



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:33 PM UTC

PDB ID : 5C2E / pdb_00005c2e
Title : PDE10 complexed with 6-chloro-N-[(2,4-dimethylthiazol-5-yl)methyl]-5-methyl-2-[2-(2-pyridyl)ethoxy]pyrimidin-4-amine
Authors : Yan, Y.
Deposited on : 2015-06-15
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

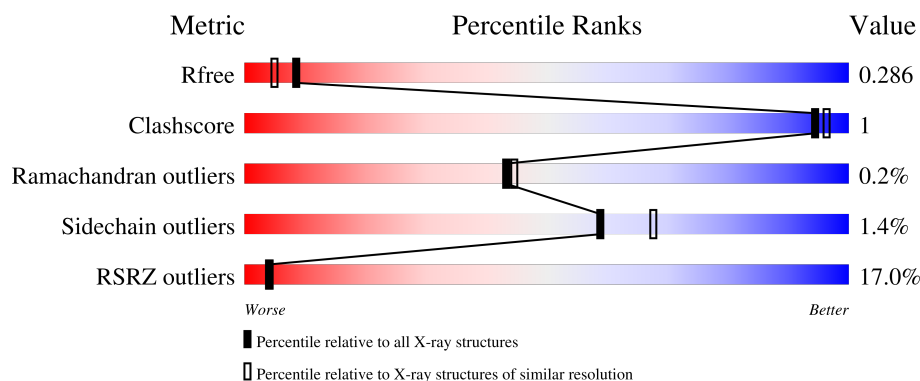
1 Overall quality at a glance

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	362	16% 84% 5% 11%
1	B	362	14% 83% 6% 11%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5388 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 cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2603	1664	443	471	25			
1	B	323	Total	C	N	O	S	0	0	0
			2612	1668	445	474	25			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	418	MET	-	initiating methionine	UNP Q9Y233
A	419	GLY	-	expression tag	UNP Q9Y233
A	420	SER	-	expression tag	UNP Q9Y233
A	421	SER	-	expression tag	UNP Q9Y233
A	422	HIS	-	expression tag	UNP Q9Y233
A	423	HIS	-	expression tag	UNP Q9Y233
A	424	HIS	-	expression tag	UNP Q9Y233
A	425	HIS	-	expression tag	UNP Q9Y233
A	426	HIS	-	expression tag	UNP Q9Y233
A	427	HIS	-	expression tag	UNP Q9Y233
A	428	SER	-	expression tag	UNP Q9Y233
A	429	SER	-	expression tag	UNP Q9Y233
A	430	GLY	-	expression tag	UNP Q9Y233
A	431	LEU	-	expression tag	UNP Q9Y233
A	432	VAL	-	expression tag	UNP Q9Y233
A	433	PRO	-	expression tag	UNP Q9Y233
A	434	ARG	-	expression tag	UNP Q9Y233
A	435	GLY	-	expression tag	UNP Q9Y233
A	436	SER	-	expression tag	UNP Q9Y233
A	437	HIS	-	expression tag	UNP Q9Y233
A	438	MET	-	expression tag	UNP Q9Y233
B	418	MET	-	initiating methionine	UNP Q9Y233
B	419	GLY	-	expression tag	UNP Q9Y233
B	420	SER	-	expression tag	UNP Q9Y233

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Chain	Residue	Modelled	Actual	Comment	Reference
B	421	SER	-	expression tag	UNP Q9Y233
B	422	HIS	-	expression tag	UNP Q9Y233
B	423	HIS	-	expression tag	UNP Q9Y233
B	424	HIS	-	expression tag	UNP Q9Y233
B	425	HIS	-	expression tag	UNP Q9Y233
B	426	HIS	-	expression tag	UNP Q9Y233
B	427	HIS	-	expression tag	UNP Q9Y233
B	428	SER	-	expression tag	UNP Q9Y233
B	429	SER	-	expression tag	UNP Q9Y233
B	430	GLY	-	expression tag	UNP Q9Y233
B	431	LEU	-	expression tag	UNP Q9Y233
B	432	VAL	-	expression tag	UNP Q9Y233
B	433	PRO	-	expression tag	UNP Q9Y233
B	434	ARG	-	expression tag	UNP Q9Y233
B	435	GLY	-	expression tag	UNP Q9Y233
B	436	SER	-	expression tag	UNP Q9Y233
B	437	HIS	-	expression tag	UNP Q9Y233
B	438	MET	-	expression tag	UNP Q9Y233

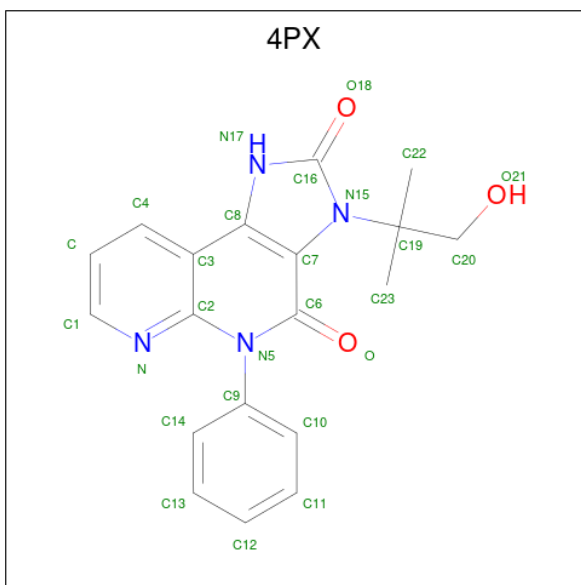
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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

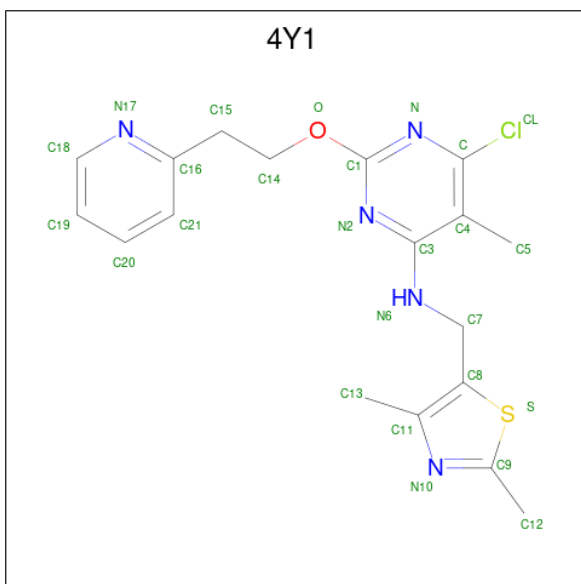
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0

- Molecule 4 is 3-(1-hydroxy-2-methylpropan-2-yl)-5-phenyl-3,5-dihydro-1H-imidazo[4,5-c][1,8]naphthyridine-2,4-dione (CCD ID: 4PX) (formula: C₁₉H₁₈N₄O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			26	19	4	3		

- Molecule 5 is 6-chloro-N-[(2,4-dimethyl-1,3-thiazol-5-yl)methyl]-5-methyl-2-[2-(pyridin-2-yl)ethoxy]pyrimidin-4-amine (CCD ID: 4Y1) (formula: $C_{18}H_{20}ClN_5OS$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	Cl	N	O	S	0
			26	18	1	5	1	1	0

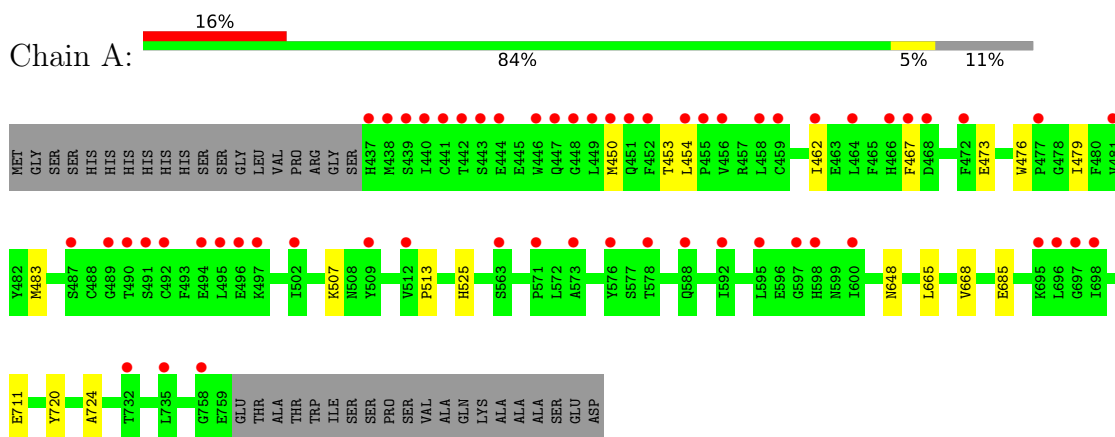
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	63	Total 63	O 63	0	0
6	B	54	Total 54	O 54	0	0

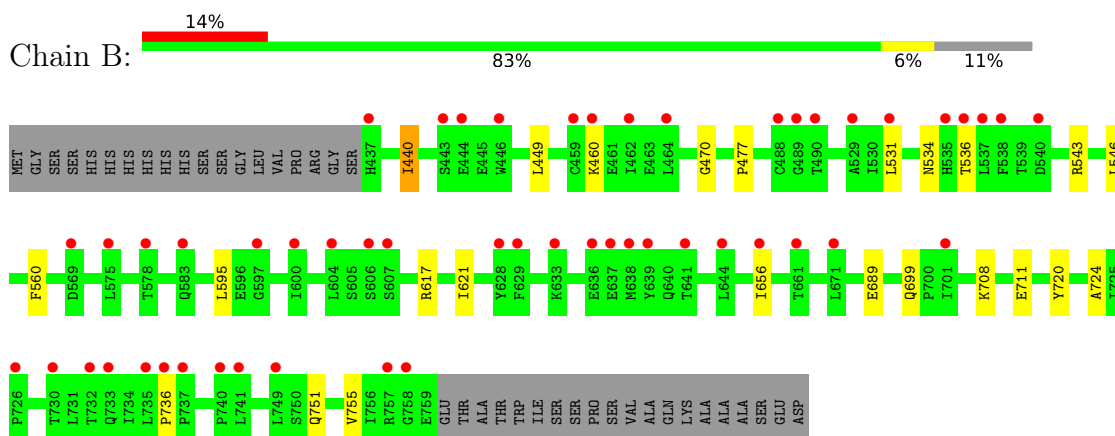
3 Residue-property plots [i](#)

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: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A



- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.50Å 81.35Å 158.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.96 – 2.10 40.96 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.1 (40.96-2.10) 97.8 (40.96-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.67 (at 2.10Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, R_{free}	0.249 , 0.280 (Not available) , 0.286	Depositor DCC
R_{free} test set	1934 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.955	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5388	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 4PX, MG, 4Y1

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	0.76	0/2668	1.36	3/3615 (0.1%)
1	B	0.77	0/2677	1.40	9/3626 (0.2%)
All	All	0.76	0/5345	1.38	12/7241 (0.2%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	708	LYS	CA-C-N	6.59	129.11	120.28
1	B	708	LYS	C-N-CA	6.59	129.11	120.28
1	A	648	ASN	CA-CB-CG	5.87	118.47	112.60
1	B	711	GLU	CA-C-N	5.74	125.94	120.43
1	B	711	GLU	C-N-CA	5.74	125.94	120.43
1	A	711	GLU	CA-C-N	5.36	124.62	120.33
1	A	711	GLU	C-N-CA	5.36	124.62	120.33
1	B	460	LYS	CA-C-N	5.22	127.53	120.38
1	B	460	LYS	C-N-CA	5.22	127.53	120.38
1	B	736	PRO	N-CA-C	5.08	116.89	110.70
1	B	534	ASN	CA-C-N	5.03	127.53	120.28
1	B	534	ASN	C-N-CA	5.03	127.53	120.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2603	0	2552	6	0
1	B	2612	0	2567	8	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	26	0	18	0	0
5	B	26	0	20	0	0
6	A	63	0	0	0	0
6	B	54	0	0	0	0
All	All	5388	0	5157	14	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 1.

All (14) 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:531:LEU:HD22	1:B:543:ARG:HG2	1.94	0.49
1:A:473:GLU:HA	1:A:476:TRP:CE2	2.49	0.48
1:B:751:GLN:O	1:B:755:VAL:HG23	2.16	0.45
1:B:560:PHE:HD2	1:B:689:GLU:HG3	1.81	0.45
1:A:479:ILE:O	1:A:483:MET:HG3	2.17	0.44
1:A:720:TYR:HA	1:A:724:ALA:HB3	1.99	0.44
1:A:513:PRO:HD2	1:A:685:GLU:HG3	1.98	0.44
1:A:665:LEU:O	1:A:668:VAL:HG22	2.19	0.43
1:B:440:ILE:HG22	1:B:595:LEU:HD13	2.02	0.42
1:B:546:LEU:HD21	1:B:656:ILE:HG23	2.01	0.42
1:B:449:LEU:HD13	1:B:477:PRO:HB2	2.01	0.42
1:B:617:ARG:O	1:B:621:ILE:HG12	2.21	0.41
1:A:467:PHE:HB3	1:A:525:HIS:CE1	2.56	0.41
1:B:720:TYR:HA	1:B:724:ALA:HB3	2.02	0.41

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	321/362 (89%)	309 (96%)	12 (4%)	0	100	100
1	B	321/362 (89%)	312 (97%)	8 (2%)	1 (0%)	36	36
All	All	642/724 (89%)	621 (97%)	20 (3%)	1 (0%)	43	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	470	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	287/323 (89%)	282 (98%)	5 (2%)	53	62
1	B	290/323 (90%)	287 (99%)	3 (1%)	68	76
All	All	577/646 (89%)	569 (99%)	8 (1%)	59	67

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

Mol	Chain	Res	Type
1	A	450	MET
1	A	453	THR
1	A	454	LEU
1	A	462	ILE
1	A	507	LYS

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Mol	Chain	Res	Type
1	B	440	ILE
1	B	536	THR
1	B	699	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	516	ASN
1	A	532	GLN
1	A	566	GLN
1	A	594	GLN
1	A	645	ASN
1	A	716	GLN
1	A	733	GLN
1	A	751	GLN
1	B	447	GLN
1	B	594	GLN
1	B	640	GLN
1	B	645	ASN
1	B	733	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 6 ligands modelled in this entry, 4 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
5	4Y1	B	803	-	26,28,28	1.34	2 (7%)	26,38,38	1.83	5 (19%)
4	4PX	A	803	-	27,29,29	0.96	2 (7%)	32,44,44	1.33	4 (12%)

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
5	4Y1	B	803	-	-	2/11/11/11	0/3/3/3
4	4PX	A	803	-	-	3/13/13/13	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	803	4Y1	C3-N6	4.60	1.41	1.34
5	B	803	4Y1	O-C1	4.02	1.38	1.34
4	A	803	4PX	C9-N5	-2.57	1.40	1.44
4	A	803	4PX	C7-C6	2.36	1.48	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	803	4Y1	C7-N6-C3	-5.73	114.51	122.23
5	B	803	4Y1	C14-O-C1	-3.95	112.03	117.80
4	A	803	4PX	C22-C19-C20	-3.56	102.90	109.21
5	B	803	4Y1	C8-C7-N6	3.43	119.34	112.34
4	A	803	4PX	C4-C3-C2	2.91	120.10	117.23
4	A	803	4PX	O-C6-C7	-2.48	121.30	126.38
4	A	803	4PX	N-C2-N5	2.29	120.61	117.52
5	B	803	4Y1	N6-C3-N2	2.28	121.38	118.33
5	B	803	4Y1	C4-C-CL	2.17	121.94	119.24

There are no chirality outliers.

All (5) torsion outliers are listed below:

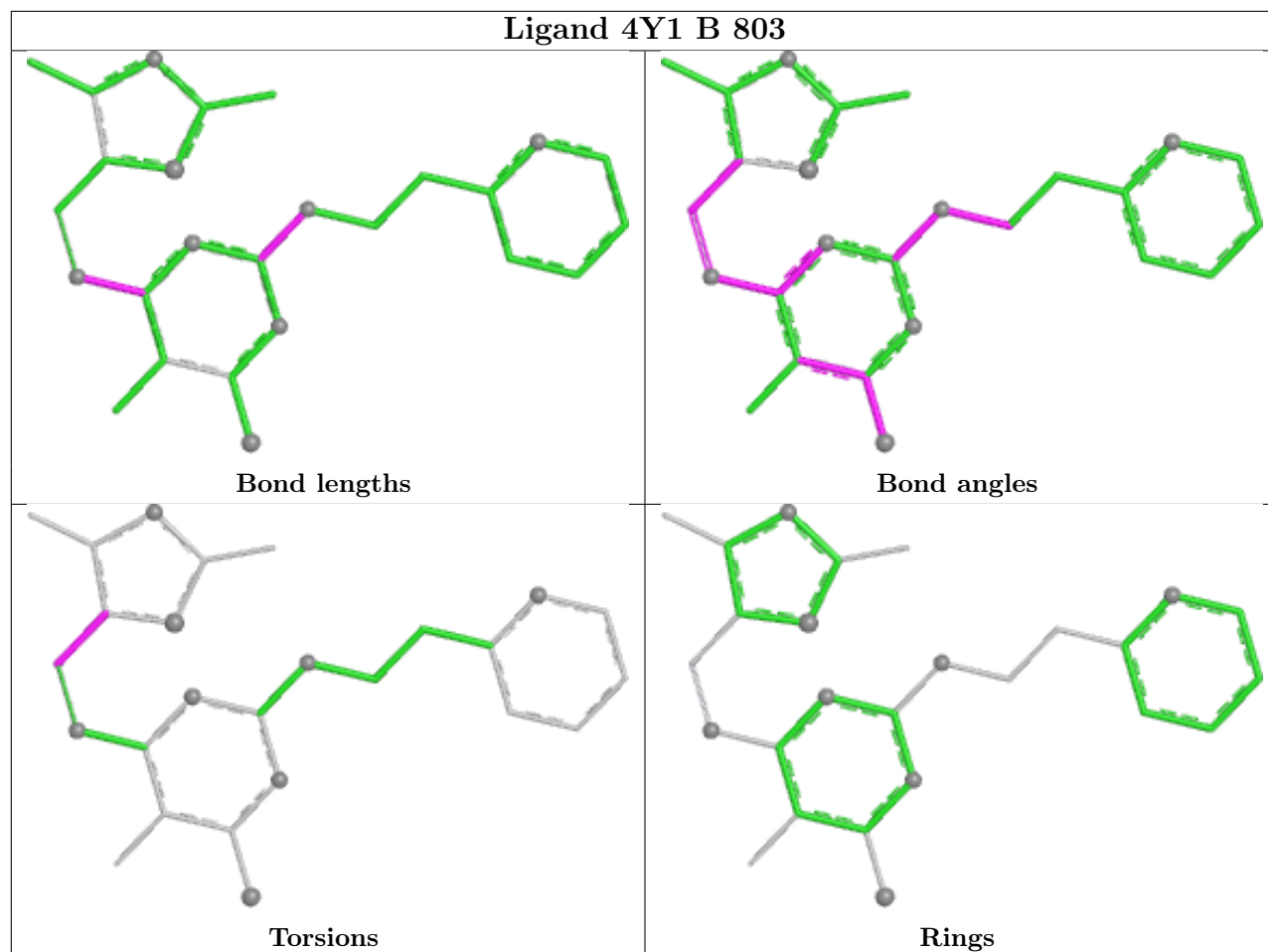
Mol	Chain	Res	Type	Atoms
4	A	803	4PX	C20-C19-N15-C16
5	B	803	4Y1	N6-C7-C8-S
4	A	803	4PX	C22-C19-N15-C16
4	A	803	4PX	C23-C19-N15-C16
5	B	803	4Y1	N6-C7-C8-C11

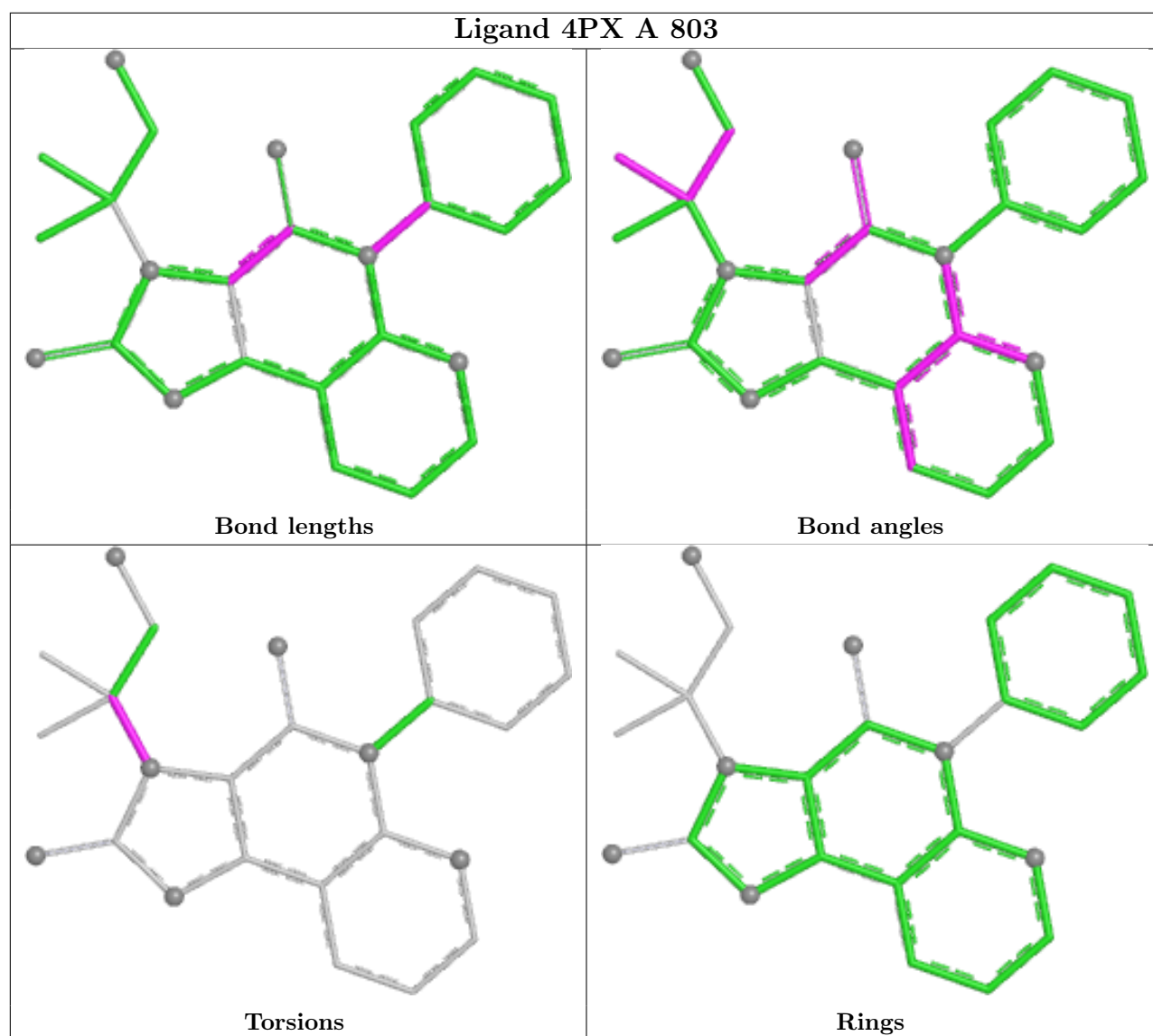
There are no ring outliers.

No monomer is involved in short contacts.

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.

Ligand 4Y1 B 803





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	323/362 (89%)	1.11	58 (17%) 3 3	26, 44, 71, 90	0
1	B	323/362 (89%)	1.24	52 (16%) 4 5	32, 49, 72, 98	0
All	All	646/724 (89%)	1.17	110 (17%) 4 4	26, 46, 72, 98	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	443	SER	5.4
1	A	459	CYS	4.5
1	A	496	GLU	4.2
1	A	456	VAL	4.1
1	A	439	SER	4.0
1	B	443	SER	3.8
1	A	491	SER	3.8
1	B	488	CYS	3.7
1	A	441	CYS	3.6
1	B	637	GLU	3.5
1	A	451	GLN	3.5
1	A	446	TRP	3.4
1	A	449	LEU	3.4
1	B	460	LYS	3.4
1	B	489	GLY	3.3
1	A	698	ILE	3.3
1	B	644	LEU	3.3
1	B	538	PHE	3.3
1	B	459	CYS	3.2
1	A	442	THR	3.2
1	B	633	LYS	3.1
1	A	563	SER	3.1
1	A	440	ILE	3.0
1	A	464	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	464	LEU	3.0
1	B	740	PRO	3.0
1	A	697	GLY	3.0
1	A	495	LEU	2.9
1	A	447	GLN	2.9
1	A	458	LEU	2.9
1	A	598	HIS	2.9
1	A	758	GLY	2.9
1	B	749	LEU	2.9
1	A	450	MET	2.9
1	A	462	ILE	2.8
1	B	606	SER	2.8
1	B	736	PRO	2.8
1	B	535	HIS	2.8
1	A	695	LYS	2.8
1	A	487	SER	2.7
1	A	437	HIS	2.7
1	B	628	TYR	2.7
1	B	741	LEU	2.7
1	B	638	MET	2.7
1	A	732	THR	2.7
1	A	455	PRO	2.7
1	A	502	ILE	2.7
1	B	569	ASP	2.6
1	B	671	LEU	2.6
1	A	481	VAL	2.6
1	B	730	THR	2.6
1	B	607	SER	2.6
1	B	629	PHE	2.5
1	A	512	VAL	2.5
1	A	597	GLY	2.5
1	B	578	THR	2.5
1	B	537	LEU	2.5
1	B	604	LEU	2.5
1	A	592	ILE	2.5
1	B	540	ASP	2.5
1	B	536	THR	2.5
1	B	732	THR	2.5
1	A	452	PHE	2.5
1	B	733	GLN	2.4
1	A	588	GLN	2.4
1	A	438	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	571	PRO	2.4
1	B	737	PRO	2.4
1	B	444	GLU	2.3
1	A	494	GLU	2.3
1	A	573	ALA	2.3
1	B	641	THR	2.3
1	A	448	GLY	2.3
1	B	575	LEU	2.3
1	B	757	ARG	2.3
1	A	468	ASP	2.3
1	A	497	LYS	2.3
1	B	758	GLY	2.3
1	B	437	HIS	2.2
1	B	462	ILE	2.2
1	B	656	ILE	2.2
1	A	509	TYR	2.2
1	B	600	ILE	2.2
1	A	696	LEU	2.2
1	A	466	HIS	2.2
1	B	639	TYR	2.2
1	A	444	GLU	2.2
1	A	576	TYR	2.2
1	B	446	TRP	2.2
1	B	661	THR	2.2
1	B	726	PRO	2.1
1	A	472	PHE	2.1
1	B	583	GLN	2.1
1	B	735	LEU	2.1
1	B	490	THR	2.1
1	B	701	ILE	2.1
1	B	529	ALA	2.1
1	B	531	LEU	2.1
1	A	467	PHE	2.1
1	A	595	LEU	2.1
1	A	454	LEU	2.0
1	A	492	CYS	2.0
1	A	477	PRO	2.0
1	A	490	THR	2.0
1	A	489	GLY	2.0
1	A	600	ILE	2.0
1	B	636	GLU	2.0
1	A	735	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	578	THR	2.0
1	B	597	GLY	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](#)

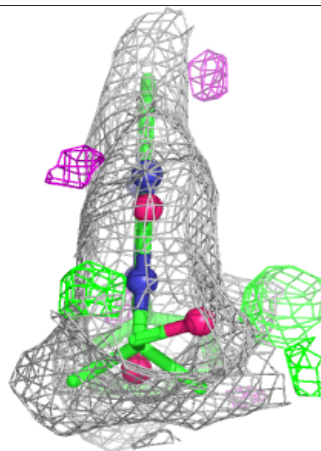
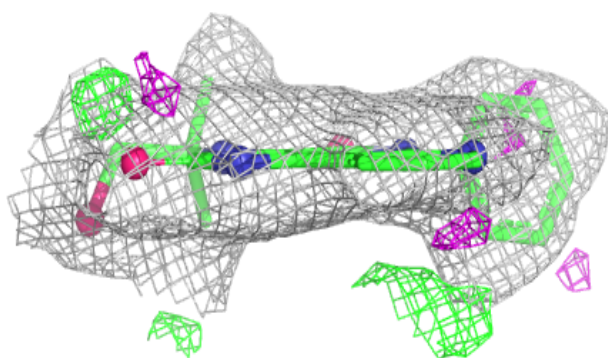
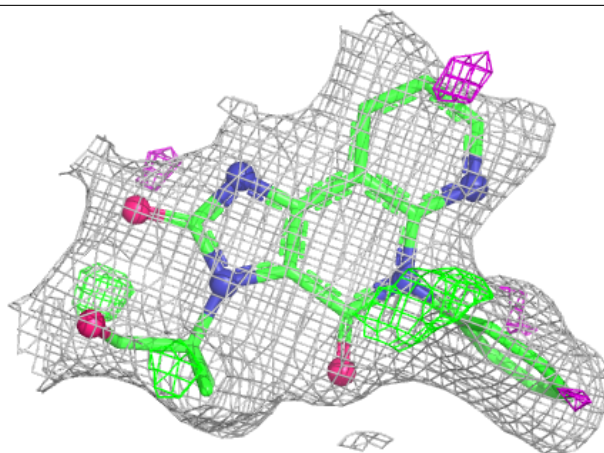
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	4PX	A	803	26/26	0.84	0.13	43,47,50,54	0
5	4Y1	B	803	26/26	0.89	0.11	32,39,47,49	0
3	MG	B	802	1/1	0.96	0.04	42,42,42,42	0
2	ZN	B	801	1/1	0.97	0.05	60,60,60,60	0
3	MG	A	802	1/1	0.99	0.02	29,29,29,29	0
2	ZN	A	801	1/1	0.99	0.04	44,44,44,44	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.

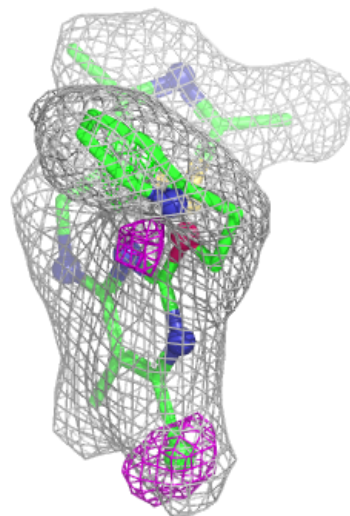
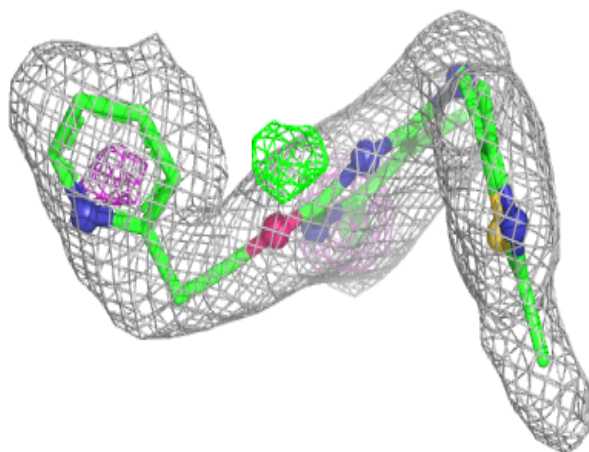
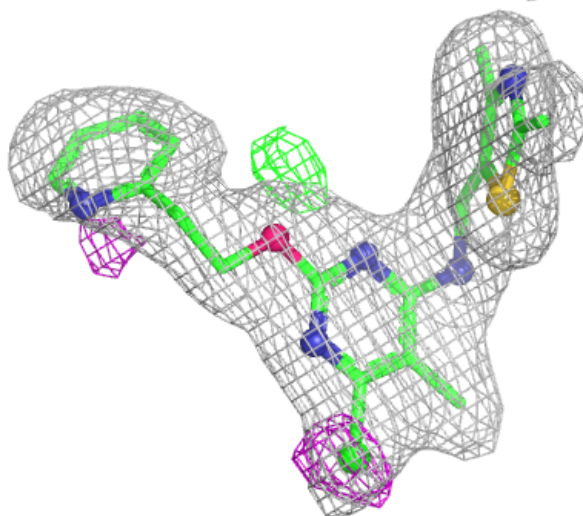
Electron density around 4PX A 803:

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



Electron density around 4Y1 B 803:

$2mF_o-DF_c$ (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.