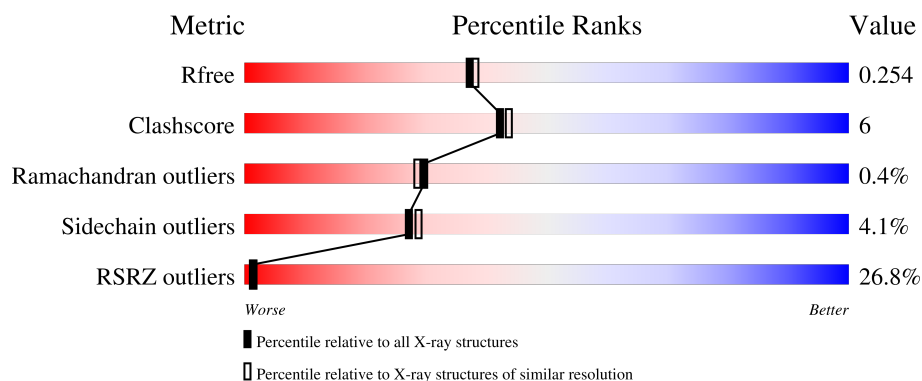
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	286	28% 72% 18% • 7%
1	B	286	22% 83% 9% • 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4543 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.

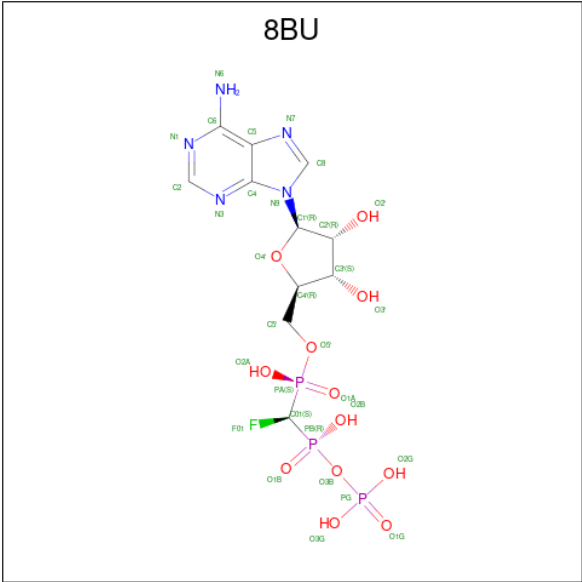
- Molecule 1 is a protein called Proto-oncogene tyrosine-protein kinase Src.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2145	1378	359	391	17			
1	B	267	Total	C	N	O	S	0	0	0
			2145	1378	359	391	17			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	248	GLY	-	expression tag	UNP P00523
A	249	HIS	-	expression tag	UNP P00523
A	250	MET	-	expression tag	UNP P00523
B	248	GLY	-	expression tag	UNP P00523
B	249	HIS	-	expression tag	UNP P00523
B	250	MET	-	expression tag	UNP P00523

- Molecule 2 is [(2R,3S,4R,5R)-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-[(S)-fluoranyl-[oxidanyl(phosphonooxy)phosphoryl]methyl]phosphinic acid (CCD ID: 8BU) (formula: C₁₁H₁₇FN₅O₁₂P₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	P	0	0
			32	11	1	5	12	3		
2	B	1	Total	C	F	N	O	P	0	0
			32	11	1	5	12	3		

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

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

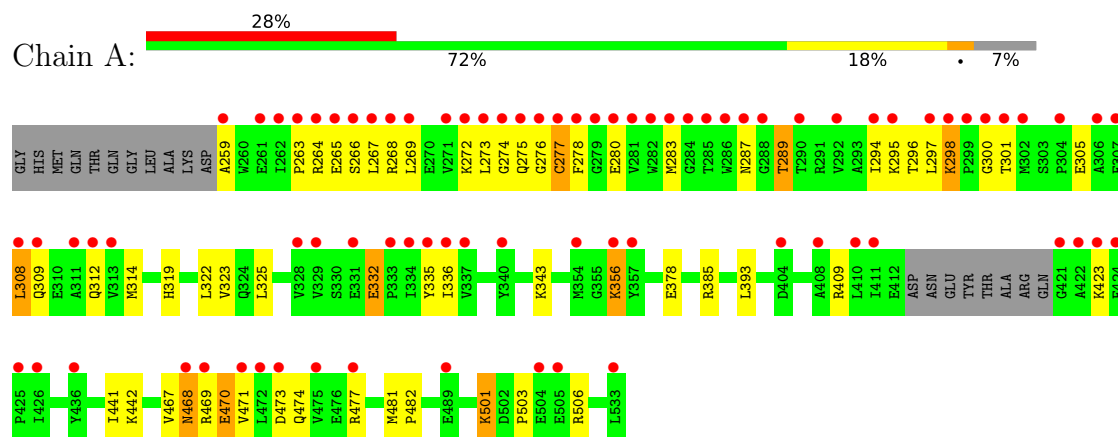
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	91	Total	O	0	0
			91	91		
4	B	96	Total	O	0	0
			96	96		

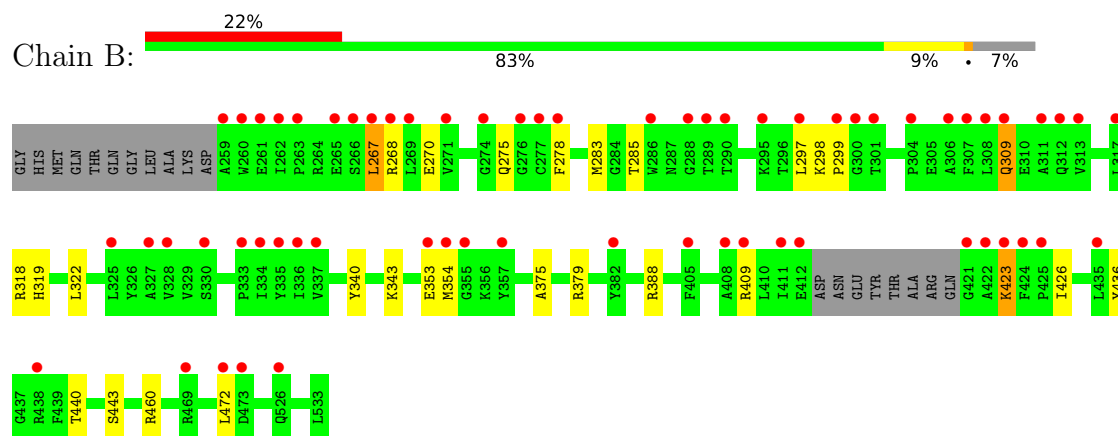
3 Residue-property plots [i](#)

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: Proto-oncogene tyrosine-protein kinase Src



- Molecule 1: Proto-oncogene tyrosine-protein kinase Src



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	42.29Å 63.69Å 73.81Å 79.07° 89.23° 89.24°	Depositor
Resolution (Å)	43.45 – 2.10 43.45 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.7 (43.45-2.10) 93.7 (43.45-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.218 , 0.246 0.227 , 0.254	Depositor DCC
R_{free} test set	1985 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4543	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.08% 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, 8BU

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	0.37	0/2197	0.85	4/2973 (0.1%)
1	B	0.32	0/2197	0.77	2/2973 (0.1%)
All	All	0.35	0/4394	0.81	6/5946 (0.1%)

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	A	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	278	PHE	N-CA-C	-7.11	103.71	112.88
1	A	468	ASN	N-CA-C	6.90	119.68	111.33
1	A	470	GLU	N-CA-C	-6.03	104.83	111.82
1	B	298	LYS	CA-C-N	5.56	125.88	119.93
1	B	298	LYS	C-N-CA	5.56	125.88	119.93
1	A	332	GLU	N-CA-C	5.36	116.42	109.72

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	298	LYS	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2145	0	2139	37	0
1	B	2145	0	2139	17	0
2	A	32	0	0	1	0
2	B	32	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	91	0	0	4	1
4	B	96	0	0	6	1
All	All	4543	0	4278	54	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 6.

All (54) 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:B:460:ARG:NH1	4:B:703:HOH:O	2.07	0.85
1:A:501:LYS:O	4:A:701:HOH:O	2.00	0.79
1:B:436:TYR:OH	4:B:702:HOH:O	2.06	0.73
1:A:343:LYS:O	4:A:702:HOH:O	2.08	0.69
1:A:297:LEU:HD21	1:A:301:THR:H	1.60	0.67
1:A:264:ARG:HE	1:A:335:TYR:HE2	1.41	0.67
1:B:270:GLU:OE2	1:B:285:THR:OG1	2.16	0.59
1:A:274:GLY:HA3	2:A:601:8BU:C5'	2.36	0.56
1:A:423:LYS:HB3	4:A:756:HOH:O	2.05	0.55
1:B:309:GLN:N	1:B:309:GLN:OE1	2.42	0.53
1:A:263:PRO:O	1:A:266:SER:OG	2.26	0.53
1:A:470:GLU:O	1:A:474:GLN:HG2	2.08	0.53
1:A:378:GLU:HG3	1:A:441:ILE:HG12	1.91	0.52
1:A:305:GLU:HG3	1:A:308:LEU:HD23	1.92	0.52
1:A:259:ALA:HB3	4:A:703:HOH:O	2.11	0.51
1:B:319:HIS:HB3	1:B:322:LEU:HG	1.91	0.51
1:A:503:PRO:HA	1:A:506:ARG:CZ	2.41	0.51
1:A:473:ASP:O	1:A:477:ARG:HG3	2.11	0.50
1:A:468:ASN:O	1:A:471:VAL:HB	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:GLU:HA	1:A:308:LEU:HB3	1.94	0.49
1:B:440:THR:O	1:B:443:SER:OG	2.31	0.48
1:B:426:ILE:H	1:B:426:ILE:HD12	1.78	0.48
1:A:269:LEU:H	1:A:269:LEU:HD12	1.79	0.48
1:A:264:ARG:HA	1:A:267:LEU:HD13	1.96	0.47
1:B:343:LYS:O	4:B:704:HOH:O	2.20	0.47
1:A:273:LEU:HD11	1:A:283:MET:HB2	1.97	0.46
1:A:287:ASN:HB2	1:A:289:THR:HG22	1.98	0.45
1:A:442:LYS:NZ	1:A:506:ARG:O	2.46	0.45
1:A:314:MET:HE2	1:A:325:LEU:HB2	1.99	0.45
1:B:423:LYS:HB2	1:B:423:LYS:HE2	1.74	0.45
1:B:278:PHE:HZ	2:B:601:8BU:O2B	2.01	0.44
1:A:305:GLU:O	1:A:308:LEU:HB3	2.17	0.44
1:B:267:LEU:HA	1:B:285:THR:O	2.17	0.44
1:A:467:VAL:O	1:A:471:VAL:HG23	2.18	0.44
1:A:297:LEU:HD23	1:A:298:LYS:O	2.18	0.43
1:A:263:PRO:HB2	1:A:265:GLU:HG2	2.00	0.43
1:B:388:ARG:NH1	4:B:713:HOH:O	2.45	0.43
1:A:272:LYS:HD2	1:A:280:GLU:OE2	2.19	0.43
1:B:297:LEU:O	1:B:299:PRO:HD3	2.19	0.43
1:A:287:ASN:C	1:A:289:THR:H	2.27	0.42
1:A:276:GLY:O	1:A:277:CYS:HB2	2.19	0.42
1:B:283:MET:HG3	1:B:340:TYR:CE1	2.54	0.42
1:A:269:LEU:HG	1:A:294:ILE:HD13	2.02	0.41
1:A:385:ARG:HH12	1:A:409:ARG:HH21	1.68	0.41
1:A:385:ARG:NH1	1:A:409:ARG:HH21	2.18	0.41
1:B:353:GLU:OE2	4:B:705:HOH:O	2.22	0.41
1:B:375:ALA:O	1:B:379:ARG:HG3	2.20	0.41
1:A:295:LYS:HB3	1:A:336:ILE:HB	2.02	0.41
1:B:318:ARG:NH2	4:B:717:HOH:O	2.53	0.41
1:A:319:HIS:HB3	1:A:322:LEU:HG	2.02	0.41
1:A:273:LEU:CD1	1:A:283:MET:HB2	2.50	0.40
1:A:323:VAL:HG21	1:A:393:LEU:HD12	2.02	0.40
1:A:356:LYS:HB3	1:A:356:LYS:HE3	1.64	0.40
1:A:481:MET:HA	1:A:482:PRO:HD3	1.92	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)
4:A:786:HOH:O	4:B:784:HOH:O[1_554]	2.11	0.09

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	263/286 (92%)	246 (94%)	15 (6%)	2 (1%)	16	12
1	B	263/286 (92%)	251 (95%)	12 (5%)	0	100	100
All	All	526/572 (92%)	497 (94%)	27 (5%)	2 (0%)	30	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	268	ARG
1	A	300	GLY

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	230/245 (94%)	219 (95%)	11 (5%)	23	23
1	B	230/245 (94%)	222 (96%)	8 (4%)	32	35
All	All	460/490 (94%)	441 (96%)	19 (4%)	27	29

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	275	GLN
1	A	277	CYS
1	A	289	THR
1	A	296	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	308	LEU
1	A	309	GLN
1	A	312	GLN
1	A	332	GLU
1	A	356	LYS
1	A	469	ARG
1	A	501	LYS
1	B	267	LEU
1	B	268	ARG
1	B	275	GLN
1	B	309	GLN
1	B	354	MET
1	B	409	ARG
1	B	423	LYS
1	B	472	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	312	GLN
1	A	528	GLN

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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	8BU	B	601	3	30,34,34	1.79	8 (26%)	47,54,54	2.56	13 (27%)
2	8BU	A	601	3	30,34,34	1.69	6 (20%)	47,54,54	2.37	17 (36%)

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	8BU	B	601	3	-	5/19/44/44	0/3/3/3
2	8BU	A	601	3	-	4/19/44/44	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	8BU	C5-C4	5.38	1.48	1.39
2	B	601	8BU	C5-C4	4.37	1.46	1.39
2	B	601	8BU	C5-N7	-3.94	1.31	1.39
2	B	601	8BU	C8-N9	-3.41	1.31	1.37
2	A	601	8BU	C5-N7	-2.93	1.33	1.39
2	B	601	8BU	PB-O2B	-2.81	1.50	1.56
2	A	601	8BU	PA-O5'	2.75	1.61	1.57
2	A	601	8BU	C5-C6	2.67	1.48	1.41
2	B	601	8BU	C5-C6	2.51	1.48	1.41
2	B	601	8BU	PA-O2A	-2.18	1.51	1.56
2	A	601	8BU	PB-O3B	2.13	1.60	1.58
2	A	601	8BU	PB-O2B	-2.08	1.51	1.56
2	B	601	8BU	C6-N1	-2.05	1.30	1.35
2	B	601	8BU	C4-N9	-2.03	1.33	1.37

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	8BU	C5-C4-N3	-9.71	113.35	126.72
2	A	601	8BU	C5-C4-N3	-7.98	115.74	126.72
2	B	601	8BU	N3-C4-N9	7.21	139.44	127.17
2	B	601	8BU	C4-C5-N7	-6.21	103.48	110.58
2	A	601	8BU	N3-C4-N9	6.00	137.37	127.17
2	A	601	8BU	C4-C5-N7	-5.35	104.47	110.58
2	B	601	8BU	C5-N7-C8	4.81	111.01	103.45
2	A	601	8BU	C5-N7-C8	4.33	110.25	103.45
2	B	601	8BU	C2-N3-C4	3.74	120.97	111.83
2	B	601	8BU	C6-C5-C4	3.34	121.74	117.18
2	A	601	8BU	C2-N3-C4	3.33	119.96	111.83
2	A	601	8BU	O2A-PA-O1A	2.96	118.78	111.58
2	B	601	8BU	O4'-C1'-N9	2.89	113.63	108.09
2	A	601	8BU	PB-O3B-PG	-2.88	122.14	132.45
2	A	601	8BU	O4'-C1'-N9	2.81	113.49	108.09
2	A	601	8BU	O1A-PA-C01	-2.77	106.33	113.19
2	A	601	8BU	C6-C5-C4	2.68	120.84	117.18
2	A	601	8BU	N9-C8-N7	-2.62	110.22	113.94
2	B	601	8BU	N9-C8-N7	-2.62	110.22	113.94
2	A	601	8BU	PA-O5'-C5'	-2.56	116.10	122.69
2	B	601	8BU	O3'-C3'-C2'	-2.46	103.94	111.82
2	B	601	8BU	PB-O3B-PG	-2.42	123.77	132.45
2	B	601	8BU	PA-O5'-C5'	-2.39	116.56	122.69
2	B	601	8BU	O2'-C2'-C3'	-2.32	104.39	111.82
2	A	601	8BU	C4-N9-C8	2.31	108.16	105.74
2	B	601	8BU	C4-N9-C8	2.22	108.06	105.74
2	A	601	8BU	C2'-C1'-N9	-2.08	108.14	113.30
2	A	601	8BU	C3'-C2'-C1'	2.04	105.33	101.46
2	A	601	8BU	O2B-PB-O1B	2.03	116.52	111.58
2	A	601	8BU	O5'-PA-O1A	-2.00	110.23	115.06

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	8BU	PA-C01-PB-O1B
2	B	601	8BU	PA-C01-PB-O1B
2	B	601	8BU	PA-C01-PB-O2B
2	B	601	8BU	O4'-C4'-C5'-O5'
2	B	601	8BU	C3'-C4'-C5'-O5'
2	A	601	8BU	C5'-O5'-PA-O2A
2	A	601	8BU	C4'-C5'-O5'-PA
2	B	601	8BU	C5'-O5'-PA-C01

Continued on next page...

Continued from previous page...

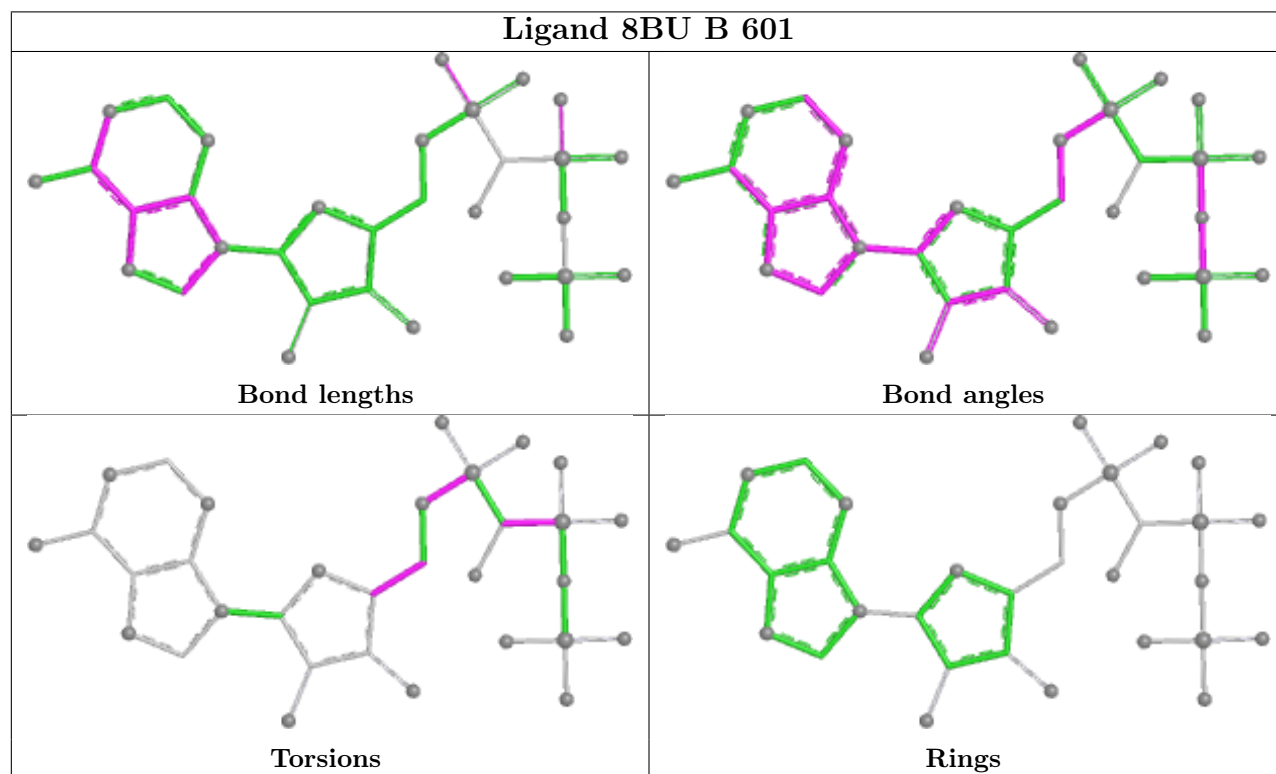
Mol	Chain	Res	Type	Atoms
2	A	601	8BU	PG-O3B-PB-O2B

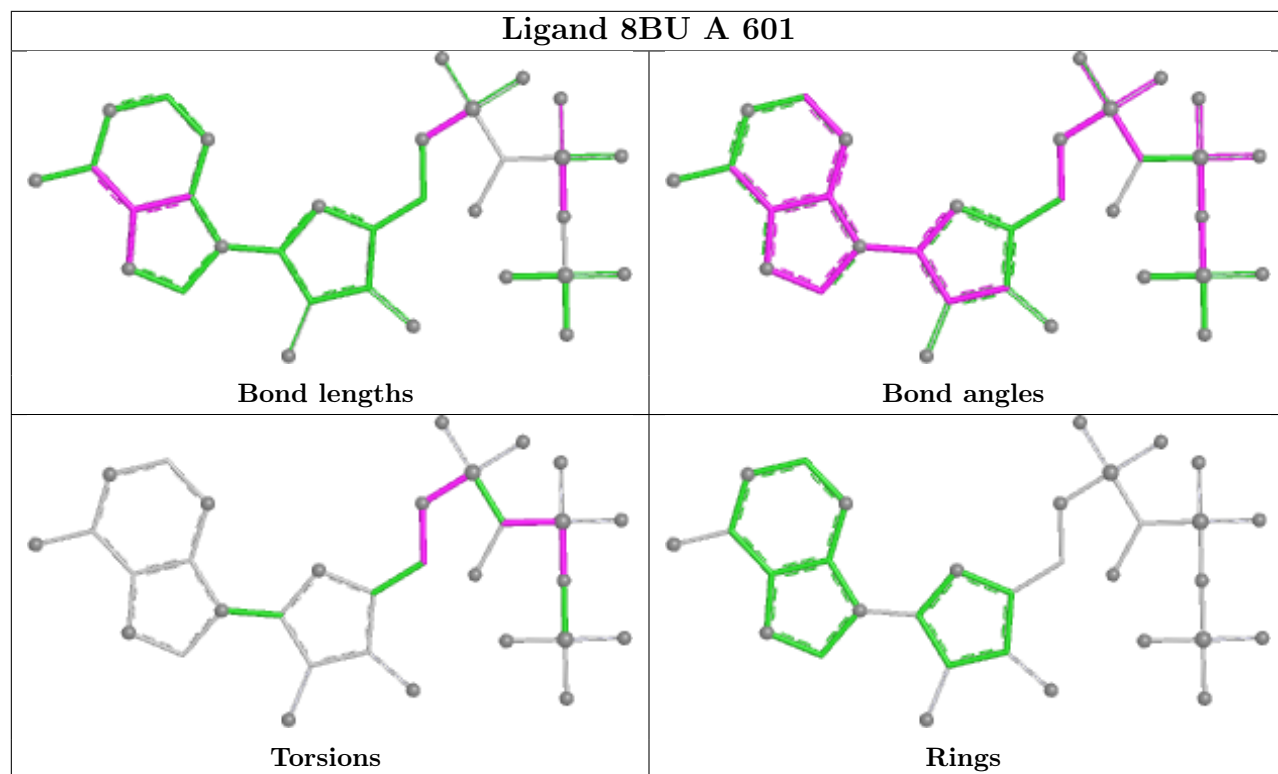
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	8BU	1	0
2	A	601	8BU	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](#)

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	267/286 (93%)	1.41	80 (29%)	1 1	27, 49, 104, 121	0
1	B	267/286 (93%)	1.20	63 (23%)	2 2	27, 50, 89, 114	0
All	All	534/572 (93%)	1.31	143 (26%)	1 1	27, 49, 98, 121	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	277	CYS	12.1
1	A	273	LEU	5.8
1	A	422	ALA	5.7
1	A	259	ALA	5.6
1	A	308	LEU	5.5
1	A	472	LEU	5.3
1	B	327	ALA	5.2
1	B	278	PHE	5.2
1	A	424	PHE	5.2
1	A	276	GLY	5.0
1	B	424	PHE	5.0
1	A	278	PHE	5.0
1	B	422	ALA	5.0
1	A	334	ILE	4.9
1	B	277	CYS	4.8
1	A	333	PRO	4.7
1	A	269	LEU	4.6
1	A	263	PRO	4.6
1	A	267	LEU	4.4
1	A	297	LEU	4.3
1	A	271	VAL	4.2
1	A	285	THR	4.2
1	A	423	LYS	4.1
1	B	421	GLY	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	354	MET	4.0
1	B	411	ILE	4.0
1	A	284	GLY	4.0
1	B	259	ALA	3.9
1	B	306	ALA	3.8
1	A	421	GLY	3.8
1	A	328	VAL	3.8
1	A	411	ILE	3.6
1	B	308	LEU	3.6
1	B	423	LYS	3.6
1	A	274	GLY	3.6
1	A	469	ARG	3.5
1	B	260	TRP	3.5
1	A	336	ILE	3.5
1	A	279	GLY	3.5
1	A	281	VAL	3.5
1	A	262	ILE	3.4
1	A	307	PHE	3.4
1	A	301	THR	3.4
1	A	302	MET	3.4
1	B	438	ARG	3.3
1	B	357	TYR	3.3
1	B	263	PRO	3.3
1	B	299	PRO	3.3
1	A	286	TRP	3.3
1	B	353	GLU	3.3
1	A	299	PRO	3.2
1	B	268	ARG	3.2
1	A	329	VAL	3.2
1	A	292	VAL	3.2
1	B	328	VAL	3.2
1	B	337	VAL	3.2
1	B	267	LEU	3.1
1	A	312	GLN	3.1
1	A	266	SER	3.1
1	A	354	MET	3.1
1	A	283	MET	3.0
1	A	335	TYR	3.0
1	B	265	GLU	2.9
1	A	471	VAL	2.9
1	A	357	TYR	2.9
1	A	282	TRP	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	330	SER	2.9
1	B	276	GLY	2.9
1	B	405	PHE	2.9
1	B	297	LEU	2.8
1	B	472	LEU	2.8
1	B	473	ASP	2.8
1	B	412	GLU	2.8
1	A	298	LYS	2.8
1	B	336	ILE	2.8
1	B	425	PRO	2.7
1	A	426	ILE	2.7
1	A	306	ALA	2.7
1	B	312	GLN	2.7
1	B	469	ARG	2.7
1	A	287	ASN	2.6
1	A	468	ASN	2.6
1	B	301	THR	2.6
1	B	304	PRO	2.6
1	B	435	LEU	2.6
1	A	340	TYR	2.6
1	B	382	TYR	2.6
1	A	295	LYS	2.6
1	B	307	PHE	2.6
1	B	355	GLY	2.6
1	A	275	GLN	2.5
1	B	309	GLN	2.5
1	A	268	ARG	2.5
1	A	473	ASP	2.5
1	A	309	GLN	2.5
1	A	313	VAL	2.5
1	B	300	GLY	2.5
1	A	477	ARG	2.5
1	B	317	LEU	2.5
1	A	288	GLY	2.5
1	B	262	ILE	2.5
1	B	334	ILE	2.5
1	A	265	GLU	2.5
1	A	331	GLU	2.5
1	B	408	ALA	2.5
1	A	264	ARG	2.5
1	A	304	PRO	2.4
1	A	408	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	533	LEU	2.4
1	A	337	VAL	2.4
1	A	475	VAL	2.4
1	B	290	THR	2.4
1	A	272	LYS	2.4
1	A	505	GLU	2.4
1	B	271	VAL	2.4
1	A	425	PRO	2.4
1	A	300	GLY	2.3
1	B	295	LYS	2.3
1	B	286	TRP	2.3
1	A	436	TYR	2.3
1	B	288	GLY	2.3
1	A	489	GLU	2.3
1	B	333	PRO	2.3
1	A	294	ILE	2.3
1	B	313	VAL	2.3
1	A	410	LEU	2.3
1	A	261	GLU	2.2
1	B	274	GLY	2.2
1	B	261	GLU	2.2
1	B	526	GLN	2.2
1	B	335	TYR	2.2
1	A	290	THR	2.2
1	A	280	GLU	2.1
1	A	504	GLU	2.1
1	B	311	ALA	2.1
1	B	409	ARG	2.1
1	B	266	SER	2.1
1	B	269	LEU	2.1
1	A	311	ALA	2.1
1	A	404	ASP	2.0
1	A	356	LYS	2.0
1	B	325	LEU	2.0
1	B	289	THR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

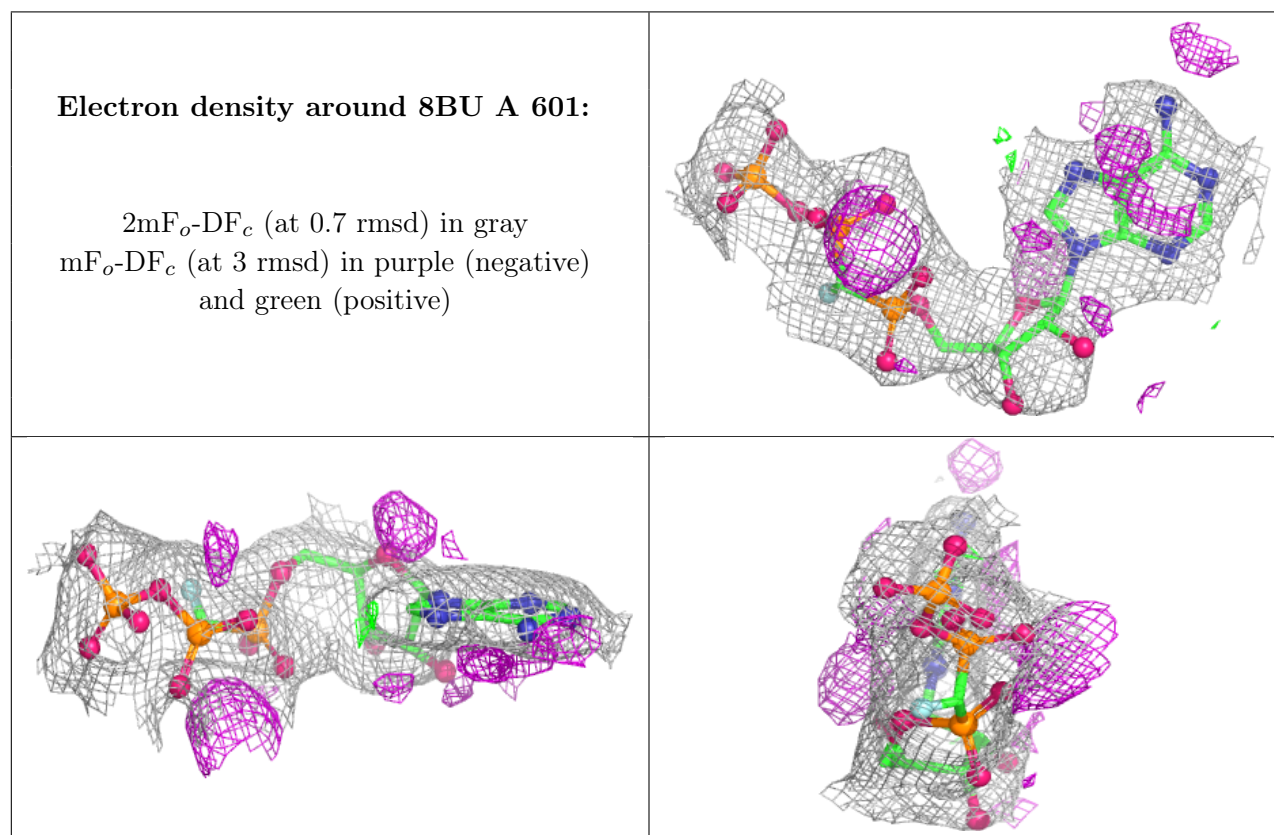
There are no oligosaccharides in this entry.

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.

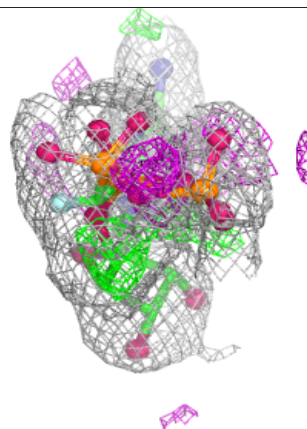
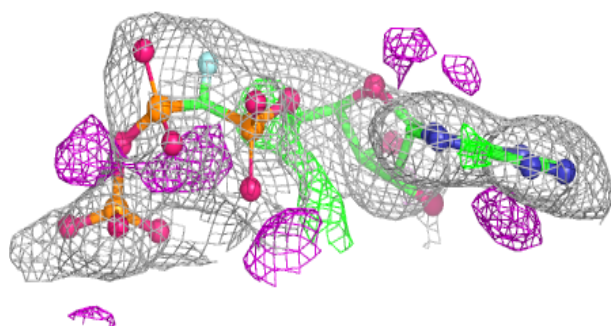
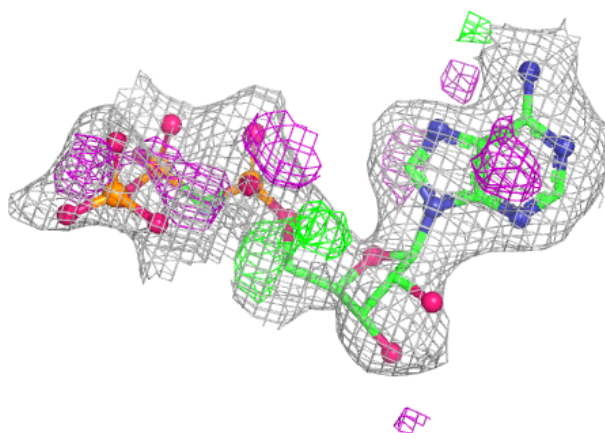
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	8BU	A	601	32/32	0.79	0.17	52,98,137,177	0
2	8BU	B	601	32/32	0.80	0.15	38,89,156,180	0
3	MG	A	602	1/1	0.89	0.35	30,30,30,30	0
3	MG	B	602	1/1	0.96	0.30	30,30,30,30	0

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 8BU B 601:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.