



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:41 PM UTC

PDB ID : 6WIW / pdb_00006wiw
Title : c-Src Bound to ATP-Competitive Inhibitor I14
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Deposited on : 2020-04-10
Resolution : 2.30 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

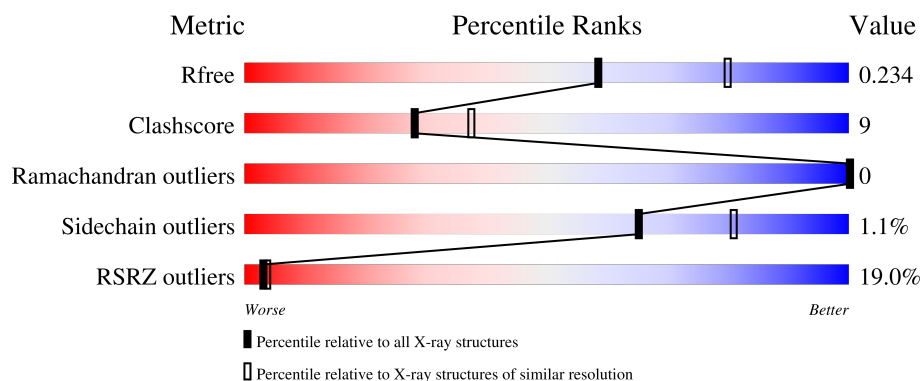
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	
1	B	286	

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
2	I14	A	601	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8643 atoms, of which 4190 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.

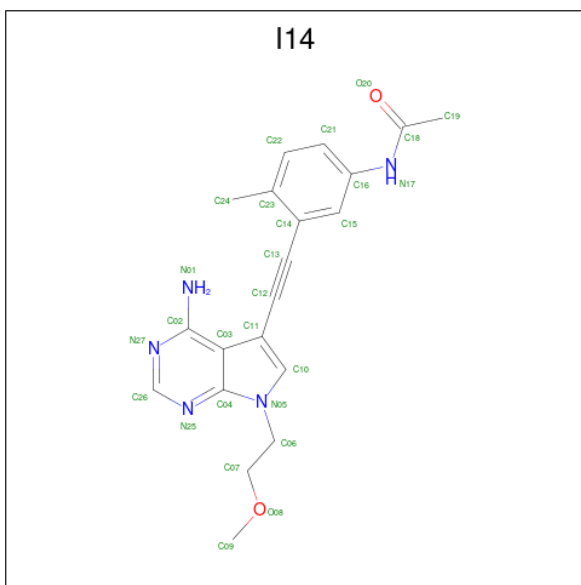
- Molecule 1 is a protein called Proto-oncogene tyrosine-protein kinase Src.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	255	Total	C	H	N	O	S	0	0	0
			4094	1315	2042	343	377	17			
1	B	262	Total	C	H	N	O	S	0	0	0
			4213	1353	2106	353	384	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 N-(3-{[4-amino-7-(2-methoxyethyl)-7H-pyrrolo[2,3-d]pyrimidin-5-yl]ethynyl}-4-methylphenyl)acetamide (CCD ID: I14) (formula: C₂₀H₂₁N₅O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 20	H 21	N 5	O 2	0	0
2	B	1	Total 48	C 20	H 21	N 5	O 2	0	0

- Molecule 3 is water.

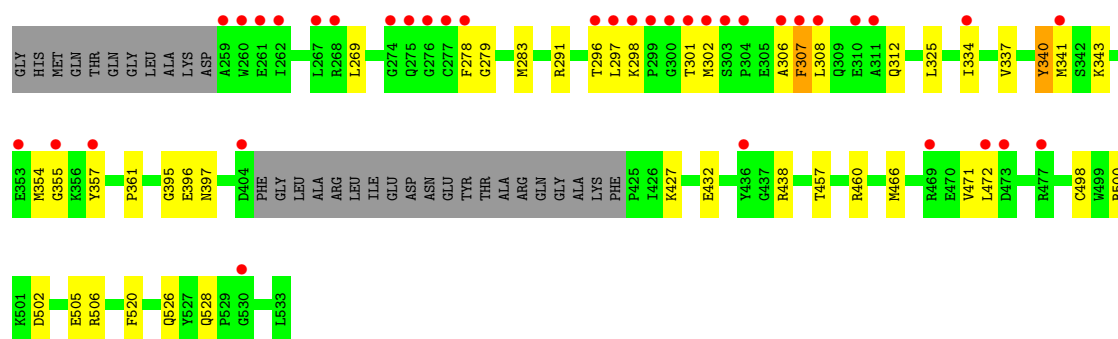
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	113	Total O 113 113	0	0
3	B	127	Total O 127 127	0	0

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.

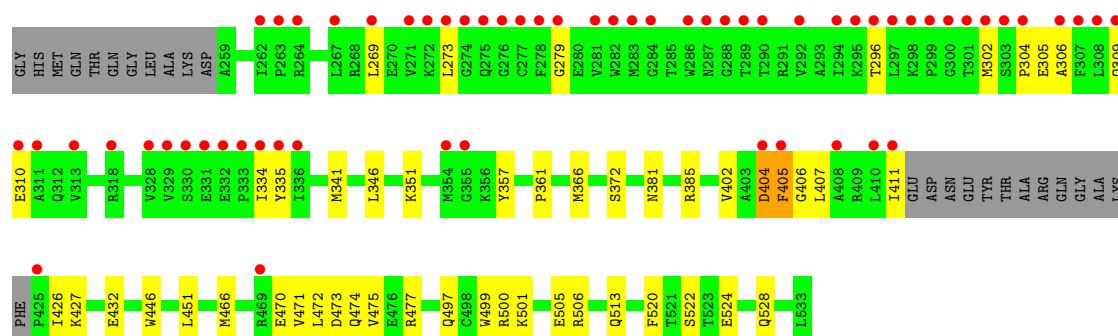
- Molecule 1: Proto-oncogene tyrosine-protein kinase Src

Chain A: 



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

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	42.15Å 63.87Å 74.88Å 78.24° 89.67° 90.21°	Depositor
Resolution (Å)	34.87 – 2.30 34.87 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.9 (34.87-2.30) 90.9 (34.87-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.205 , 0.235 0.206 , 0.234	Depositor DCC
R_{free} test set	1471 reflections (4.31%)	wwPDB-VP
Wilson B-factor (Å ²)	30.1	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8643	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.35% 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: I14

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	0.70	1/2102 (0.0%)	0.83	4/2846 (0.1%)
1	B	0.67	0/2158	0.84	4/2921 (0.1%)
All	All	0.68	1/4260 (0.0%)	0.84	8/5767 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	341	MET	C-O	-5.05	1.17	1.24

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	405	PHE	N-CA-C	-10.35	98.60	112.26
1	B	404	ASP	O-C-N	-8.55	111.22	122.59
1	A	341	MET	CA-C-N	8.39	132.37	120.28
1	A	341	MET	C-N-CA	8.39	132.37	120.28
1	A	340	TYR	CA-C-N	8.16	137.13	121.54
1	A	340	TYR	C-N-CA	8.16	137.13	121.54
1	B	404	ASP	CA-C-N	8.06	135.20	122.86
1	B	404	ASP	C-N-CA	8.06	135.20	122.86

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	2052	2042	2041	33	2
1	B	2107	2106	2104	37	1
2	A	27	21	0	2	0
2	B	27	21	0	6	0
3	A	113	0	0	9	1
3	B	127	0	0	8	1
All	All	4453	4190	4145	74	4

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 9.

All (74) 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:457:THR:O	3:A:701:HOH:O	2.00	0.78
1:A:302:MET:HE2	1:A:306:ALA:HB1	1.70	0.74
1:A:396:GLU:OE2	3:A:703:HOH:O	2.07	0.73
1:A:302:MET:HE2	1:A:306:ALA:CB	2.20	0.72
1:A:427:LYS:HE3	3:B:744:HOH:O	1.89	0.72
1:B:505:GLU:OE1	3:B:701:HOH:O	2.07	0.71
1:B:273:LEU:O	3:B:702:HOH:O	2.10	0.70
1:A:526:GLN:HB2	3:A:704:HOH:O	1.95	0.67
1:B:302:MET:HE2	1:B:306:ALA:HB1	1.77	0.67
1:A:340:TYR:O	3:A:705:HOH:O	2.14	0.65
1:A:298:LYS:HD3	1:A:301:THR:HG21	1.81	0.62
1:B:474:GLN:OE1	1:B:477:ARG:NH1	2.35	0.59
1:A:472:LEU:C	1:A:472:LEU:HD23	2.28	0.59
1:A:308:LEU:O	1:A:312:GLN:HG2	2.05	0.56
1:B:470:GLU:OE2	3:B:703:HOH:O	2.18	0.56
1:B:341:MET:H	2:B:601:I14:C26	2.20	0.55
1:B:472:LEU:HD23	1:B:472:LEU:C	2.33	0.54
1:B:501:LYS:HD3	3:B:756:HOH:O	2.08	0.54
1:A:355:GLY:HA3	3:A:711:HOH:O	2.06	0.54
1:B:426:ILE:CD1	1:B:472:LEU:HB2	2.37	0.53
1:B:466:MET:CE	1:B:471:VAL:HA	2.37	0.53
1:B:451:LEU:O	1:B:451:LEU:HD23	2.08	0.53
1:A:502:ASP:HB3	1:A:505:GLU:HG3	1.90	0.53
1:B:385:ARG:HD3	1:B:407:LEU:O	2.09	0.53
1:B:427:LYS:HG3	3:B:743:HOH:O	2.08	0.52
1:B:341:MET:O	2:B:601:I14:C26	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:601:I14:N25	2:A:601:I14:C07	2.73	0.51
2:B:601:I14:N01	2:B:601:I14:C12	2.74	0.50
1:B:279:GLY:HA3	1:B:296:THR:O	2.11	0.50
1:A:357:TYR:OH	3:A:706:HOH:O	2.19	0.49
1:B:404:ASP:H	2:B:601:I14:C18	2.25	0.49
1:A:279:GLY:HA3	1:A:296:THR:O	2.13	0.49
1:B:302:MET:HE2	1:B:306:ALA:CB	2.42	0.48
1:A:283:MET:SD	1:A:291:ARG:HD3	2.54	0.48
1:A:526:GLN:N	3:A:704:HOH:O	2.08	0.47
1:A:297:LEU:HB2	1:A:307:PHE:CE2	2.49	0.47
1:B:361:PRO:HA	1:B:520:PHE:CE2	2.50	0.47
1:A:278:PHE:CD1	1:A:302:MET:SD	3.09	0.46
1:A:269:LEU:HD12	1:A:269:LEU:N	2.31	0.46
1:A:526:GLN:CA	3:A:704:HOH:O	2.59	0.45
1:B:310:GLU:OE2	2:B:601:I14:N17	2.49	0.45
1:A:302:MET:CE	1:A:306:ALA:HB1	2.44	0.45
1:B:432:GLU:OE2	1:B:506:ARG:NH2	2.47	0.45
1:A:343:LYS:HD3	1:A:395:GLY:O	2.17	0.45
1:A:283:MET:HG3	1:A:340:TYR:CE1	2.52	0.45
1:B:273:LEU:C	3:B:702:HOH:O	2.58	0.45
1:B:310:GLU:HB2	1:B:406:GLY:HA2	1.97	0.45
1:B:471:VAL:O	1:B:475:VAL:HG13	2.17	0.44
1:B:426:ILE:HD13	1:B:472:LEU:HB2	2.00	0.44
1:B:346:LEU:HD13	1:B:366:MET:HE2	2.00	0.44
1:A:500:ARG:HD3	1:A:505:GLU:HB3	2.00	0.44
1:B:426:ILE:CD1	1:B:472:LEU:HD12	2.48	0.44
1:A:325:LEU:HD12	1:A:337:VAL:O	2.19	0.43
1:B:522:SER:HB2	3:B:711:HOH:O	2.18	0.43
1:A:472:LEU:C	1:A:472:LEU:CD2	2.92	0.43
2:B:601:I14:N25	2:B:601:I14:C07	2.82	0.43
1:A:354:MET:HB3	1:A:354:MET:HE3	1.80	0.42
1:A:466:MET:CE	1:A:471:VAL:HA	2.50	0.42
2:A:601:I14:N01	2:A:601:I14:C12	2.82	0.42
1:B:426:ILE:HD11	1:B:472:LEU:HB2	2.01	0.42
1:B:269:LEU:HD21	1:B:335:TYR:HE2	1.84	0.42
1:B:446:TRP:CE3	1:B:499:TRP:HA	2.55	0.42
1:A:432:GLU:OE2	1:A:506:ARG:NH2	2.50	0.42
1:A:460:ARG:NH2	3:A:729:HOH:O	2.52	0.42
1:A:297:LEU:HD23	1:A:334:ILE:HD12	2.01	0.41
1:B:304:PRO:CB	1:B:334:ILE:HD11	2.50	0.41
1:B:305:GLU:O	1:B:309:GLN:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:497:GLN:HA	1:B:500:ARG:HD2	2.01	0.41
1:A:361:PRO:HA	1:A:520:PHE:CE2	2.56	0.41
1:B:372:SER:HA	1:B:513:GLN:OE1	2.21	0.41
1:B:381:ASN:HB3	1:B:411:ILE:HD12	2.03	0.41
1:B:466:MET:HE2	1:B:471:VAL:HA	2.04	0.40
1:B:402:VAL:HG12	1:B:405:PHE:HE1	1.86	0.40
1:A:498:CYS:O	1:A:506:ARG:HG2	2.21	0.40

All (4) 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:B:357:TYR:OH	1:B:473:ASP:OD1[1_655]	1.77	0.43
3:A:762:HOH:O	3:B:799:HOH:O[1_565]	1.95	0.25
1:A:397:ASN:OD1	1:A:438:ARG:NH1[1_455]	2.06	0.14
1:A:397:ASN:OD1	1:A:438:ARG:HH11[1_455]	1.60	0.00

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	251/286 (88%)	249 (99%)	2 (1%)	0	100	100
1	B	258/286 (90%)	254 (98%)	4 (2%)	0	100	100
All	All	509/572 (89%)	503 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	222/245 (91%)	220 (99%)	2 (1%)	70	84
1	B	227/245 (93%)	224 (99%)	3 (1%)	61	77
All	All	449/490 (92%)	444 (99%)	5 (1%)	65	81

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	307	PHE
1	A	528	GLN
1	B	351	LYS
1	B	524	GLU
1	B	528	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	324	GLN
1	A	526	GLN
1	B	312	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

2 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
2	I14	A	601	-	28,29,29	2.36	13 (46%)	32,40,40	3.19	19 (59%)
2	I14	B	601	-	28,29,29	2.32	13 (46%)	32,40,40	2.66	13 (40%)

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	I14	A	601	-	-	4/12/13/13	0/3/3/3
2	I14	B	601	-	-	4/12/13/13	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	I14	C14-C13	5.63	1.54	1.43
2	B	601	I14	C03-C04	-5.09	1.34	1.40
2	A	601	I14	C03-C04	-5.01	1.34	1.40
2	B	601	I14	C12-C13	-4.97	1.12	1.20
2	A	601	I14	C12-C11	3.43	1.50	1.43
2	B	601	I14	O20-C18	-3.32	1.15	1.23
2	B	601	I14	C04-N05	-3.29	1.33	1.37
2	A	601	I14	C04-N05	-3.27	1.33	1.37
2	A	601	I14	O20-C18	-3.20	1.16	1.23
2	B	601	I14	C02-N27	-3.01	1.27	1.35
2	A	601	I14	C02-N27	-3.00	1.27	1.35
2	A	601	I14	C26-N25	-2.85	1.28	1.33
2	B	601	I14	C18-N17	2.83	1.41	1.36
2	B	601	I14	C26-N25	-2.83	1.28	1.33
2	B	601	I14	C15-C16	-2.71	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	I14	C02-N01	2.70	1.41	1.34
2	A	601	I14	C02-N01	2.70	1.41	1.34
2	A	601	I14	C22-C21	-2.60	1.34	1.38
2	A	601	I14	C18-N17	2.47	1.40	1.36
2	A	601	I14	C03-C02	-2.44	1.39	1.42
2	B	601	I14	C03-C02	-2.42	1.39	1.42
2	A	601	I14	C22-C23	-2.21	1.35	1.39
2	B	601	I14	C14-C13	2.19	1.47	1.43
2	B	601	I14	C24-C23	2.10	1.54	1.51
2	A	601	I14	C26-N27	-2.10	1.30	1.33
2	B	601	I14	C26-N27	-2.07	1.30	1.33

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	I14	C03-C04-N25	-7.43	119.09	126.97
2	B	601	I14	C03-C04-N25	-7.38	119.14	126.97
2	A	601	I14	C24-C23-C22	-5.42	109.84	120.28
2	A	601	I14	N25-C04-N05	5.31	133.44	126.87
2	B	601	I14	N25-C04-N05	5.25	133.37	126.87
2	A	601	I14	C22-C23-C14	5.09	123.46	117.80
2	B	601	I14	N27-C26-N25	-4.90	121.16	128.58
2	A	601	I14	C19-C18-N17	4.90	122.32	114.95
2	A	601	I14	N27-C26-N25	-4.90	121.17	128.58
2	B	601	I14	C10-C11-C12	4.79	138.50	127.41
2	A	601	I14	C24-C23-C14	4.11	126.70	121.44
2	A	601	I14	C26-N25-C04	3.69	120.83	111.83
2	B	601	I14	C26-N25-C04	3.67	120.80	111.83
2	A	601	I14	C21-C16-N17	-3.64	108.19	120.41
2	A	601	I14	C10-C11-C12	3.60	135.75	127.41
2	A	601	I14	C06-N05-C04	-3.39	121.09	126.63
2	B	601	I14	C06-N05-C04	-3.35	121.15	126.63
2	B	601	I14	C21-C22-C23	-2.92	117.62	121.98
2	A	601	I14	C02-C03-C04	2.84	117.87	115.74
2	B	601	I14	C02-C03-C04	2.83	117.86	115.74
2	A	601	I14	O20-C18-N17	-2.73	119.32	123.06
2	A	601	I14	C15-C16-N17	2.72	128.96	120.13
2	B	601	I14	C23-C14-C13	-2.66	116.94	120.46
2	A	601	I14	C21-C16-C15	2.64	122.84	119.66
2	B	601	I14	C13-C12-C11	-2.51	170.58	176.41
2	A	601	I14	C03-C02-N01	-2.46	120.15	123.40
2	B	601	I14	C03-C02-N01	-2.43	120.19	123.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	I14	C15-C14-C23	-2.43	116.38	121.44
2	A	601	I14	C14-C13-C12	-2.42	169.51	175.82
2	B	601	I14	C16-N17-C18	2.41	132.48	127.98
2	A	601	I14	O20-C18-C19	-2.14	118.25	122.05
2	B	601	I14	C07-C06-N05	2.10	119.57	112.30

There are no chirality outliers.

All (8) torsion outliers are listed below:

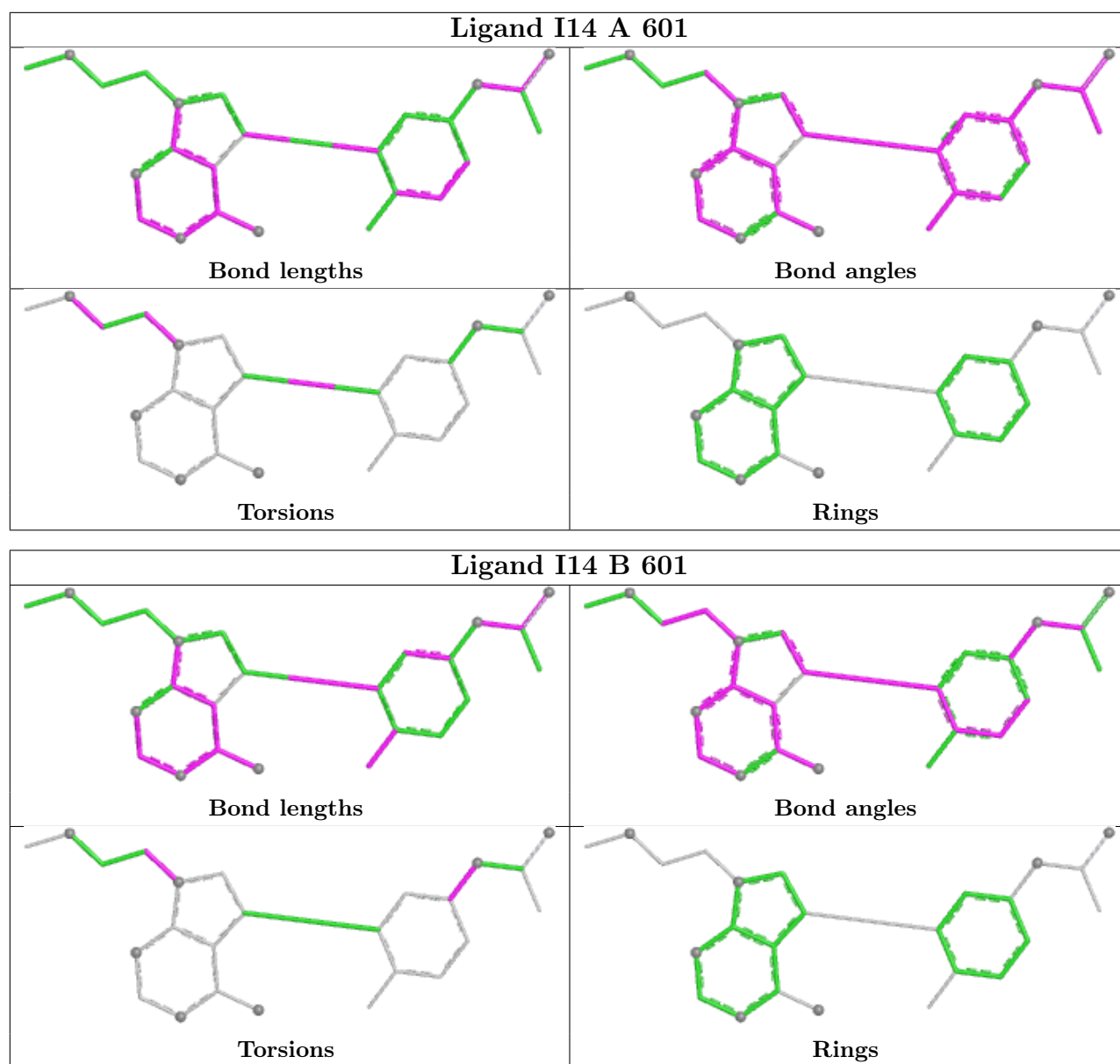
Mol	Chain	Res	Type	Atoms
2	A	601	I14	C07-C06-N05-C04
2	A	601	I14	C07-C06-N05-C10
2	B	601	I14	C07-C06-N05-C04
2	B	601	I14	C07-C06-N05-C10
2	B	601	I14	C15-C16-N17-C18
2	B	601	I14	C21-C16-N17-C18
2	A	601	I14	C11-C12-C13-C14
2	A	601	I14	C06-C07-O08-C09

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	I14	2	0
2	B	601	I14	6	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	255/286 (89%)	0.73	37 (14%) 6 7	24, 44, 110, 135	0
1	B	262/286 (91%)	0.85	61 (23%) 2 2	22, 41, 129, 164	0
All	All	517/572 (90%)	0.79	98 (18%) 3 4	22, 42, 119, 164	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	288	GLY	5.8
1	B	274	GLY	4.9
1	A	278	PHE	4.9
1	B	303	SER	4.8
1	B	267	LEU	4.7
1	A	308	LEU	4.7
1	B	273	LEU	4.7
1	B	269	LEU	4.6
1	A	307	PHE	4.5
1	B	334	ILE	4.5
1	A	259	ALA	4.5
1	B	308	LEU	4.4
1	A	301	THR	4.4
1	A	311	ALA	4.3
1	A	277	CYS	4.1
1	A	472	LEU	4.0
1	B	287	ASN	4.0
1	B	299	PRO	3.9
1	B	284	GLY	3.9
1	B	410	LEU	3.8
1	B	304	PRO	3.7
1	B	277	CYS	3.7
1	B	296	THR	3.7
1	A	306	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	282	TRP	3.6
1	B	271	VAL	3.6
1	B	292	VAL	3.6
1	B	301	THR	3.6
1	B	328	VAL	3.6
1	B	311	ALA	3.5
1	B	411	ILE	3.5
1	A	473	ASP	3.5
1	B	335	TYR	3.5
1	A	296	THR	3.4
1	B	333	PRO	3.4
1	B	405	PHE	3.3
1	A	404	ASP	3.3
1	A	276	GLY	3.3
1	B	354	MET	3.2
1	B	272	LYS	3.2
1	B	278	PHE	3.2
1	B	302	MET	3.2
1	B	330	SER	3.2
1	A	297	LEU	3.2
1	B	332	GLU	3.1
1	B	297	LEU	3.1
1	B	300	GLY	3.1
1	B	307	PHE	3.1
1	B	309	GLN	3.1
1	A	304	PRO	3.1
1	B	336	ILE	3.0
1	A	300	GLY	3.0
1	A	355	GLY	2.9
1	A	299	PRO	2.9
1	B	469	ARG	2.9
1	B	281	VAL	2.9
1	B	283	MET	2.7
1	B	306	ALA	2.7
1	A	302	MET	2.6
1	A	477	ARG	2.6
1	B	286	TRP	2.6
1	B	425	PRO	2.6
1	A	469	ARG	2.5
1	A	275	GLN	2.5
1	A	268	ARG	2.5
1	B	408	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	530	GLY	2.5
1	B	263	PRO	2.5
1	A	262	ILE	2.5
1	A	261	GLU	2.4
1	B	294	ILE	2.4
1	A	267	LEU	2.4
1	B	329	VAL	2.4
1	B	275	GLN	2.4
1	A	353	GLU	2.4
1	A	310	GLU	2.4
1	B	276	GLY	2.3
1	B	295	LYS	2.3
1	B	298	LYS	2.3
1	B	289	THR	2.3
1	A	334	ILE	2.3
1	B	331	GLU	2.3
1	B	279	GLY	2.3
1	A	298	LYS	2.3
1	B	262	ILE	2.3
1	B	318	ARG	2.3
1	A	303	SER	2.3
1	B	264	ARG	2.2
1	A	341	MET	2.2
1	B	313	VAL	2.1
1	B	355	GLY	2.1
1	A	357	TYR	2.1
1	A	436	TYR	2.1
1	B	290	THR	2.1
1	B	310	GLU	2.1
1	A	274	GLY	2.1
1	A	260	TRP	2.1
1	B	404	ASP	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](#)

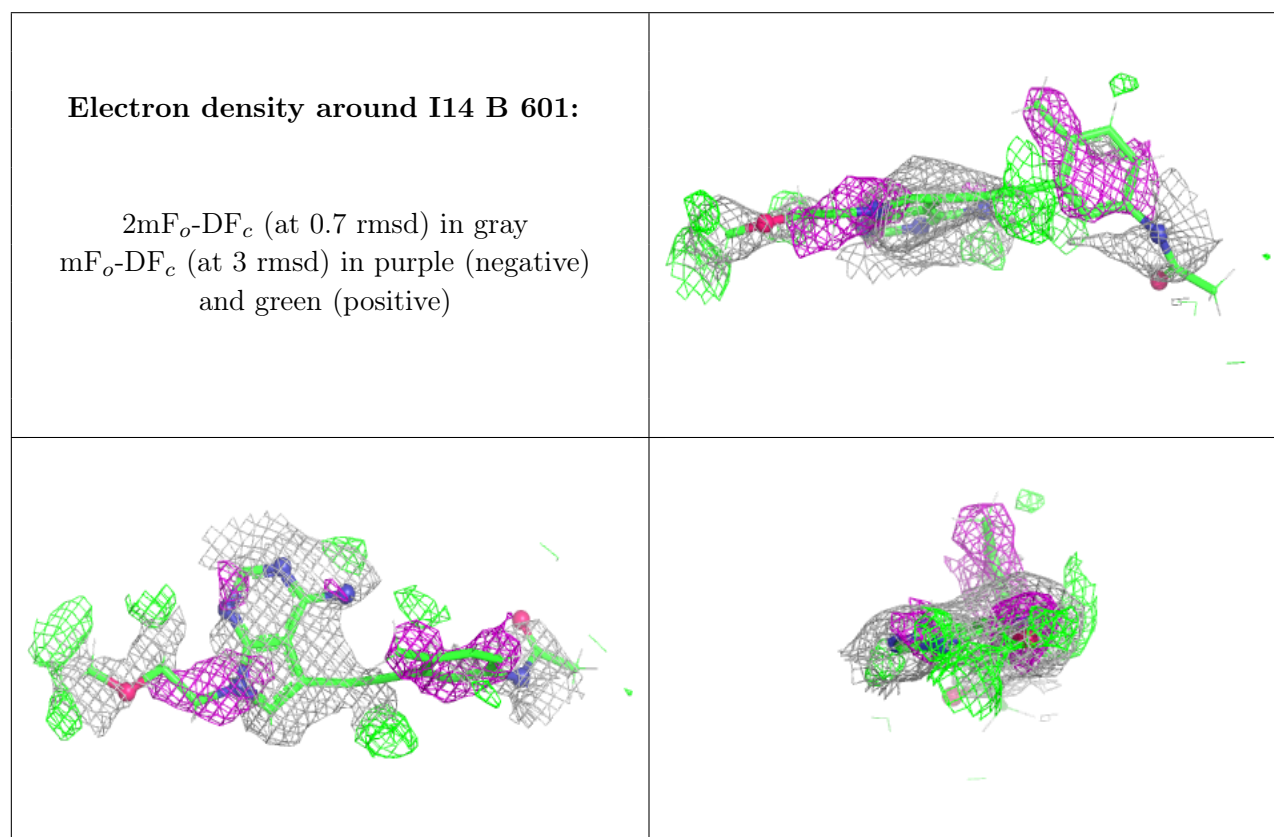
There are no oligosaccharides in this entry.

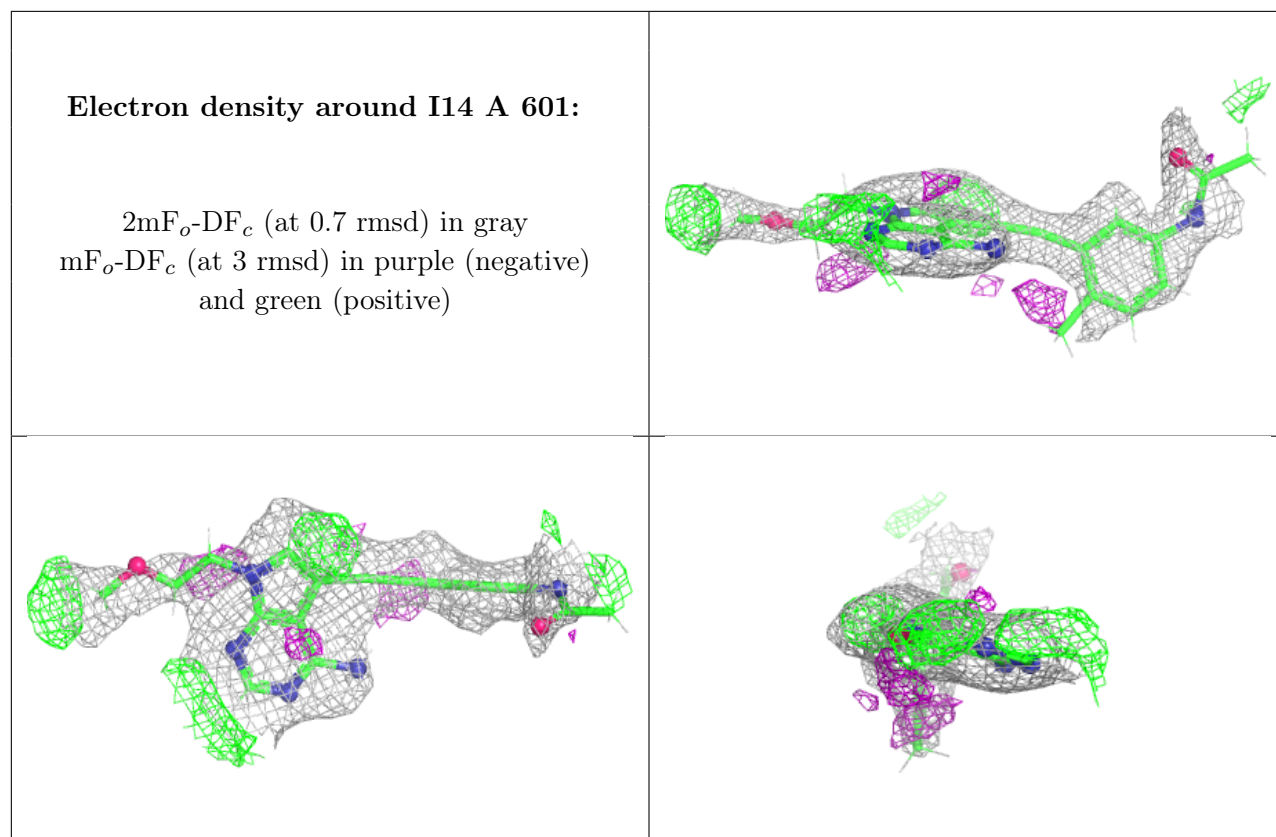
6.4 Ligands ⓘ

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
2	I14	B	601	27/27	0.50	0.25	48,69,92,93	0
2	I14	A	601	27/27	0.77	0.21	48,69,92,93	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.