WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2023 – 01:49 AM JST

PDB ID	:	6KE0
Title	:	Crystal structure of PDE10A in complex with a triazolopyrimidine inhibitor
Authors	:	Amano, Y.; Honbou, K.
Deposited on	:	2019-07-03
Resolution	:	2.95 Å(reported)

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
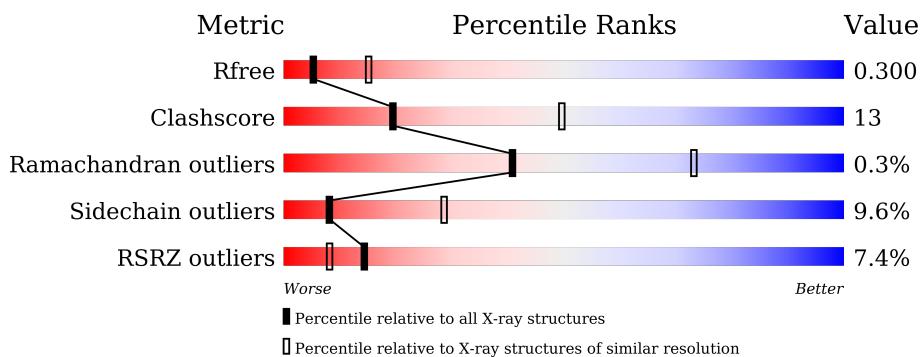
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
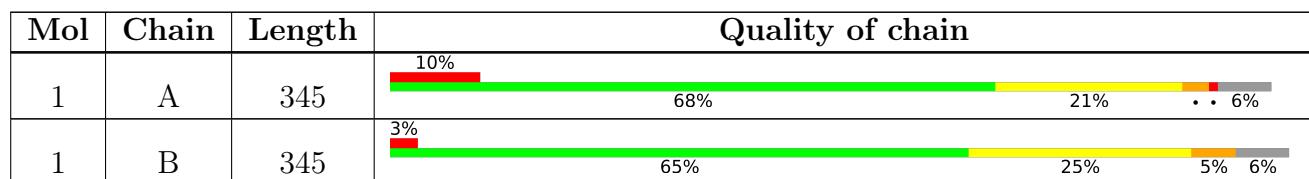
The reported resolution of this entry is 2.95 Å.

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	Percentile Ranks	Value
Rfree		0.300
Clashscore		13
Ramachandran outliers		0.3%
Sidechain outliers		9.6%
RSRZ outliers		7.4%

Worse _____ *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	10% / 68% 21% · · 6%
1	B	345	3% / 65% 25% 5% 6%

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2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 5289 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 2629	C 1678	N 447	O 479	S 25	0	0	0
1	B	324	Total 2629	C 1678	N 447	O 479	S 25	0	0	0

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 1	Zn 1	0	0
2	B	1	Total 1	Zn 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).
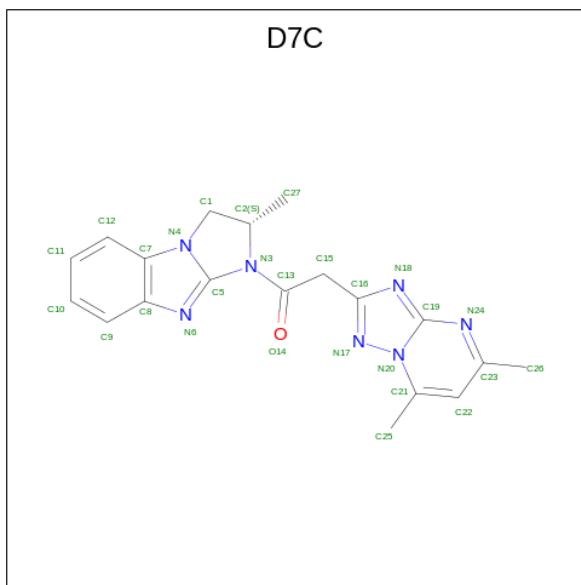
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Mg 1	0	0

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

- Molecule 4 is 2-(5,7-dimethyl-[1,2,4]triazolo[1,5-a]pyrimidin-2-yl)-1-[(2S)-2-methyl-1,2-dihyd roimidazo[1,2-a]benzimidazol-3-yl]ethanone (three-letter code: D7C) (formula: $C_{19}H_{19}N_7O$) (labeled as "Ligand of Interest" by depositor).
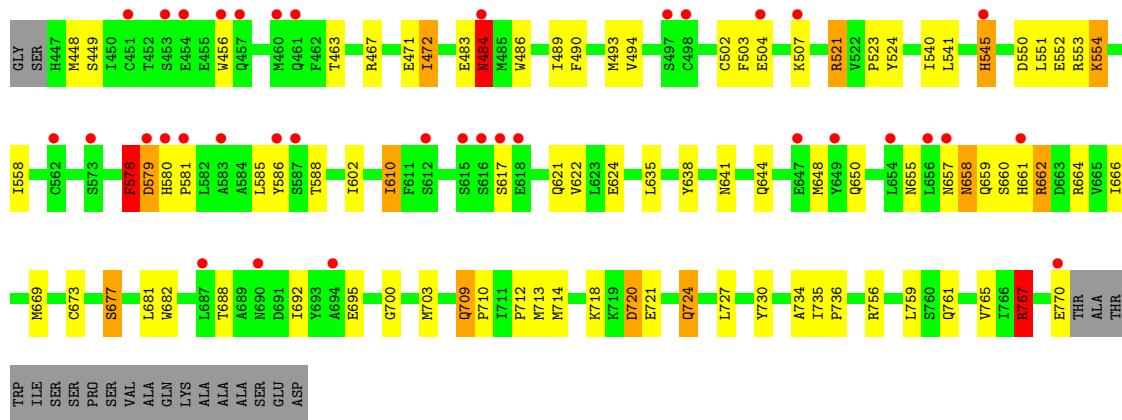
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			27	19	7	1		
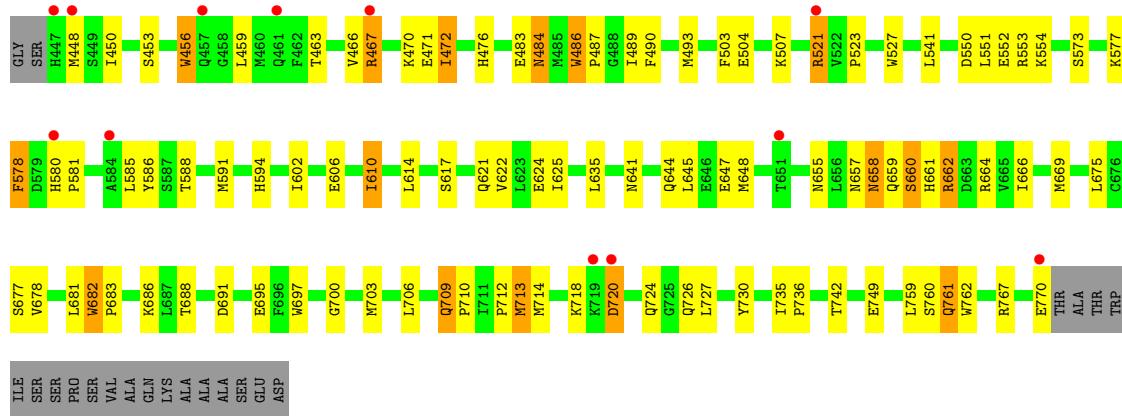
3 Residue-property plots ⓘ

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

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4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	50.40Å 81.55Å 160.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.91 – 2.95 29.91 – 2.95	Depositor EDS
% Data completeness (in resolution range)	91.9 (29.91-2.95) 92.1 (29.91-2.95)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.74 (at 2.95Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.251 , 0.302 0.248 , 0.300	Depositor DCC
R_{free} test set	674 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	55.2	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 25.6	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	5289	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: MG, ZN, D7C

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	0.67	3/2694 (0.1%)	0.81	8/3647 (0.2%)
1	B	0.64	5/2694 (0.2%)	0.77	9/3647 (0.2%)
All	All	0.66	8/5388 (0.1%)	0.79	17/7294 (0.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	545	HIS	CE1-NE2	7.95	1.50	1.32
1	A	545	HIS	CG-CD2	7.68	1.48	1.35
1	B	456	TRP	CD2-CE2	5.67	1.48	1.41
1	A	456	TRP	CD2-CE2	5.62	1.48	1.41
1	B	697	TRP	CD2-CE2	5.56	1.48	1.41
1	B	682	TRP	CD2-CE2	5.21	1.47	1.41
1	B	527	TRP	CD2-CE2	5.09	1.47	1.41
1	B	486	TRP	CD2-CE2	5.04	1.47	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	579	ASP	N-CA-C	-8.70	87.52	111.00
1	B	467	ARG	NE-CZ-NH2	-8.37	116.11	120.30
1	B	467	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	A	767	ARG	NE-CZ-NH2	7.73	124.17	120.30
1	A	467	ARG	NE-CZ-NH1	-7.56	116.52	120.30
1	B	578	PHE	CB-CG-CD1	-7.41	115.62	120.80
1	B	578	PHE	CB-CA-C	-7.39	95.63	110.40
1	B	767	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	467	ARG	NE-CZ-NH2	6.91	123.75	120.30
1	A	713	MET	CG-SD-CE	6.83	111.13	100.20
1	A	578	PHE	C-N-CA	6.49	137.93	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	484	ASN	CB-CA-C	-5.72	98.97	110.40
1	A	767	ARG	NH1-CZ-NH2	-5.58	113.26	119.40
1	B	767	ARG	NH1-CZ-NH2	-5.52	113.33	119.40
1	B	713	MET	CG-SD-CE	5.34	108.74	100.20
1	B	767	ARG	NE-CZ-NH2	5.23	122.92	120.30
1	B	578	PHE	CB-CG-CD2	5.13	124.39	120.80

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	2629	0	2588	70	1
1	B	2629	0	2588	78	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	27	0	0	1	0
All	All	5289	0	5176	134	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 13.

All (134) 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:724:GLN:CG	1:B:683:PRO:HG3	1.97	0.94
1:A:502:CYS:SG	1:A:554:LYS:HD2	2.07	0.94
1:A:724:GLN:HG2	1:B:683:PRO:HG3	1.48	0.92
1:A:724:GLN:OE1	1:B:682:TRP:HB3	1.71	0.90
1:B:484:ASN:H	1:B:484:ASN:HD22	1.25	0.85
1:B:761:GLN:HE21	1:B:761:GLN:HA	1.41	0.84
1:A:550:ASP:O	1:A:554:LYS:HG3	1.78	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:ARG:HH11	1:A:521:ARG:HG3	1.49	0.77
1:A:641:ASN:HD22	1:A:664:ARG:HH11	1.32	0.76
1:B:472:ILE:HD11	1:B:489:ILE:HG23	1.65	0.76
1:B:648:MET:SD	1:B:661:HIS:CD2	2.80	0.75
1:A:724:GLN:HG3	1:B:683:PRO:CG	2.17	0.73
1:A:641:ASN:HD22	1:A:664:ARG:NH1	1.86	0.73
1:B:521:ARG:HH11	1:B:521:ARG:HG3	1.54	0.72
1:B:484:ASN:HD22	1:B:484:ASN:N	1.88	0.71
1:A:484:ASN:HD22	1:A:484:ASN:H	1.38	0.71
1:A:484:ASN:H	1:A:484:ASN:ND2	1.87	0.71
1:A:580:HIS:ND1	1:A:581:PRO:HD2	2.07	0.70
1:A:767:ARG:HD2	1:B:476:HIS:NE2	2.06	0.69
1:A:648:MET:SD	1:A:661:HIS:CD2	2.87	0.68
1:A:578:PHE:HZ	1:A:703:MET:HG2	1.59	0.68
1:A:709:GLN:HE21	1:A:710:PRO:HD2	1.59	0.67
1:A:580:HIS:CG	1:A:581:PRO:HD2	2.28	0.67
1:A:756:ARG:HH22	1:B:484:ASN:HD21	1.41	0.67
1:B:648:MET:SD	1:B:661:HIS:HD2	2.17	0.67
1:A:472:ILE:HD11	1:A:489:ILE:HG23	1.77	0.65
1:A:727:LEU:HD23	1:B:683:PRO:HG2	1.76	0.65
1:A:448:MET:HE2	1:A:602:ILE:HG13	1.78	0.65
1:B:580:HIS:CG	1:B:581:PRO:HD2	2.31	0.65
1:A:484:ASN:HD22	1:A:484:ASN:N	1.96	0.64
1:A:724:GLN:CG	1:B:683:PRO:CG	2.72	0.64
1:B:641:ASN:HD22	1:B:664:ARG:NH1	1.95	0.64
1:A:724:GLN:HG3	1:B:683:PRO:HG3	1.73	0.63
1:B:580:HIS:ND1	1:B:581:PRO:HD2	2.14	0.62
1:A:650:GLN:OE1	1:B:521:ARG:NH2	2.33	0.61
1:B:504:GLU:HG3	1:B:507:LYS:HB2	1.80	0.61
1:A:677:SER:HB3	1:A:688:THR:HG21	1.81	0.61
1:B:641:ASN:HD22	1:B:664:ARG:HH11	1.48	0.60
1:A:682:TRP:NE1	1:A:770:GLU:OE2	2.35	0.60
1:A:648:MET:SD	1:A:661:HIS:HD2	2.25	0.60
1:B:709:GLN:HE21	1:B:710:PRO:HD2	1.66	0.60
1:A:712:PRO:HB3	1:A:718:LYS:HD3	1.83	0.59
1:B:658:ASN:C	1:B:658:ASN:HD22	2.04	0.59
1:B:700:GLY:HA3	1:B:714:MET:O	2.03	0.58
1:B:720:ASP:OD1	1:B:720:ASP:N	2.35	0.58
1:A:504:GLU:HG3	1:A:507:LYS:HB2	1.86	0.57
1:A:523:PRO:HD2	1:A:695:GLU:HG2	1.86	0.57
1:A:545:HIS:O	1:A:545:HIS:HD2	1.88	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:523:PRO:HD2	1:B:695:GLU:HG2	1.87	0.57
1:A:735:ILE:HB	1:A:736:PRO:HD3	1.87	0.56
1:A:448:MET:CE	1:A:602:ILE:HG13	2.35	0.56
1:A:540:ILE:HD12	1:A:673:CYS:SG	2.45	0.56
1:A:521:ARG:HH11	1:A:521:ARG:CG	2.16	0.56
1:A:727:LEU:HD23	1:B:683:PRO:CG	2.35	0.56
1:A:720:ASP:OD1	1:A:720:ASP:N	2.28	0.56
1:B:658:ASN:HD22	1:B:659:GLN:N	2.04	0.55
1:A:730:TYR:HB3	1:A:759:LEU:HD12	1.88	0.55
1:B:483:GLU:HA	1:B:486:TRP:CE2	2.42	0.55
1:A:545:HIS:O	1:A:545:HIS:CD2	2.60	0.55
1:B:541:LEU:HD22	1:B:553:ARG:HG2	1.89	0.54
1:B:484:ASN:H	1:B:484:ASN:ND2	1.99	0.54
1:B:712:PRO:HB3	1:B:718:LYS:HD3	1.90	0.54
1:B:761:GLN:HA	1:B:761:GLN:NE2	2.17	0.53
1:B:552:GLU:OE2	1:B:662:ARG:NE	2.35	0.53
1:B:448:MET:HE2	1:B:602:ILE:HG13	1.89	0.53
1:B:658:ASN:C	1:B:658:ASN:ND2	2.61	0.53
1:B:730:TYR:CB	1:B:759:LEU:HD12	2.39	0.53
1:B:521:ARG:HH11	1:B:521:ARG:CG	2.20	0.52
1:A:730:TYR:CB	1:A:759:LEU:HD12	2.39	0.52
1:A:490:PHE:HA	1:A:493:MET:HE2	1.92	0.52
1:A:666:ILE:O	1:A:669:MET:HB2	2.09	0.52
1:B:448:MET:CE	1:B:602:ILE:HG13	2.40	0.50
1:A:655:ASN:ND2	1:A:657:ASN:H	2.10	0.50
1:A:700:GLY:HA3	1:A:714:MET:O	2.12	0.50
1:B:503:PHE:CZ	1:B:554:LYS:HE3	2.46	0.50
1:A:641:ASN:ND2	1:A:664:ARG:HH11	2.03	0.50
1:B:662:ARG:HG3	1:B:662:ARG:HH11	1.77	0.49
1:A:658:ASN:HD22	1:A:659:GLN:N	2.10	0.49
1:B:550:ASP:O	1:B:554:LYS:HG3	2.12	0.49
1:B:682:TRP:CZ2	1:B:686:LYS:HE2	2.47	0.49
1:B:730:TYR:HB3	1:B:759:LEU:HD12	1.94	0.49
1:A:730:TYR:HB3	1:A:759:LEU:CD1	2.43	0.49
1:A:730:TYR:HA	1:A:734:ALA:HB3	1.95	0.49
1:B:735:ILE:HB	1:B:736:PRO:HD3	1.94	0.49
1:A:658:ASN:HD22	1:A:658:ASN:C	2.15	0.48
1:A:724:GLN:OE1	1:B:683:PRO:HD3	2.13	0.48
1:B:666:ILE:O	1:B:669:MET:HB2	2.13	0.48
1:B:484:ASN:N	1:B:484:ASN:ND2	2.60	0.48
1:B:730:TYR:HB3	1:B:759:LEU:CD1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:PHE:HA	1:B:493:MET:HE2	1.95	0.48
1:A:503:PHE:CD1	1:A:610:ILE:HB	2.50	0.47
1:B:503:PHE:CD1	1:B:610:ILE:HB	2.49	0.47
1:A:578:PHE:CZ	1:A:703:MET:HG2	2.43	0.47
1:A:490:PHE:O	1:A:494:VAL:HG23	2.15	0.47
1:B:742:THR:OG1	1:B:749:GLU:HA	2.15	0.47
1:A:552:GLU:OE2	1:A:662:ARG:NE	2.42	0.46
4:A:803:D7C:C15	4:A:803:D7C:N6	2.79	0.46
1:B:644:GLN:HG3	1:B:664:ARG:CZ	2.47	0.45
1:B:688:THR:O	1:B:691:ASP:HB2	2.17	0.45
1:A:521:ARG:CG	1:A:521:ARG:NH1	2.79	0.45
1:A:641:ASN:HA	1:A:664:ARG:NH1	2.32	0.45
1:A:541:LEU:HD22	1:A:553:ARG:HG2	1.99	0.45
1:B:573:SER:O	1:B:577:LYS:HB2	2.17	0.45
1:A:483:GLU:HA	1:A:486:TRP:CE2	2.53	0.44
1:B:641:ASN:ND2	1:B:664:ARG:HH11	2.14	0.44
1:B:645:LEU:HD11	1:B:664:ARG:O	2.18	0.44
1:B:655:ASN:ND2	1:B:657:ASN:H	2.16	0.44
1:B:453:SER:HA	1:B:456:TRP:CD1	2.53	0.44
1:A:727:LEU:HD23	1:B:683:PRO:HD2	2.00	0.43
1:B:641:ASN:HA	1:B:664:ARG:NH1	2.33	0.43
1:B:677:SER:CB	1:B:688:THR:HG21	2.48	0.43
1:A:484:ASN:ND2	1:A:484:ASN:N	2.54	0.43
1:B:551:LEU:HD12	1:B:551:LEU:HA	1.92	0.43
1:B:578:PHE:CZ	1:B:703:MET:HG2	2.54	0.43
1:B:658:ASN:HD21	1:B:660:SER:HB3	1.83	0.43
1:B:726:GLN:O	1:B:727:LEU:C	2.58	0.43
1:B:521:ARG:CG	1:B:521:ARG:NH1	2.82	0.42
1:A:658:ASN:C	1:A:658:ASN:ND2	2.71	0.42
1:B:578:PHE:CE1	1:B:706:LEU:HD13	2.54	0.42
1:B:682:TRP:NE1	1:B:770:GLU:OE2	2.52	0.42
1:A:724:GLN:HG3	1:B:683:PRO:HG2	1.98	0.42
1:B:675:LEU:O	1:B:678:VAL:HG22	2.20	0.42
1:A:724:GLN:HE21	1:A:724:GLN:HB2	1.69	0.41
1:B:459:LEU:HD13	1:B:487:PRO:HB2	2.02	0.41
1:B:504:GLU:H	1:B:504:GLU:HG2	1.62	0.41
1:A:524:TYR:CD2	1:A:692:ILE:HD13	2.55	0.41
1:B:726:GLN:HG3	1:B:762:TRP:CE2	2.56	0.41
1:A:551:LEU:HD12	1:A:551:LEU:HA	1.87	0.41
1:A:558:ILE:HD13	1:A:558:ILE:HA	1.94	0.41
1:B:591:MET:O	1:B:594:HIS:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:PHE:HE1	1:B:706:LEU:HD13	1.87	0.40
1:A:721:GLU:OE1	1:B:770:GLU:OE1	2.39	0.40
1:A:644:GLN:HG3	1:A:664:ARG:CZ	2.52	0.40
1:A:761:GLN:O	1:A:765:VAL:HG23	2.21	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]	2.19	0.01

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	322/345 (93%)	305 (95%)	17 (5%)	0	100	100
1	B	322/345 (93%)	300 (93%)	20 (6%)	2 (1%)	25	60
All	All	644/690 (93%)	605 (94%)	37 (6%)	2 (0%)	41	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	647	GLU
1	B	625	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	293/308 (95%)	266 (91%)	27 (9%)	9	30
1	B	293/308 (95%)	264 (90%)	29 (10%)	8	27
All	All	586/616 (95%)	530 (90%)	56 (10%)	8	28

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	463	THR
1	A	471	GLU
1	A	472	ILE
1	A	484	ASN
1	A	521	ARG
1	A	554	LYS
1	A	578	PHE
1	A	579	ASP
1	A	585	LEU
1	A	586	TYR
1	A	588	THR
1	A	610	ILE
1	A	617	SER
1	A	621	GLN
1	A	622	VAL
1	A	624	GLU
1	A	635	LEU
1	A	638	TYR
1	A	658	ASN
1	A	660	SER
1	A	662	ARG
1	A	677	SER
1	A	681	LEU
1	A	709	GLN
1	A	720	ASP
1	A	724	GLN
1	A	767	ARG
1	B	450	ILE
1	B	463	THR
1	B	466	VAL
1	B	467	ARG
1	B	470	LYS
1	B	471	GLU

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Mol	Chain	Res	Type
1	B	472	ILE
1	B	484	ASN
1	B	521	ARG
1	B	585	LEU
1	B	586	TYR
1	B	588	THR
1	B	606	GLU
1	B	610	ILE
1	B	617	SER
1	B	621	GLN
1	B	622	VAL
1	B	624	GLU
1	B	635	LEU
1	B	658	ASN
1	B	660	SER
1	B	662	ARG
1	B	681	LEU
1	B	709	GLN
1	B	713	MET
1	B	720	ASP
1	B	724	GLN
1	B	760	SER
1	B	761	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	484	ASN
1	A	545	HIS
1	A	641	ASN
1	A	655	ASN
1	A	658	ASN
1	A	690	ASN
1	A	709	GLN
1	A	726	GLN
1	A	761	GLN
1	B	484	ASN
1	B	495	HIS
1	B	641	ASN
1	B	655	ASN
1	B	658	ASN
1	B	709	GLN

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Mol	Chain	Res	Type
1	B	724	GLN
1	B	726	GLN
1	B	761	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	D7C	A	803	-	21,31,31	1.80	5 (23%)	21,47,47	2.88	8 (38%)

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	D7C	A	803	-	-	1/8/20/20	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	803	D7C	C22-C23	5.45	1.49	1.38
4	A	803	D7C	C2-N3	-3.82	1.44	1.48
4	A	803	D7C	C19-N18	-2.18	1.32	1.35
4	A	803	D7C	C5-N6	-2.08	1.31	1.35
4	A	803	D7C	C15-C16	-2.06	1.47	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	803	D7C	C5-N3-C13	-8.97	120.89	131.60
4	A	803	D7C	C21-C22-C23	-4.36	113.49	119.27
4	A	803	D7C	C22-C23-N24	4.01	127.31	122.57
4	A	803	D7C	C26-C23-C22	-3.70	116.16	121.81
4	A	803	D7C	C11-C12-C7	-2.78	114.12	119.44
4	A	803	D7C	C10-C9-C8	-2.45	116.56	120.08
4	A	803	D7C	C2-N3-C13	2.28	124.12	119.27
4	A	803	D7C	C12-C7-C8	2.18	124.85	121.30

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	803	D7C	C13-C15-C16-N18
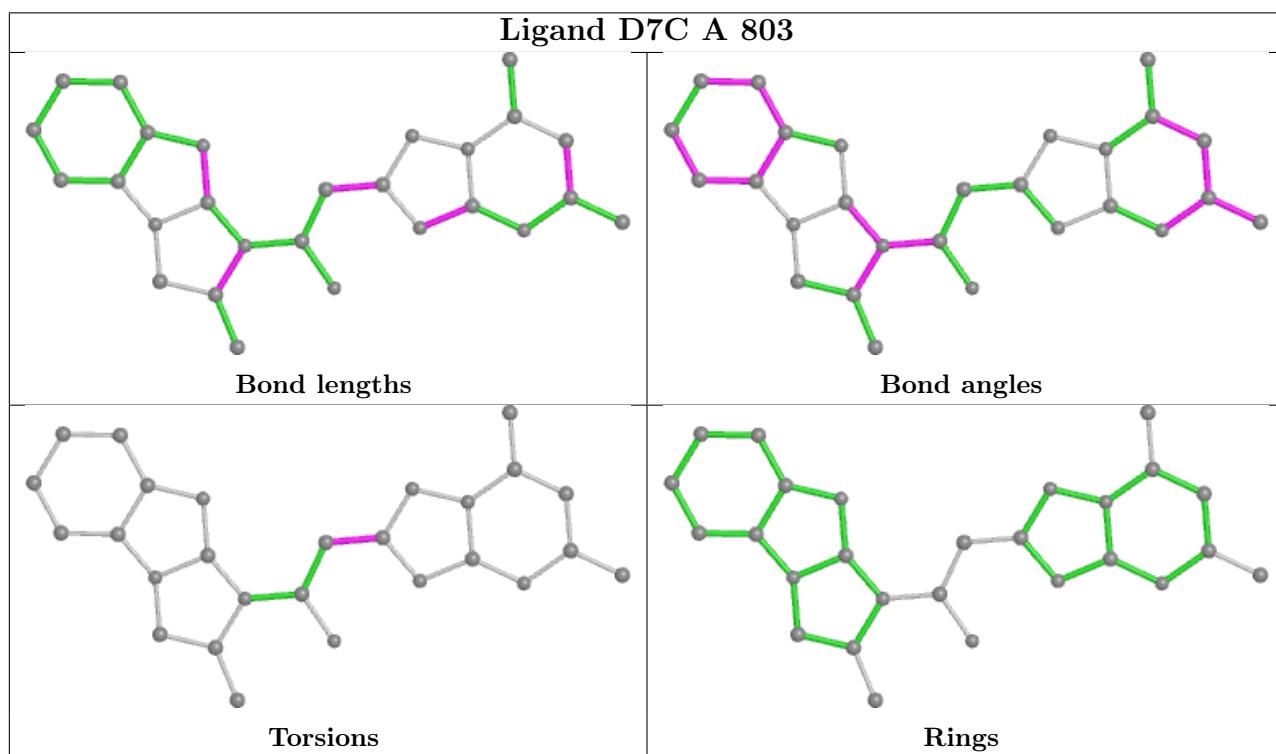
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	803	D7C	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 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.

Ligand D7C A 803

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	324/345 (93%)	0.62	36 (11%)	5	3	29, 49, 82, 112	0
1	B	324/345 (93%)	0.36	12 (3%)	41	27	27, 44, 73, 105	0
All	All	648/690 (93%)	0.49	48 (7%)	14	8	27, 46, 81, 112	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	770	GLU	4.1
1	B	584	ALA	4.1
1	B	447	HIS	4.0
1	B	770	GLU	3.7
1	B	467	ARG	3.2
1	A	456	TRP	3.1
1	A	654	LEU	3.1
1	A	615	SER	3.1
1	B	720	ASP	3.0
1	A	457	GLN	2.9
1	A	587	SER	2.8
1	A	661	HIS	2.8
1	A	657	ASN	2.7
1	A	579	ASP	2.7
1	A	454	GLU	2.7
1	A	580	HIS	2.7
1	A	618	GLU	2.6
1	A	616	SER	2.6
1	A	460	MET	2.5
1	A	507	LYS	2.5
1	A	461	GLN	2.4
1	B	461	GLN	2.4
1	A	545	HIS	2.4
1	B	719	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	649	TYR	2.4
1	B	651	THR	2.3
1	B	448	MET	2.3
1	A	562	CYS	2.3
1	A	612	SER	2.3
1	A	583	ALA	2.3
1	A	451	CYS	2.3
1	A	453	SER	2.3
1	B	580	HIS	2.2
1	A	497	SER	2.2
1	A	656	LEU	2.2
1	A	694	ALA	2.2
1	A	498	CYS	2.2
1	A	581	PRO	2.2
1	A	617	SER	2.2
1	A	573	SER	2.2
1	A	690	ASN	2.1
1	A	586	TYR	2.1
1	B	521	ARG	2.1
1	B	457	GLN	2.1
1	A	687	LEU	2.1
1	A	504	GLU	2.1
1	A	647	GLU	2.0
1	A	484	ASN	2.0

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 ⓘ
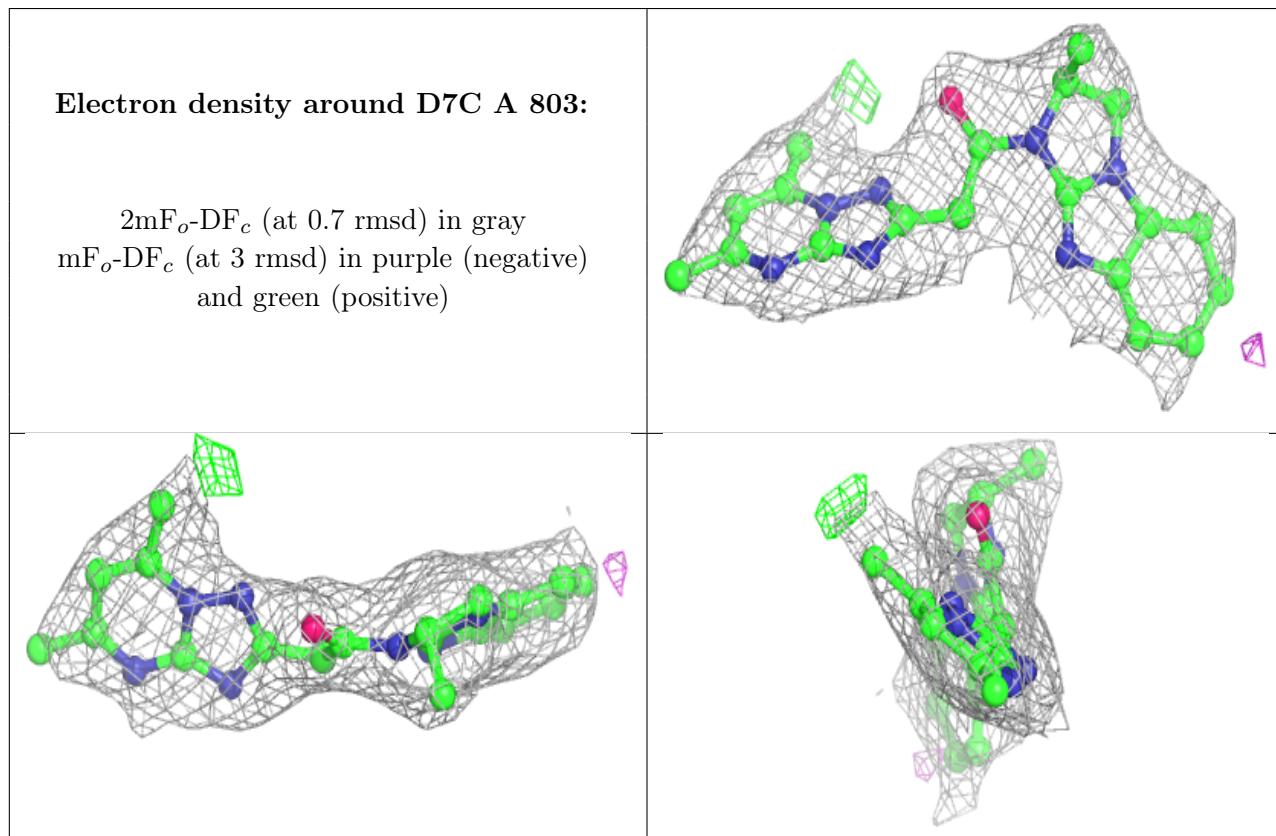
There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	A	802	1/1	0.80	0.57	39,39,39,39	0
3	MG	B	802	1/1	0.89	0.67	34,34,34,34	0
4	D7C	A	803	27/27	0.93	0.18	36,41,43,44	0
2	ZN	A	801	1/1	0.94	0.14	44,44,44,44	0
2	ZN	B	801	1/1	0.99	0.19	38,38,38,38	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 D7C A 803:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.