Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2023 – 01:25 AM JST

PDB ID	:	6KDX
Title	:	Crystal structure of PDE10A in complex with a triazolopyrimidine inhibitor
Authors	:	Amano, Y.; Honbou, K.
Deposited on	:	2019-07-03
Resolution	:	2.44 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:

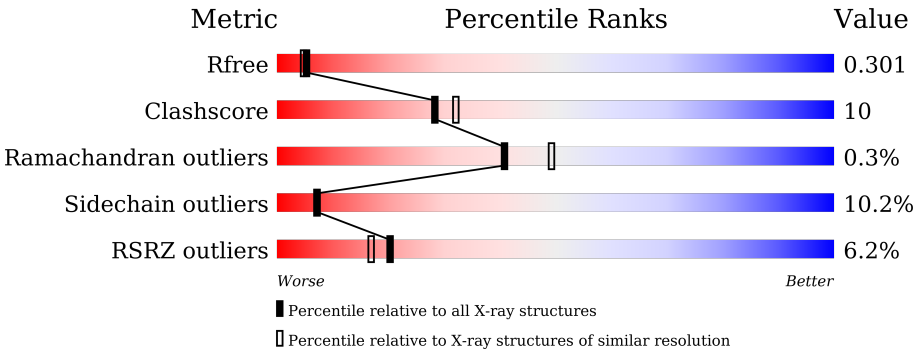
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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}	130704	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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 <=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	345	7% 65% 25% • • 6%
1	B	345	5% 67% 23% • 6%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5306 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	324	Total	C	N	O	S	0	0	0
			2629	1678	447	479	25			
1	B	324	Total	C	N	O	S	0	0	0
			2629	1678	447	479	25			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	445	GLY	-	expression tag	UNP Q9Y233
A	446	SER	-	expression tag	UNP Q9Y233
A	447	HIS	-	expression tag	UNP Q9Y233
A	448	MET	-	expression tag	UNP Q9Y233
B	445	GLY	-	expression tag	UNP Q9Y233
B	446	SER	-	expression tag	UNP Q9Y233
B	447	HIS	-	expression tag	UNP Q9Y233
B	448	MET	-	expression tag	UNP Q9Y233

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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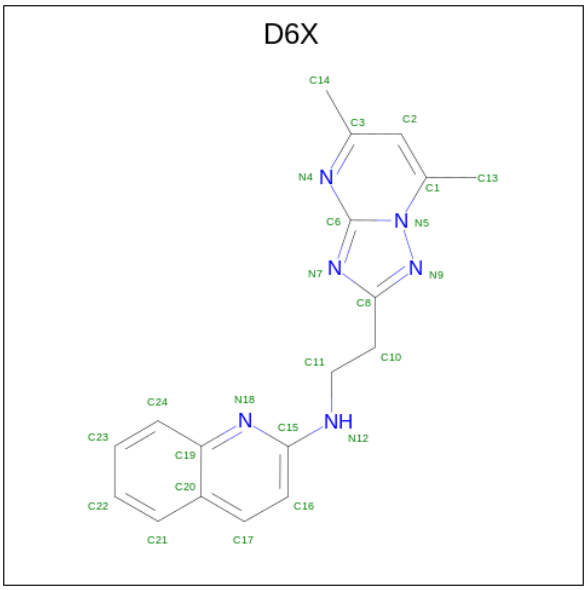
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0

- Molecule 4 is N-[2-(5,7-dimethyl-[1,2,4]triazolo[1,5-a]pyrimidin-2-yl)ethyl]quinolin-2-amine (three-letter code: D6X) (formula: $C_{18}H_{18}N_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N 24 18 6	0	0

- Molecule 5 is water.

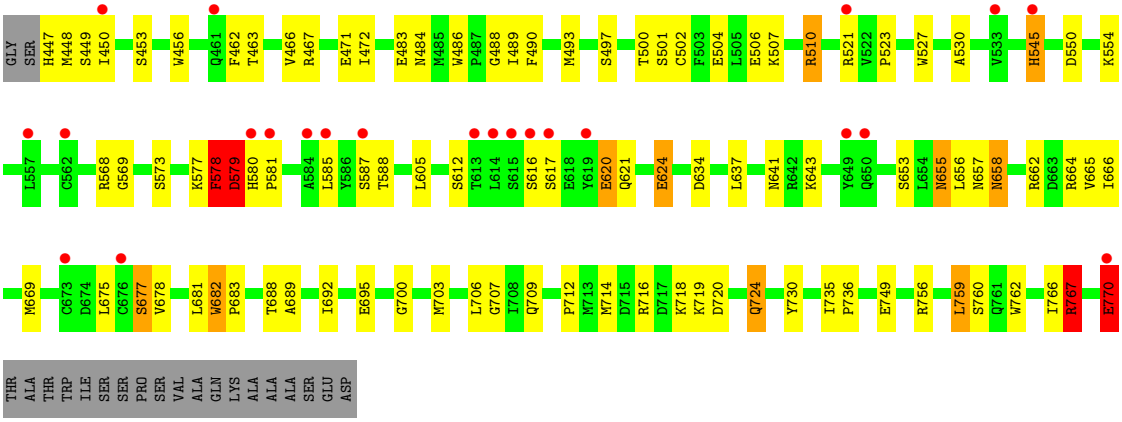
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	11	Total O 11 11	0	0
5	B	9	Total O 9 9	0	0

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.

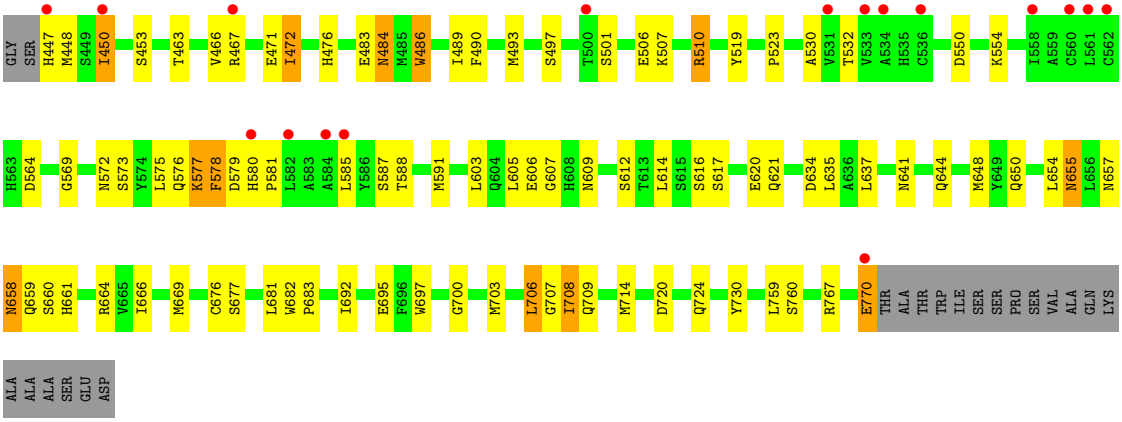
• Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A

Chain A:



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

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	50.42Å 81.44Å 159.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.66 – 2.44 26.66 – 2.44	Depositor EDS
% Data completeness (in resolution range)	91.1 (26.66-2.44) 91.2 (26.66-2.44)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.14 (at 2.44Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.241 , 0.301 0.241 , 0.301	Depositor DCC
R_{free} test set	1187 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	49.7	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 36.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5306	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: D6X, MG, ZN

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	0.85	9/2694 (0.3%)	0.94	12/3647 (0.3%)
1	B	0.82	5/2694 (0.2%)	0.92	12/3647 (0.3%)
All	All	0.84	14/5388 (0.3%)	0.93	24/7294 (0.3%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	545	HIS	CE1-NE2	10.59	1.57	1.32
1	A	770	GLU	CD-OE2	8.30	1.34	1.25
1	A	620	GLU	C-O	7.86	1.38	1.23
1	B	697	TRP	CD2-CE2	7.17	1.50	1.41
1	B	577	LYS	CE-NZ	6.55	1.65	1.49
1	A	471	GLU	CD-OE1	-6.53	1.18	1.25
1	A	620	GLU	CD-OE1	6.33	1.32	1.25
1	B	471	GLU	CD-OE1	-6.32	1.18	1.25
1	B	770	GLU	CD-OE2	5.97	1.32	1.25
1	A	456	TRP	CD2-CE2	5.71	1.48	1.41
1	A	682	TRP	CD2-CE2	5.29	1.47	1.41
1	B	486	TRP	CD2-CE2	5.24	1.47	1.41
1	A	471	GLU	CD-OE2	-5.10	1.20	1.25
1	A	762	TRP	CD2-CE2	5.03	1.47	1.41

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	467	ARG	NE-CZ-NH2	10.35	125.48	120.30
1	A	484	ASN	CB-CA-C	-9.58	91.23	110.40
1	B	467	ARG	NE-CZ-NH1	9.46	125.03	120.30
1	B	467	ARG	NE-CZ-NH2	-9.29	115.66	120.30
1	B	578	PHE	CB-CA-C	-8.70	93.00	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	720	ASP	CB-CG-OD1	-8.26	110.86	118.30
1	A	720	ASP	CB-CG-OD2	7.63	125.17	118.30
1	A	467	ARG	NE-CZ-NH1	-7.53	116.54	120.30
1	A	579	ASP	N-CA-C	-7.41	90.99	111.00
1	A	767	ARG	NE-CZ-NH2	7.38	123.99	120.30
1	B	564	ASP	CB-CG-OD1	7.32	124.89	118.30
1	B	720	ASP	CB-CG-OD1	-7.15	111.87	118.30
1	B	767	ARG	NE-CZ-NH2	7.07	123.84	120.30
1	B	720	ASP	CB-CG-OD2	6.84	124.46	118.30
1	B	471	GLU	OE1-CD-OE2	-6.02	116.08	123.30
1	A	578	PHE	C-N-CA	5.88	136.39	121.70
1	B	578	PHE	CB-CG-CD1	-5.70	116.81	120.80
1	B	767	ARG	NH1-CZ-NH2	-5.64	113.20	119.40
1	A	471	GLU	OE1-CD-OE2	-5.56	116.63	123.30
1	A	578	PHE	N-CA-C	5.50	125.85	111.00
1	A	767	ARG	NH1-CZ-NH2	-5.38	113.49	119.40
1	B	767	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	B	692	ILE	CG1-CB-CG2	-5.26	99.84	111.40
1	A	578	PHE	CB-CG-CD1	-5.17	117.18	120.80

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	2629	0	2588	60	1
1	B	2629	0	2588	52	1
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	24	0	0	0	0
5	A	11	0	0	2	0
5	B	9	0	0	0	0
All	All	5306	0	5176	102	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 10.

All (102) 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:580:HIS:ND1	5:A:901:HOH:O	1.68	1.26
1:A:724:GLN:OE1	1:B:683:PRO:HD3	1.33	1.26
1:A:724:GLN:HG3	1:B:683:PRO:HG3	1.30	1.08
1:A:641:ASN:HD22	1:A:664:ARG:HH11	1.09	0.99
1:A:724:GLN:OE1	1:B:682:TRP:HB3	1.64	0.97
1:B:523:PRO:HD2	1:B:695:GLU:HG3	1.48	0.94
1:A:502:CYS:SG	1:A:554:LYS:HD2	2.11	0.91
1:B:472:ILE:HD11	1:B:489:ILE:HG23	1.61	0.83
1:A:724:GLN:HG3	1:B:683:PRO:CG	2.08	0.82
1:B:573:SER:O	1:B:577:LYS:HB2	1.81	0.81
1:A:655:ASN:ND2	1:A:657:ASN:H	1.79	0.79
1:A:641:ASN:HD22	1:A:664:ARG:NH1	1.80	0.79
1:A:578:PHE:HZ	1:A:703:MET:HG2	1.48	0.78
1:A:677:SER:OG	1:A:688:THR:HG21	1.84	0.78
1:A:573:SER:O	1:A:577:LYS:HB2	1.84	0.77
1:B:658:ASN:C	1:B:658:ASN:HD22	1.88	0.77
1:A:730:TYR:HB3	1:A:759:LEU:HD12	1.67	0.74
1:B:641:ASN:HD22	1:B:664:ARG:HH11	1.41	0.67
1:B:655:ASN:ND2	1:B:657:ASN:H	1.93	0.67
1:A:472:ILE:HD11	1:A:489:ILE:HG23	1.78	0.65
1:A:730:TYR:CB	1:A:759:LEU:HD12	2.26	0.65
1:A:634:ASP:HB3	1:A:637:LEU:HD12	1.78	0.64
1:B:654:LEU:HD12	1:B:661:HIS:HD2	1.62	0.64
1:B:706:LEU:O	1:B:708:ILE:HG12	1.98	0.63
1:B:658:ASN:C	1:B:658:ASN:ND2	2.54	0.62
1:A:523:PRO:HD2	1:A:695:GLU:HG3	1.82	0.61
1:A:550:ASP:O	1:A:554:LYS:HG3	2.01	0.60
1:B:641:ASN:HD22	1:B:664:ARG:NH1	2.00	0.60
1:A:716:ARG:O	1:A:719:LYS:HG3	2.02	0.60
1:B:616:SER:O	1:B:620:GLU:HB2	2.03	0.59
1:B:578:PHE:CZ	1:B:703:MET:HG2	2.38	0.59
1:A:580:HIS:ND1	1:A:581:PRO:HD2	2.19	0.58
1:B:658:ASN:OD1	1:B:661:HIS:ND1	2.37	0.57
1:B:580:HIS:ND1	1:B:581:PRO:HD2	2.20	0.57
1:A:545:HIS:O	1:A:545:HIS:HD2	1.87	0.57
1:A:655:ASN:C	1:A:655:ASN:HD22	2.07	0.57
1:A:641:ASN:ND2	1:A:664:ARG:HH11	1.91	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:TRP:NE1	1:A:770:GLU:OE2	2.40	0.55
1:A:616:SER:O	1:A:620:GLU:HB2	2.07	0.54
1:B:507:LYS:HG2	1:B:607:GLY:O	2.07	0.54
1:A:527:TRP:O	1:A:530:ALA:HB3	2.07	0.54
1:B:483:GLU:HA	1:B:486:TRP:CE2	2.43	0.54
1:A:624:GLU:OE2	1:A:624:GLU:HA	2.08	0.53
1:A:767:ARG:HD2	1:B:476:HIS:NE2	2.23	0.52
1:B:730:TYR:CB	1:B:759:LEU:HD12	2.39	0.52
1:B:654:LEU:HD12	1:B:661:HIS:CD2	2.44	0.52
1:A:658:ASN:HD22	1:A:658:ASN:C	2.13	0.52
1:B:532:THR:HG22	1:B:676:CYS:SG	2.50	0.52
1:B:658:ASN:HD22	1:B:659:GLN:N	2.09	0.50
1:A:483:GLU:HA	1:A:486:TRP:CE2	2.46	0.50
1:A:756:ARG:HH22	1:B:484:ASN:HD21	1.60	0.50
1:B:730:TYR:HB3	1:B:759:LEU:CD1	2.41	0.49
1:B:634:ASP:HB3	1:B:637:LEU:HD12	1.94	0.49
1:A:507:LYS:NZ	1:A:612:SER:HB2	2.28	0.48
1:A:578:PHE:CZ	1:A:703:MET:HG2	2.39	0.48
1:B:506:GLU:OE1	1:B:510:ARG:NH2	2.45	0.48
1:B:658:ASN:OD1	1:B:661:HIS:CE1	2.66	0.48
1:B:572:ASN:O	1:B:576:GLN:HG3	2.13	0.48
1:A:506:GLU:OE1	1:A:510:ARG:NH2	2.46	0.48
1:B:700:GLY:HA3	1:B:714:MET:O	2.14	0.48
1:A:724:GLN:CD	1:B:683:PRO:HD3	2.26	0.48
1:A:756:ARG:HH22	1:B:484:ASN:ND2	2.11	0.47
1:A:655:ASN:ND2	1:A:655:ASN:C	2.67	0.47
1:A:766:ILE:HG21	1:B:681:LEU:HD22	1.97	0.47
1:A:490:PHE:HA	1:A:493:MET:HE2	1.97	0.46
1:B:644:GLN:O	1:B:648:MET:HG3	2.16	0.46
1:A:724:GLN:HE21	1:A:724:GLN:HB2	1.54	0.46
1:A:689:ALA:O	1:A:692:ILE:HG22	2.15	0.46
1:A:450:ILE:HG23	1:A:605:LEU:HD13	1.98	0.46
1:B:609:ASN:HB3	1:B:612:SER:OG	2.16	0.46
1:A:724:GLN:OE1	1:B:683:PRO:CD	2.29	0.45
1:B:603:LEU:HA	1:B:603:LEU:HD23	1.77	0.45
1:A:655:ASN:HD22	1:A:657:ASN:H	1.57	0.45
1:A:545:HIS:O	1:A:545:HIS:CD2	2.68	0.45
1:B:575:LEU:HD11	1:B:591:MET:SD	2.57	0.45
1:B:484:ASN:H	1:B:484:ASN:HD22	1.63	0.44
1:A:569:GLY:HA2	1:A:695:GLU:OE2	2.18	0.44
1:B:550:ASP:O	1:B:554:LYS:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:519:TYR:CZ	1:B:530:ALA:HB2	2.52	0.44
1:B:569:GLY:HA2	1:B:695:GLU:OE2	2.18	0.43
1:A:656:LEU:HD11	1:A:665:VAL:HG21	1.99	0.43
1:A:682:TRP:HB3	1:A:683:PRO:HD3	2.01	0.43
1:B:578:PHE:HZ	1:B:703:MET:HG2	1.84	0.43
1:A:675:LEU:O	1:A:678:VAL:HG22	2.18	0.43
1:B:648:MET:SD	1:B:661:HIS:CD2	3.12	0.43
1:A:617:SER:O	1:A:621:GLN:HB2	2.19	0.42
1:B:450:ILE:HG23	1:B:605:LEU:HD13	2.01	0.42
1:A:700:GLY:HA3	1:A:714:MET:O	2.20	0.42
1:A:568:ARG:N	1:A:568:ARG:HD2	2.34	0.42
1:B:655:ASN:ND2	1:B:655:ASN:C	2.72	0.42
1:A:580:HIS:CE1	5:A:901:HOH:O	2.46	0.41
1:A:462:PHE:CD2	1:A:488:GLY:HA3	2.55	0.41
1:A:666:ILE:O	1:A:669:MET:HB2	2.20	0.41
1:A:712:PRO:HB3	1:A:718:LYS:HD3	2.03	0.41
1:B:666:ILE:O	1:B:669:MET:HB2	2.21	0.41
1:A:507:LYS:HZ1	1:A:612:SER:HB2	1.85	0.41
1:B:490:PHE:HA	1:B:493:MET:HE2	2.02	0.41
1:A:658:ASN:C	1:A:658:ASN:ND2	2.74	0.41
1:A:735:ILE:HB	1:A:736:PRO:HD3	2.03	0.41
1:B:617:SER:O	1:B:621:GLN:HB2	2.21	0.40
1:A:578:PHE:HA	1:A:579:ASP:OD1	2.22	0.40
1:B:580:HIS:CG	1:B:581:PRO:HD2	2.56	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:449:SER:OG	1:B:614:LEU:O[1_545]	1.95	0.25

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	322/345 (93%)	296 (92%)	25 (8%)	1 (0%)	41 49
1	B	322/345 (93%)	302 (94%)	19 (6%)	1 (0%)	41 49
All	All	644/690 (93%)	598 (93%)	44 (7%)	2 (0%)	41 49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	707	GLY
1	B	707	GLY

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	293/308 (95%)	261 (89%)	32 (11%)	6 6
1	B	293/308 (95%)	265 (90%)	28 (10%)	8 8
All	All	586/616 (95%)	526 (90%)	60 (10%)	7 7

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	447	HIS
1	A	448	MET
1	A	453	SER
1	A	463	THR
1	A	466	VAL
1	A	497	SER
1	A	500	THR
1	A	501	SER
1	A	504	GLU
1	A	510	ARG
1	A	521	ARG
1	A	578	PHE

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Mol	Chain	Res	Type
1	A	579	ASP
1	A	585	LEU
1	A	587	SER
1	A	588	THR
1	A	624	GLU
1	A	643	LYS
1	A	653	SER
1	A	655	ASN
1	A	658	ASN
1	A	662	ARG
1	A	677	SER
1	A	681	LEU
1	A	706	LEU
1	A	709	GLN
1	A	724	GLN
1	A	749	GLU
1	A	759	LEU
1	A	760	SER
1	A	767	ARG
1	A	770	GLU
1	B	447	HIS
1	B	448	MET
1	B	450	ILE
1	B	453	SER
1	B	463	THR
1	B	466	VAL
1	B	472	ILE
1	B	484	ASN
1	B	497	SER
1	B	501	SER
1	B	510	ARG
1	B	579	ASP
1	B	585	LEU
1	B	587	SER
1	B	588	THR
1	B	606	GLU
1	B	635	LEU
1	B	650	GLN
1	B	655	ASN
1	B	658	ASN
1	B	660	SER
1	B	677	SER

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Mol	Chain	Res	Type
1	B	706	LEU
1	B	708	ILE
1	B	709	GLN
1	B	724	GLN
1	B	760	SER
1	B	770	GLU

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	545	HIS
1	A	641	ASN
1	A	655	ASN
1	A	658	ASN
1	A	690	ASN
1	B	484	ASN
1	B	641	ASN
1	B	655	ASN
1	B	658	ASN
1	B	690	ASN
1	B	709	GLN
1	B	724	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
4	D6X	A	803	-	21,27,27	1.73	4 (19%)	25,38,38	2.70	6 (24%)

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
4	D6X	A	803	-	-	1/6/6/6	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	803	D6X	C2-C3	4.68	1.47	1.38
4	A	803	D6X	C10-C8	-3.76	1.45	1.50
4	A	803	D6X	C6-N7	-2.33	1.32	1.35
4	A	803	D6X	C15-N12	2.14	1.39	1.36

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	803	D6X	C10-C11-N12	-6.58	100.74	111.75
4	A	803	D6X	C11-N12-C15	-6.55	113.01	123.38
4	A	803	D6X	C1-C2-C3	-5.09	112.51	119.27
4	A	803	D6X	C2-C3-N4	4.59	128.00	122.57
4	A	803	D6X	C14-C3-C2	-3.76	116.07	121.81
4	A	803	D6X	C16-C15-N12	-3.59	113.32	121.04

There are no chirality outliers.

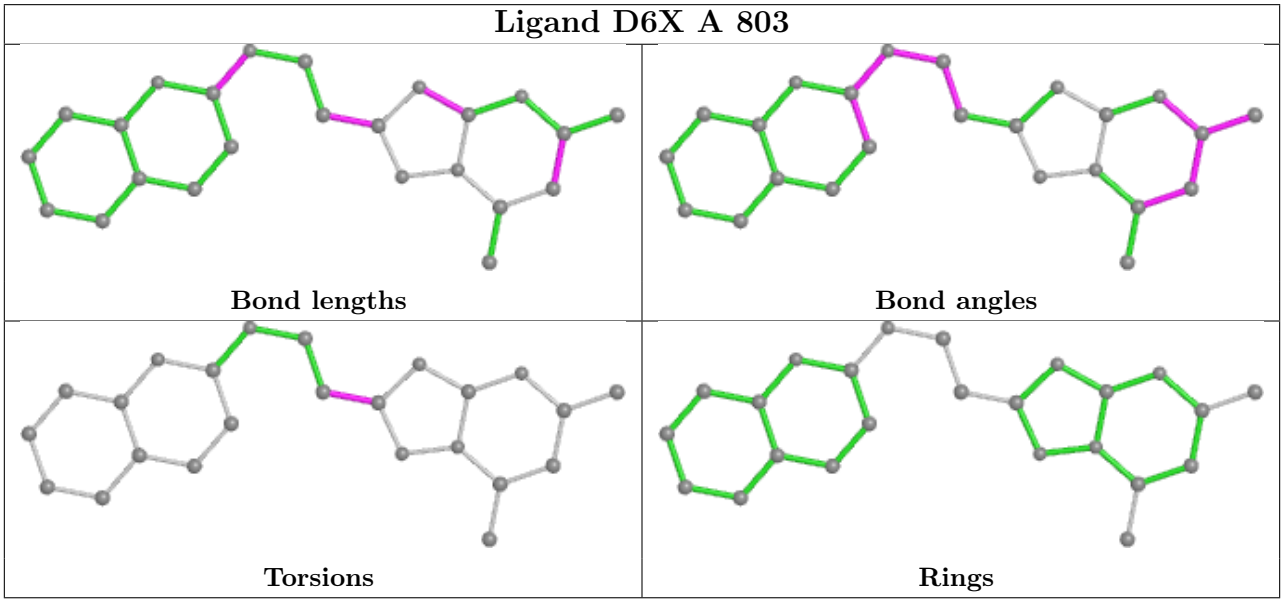
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	803	D6X	C11-C10-C8-N9

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 then 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, 95^{th} 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	324/345 (93%)	0.36	23 (7%)	16	12	33, 56, 92, 120	0
1	B	324/345 (93%)	0.15	17 (5%)	27	24	32, 51, 81, 105	0
All	All	648/690 (93%)	0.25	40 (6%)	20	17	32, 53, 88, 120	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	770	GLU	6.6
1	B	447	HIS	4.3
1	A	545	HIS	4.3
1	A	585	LEU	4.2
1	A	617	SER	3.8
1	A	587	SER	3.8
1	B	467	ARG	3.5
1	A	615	SER	3.4
1	B	584	ALA	3.2
1	A	613	THR	3.1
1	A	649	TYR	3.0
1	A	584	ALA	3.0
1	B	770	GLU	2.9
1	A	581	PRO	2.9
1	B	450	ILE	2.8
1	B	585	LEU	2.8
1	A	562	CYS	2.8
1	B	500	THR	2.7
1	A	533	VAL	2.7
1	A	461	GLN	2.7
1	B	531	VAL	2.6
1	B	561	LEU	2.6
1	B	560	CYS	2.6
1	B	582	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	557	LEU	2.4
1	A	450	ILE	2.4
1	B	580	HIS	2.4
1	A	616	SER	2.3
1	A	619	TYR	2.3
1	B	536	CYS	2.3
1	B	558	ILE	2.3
1	B	534	ALA	2.2
1	A	650	GLN	2.2
1	B	533	VAL	2.2
1	A	673	CYS	2.1
1	A	676	CYS	2.1
1	A	580	HIS	2.0
1	A	614	LEU	2.0
1	B	562	CYS	2.0
1	A	521	ARG	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 monosaccharides 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, 95^{th} 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.

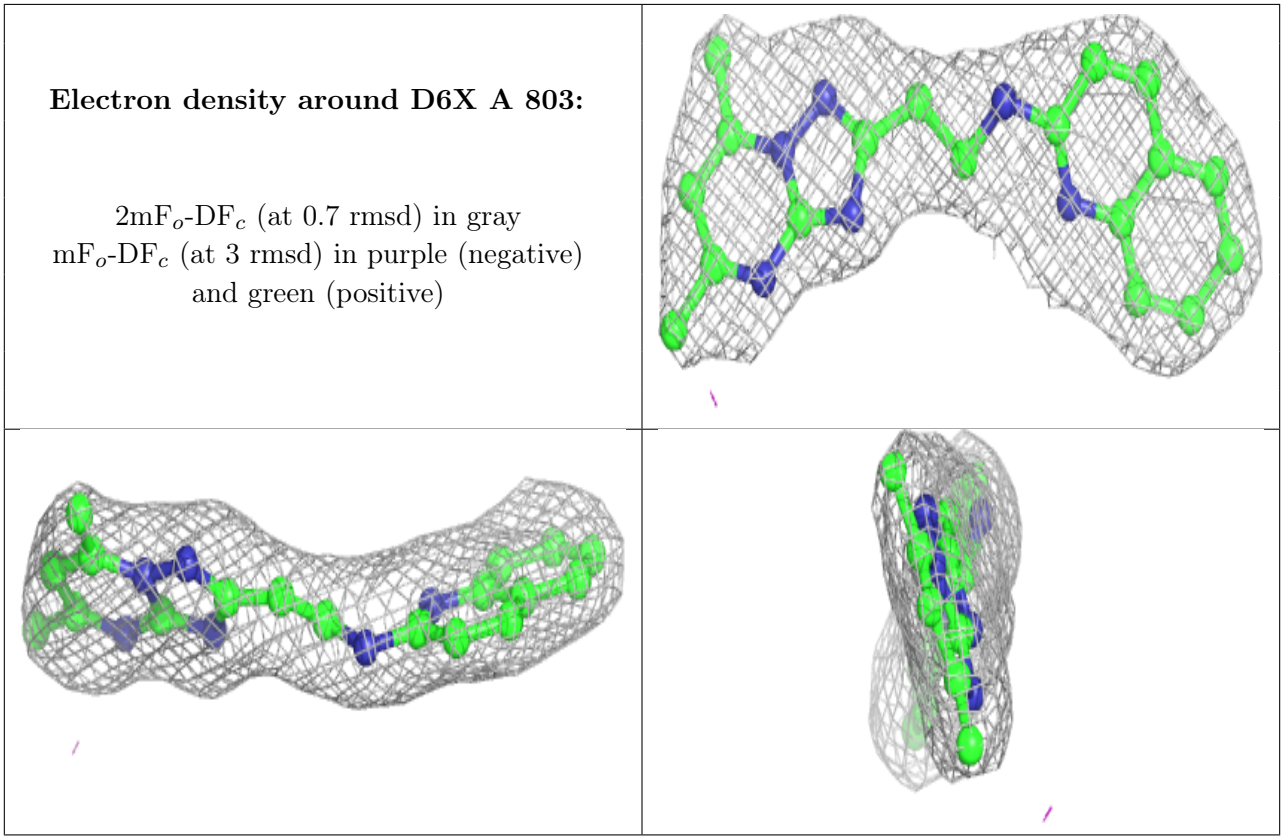
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	A	802	1/1	0.91	0.15	43,43,43,43	0
4	D6X	A	803	24/24	0.95	0.12	35,37,41,43	0
2	ZN	A	801	1/1	0.99	0.13	51,51,51,51	0
3	MG	B	802	1/1	1.00	0.16	34,34,34,34	0
2	ZN	B	801	1/1	1.00	0.14	39,39,39,39	0

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 D6X 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)



6.5 Other polymers (i)

There are no such residues in this entry.