



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:14 AM UTC

PDB ID : 8BI6 / pdb_00008bi6
Title : Crystal structure of human Choline Kinase A in complex with UNC0638
Authors : Diaz-Saez, L.; Ward, J.; Kennedy, E.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Huber, K.; Structural Genomics Consortium (SGC)
Deposited on : 2022-11-01
Resolution : 2.40 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

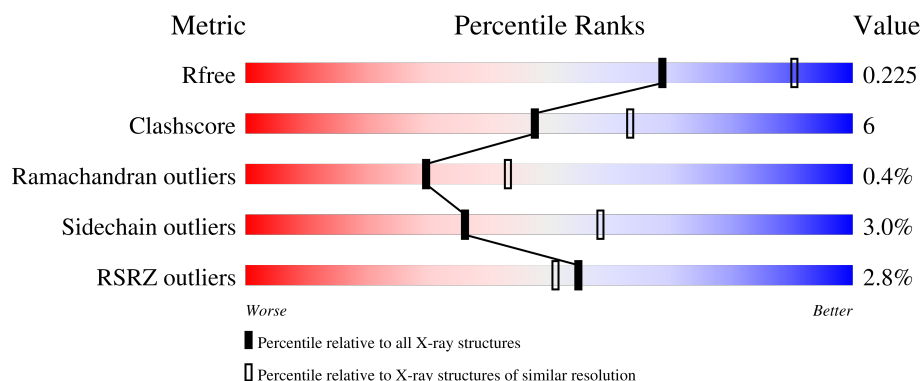
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

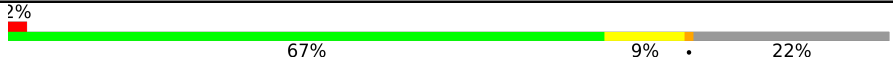
The reported resolution of this entry is 2.40 Å.

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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	457	
1	B	457	

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.

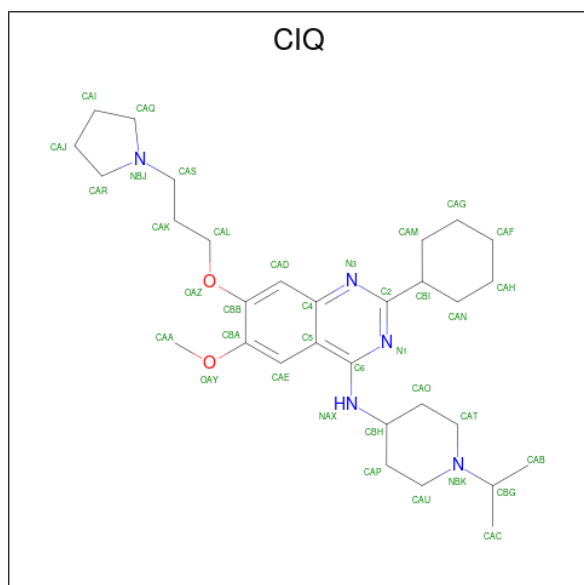
- Molecule 1 is a protein called Choline kinase alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total 2981	C 1931	N 495	O 538	S 17	6	6	0
1	B	354	Total 2973	C 1927	N 497	O 533	S 16	17	5	0

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

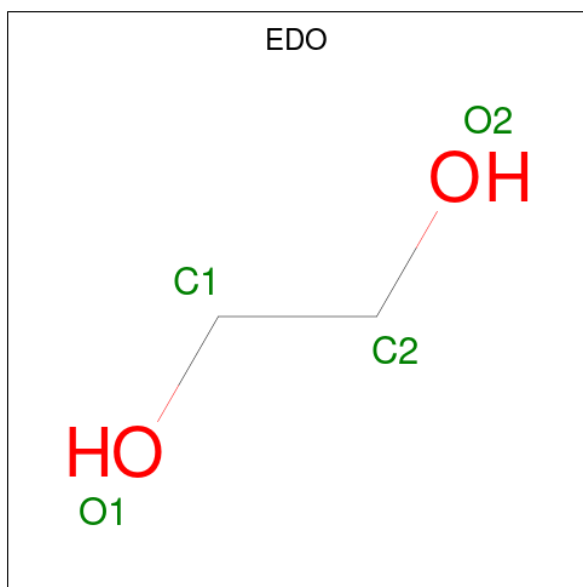
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0

- Molecule 3 is 2-cyclohexyl-6-methoxy-N-[1-(1-methylethyl)piperidin-4-yl]-7-(3-pyrrolidin-1-ylpropoxy)quinazolin-4-amine (CCD ID: CIQ) (formula: C₃₀H₄₇N₅O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			37	30	5	2		
3	B	1	Total	C	N	O	0	1
			74	60	10	4		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



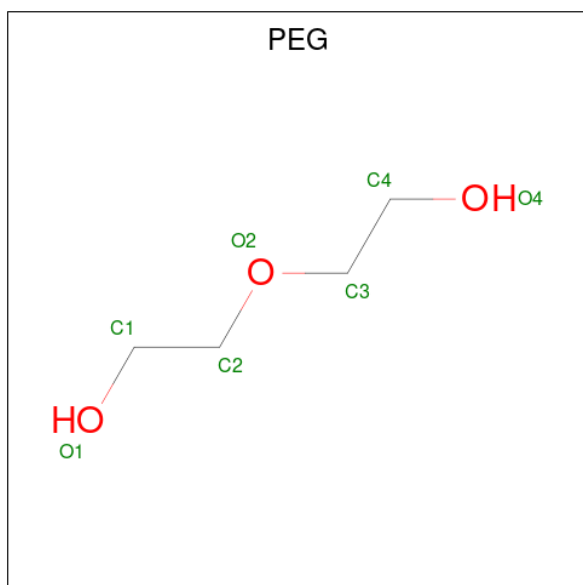
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total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

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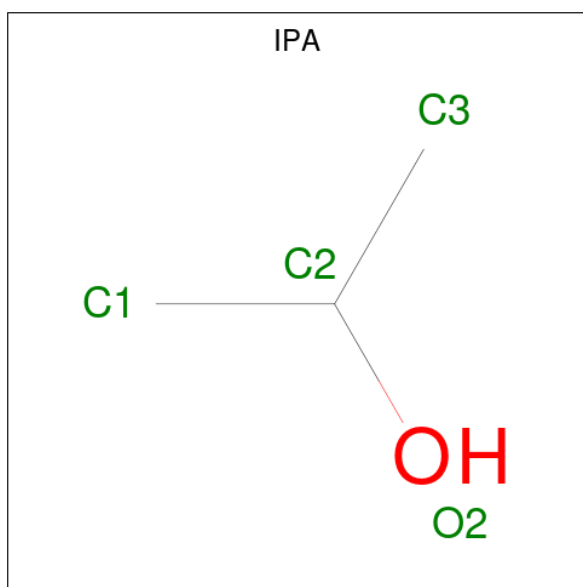
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



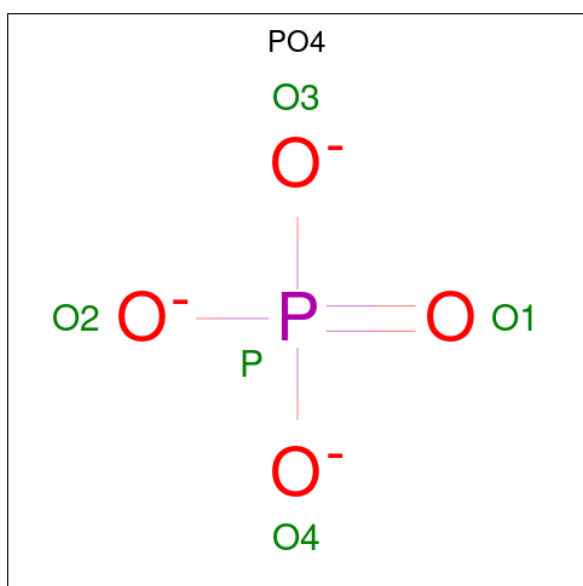
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C_3H_8O).



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

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

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

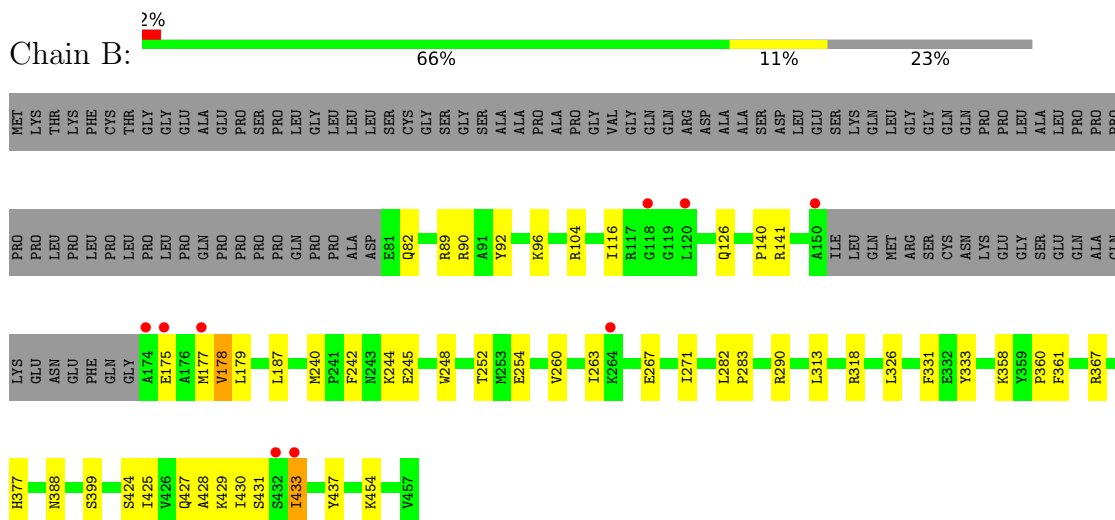
- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	2	Total	Cl	0	0
			2	2		
8	B	1	Total	Cl	0	0
			1	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	180	Total	O	0	0
			180	180		
9	B	216	Total	O	0	0
			216	216		

- Molecule 1: Choline kinase alpha



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	132.03Å 132.03Å 168.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.45 – 2.40 48.45 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.45-2.40) 100.0 (48.45-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.14 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.179 , 0.221 0.186 , 0.225	Depositor DCC
R_{free} test set	3035 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	51.0	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 35.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6556	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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: PEG, MG, PO4, EDO, IPA, CL, CIQ

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	0.65	0/3078	1.11	3/4143 (0.1%)
1	B	0.72	2/3066 (0.1%)	1.08	3/4127 (0.1%)
All	All	0.69	2/6144 (0.0%)	1.09	6/8270 (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	2
1	B	0	6
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	358	LYS	CG-CD	-11.41	1.18	1.52
1	B	429	LYS	CG-CD	11.28	1.86	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	429	LYS	CB-CG-CD	-7.00	95.19	111.30
1	A	332	GLU	CB-CG-CD	6.02	122.84	112.60
1	B	358	LYS	CB-CG-CD	5.70	124.41	111.30
1	B	82	GLN	CB-CA-C	5.66	116.27	109.31
1	A	435	PHE	CA-CB-CG	5.42	119.22	113.80
1	A	403	GLU	CB-CG-CD	5.30	121.61	112.60

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	141	ARG	Sidechain
1	A	213	ARG	Sidechain
1	B	104	ARG	Sidechain
1	B	141	ARG	Sidechain
1	B	318	ARG	Sidechain
1	B	367[A]	ARG	Sidechain
1	B	367[B]	ARG	Sidechain
1	B	89	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	2981	0	2943	32	0
1	B	2973	0	2948	25	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	37	0	47	0	0
3	B	74	0	94	16	0
4	A	28	0	42	0	0
4	B	20	0	30	2	0
5	A	14	0	20	0	0
6	A	4	0	8	2	0
6	B	4	0	8	1	0
7	A	5	0	0	0	0
7	B	15	0	0	1	0
8	A	2	0	0	0	0
8	B	1	0	0	0	0
9	A	180	0	0	5	0
9	B	216	0	0	7	0
All	All	6556	0	6140	68	0

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 (68) 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)
3:B:601[B]:CIQ:N1	3:B:601[B]:CIQ:HAPA	1.64	1.11
3:B:601[B]:CIQ:N1	3:B:601[B]:CIQ:CAP	2.34	0.91
1:A:331[A]:PHE:CD2	9:A:686:HOH:O	2.35	0.77
7:B:609:PO4:O3	9:B:701:HOH:O	2.06	0.73
3:B:601[B]:CIQ:CAI	3:B:601[B]:CIQ:CAK	2.68	0.72
1:B:116:ILE:HD11	1:B:126:GLN:HB2	1.73	0.71
1:A:178:VAL:HG22	1:B:178:VAL:HG12	1.74	0.68
3:B:601[B]:CIQ:HAD	9:B:727:HOH:O	1.96	0.66
1:A:84:GLU:HB2	1:A:85:PRO:CD	2.26	0.66
1:A:183:MET:HE1	1:A:331[A]:PHE:CD2	2.30	0.66
1:B:433:ILE:HG22	3:B:601[A]:CIQ:CAO	2.28	0.64
1:B:333:TYR:OH	3:B:601[A]:CIQ:HAS	1.99	0.63
1:B:90:ARG:NH1	9:B:702:HOH:O	2.18	0.63
1:B:175:GLU:O	1:B:179:LEU:HG	2.00	0.61
1:B:433:ILE:HG22	3:B:601[A]:CIQ:HAO	1.84	0.60
3:B:601[A]:CIQ:HAR	3:B:601[A]:CIQ:OAZ	2.02	0.60
1:A:223[B]:ASP:OD1	9:A:601:HOH:O	2.15	0.59
1:A:149:GLY:O	1:A:150:ALA:C	2.46	0.59
3:B:601[B]:CIQ:HAK	3:B:601[B]:CIQ:HAI	1.87	0.57
3:B:601[B]:CIQ:CAK	3:B:601[B]:CIQ:HAI	2.35	0.56
1:A:248:TRP:CG	1:A:335:SER:HG	2.25	0.55
1:A:183:MET:HE1	1:A:331[A]:PHE:HB2	1.90	0.54
1:B:433:ILE:HG22	3:B:601[A]:CIQ:HAOA	1.90	0.54
1:A:183:MET:HE1	1:A:331[B]:PHE:HB2	1.90	0.54
1:B:244:LYS:O	9:B:703:HOH:O	2.18	0.53
1:A:275:HIS:NE2	6:A:511:IPA:C3	2.71	0.53
1:A:357:GLU:HG3	9:A:728:HOH:O	2.08	0.53
1:B:427:GLN:O	1:B:431:SER:HB3	2.08	0.53
1:B:433:ILE:CG2	3:B:601[A]:CIQ:HAOA	2.40	0.51
1:B:254:GLU:OE1	1:B:290:ARG:NH2	2.39	0.51
1:A:308:GLN:HB3	1:A:349:GLU:HG3	1.93	0.50
1:A:331[A]:PHE:HD2	9:A:686:HOH:O	1.85	0.50
1:A:194:PRO:HD3	1:A:327:MET:HE2	1.95	0.49
1:B:454:LYS:HE2	9:B:842:HOH:O	2.13	0.49
1:A:84:GLU:HB2	1:A:85:PRO:HD2	1.95	0.48
1:B:377:HIS:ND1	4:B:604:EDO:H11	2.28	0.48
1:B:92:TYR:OH	1:B:96:LYS:HE2	2.13	0.48
1:B:140:PRO:HA	6:B:607:IPA:H2	1.96	0.48
3:B:601[B]:CIQ:HAU	9:B:762:HOH:O	2.13	0.48
3:B:601[A]:CIQ:OAZ	3:B:601[A]:CIQ:CAR	2.62	0.47
3:B:601[B]:CIQ:N1	3:B:601[B]:CIQ:CAU	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ARG:NH1	1:A:108:GLU:O	2.49	0.46
1:A:387:GLN:O	1:A:387:GLN:HG3	2.15	0.46
1:B:187:LEU:HD12	1:B:331[B]:PHE:CE2	2.51	0.45
1:B:248:TRP:O	1:B:252:THR:OG1	2.29	0.45
1:A:304:HIS:CD2	1:A:331[B]:PHE:CD1	3.05	0.45
1:A:275:HIS:NE2	6:A:511:IPA:H32	2.32	0.44
1:A:84:GLU:HB2	1:A:85:PRO:HD3	1.96	0.44
1:A:429:LYS:O	1:A:429:LYS:HD3	2.17	0.44
1:A:104:ARG:NH2	1:B:245:GLU:OE1	2.37	0.44
1:A:270:ARG:NH1	1:A:428:ALA:O	2.49	0.44
1:B:360:PRO:O	1:B:361:PHE:HB2	2.16	0.44
1:B:425:ILE:O	1:B:428:ALA:HB3	2.17	0.44
1:B:424:SER:O	1:B:437:TYR:HB3	2.18	0.43
1:A:389:ASP:OD2	9:A:602:HOH:O	2.21	0.43
1:B:282:LEU:N	1:B:283:PRO:CD	2.82	0.42
1:A:394:SER:HB3	1:A:397:GLU:OE1	2.19	0.42
1:B:313:LEU:O	1:B:326:LEU:HA	2.19	0.42
3:B:601[B]:CIQ:CAI	3:B:601[B]:CIQ:HAK	2.39	0.42
1:A:122:ASN:HA	1:A:147:LEU:O	2.20	0.42
1:A:174:ALA:O	1:A:178:VAL:HG23	2.20	0.41
1:A:183:MET:HE1	1:A:331[A]:PHE:CG	2.55	0.41
4:B:604:EDO:H21	9:B:858:HOH:O	2.20	0.41
1:A:128:SER:HB3	1:A:142:LYS:HB3	2.01	0.41
1:B:240:MET:HE3	1:B:242:PHE:CE2	2.56	0.41
1:A:84:GLU:CB	1:A:85:PRO:CD	2.95	0.41
1:A:144:LEU:C	1:A:144:LEU:HD23	2.46	0.40
1:A:313:LEU:O	1:A:326:LEU:HA	2.22	0.40

There are no symmetry-related clashes.

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	357/457 (78%)	340 (95%)	16 (4%)	1 (0%)	36	50
1	B	355/457 (78%)	344 (97%)	9 (2%)	2 (1%)	21	32
All	All	712/914 (78%)	684 (96%)	25 (4%)	3 (0%)	30	43

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	GLU
1	B	388	ASN
1	B	430	ILE

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	323/400 (81%)	312 (97%)	11 (3%)	32	54
1	B	322/400 (80%)	314 (98%)	8 (2%)	42	64
All	All	645/800 (81%)	626 (97%)	19 (3%)	36	60

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

Mol	Chain	Res	Type
1	A	86	ARG
1	A	88	ARG
1	A	128	SER
1	A	175	GLU
1	A	195	LYS
1	A	238	MET
1	A	269	SER
1	A	270	ARG
1	A	328	LEU
1	A	395	THR
1	A	429	LYS
1	B	177	MET
1	B	178	VAL

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Mol	Chain	Res	Type
1	B	260	VAL
1	B	263	ILE
1	B	267	GLU
1	B	271	ILE
1	B	399	SER
1	B	433	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	112	HIS
1	A	126	GLN
1	A	288	ASN
1	A	320	ASN
1	A	392	ASN
1	A	442	GLN
1	B	82	GLN
1	B	112	HIS
1	B	288	ASN
1	B	387	GLN
1	B	392	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](#)

Of 28 ligands modelled in this entry, 5 are monoatomic - leaving 23 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$
3	CIQ	B	601[B]	-	39,41,41	1.54	9 (23%)	53,56,56	3.08	20 (37%)
3	CIQ	B	601[A]	-	39,41,41	1.05	3 (7%)	53,56,56	2.93	21 (39%)
4	EDO	A	502	-	3,3,3	0.21	0	2,2,2	0.06	0
4	EDO	B	606	-	3,3,3	0.37	0	2,2,2	0.31	0
7	PO4	B	608	-	4,4,4	0.66	0	6,6,6	0.45	0
5	PEG	A	509	-	6,6,6	0.53	0	5,5,5	0.28	0
4	EDO	A	504	-	3,3,3	0.31	0	2,2,2	0.11	0
4	EDO	B	604	-	3,3,3	0.50	0	2,2,2	0.84	0
4	EDO	B	603	-	3,3,3	0.17	0	2,2,2	0.34	0
4	EDO	A	506	-	3,3,3	0.37	0	2,2,2	0.45	0
4	EDO	B	605	-	3,3,3	0.21	0	2,2,2	0.11	0
4	EDO	A	507	-	3,3,3	0.36	0	2,2,2	0.50	0
7	PO4	B	609	-	4,4,4	0.58	0	6,6,6	0.66	0
4	EDO	A	503	-	3,3,3	0.33	0	2,2,2	0.37	0
4	EDO	A	505	-	3,3,3	0.81	0	2,2,2	0.78	0
7	PO4	B	610	-	4,4,4	1.23	0	6,6,6	0.59	0
7	PO4	A	512	-	4,4,4	1.57	2 (50%)	6,6,6	0.58	0
4	EDO	A	508	-	3,3,3	0.19	0	2,2,2	0.63	0
6	IPA	B	607	-	3,3,3	0.54	0	3,3,3	0.42	0
4	EDO	B	602	-	3,3,3	0.62	0	2,2,2	0.71	0
3	CIQ	A	501	-	39,41,41	1.50	9 (23%)	53,56,56	2.41	15 (28%)
5	PEG	A	510	-	6,6,6	0.61	0	5,5,5	0.64	0
6	IPA	A	511	-	3,3,3	0.57	0	3,3,3	0.16	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
3	CIQ	B	601[B]	-	-	9/21/46/46	0/5/5/5
4	EDO	B	604	-	-	0/1/1/1	-
3	CIQ	B	601[A]	-	-	5/21/46/46	0/5/5/5
4	EDO	A	505	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	508	-	-	1/1/1/1	-
4	EDO	A	502	-	-	0/1/1/1	-
4	EDO	B	602	-	-	1/1/1/1	-
3	CIQ	A	501	-	-	5/21/46/46	0/5/5/5
4	EDO	A	506	-	-	0/1/1/1	-
4	EDO	B	603	-	-	1/1/1/1	-
5	PEG	A	510	-	-	3/4/4/4	-
4	EDO	B	606	-	-	1/1/1/1	-
4	EDO	B	605	-	-	1/1/1/1	-
4	EDO	A	507	-	-	0/1/1/1	-
5	PEG	A	509	-	-	2/4/4/4	-
4	EDO	A	504	-	-	1/1/1/1	-
4	EDO	A	503	-	-	1/1/1/1	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601[B]	CIQ	CAE-CBA	3.70	1.43	1.36
3	B	601[B]	CIQ	C6-N1	3.07	1.37	1.33
3	A	501	CIQ	C6-N1	3.05	1.37	1.33
3	A	501	CIQ	CAE-CBA	2.98	1.42	1.36
3	B	601[B]	CIQ	C6-C5	-2.97	1.41	1.44
3	B	601[A]	CIQ	CBH-NAX	2.78	1.52	1.46
3	B	601[B]	CIQ	CAD-C4	-2.66	1.37	1.41
3	B	601[A]	CIQ	C6-C5	-2.58	1.41	1.44
3	A	501	CIQ	CBG-NBK	2.53	1.53	1.48
3	B	601[B]	CIQ	C4-N3	-2.50	1.33	1.37
7	A	512	PO4	P-O1	2.35	1.56	1.50
3	B	601[A]	CIQ	CAE-CBA	2.29	1.40	1.36
3	A	501	CIQ	CAD-CBB	2.27	1.40	1.36
3	A	501	CIQ	C6-C5	-2.26	1.42	1.44
3	A	501	CIQ	CAN-CBI	2.20	1.58	1.53
3	A	501	CIQ	CAO-CAT	2.20	1.58	1.52
3	B	601[B]	CIQ	CAO-CAT	2.17	1.58	1.52
3	A	501	CIQ	CAO-CBH	2.14	1.56	1.52
3	A	501	CIQ	CAH-CAN	2.05	1.58	1.53
3	B	601[B]	CIQ	CAI-CAQ	-2.05	1.44	1.51
3	B	601[B]	CIQ	CAH-CAN	2.04	1.58	1.53
7	A	512	PO4	P-O4	-2.02	1.48	1.54
3	B	601[B]	CIQ	CBH-NAX	2.02	1.50	1.46

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601[B]	CIQ	C2-N3-C4	9.20	122.60	116.50
3	B	601[A]	CIQ	CAT-NBK-CBG	-9.07	98.54	113.01
3	B	601[B]	CIQ	CAS-NBJ-CAQ	-8.61	92.84	113.25
3	B	601[A]	CIQ	CAU-NBK-CBG	-8.01	100.23	113.01
3	B	601[A]	CIQ	C2-N3-C4	6.91	121.08	116.50
3	B	601[B]	CIQ	CAJ-CAR-NBJ	-6.78	95.91	103.90
3	A	501	CIQ	CAS-NBJ-CAR	-6.42	98.02	113.25
3	A	501	CIQ	C2-N3-C4	6.23	120.63	116.50
3	B	601[B]	CIQ	CAS-NBJ-CAR	-6.20	98.55	113.25
3	A	501	CIQ	N3-C2-N1	-5.92	118.00	126.21
3	A	501	CIQ	CAR-NBJ-CAQ	5.80	110.89	104.04
3	B	601[B]	CIQ	CAR-NBJ-CAQ	5.75	110.84	104.04
3	B	601[B]	CIQ	N3-C2-N1	-5.72	118.28	126.21
3	A	501	CIQ	CAU-CAP-CBH	-5.49	102.00	110.67
3	B	601[A]	CIQ	CAS-NBJ-CAQ	-5.29	100.70	113.25
3	B	601[A]	CIQ	CAG-CAM-CBI	-4.96	102.80	111.56
3	B	601[A]	CIQ	CAO-CAT-NBK	-4.93	103.83	111.42
3	A	501	CIQ	CAS-NBJ-CAQ	-4.92	101.60	113.25
3	B	601[A]	CIQ	CAS-NBJ-CAR	-4.85	101.74	113.25
3	B	601[B]	CIQ	CAP-CAU-NBK	-4.83	103.98	111.42
3	B	601[B]	CIQ	CAK-CAS-NBJ	-4.67	100.79	113.93
3	B	601[A]	CIQ	CAA-OAY-CBA	-4.62	110.74	117.51
3	B	601[B]	CIQ	OAZ-CBB-CAD	-4.45	117.89	125.20
3	B	601[A]	CIQ	N3-C2-N1	-4.43	120.07	126.21
3	B	601[A]	CIQ	CAP-CAU-NBK	-4.08	105.14	111.42
3	B	601[A]	CIQ	CAU-CAP-CBH	-3.92	104.47	110.67
3	A	501	CIQ	CAT-NBK-CBG	-3.87	106.83	113.01
3	B	601[A]	CIQ	CAL-OAZ-CBB	-3.41	109.45	117.69
3	B	601[B]	CIQ	CAG-CAM-CBI	-3.30	105.74	111.56
3	B	601[B]	CIQ	CAM-CBI-C2	-3.23	105.08	111.85
3	B	601[B]	CIQ	CAS-CAK-CAL	-3.17	101.78	112.77
3	A	501	CIQ	CAP-CAU-NBK	-2.95	106.88	111.42
3	B	601[B]	CIQ	CAU-CAP-CBH	-2.87	106.14	110.67
3	A	501	CIQ	C5-C6-N1	-2.79	117.88	122.07
3	B	601[B]	CIQ	CAT-CAO-CBH	-2.79	106.26	110.67
3	A	501	CIQ	C2-N1-C6	2.72	124.60	118.03
3	B	601[A]	CIQ	CAU-NBK-CAT	2.63	114.14	109.13
3	B	601[B]	CIQ	OAZ-CBB-CBA	2.62	121.17	115.75
3	A	501	CIQ	CAG-CAM-CBI	-2.52	107.11	111.56
3	A	501	CIQ	CAO-CAT-NBK	-2.43	107.68	111.42
3	A	501	CIQ	CAC-CBG-CAB	-2.39	105.96	112.46
3	B	601[B]	CIQ	CAF-CAG-CAM	-2.34	106.60	111.42
3	B	601[A]	CIQ	C6-C5-C4	2.21	117.17	115.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601[B]	CIQ	CAD-C4-C5	2.20	122.04	119.58
3	B	601[B]	CIQ	CAL-OAZ-CBB	2.20	123.00	117.69
3	B	601[A]	CIQ	C5-C4-N3	-2.16	120.51	122.80
3	A	501	CIQ	CAH-CAN-CBI	2.13	115.31	111.56
3	B	601[A]	CIQ	CAJ-CAI-CAQ	-2.13	99.21	105.10
3	B	601[B]	CIQ	CAA-OAY-CBA	-2.12	114.41	117.51
3	B	601[A]	CIQ	CAD-C4-C5	2.12	121.94	119.58
3	B	601[A]	CIQ	C5-C6-N1	-2.10	118.92	122.07
3	A	501	CIQ	CAK-CAS-NBJ	-2.06	108.14	113.93
3	B	601[A]	CIQ	CAS-CAK-CAL	-2.06	105.62	112.77
3	B	601[A]	CIQ	CAP-CBH-CAO	-2.06	107.25	110.80
3	B	601[A]	CIQ	CAT-CAO-CBH	-2.03	107.47	110.67
3	B	601[B]	CIQ	OAZ-CAL-CAK	-2.03	100.84	108.30

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	CIQ	CAK-CAS-NBJ-CAR
3	B	601[A]	CIQ	CAL-CAK-CAS-NBJ
3	B	601[B]	CIQ	CAK-CAS-NBJ-CAR
3	B	601[B]	CIQ	CAP-CBH-NAX-C6
5	A	510	PEG	O2-C3-C4-O4
3	A	501	CIQ	CAS-CAK-CAL-OAZ
3	B	601[A]	CIQ	N3-C2-CBI-CAM
3	B	601[A]	CIQ	CAK-CAL-OAZ-CBB
3	B	601[A]	CIQ	CBA-CBB-OAZ-CAL
5	A	509	PEG	O1-C1-C2-O2
5	A	510	PEG	O1-C1-C2-O2
3	B	601[B]	CIQ	CAK-CAL-OAZ-CBB
4	A	504	EDO	O1-C1-C2-O2
4	B	605	EDO	O1-C1-C2-O2
3	A	501	CIQ	CAC-CBG-NBK-CAU
3	B	601[B]	CIQ	CAB-CBG-NBK-CAU
4	A	508	EDO	O1-C1-C2-O2
3	B	601[B]	CIQ	CAD-CBB-OAZ-CAL
3	B	601[A]	CIQ	CAD-CBB-OAZ-CAL
3	B	601[B]	CIQ	N1-C2-CBI-CAN
4	B	602	EDO	O1-C1-C2-O2
5	A	510	PEG	C1-C2-O2-C3
4	A	503	EDO	O1-C1-C2-O2
5	A	509	PEG	C4-C3-O2-C2

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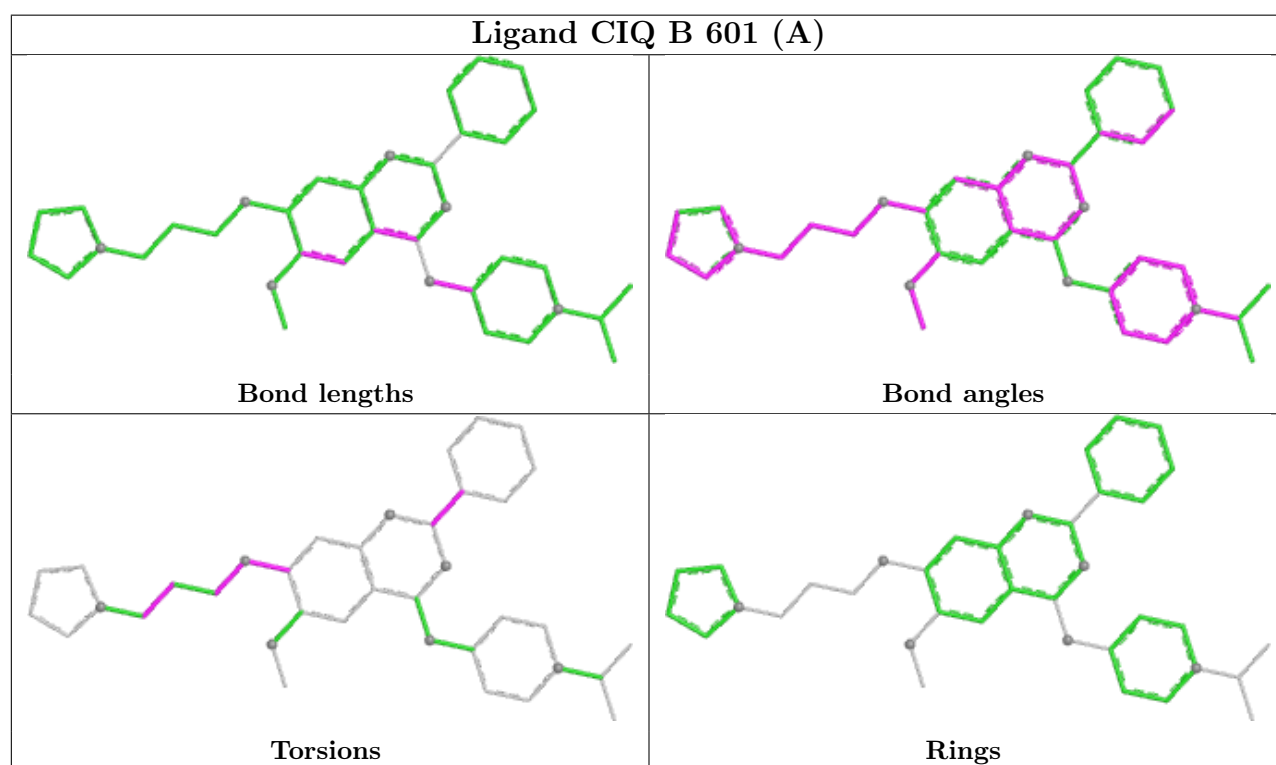
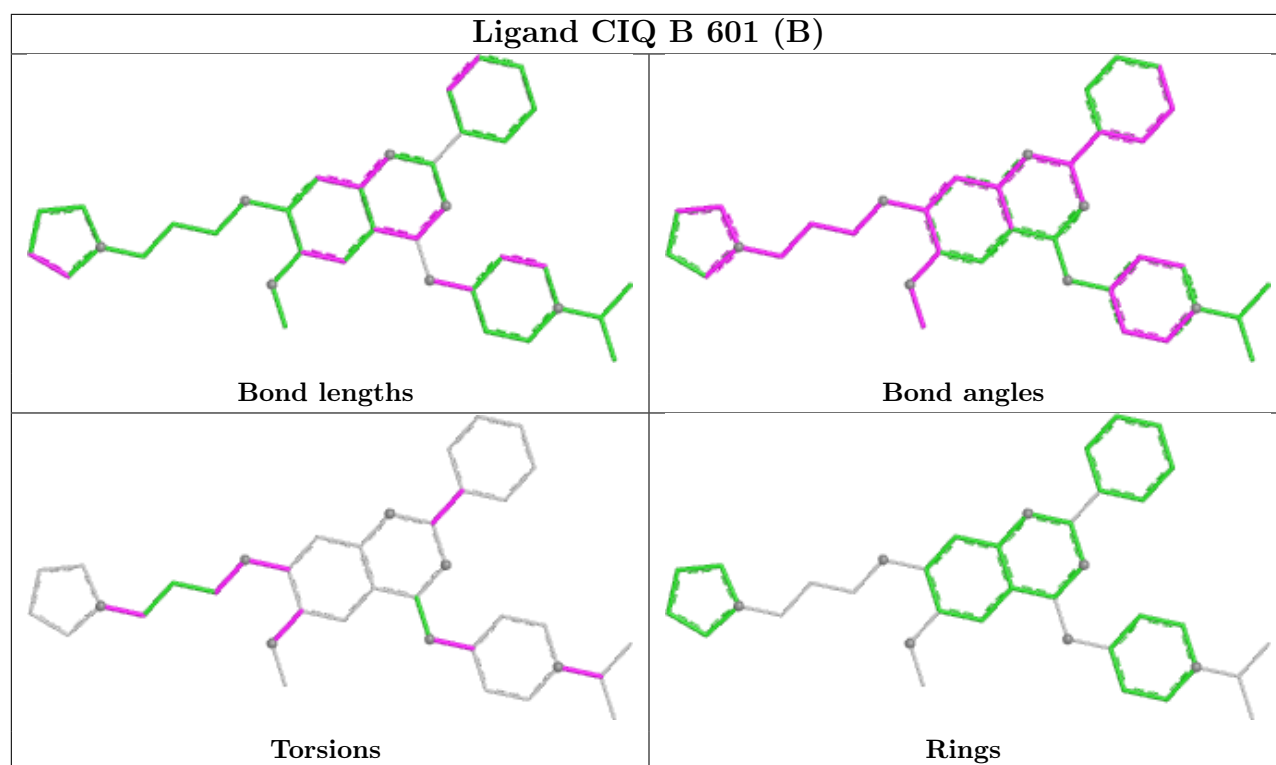
Mol	Chain	Res	Type	Atoms
3	B	601[B]	CIQ	CBB-CBA-OAY-CAA
4	A	505	EDO	O1-C1-C2-O2
4	B	603	EDO	O1-C1-C2-O2
3	A	501	CIQ	CAK-CAS-NBJ-CAQ
3	B	601[B]	CIQ	CAE-CBA-OAY-CAA
4	B	606	EDO	O1-C1-C2-O2
3	B	601[B]	CIQ	CBA-CBB-OAZ-CAL
3	A	501	CIQ	N3-C2-CBI-CAM

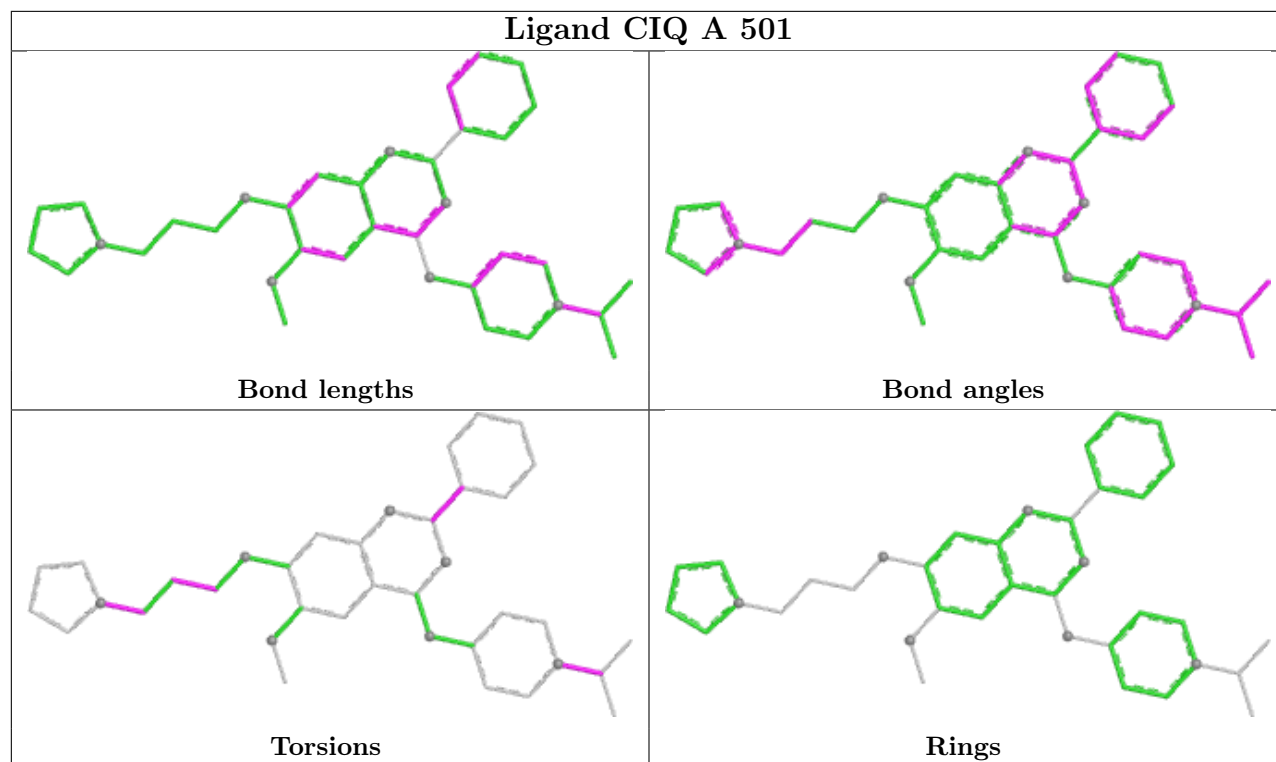
There are no ring outliers.

6 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601[B]	CIQ	9	0
3	B	601[A]	CIQ	7	0
4	B	604	EDO	2	0
7	B	609	PO4	1	0
6	B	607	IPA	1	0
6	A	511	IPA	2	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	355/457 (77%)	0.16	11 (3%) 51 47	25, 51, 110, 143	8 (2%)
1	B	354/457 (77%)	0.04	9 (2%) 58 54	22, 52, 99, 137	10 (2%)
All	All	709/914 (77%)	0.10	20 (2%) 55 51	22, 52, 106, 143	18 (2%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	174	ALA	6.5
1	A	150	ALA	6.4
1	A	174	ALA	4.9
1	A	433	ILE	4.1
1	A	177[A]	MET	4.1
1	A	120	LEU	4.1
1	B	150	ALA	3.6
1	A	87	THR	3.4
1	B	120	LEU	3.3
1	B	433	ILE	3.3
1	A	85	PRO	3.0
1	B	177	MET	2.8
1	A	117	ARG	2.7
1	B	175	GLU	2.6
1	B	118	GLY	2.5
1	B	264	LYS	2.5
1	A	149	GLY	2.4
1	A	86	ARG	2.4
1	A	134	ALA	2.4
1	B	432	SER	2.1

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 ⓘ

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($\text{\AA}^2$)	Q<0.9
4	EDO	B	604	4/4	0.82	0.23	57,57,63,84	0
4	EDO	A	507	4/4	0.83	0.30	78,87,87,89	0
6	IPA	A	511	4/4	0.83	0.28	74,83,88,90	0
6	IPA	B	607	4/4	0.85	0.22	49,66,68,70	0
7	PO4	A	512	5/5	0.85	0.13	72,81,87,113	0
7	PO4	B	610	5/5	0.85	0.16	64,79,96,102	0
4	EDO	A	506	4/4	0.86	0.27	74,84,88,89	0
7	PO4	B	608	5/5	0.86	0.12	102,103,119,123	0
5	PEG	A	509	7/7	0.86	0.23	79,83,89,92	0
7	PO4	B	609	5/5	0.87	0.17	108,113,117,129	0
5	PEG	A	510	7/7	0.87	0.23	68,77,86,93	0
4	EDO	B	605	4/4	0.88	0.18	65,69,76,85	0
4	EDO	A	505	4/4	0.89	0.20	60,70,70,74	0
4	EDO	B	606	4/4	0.89	0.21	65,72,87,89	0
3	CIQ	B	601[A]	37/37	0.89	0.35	88,103,154,160	37
3	CIQ	B	601[B]	37/37	0.89	0.35	39,70,97,98	37
4	EDO	A	504	4/4	0.89	0.24	60,65,75,76	0
4	EDO	A	508	4/4	0.90	0.14	77,84,87,87	0
4	EDO	A	503	4/4	0.90	0.29	54,68,69,80	0
8	CL	A	513	1/1	0.91	0.17	81,81,81,81	0
8	CL	A	514	1/1	0.91	0.15	85,85,85,85	0
3	CIQ	A	501	37/37	0.92	0.17	63,83,117,123	0
4	EDO	B	603	4/4	0.93	0.14	60,62,69,70	0
4	EDO	B	602	4/4	0.93	0.16	54,66,71,81	0
8	CL	B	611	1/1	0.95	0.14	84,84,84,84	0
2	MG	A	500	1/1	0.97	0.08	44,44,44,44	0
4	EDO	A	502	4/4	0.97	0.11	41,51,54,54	0

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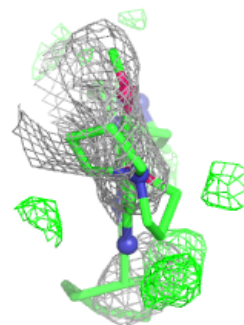
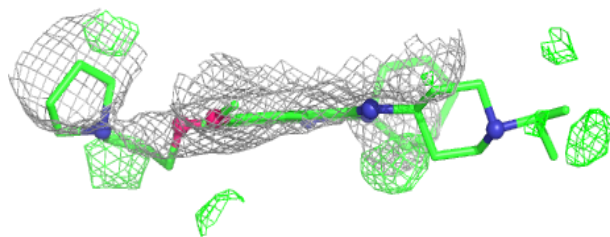
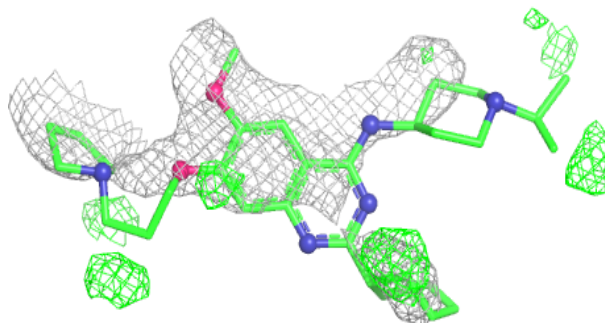
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	B	600	1/1	0.99	0.05	47,47,47,47	0

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.

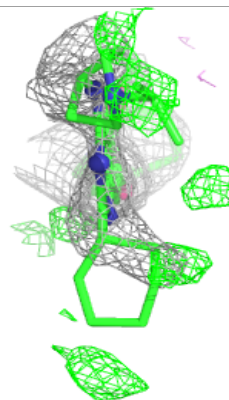
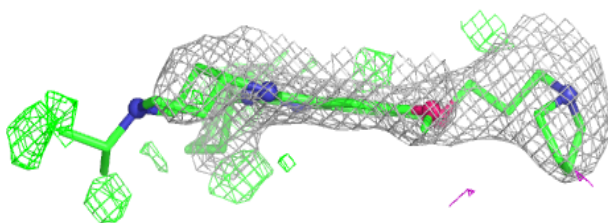
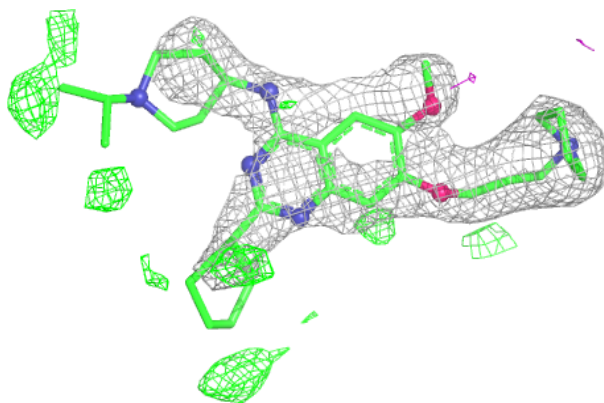
Electron density around CIQ B 601 (A):

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

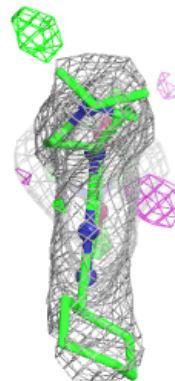
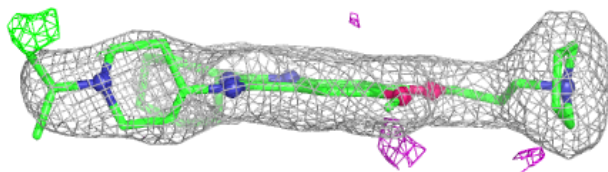
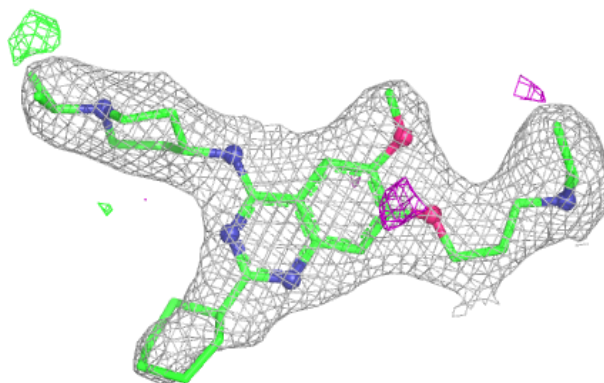


Electron density around CIQ B 601 (B):

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

**Electron density around CIQ A 501:**

$2mF_o-DF_c$ (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.