



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 07:36 PM UTC

PDB ID : 8K79 / pdb_00008k79
Title : Crystal structure of c-SRC kinase domain bound by TPX-0022
Authors : Qu, L.Z.; Chen, Y.H.
Deposited on : 2023-07-26
Resolution : 2.80 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

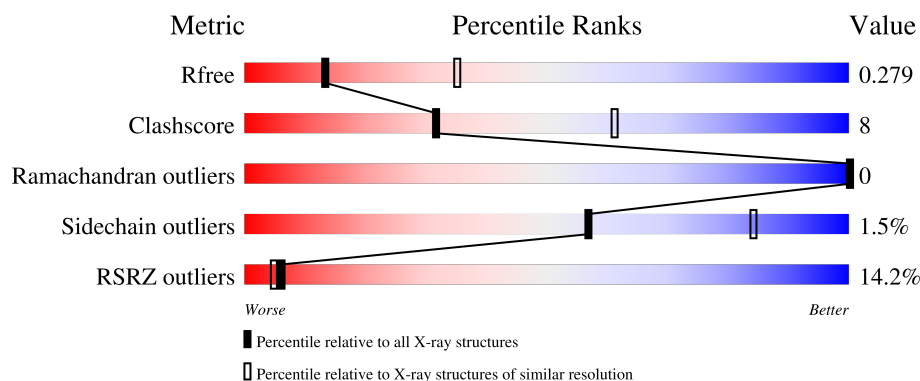
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	14% 73% 18% 8%
1	B	286	11% 71% 14% 15%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4085 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.

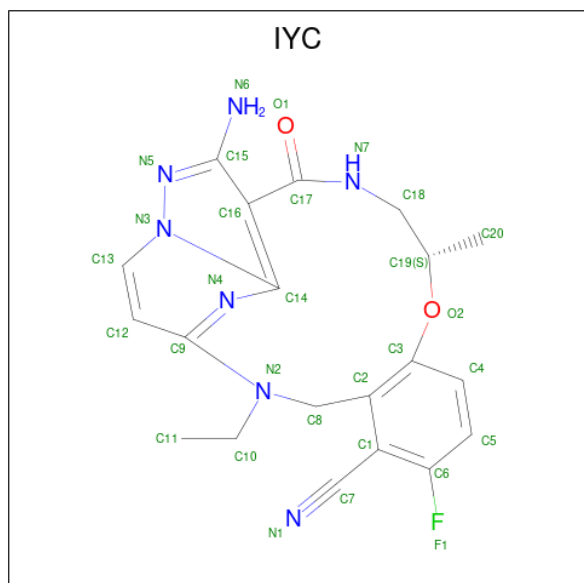
- Molecule 1 is a protein called Proto-oncogene tyrosine-protein kinase Src.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2046	1315	336	379	16			
1	B	244	Total	C	N	O	S	0	0	0
			1895	1221	311	348	15			

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 Elzovantinib (CCD ID: IYC) (formula: C₂₀H₂₀FN₇O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			30	20	1	7	2		
2	B	1	Total	C	F	N	O	0	0
			30	20	1	7	2		

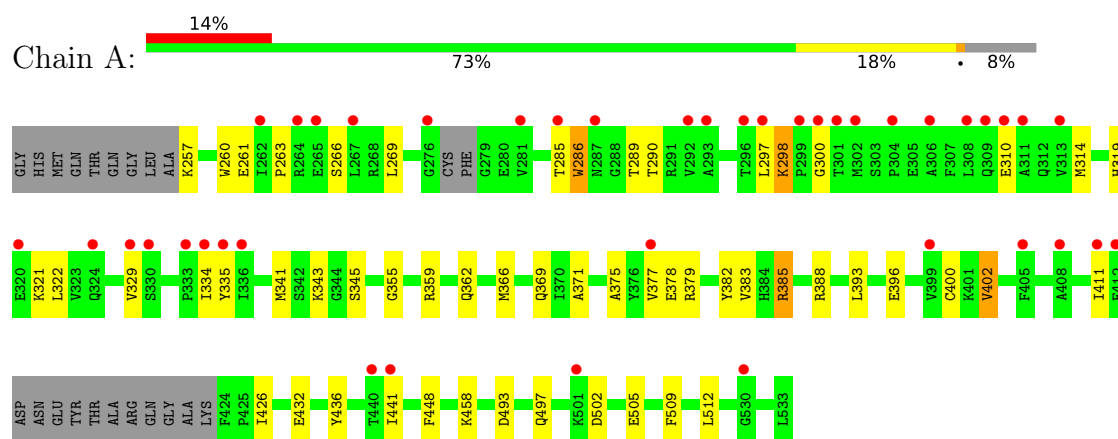
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	45	Total	O	0	0
			45	45		
3	B	39	Total	O	0	0
			39	39		

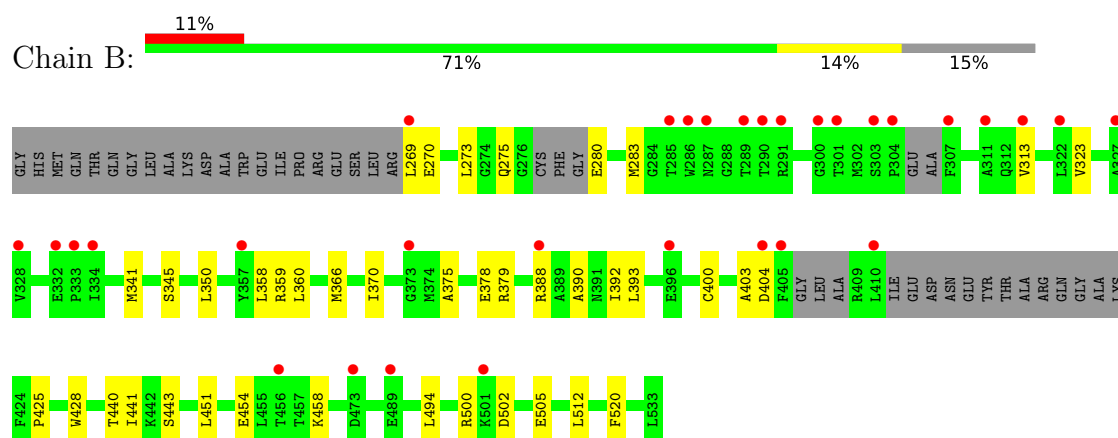
3 Residue-property plots [i](#)

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	41.86Å 63.06Å 73.08Å 100.48° 91.10° 90.22°	Depositor
Resolution (Å)	25.00 – 2.80 25.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (25.00-2.80) 99.6 (25.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.28Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.241 , 0.277 0.242 , 0.279	Depositor DCC
R_{free} test set	2018 reflections (6.39%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-l	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	4085	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.07% 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: IYC

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	0.54	1/2095 (0.0%)	0.62	8/2846 (0.3%)
1	B	0.25	0/1940	0.43	3/2635 (0.1%)
All	All	0.43	1/4035 (0.0%)	0.53	11/5481 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	286	TRP	CA-C	-5.80	1.45	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	270	GLU	N-CA-C	12.28	130.34	111.56
1	A	300	GLY	N-CA-C	-9.58	90.48	113.18
1	A	426	ILE	N-CA-C	8.23	120.00	110.62
1	A	260	TRP	N-CA-C	-7.17	104.39	113.72
1	A	289	THR	CA-C-N	-6.80	113.53	123.05
1	A	289	THR	C-N-CA	-6.80	113.53	123.05
1	B	404	ASP	N-CA-C	6.46	120.56	111.52
1	A	298	LYS	N-CA-C	-5.88	101.07	109.24
1	B	270	GLU	CB-CA-C	-5.73	100.31	111.03
1	A	289	THR	CB-CA-C	-5.42	101.33	110.44
1	A	385	ARG	N-CA-C	5.01	121.46	110.80

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	2046	0	1969	30	1
1	B	1895	0	1811	31	1
2	A	30	0	0	1	0
2	B	30	0	0	3	0
3	A	45	0	0	1	0
3	B	39	0	0	0	0
All	All	4085	0	3780	63	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 8.

All (63) 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:388:ARG:HH22	1:B:425:PRO:CB	1.54	1.20
1:B:388:ARG:NH2	1:B:425:PRO:CB	2.05	1.20
1:B:388:ARG:HH21	1:B:425:PRO:CG	1.54	1.17
1:B:388:ARG:NH2	1:B:425:PRO:CG	2.07	1.17
1:B:388:ARG:NH2	1:B:425:PRO:HG3	1.60	1.14
1:B:388:ARG:HH22	1:B:425:PRO:HB3	1.12	1.08
1:B:388:ARG:HH21	1:B:425:PRO:HG3	1.10	0.98
1:A:377:VAL:CG2	1:A:382:TYR:HB2	1.99	0.93
1:A:343:LYS:NZ	1:A:396:GLU:OE2	2.14	0.80
1:A:377:VAL:HG23	1:A:382:TYR:HB2	1.70	0.73
1:B:502:ASP:HB3	1:B:505:GLU:HG3	1.73	0.70
1:B:388:ARG:NH2	1:B:425:PRO:HB2	2.06	0.69
1:A:329:VAL:HB	1:A:335:TYR:HB2	1.77	0.65
1:A:377:VAL:HG22	1:A:382:TYR:HB2	1.79	0.65
1:A:502:ASP:HB3	1:A:505:GLU:HG3	1.81	0.63
1:B:500:ARG:NH1	1:B:505:GLU:O	2.34	0.61
1:A:319:HIS:HB3	1:A:322:LEU:HG	1.82	0.60
1:B:273:LEU:HD11	1:B:283:MET:HB3	1.82	0.59
1:B:370:ILE:HD13	1:B:451:LEU:HD21	1.85	0.59
1:B:388:ARG:NH2	1:B:425:PRO:HB3	1.89	0.57
1:B:358:LEU:O	1:B:359:ARG:NH1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:LYS:HD2	1:A:369:GLN:HB3	1.87	0.55
1:A:362:GLN:O	1:A:366:MET:HG3	2.07	0.55
1:B:388:ARG:HD2	1:B:390:ALA:HB3	1.89	0.55
1:A:355:GLY:O	1:A:458:LYS:HE2	2.08	0.54
2:A:601:IYC:N4	2:A:601:IYC:N7	2.54	0.53
1:A:341:MET:HG3	1:A:393:LEU:HB3	1.90	0.52
2:B:601:IYC:N4	2:B:601:IYC:N7	2.58	0.52
1:A:322:LEU:HD22	1:A:402:VAL:HG22	1.91	0.51
1:B:378:GLU:HG3	1:B:441:ILE:HG12	1.92	0.51
1:A:269:LEU:HD11	1:A:335:TYR:HE2	1.76	0.50
1:B:366:MET:HG2	1:B:400:CYS:SG	2.52	0.49
1:A:378:GLU:HG3	1:A:441:ILE:HG12	1.94	0.49
1:B:323:VAL:HG21	1:B:393:LEU:HD12	1.95	0.48
1:A:432:GLU:HA	1:A:436:TYR:HD2	1.79	0.48
1:A:366:MET:HE2	1:A:400:CYS:SG	2.53	0.48
1:A:383:VAL:HG12	1:A:385:ARG:HG3	1.96	0.47
1:A:310:GLU:HG2	1:A:314:MET:HE2	1.96	0.47
1:B:350:LEU:HD22	1:B:458:LYS:HA	1.96	0.47
1:A:286:TRP:HB3	1:A:290:THR:HB	1.97	0.46
1:B:494:LEU:HD11	1:B:512:LEU:HD23	1.97	0.46
1:B:440:THR:O	1:B:443:SER:OG	2.33	0.46
1:B:388:ARG:O	1:B:392:ILE:HG12	2.16	0.46
1:A:509:PHE:HA	1:A:512:LEU:HB2	1.98	0.45
1:B:275:GLN:HA	1:B:280:GLU:HA	1.97	0.45
1:A:493:ASP:O	1:A:497:GLN:HG3	2.17	0.44
1:A:377:VAL:CG2	1:A:382:TYR:CB	2.87	0.44
1:B:403:ALA:HB1	2:B:601:IYC:N1	2.33	0.43
1:B:388:ARG:CD	1:B:390:ALA:HB3	2.48	0.43
1:A:263:PRO:HG2	1:A:266:SER:HB2	1.99	0.43
1:A:371:ALA:HB2	1:A:448:PHE:CZ	2.53	0.42
1:A:297:LEU:HB3	1:A:334:ILE:HB	2.01	0.42
1:B:375:ALA:O	1:B:379:ARG:HG3	2.20	0.42
1:B:359:ARG:HA	1:B:359:ARG:HD3	1.89	0.42
1:B:341:MET:O	2:B:601:IYC:N6	2.53	0.41
1:B:428:TRP:HZ2	1:B:454:GLU:OE2	2.03	0.41
1:A:359:ARG:HA	1:A:359:ARG:HD3	1.90	0.41
1:A:375:ALA:O	1:A:379:ARG:HG3	2.20	0.41
1:B:345:SER:HA	1:B:393:LEU:HD23	2.03	0.41
1:B:360:LEU:HD23	1:B:520:PHE:HE1	1.86	0.41
1:A:383:VAL:HG23	1:A:411:ILE:HG22	2.03	0.40
1:A:377:VAL:HG22	1:A:377:VAL:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:ARG:NH2	3:A:712:HOH:O	2.54	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:257:LYS:O	1:B:269:LEU:CD2[1_554]	1.41	0.79

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	258/286 (90%)	245 (95%)	13 (5%)	0	100	100
1	B	234/286 (82%)	222 (95%)	12 (5%)	0	100	100
All	All	492/572 (86%)	467 (95%)	25 (5%)	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	210/245 (86%)	205 (98%)	5 (2%)	43	77
1	B	195/245 (80%)	194 (100%)	1 (0%)	81	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	405/490 (83%)	399 (98%)	6 (2%)	57 84

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

Mol	Chain	Res	Type
1	A	261	GLU
1	A	285	THR
1	A	298	LYS
1	A	345	SER
1	A	402	VAL
1	B	313	VAL

Sometimes 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 ⓘ

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

5.5 Carbohydrates ⓘ

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	IYC	B	601	-	33,33,33	3.35	11 (33%)	37,48,48	2.07	8 (21%)
2	IYC	A	601	-	33,33,33	3.31	11 (33%)	37,48,48	2.21	8 (21%)

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	IYC	B	601	-	-	7/23/25/25	0/3/4/4
2	IYC	A	601	-	-	8/23/25/25	0/3/4/4

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	IYC	N3-N5	12.48	1.51	1.37
2	A	601	IYC	N3-N5	12.15	1.51	1.37
2	B	601	IYC	C16-C15	-6.74	1.29	1.43
2	A	601	IYC	C16-C15	-6.65	1.29	1.43
2	B	601	IYC	C17-N7	6.26	1.44	1.33
2	A	601	IYC	C17-N7	5.88	1.43	1.33
2	A	601	IYC	C16-C14	-5.57	1.25	1.44
2	B	601	IYC	C16-C14	-5.51	1.25	1.44
2	A	601	IYC	C1-C7	5.07	1.52	1.44
2	B	601	IYC	C1-C7	4.80	1.51	1.44
2	A	601	IYC	C15-N6	4.24	1.44	1.34
2	B	601	IYC	C15-N6	4.15	1.44	1.34
2	B	601	IYC	C9-N2	3.64	1.44	1.37
2	A	601	IYC	C9-N2	3.63	1.44	1.37
2	B	601	IYC	C9-N4	3.49	1.39	1.33
2	A	601	IYC	C9-N4	3.35	1.39	1.33
2	B	601	IYC	O1-C17	-2.90	1.18	1.23
2	A	601	IYC	O1-C17	-2.75	1.18	1.23
2	A	601	IYC	C1-C2	-2.49	1.38	1.40
2	B	601	IYC	C15-N5	2.18	1.37	1.33
2	B	601	IYC	C1-C2	-2.17	1.38	1.40
2	A	601	IYC	C15-N5	2.05	1.37	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	IYC	O2-C3-C2	6.93	117.81	114.02
2	A	601	IYC	C16-C14-N3	-6.42	102.95	107.27
2	B	601	IYC	C16-C14-N3	-6.23	103.08	107.27
2	B	601	IYC	O2-C3-C2	5.83	117.21	114.02
2	B	601	IYC	O2-C19-C18	4.49	111.15	106.13
2	A	601	IYC	C19-C18-N7	-4.31	106.58	112.92
2	A	601	IYC	N3-C14-N4	3.54	126.23	121.96
2	A	601	IYC	C13-N3-N5	3.44	131.32	124.70
2	B	601	IYC	C19-C18-N7	-3.30	108.07	112.92
2	B	601	IYC	N3-C14-N4	3.14	125.75	121.96
2	B	601	IYC	C13-N3-N5	3.02	130.50	124.70
2	B	601	IYC	C6-C1-C2	2.60	119.96	116.50
2	A	601	IYC	O2-C19-C18	2.54	108.96	106.13
2	A	601	IYC	C6-C1-C2	2.29	119.54	116.50
2	B	601	IYC	C2-C8-N2	2.23	116.13	112.55
2	A	601	IYC	C20-C19-C18	-2.08	107.41	111.42

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	IYC	N7-C18-C19-O2
2	A	601	IYC	N7-C18-C19-C20
2	B	601	IYC	C14-C16-C17-O1
2	B	601	IYC	C14-C16-C17-N7
2	B	601	IYC	N7-C18-C19-O2
2	B	601	IYC	N7-C18-C19-C20
2	A	601	IYC	C14-C16-C17-O1
2	A	601	IYC	C14-C16-C17-N7
2	B	601	IYC	C18-C19-O2-C3
2	A	601	IYC	C2-C8-N2-C10
2	B	601	IYC	C2-C8-N2-C10
2	A	601	IYC	C20-C19-O2-C3
2	A	601	IYC	C2-C8-N2-C9
2	A	601	IYC	C15-C16-C17-O1
2	B	601	IYC	C2-C8-N2-C9

There are no ring outliers.

2 monomers are involved in 4 short contacts:

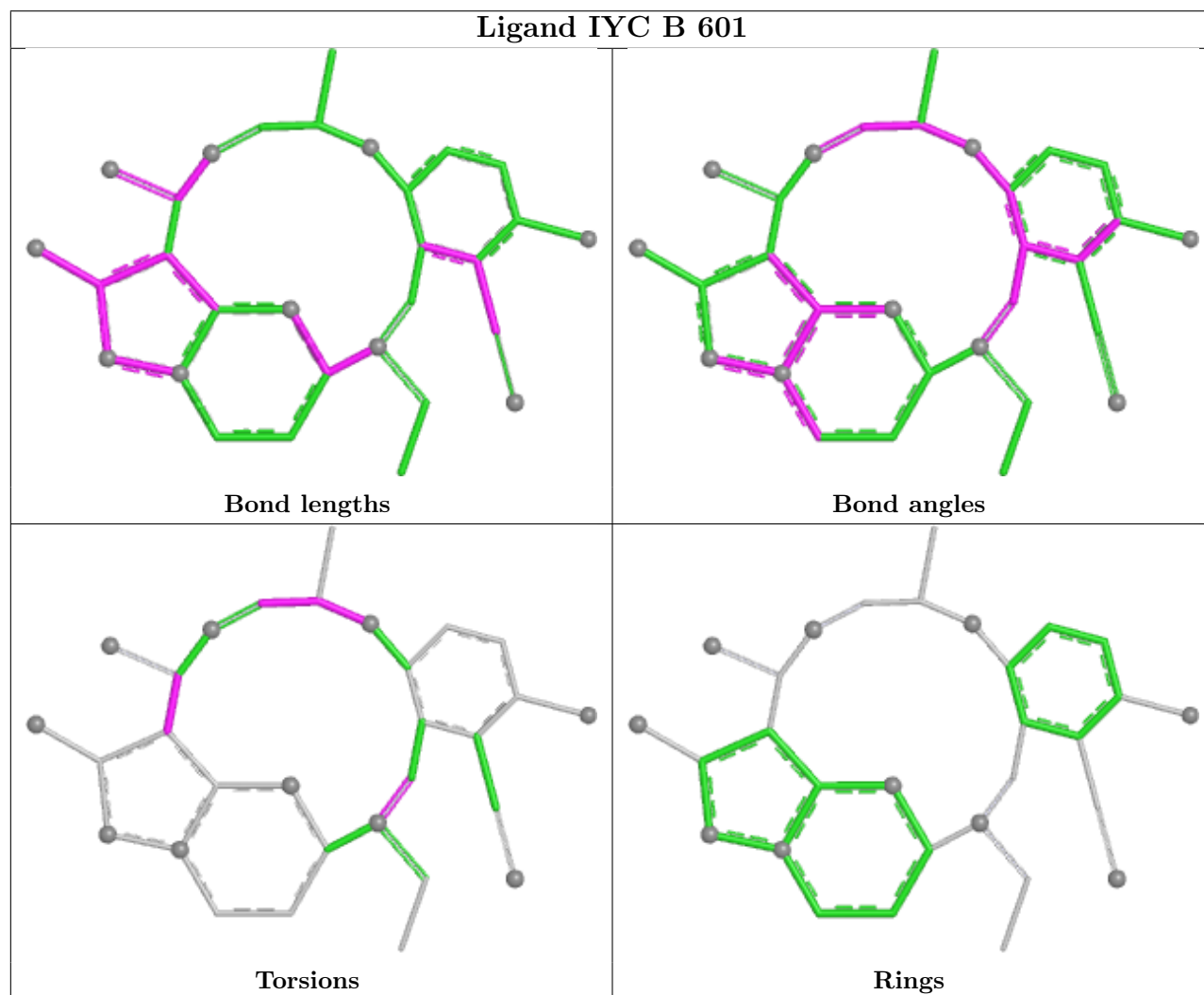
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	IYC	3	0

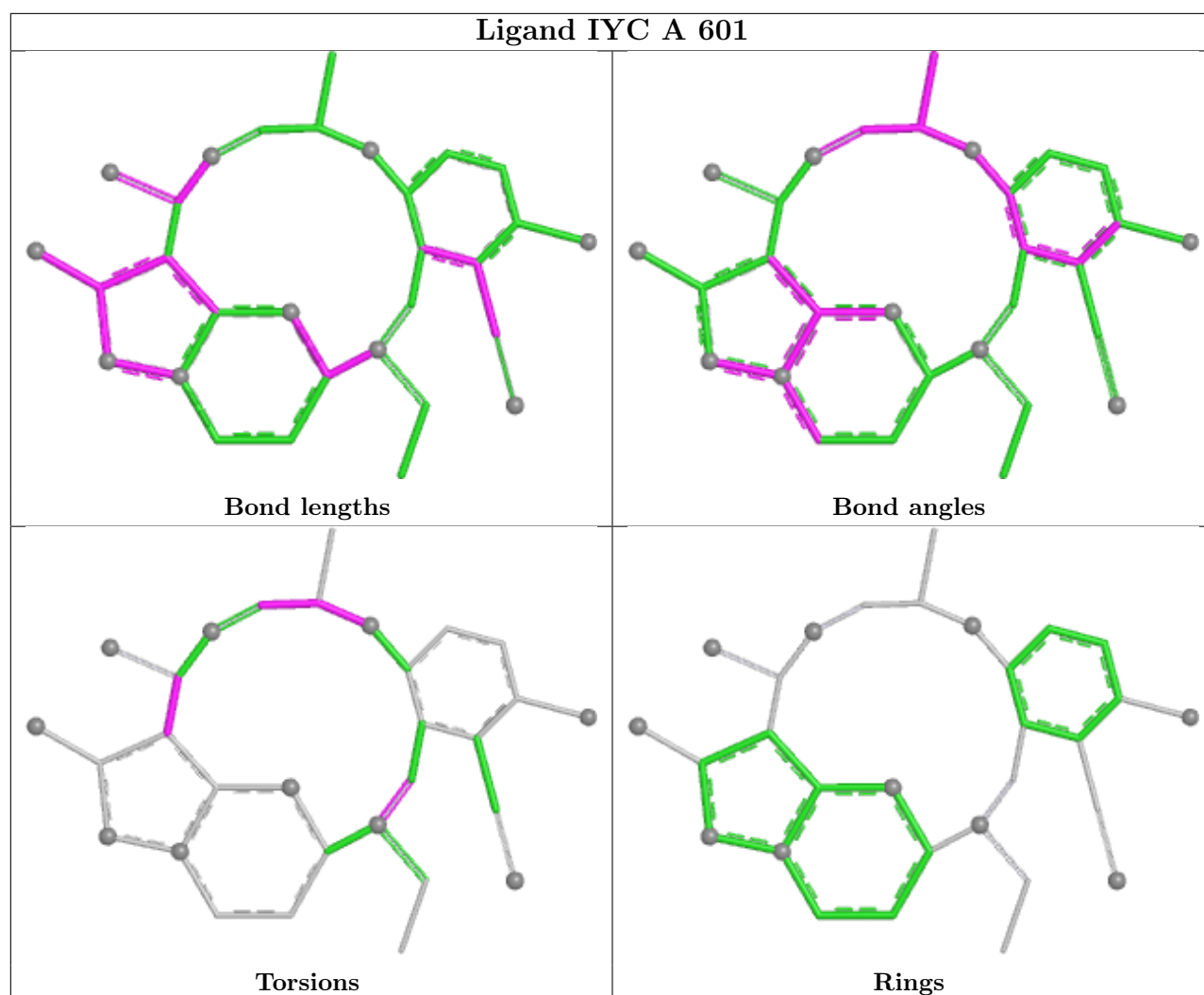
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	IYC	1	0

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	264/286 (92%)	0.96	41 (15%) 5 4	5, 18, 51, 74	0
1	B	244/286 (85%)	0.92	31 (12%) 8 6	4, 16, 49, 65	0
All	All	508/572 (88%)	0.94	72 (14%) 6 5	4, 17, 51, 74	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	441	ILE	4.9
1	B	404	ASP	4.8
1	A	377	VAL	4.4
1	B	307	PHE	4.3
1	A	408	ALA	4.3
1	B	410	LEU	4.2
1	B	304	PRO	3.8
1	A	265	GLU	3.8
1	A	276	GLY	3.5
1	A	299	PRO	3.5
1	A	301	THR	3.4
1	A	306	ALA	3.4
1	A	411	ILE	3.3
1	A	308	LEU	3.2
1	A	333	PRO	3.2
1	B	285	THR	3.2
1	A	311	ALA	3.1
1	A	267	LEU	3.0
1	A	310	GLU	2.9
1	B	287	ASN	2.9
1	A	302	MET	2.9
1	A	412	GLU	2.9
1	A	329	VAL	2.9
1	B	333	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	440	THR	2.8
1	B	332	GLU	2.8
1	A	287	ASN	2.8
1	B	388	ARG	2.7
1	A	530	GLY	2.7
1	B	303	SER	2.6
1	A	264	ARG	2.6
1	B	396	GLU	2.6
1	B	286	TRP	2.6
1	A	501	LYS	2.5
1	B	313	VAL	2.5
1	B	289	THR	2.5
1	B	290	THR	2.5
1	B	405	PHE	2.5
1	A	293	ALA	2.5
1	A	313	VAL	2.4
1	A	296	THR	2.4
1	A	304	PRO	2.4
1	A	399	VAL	2.3
1	A	330	SER	2.3
1	A	300	GLY	2.3
1	A	297	LEU	2.3
1	B	456	THR	2.3
1	A	335	TYR	2.3
1	A	309	GLN	2.3
1	A	405	PHE	2.2
1	A	320	GLU	2.2
1	B	322	LEU	2.2
1	B	291	ARG	2.2
1	B	311	ALA	2.2
1	A	292	VAL	2.2
1	B	328	VAL	2.1
1	B	373	GLY	2.1
1	A	262	ILE	2.1
1	A	324	GLN	2.1
1	B	269	LEU	2.1
1	B	357	TYR	2.1
1	B	473	ASP	2.1
1	A	285	THR	2.1
1	A	334	ILE	2.1
1	B	489	GLU	2.1
1	B	300	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	336	ILE	2.0
1	B	334	ILE	2.0
1	B	327	ALA	2.0
1	A	281	VAL	2.0
1	B	301	THR	2.0
1	B	501	LYS	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](#)

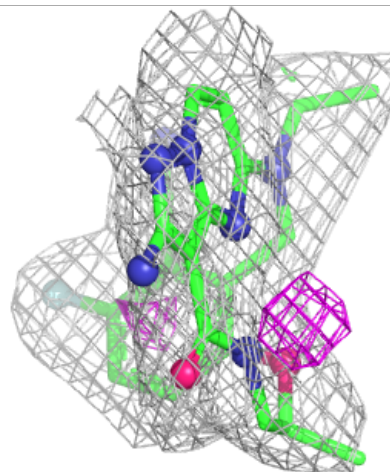
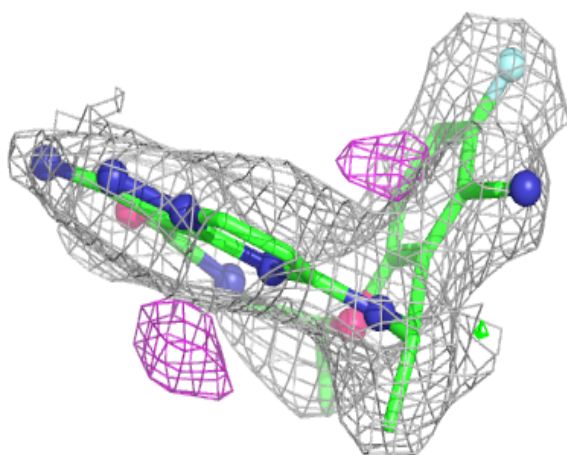
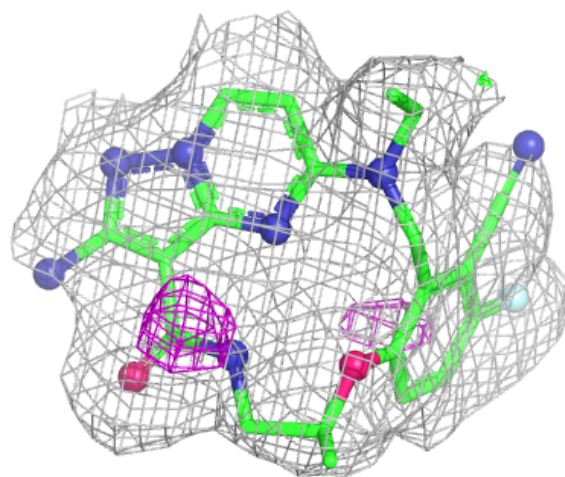
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	IYC	B	601	30/30	0.83	0.15	17,27,34,46	0
2	IYC	A	601	30/30	0.87	0.16	15,27,38,58	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.

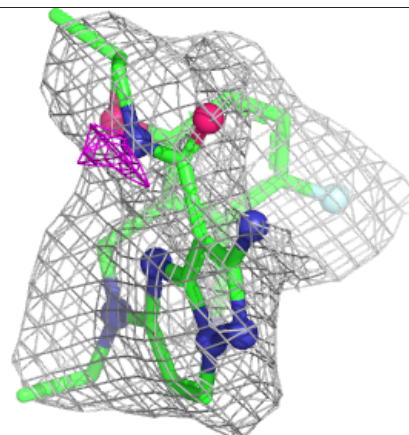
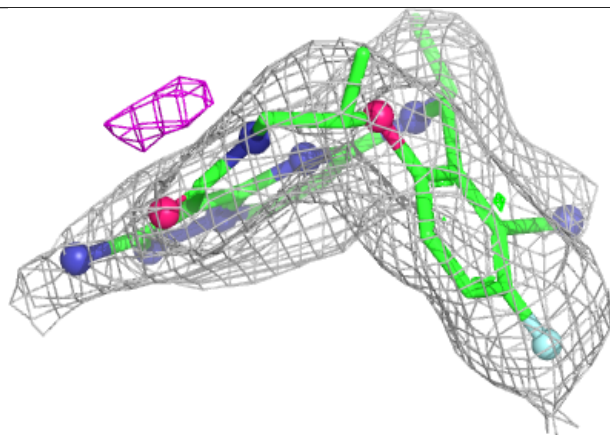
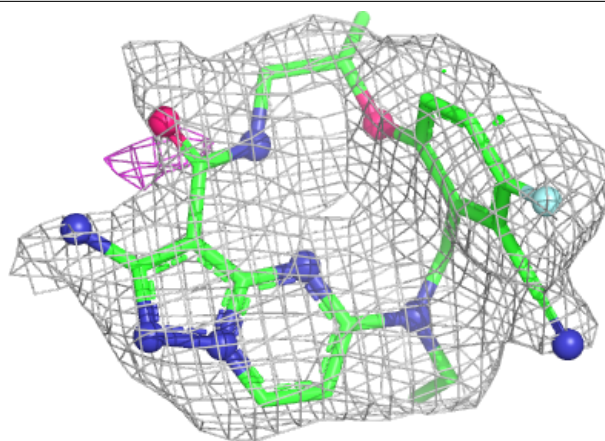
Electron density around IYC B 601:

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



Electron density around IYC A 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 [i](#)

There are no such residues in this entry.