



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:45 PM UTC

PDB ID : 9EYX / pdb_00009eyx
Title : Human PRMT5 in complex with AZ compound 28
Authors : Debreczeni, J.
Deposited on : 2024-04-09
Resolution : 2.20 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

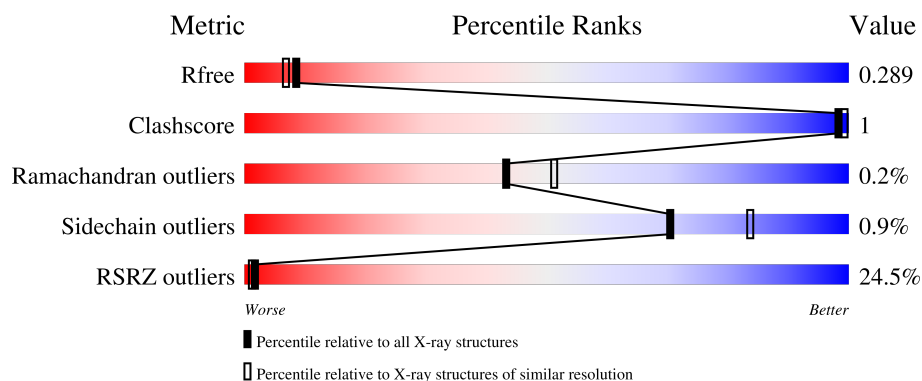
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	637	14% 95% ..
2	B	342	41% 87% • 11%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7369 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.

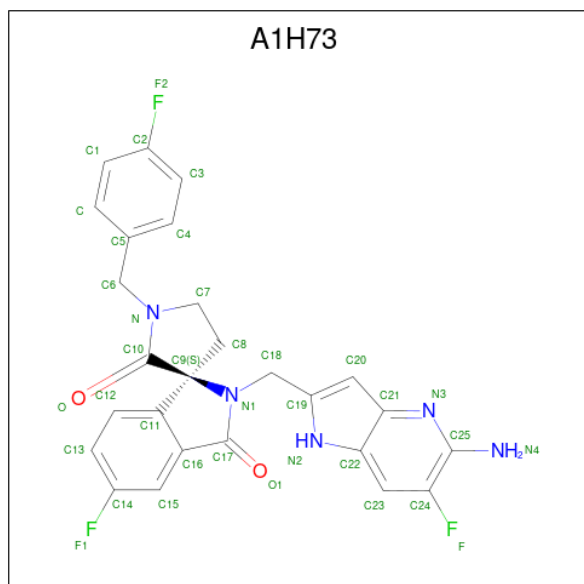
- Molecule 1 is a protein called Protein arginine N-methyltransferase 5, N-terminally processed.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	625	Total	C	N	O	S	0	0	0
			4970	3175	848	925	22			

- Molecule 2 is a protein called Methylosome protein WDR77.

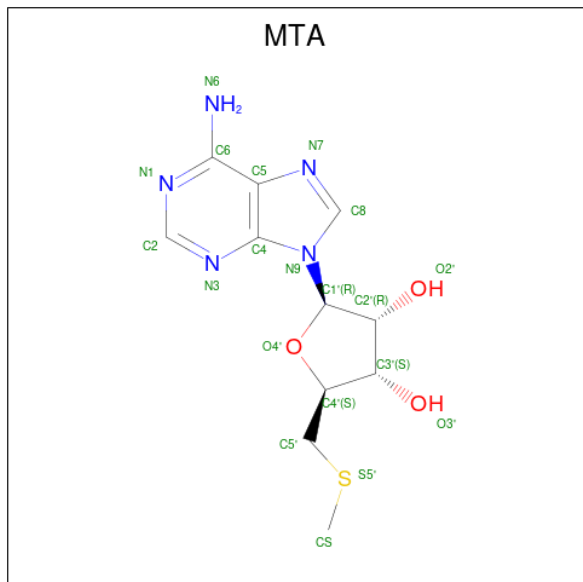
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	303	Total	C	N	O	S	0	0	0
			2269	1427	387	443	12			

- Molecule 3 is (3 {S})-2-[(5-azanyl-6-fluoranyl-1 {H}-pyrrolo[3,2-b]pyridin-2-yl)methyl]-6-fluoranyl-1'-[(4-fluorophenyl)methyl]spiro[isindole-3,3'-pyrrolidine]-1,2'-dione (CCD ID: A1H73) (formula: C₂₆H₂₀F₃N₅O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			36	26	3	5	2		

- Molecule 4 is 5'-DEOXY-5'-METHYLTHIOADENOSINE (CCD ID: MTA) (formula: $C_{11}H_{15}N_5O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			20	11	5	3	1		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		

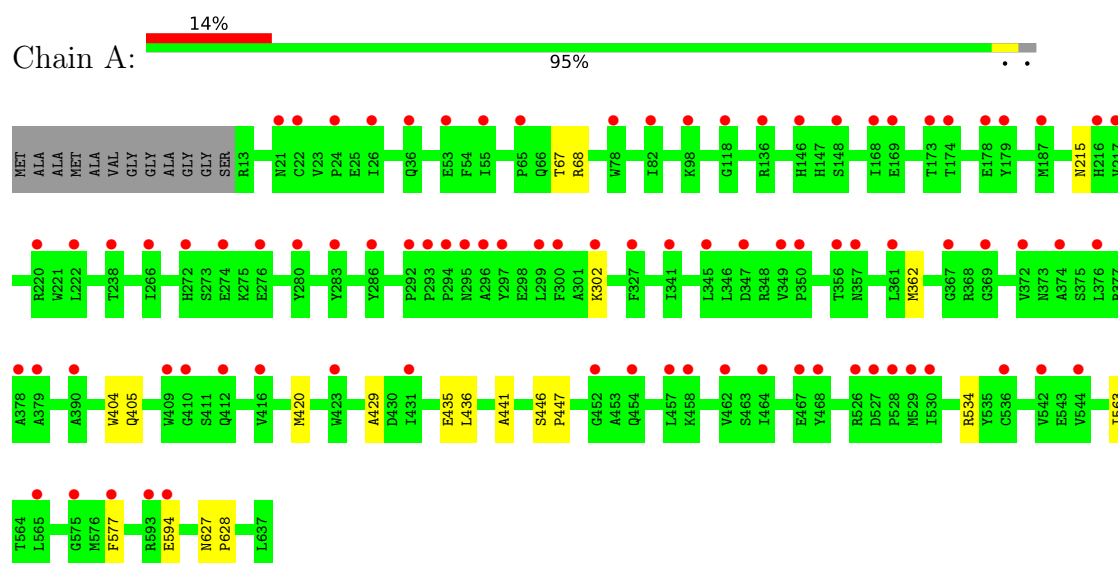
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	54	Total 54	O 54	0	0
6	B	15	Total 15	O 15	0	0

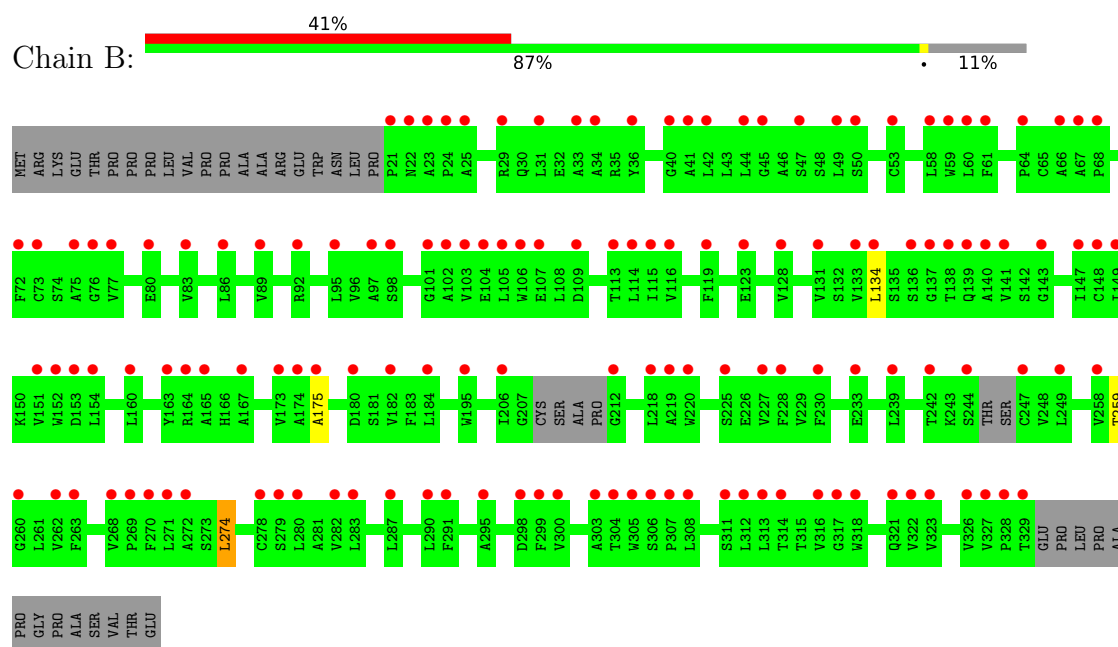
3 Residue-property plots [i](#)

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: Protein arginine N-methyltransferase 5, N-terminally processed



- Molecule 2: Methylosome protein WDR77



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	102.12Å 139.12Å 178.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	46.7 (20.00-2.20) 46.7 (20.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.21Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.269 , 0.288 0.269 , 0.289	Depositor DCC
R_{free} test set	1579 reflections (2.46%)	wwPDB-VP
Wilson B-factor (Å ²)	43.7	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 25.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	7369	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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: A1H73, SO4, MTA

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	0.45	0/5108	0.81	0/6967
2	B	0.48	0/2322	0.76	0/3173
All	All	0.46	0/7430	0.79	0/10140

There are no bond length outliers.

There are no bond angle outliers.

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	4970	0	4773	7	0
2	B	2269	0	2157	2	0
3	A	36	0	0	1	0
4	A	20	0	15	0	0
5	A	5	0	0	0	0
6	A	54	0	0	0	0
6	B	15	0	0	0	0
All	All	7369	0	6945	9	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 (9) 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:446:SER:N	1:A:447:PRO:CD	2.78	0.47
1:A:627:ASN:N	1:A:628:PRO:CD	2.78	0.47
2:B:134:LEU:HD23	2:B:175:ALA:HB1	1.97	0.46
1:A:420:MET:HE1	1:A:436:LEU:HD11	2.01	0.42
1:A:534:ARG:HH11	1:A:534:ARG:HG3	1.84	0.42
2:B:259:THR:HB	2:B:274:LEU:HD12	2.01	0.42
1:A:67:THR:OG1	1:A:68:ARG:N	2.48	0.42
1:A:362:MET:SD	1:A:429:ALA:HB2	2.61	0.41
1:A:435:GLU:O	3:A:701:A1H73:N4	2.54	0.41

There are no symmetry-related clashes.

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	623/637 (98%)	595 (96%)	26 (4%)	2 (0%)	36	42
2	B	297/342 (87%)	276 (93%)	21 (7%)	0	100	100
All	All	920/979 (94%)	871 (95%)	47 (5%)	2 (0%)	43	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	441	ALA
1	A	302	LYS

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	536/562 (95%)	530 (99%)	6 (1%)	65	79
2	B	248/290 (86%)	247 (100%)	1 (0%)	84	92
All	All	784/852 (92%)	777 (99%)	7 (1%)	70	84

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	215	ASN
1	A	404	TRP
1	A	405	GLN
1	A	563	ILE
1	A	577	PHE
1	A	594	GLU
2	B	274	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	79	ASN
1	A	128	GLN
1	A	270	ASN
1	A	338	GLN
1	A	532	ASN
2	B	78	GLN
2	B	221	HIS
2	B	224	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	A1H73	A	701	-	39,41,41	0.22	0	49,63,63	0.52	0
5	SO4	A	703	-	4,4,4	0.34	0	6,6,6	0.08	0
4	MTA	A	702	-	22,22,22	0.23	0	32,32,32	0.35	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	A1H73	A	701	-	-	0/8/44/44	0/6/6/6
4	MTA	A	702	-	-	0/7/23/23	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

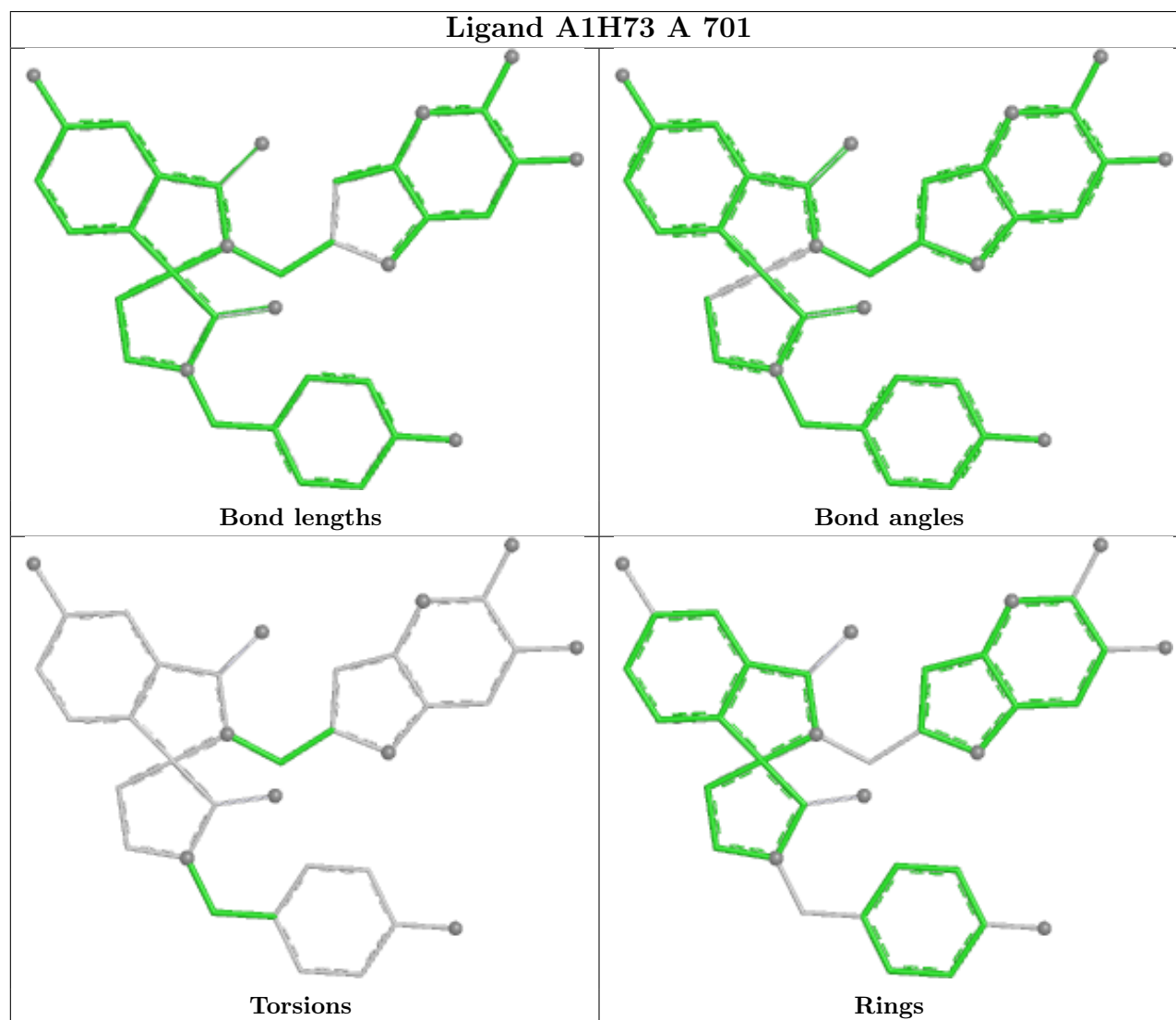
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	A1H73	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

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(Å ²)	Q<0.9
1	A	625/637 (98%)	1.05	87 (13%) 6 5	25, 52, 92, 110	0
2	B	303/342 (88%)	2.01	140 (46%) 0 0	49, 74, 100, 119	0
All	All	928/979 (94%)	1.36	227 (24%) 2 1	25, 62, 96, 119	0

All (227) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	296	ALA	6.6
1	A	530	ILE	5.3
2	B	247	CYS	5.1
2	B	59	TRP	4.9
2	B	103	VAL	4.6
2	B	60	LEU	4.6
2	B	102	ALA	4.5
2	B	22	ASN	4.5
2	B	322	VAL	4.5
2	B	147	ILE	4.5
1	A	345	LEU	4.4
2	B	314	THR	4.3
1	A	294	PRO	4.1
2	B	114	LEU	4.1
2	B	312	LEU	4.0
2	B	280	LEU	4.0
2	B	61	PHE	4.0
1	A	409	TRP	3.9
2	B	106	TRP	3.9
1	A	174	THR	3.9
1	A	297	TYR	3.9
2	B	72	PHE	3.9
2	B	282	VAL	3.9
2	B	116	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	378	ALA	3.8
2	B	50	SER	3.8
2	B	134	LEU	3.8
2	B	272	ALA	3.8
2	B	303	ALA	3.8
1	A	217	VAL	3.8
1	A	372	VAL	3.8
2	B	218	LEU	3.7
2	B	113	THR	3.7
2	B	41	ALA	3.7
2	B	44	LEU	3.6
1	A	21	ASN	3.6
2	B	300	VAL	3.6
1	A	293	PRO	3.6
2	B	279	SER	3.5
1	A	462	VAL	3.5
1	A	390	ALA	3.5
2	B	34	ALA	3.5
1	A	179	TYR	3.5
2	B	49	LEU	3.5
2	B	31	LEU	3.4
2	B	137	GLY	3.4
1	A	356	THR	3.3
2	B	326	VAL	3.3
1	A	565	LEU	3.3
2	B	128	VAL	3.3
2	B	329	THR	3.2
2	B	77	VAL	3.2
1	A	169	GLU	3.2
2	B	152	TRP	3.2
1	A	452	GLY	3.2
2	B	33	ALA	3.2
1	A	78	TRP	3.2
2	B	249	LEU	3.2
1	A	529	MET	3.2
1	A	577	PHE	3.1
1	A	36	GLN	3.1
2	B	290	LEU	3.1
2	B	25	ALA	3.1
2	B	66	ALA	3.1
2	B	308	LEU	3.1
2	B	269	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	115	ILE	3.0
1	A	148	SER	3.0
1	A	593	ARG	3.0
2	B	139	GLN	3.0
1	A	575	GLY	2.9
2	B	298	ASP	2.9
1	A	292	PRO	2.9
1	A	146	HIS	2.9
1	A	376	LEU	2.9
2	B	316	VAL	2.9
1	A	187	MET	2.9
2	B	233	GLU	2.9
1	A	299	LEU	2.9
2	B	42	LEU	2.9
2	B	271	LEU	2.9
2	B	136	SER	2.8
2	B	311	SER	2.8
2	B	36	TYR	2.8
2	B	148	CYS	2.8
2	B	149	ILE	2.8
2	B	164	ARG	2.8
2	B	58	LEU	2.8
2	B	327	VAL	2.8
2	B	21	PRO	2.8
2	B	262	VAL	2.8
2	B	323	VAL	2.8
1	A	168	ILE	2.8
1	A	302	LYS	2.8
2	B	219	ALA	2.8
2	B	131	VAL	2.8
1	A	341	ILE	2.7
2	B	304	THR	2.7
2	B	268	VAL	2.7
1	A	454	GLN	2.7
1	A	416	VAL	2.7
2	B	212	GLY	2.7
2	B	244	SER	2.7
1	A	464	ILE	2.7
1	A	379	ALA	2.6
2	B	318	TRP	2.6
1	A	526	ARG	2.6
2	B	313	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	119	PHE	2.6
2	B	263	PHE	2.6
2	B	306	SER	2.6
1	A	222	LEU	2.6
2	B	92	ARG	2.6
2	B	141	VAL	2.6
2	B	47	SER	2.6
2	B	163	TYR	2.6
2	B	86	LEU	2.5
1	A	295	ASN	2.5
1	A	98	LYS	2.5
2	B	151	VAL	2.5
2	B	160	LEU	2.5
2	B	175	ALA	2.5
1	A	173	THR	2.5
2	B	270	PHE	2.5
2	B	206	ILE	2.5
2	B	140	ALA	2.5
2	B	167	ALA	2.5
1	A	274	GLU	2.4
2	B	53	CYS	2.4
1	A	349	VAL	2.4
1	A	594	GLU	2.4
2	B	104	GLU	2.4
1	A	536	CYS	2.4
2	B	299	PHE	2.4
2	B	305	TRP	2.4
1	A	283	TYR	2.4
1	A	65	PRO	2.4
1	A	374	ALA	2.4
1	A	266	ILE	2.4
2	B	195	TRP	2.4
1	A	272	HIS	2.4
1	A	412	GLN	2.4
1	A	300	PHE	2.4
1	A	542	VAL	2.4
2	B	291	PHE	2.4
2	B	40	GLY	2.3
2	B	75	ALA	2.3
2	B	295	ALA	2.3
2	B	242	THR	2.3
2	B	283	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	53	GLU	2.3
1	A	544	VAL	2.3
2	B	153	ASP	2.3
1	A	350	PRO	2.3
2	B	68	PRO	2.3
1	A	369	GLY	2.3
1	A	468	TYR	2.3
2	B	143	GLY	2.3
2	B	67	ALA	2.3
1	A	431	ILE	2.3
1	A	357	ASN	2.3
1	A	280	TYR	2.3
1	A	286	TYR	2.3
2	B	23	ALA	2.3
2	B	258	VAL	2.3
2	B	45	GLY	2.2
2	B	76	GLY	2.2
2	B	317	GLY	2.2
2	B	89	VAL	2.2
2	B	95	LEU	2.2
2	B	133	VAL	2.2
2	B	182	VAL	2.2
1	A	347	ASP	2.2
1	A	22	CYS	2.2
2	B	73	CYS	2.2
2	B	328	PRO	2.2
2	B	101	GLY	2.2
2	B	98	SER	2.2
2	B	225	SER	2.2
1	A	55	ILE	2.2
2	B	228	PHE	2.2
2	B	64	PRO	2.2
1	A	216	HIS	2.2
1	A	276	GLU	2.2
1	A	467	GLU	2.2
1	A	220	ARG	2.2
2	B	105	LEU	2.2
2	B	83	VAL	2.2
2	B	307	PRO	2.2
1	A	178	GLU	2.2
1	A	410	GLY	2.2
2	B	97	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	26	ILE	2.1
2	B	109	ASP	2.1
1	A	528	PRO	2.1
2	B	24	PRO	2.1
2	B	278	CYS	2.1
2	B	138	THR	2.1
1	A	136	ARG	2.1
1	A	361	LEU	2.1
1	A	457	LEU	2.1
1	A	458	LYS	2.1
2	B	184	LEU	2.1
1	A	367	GLY	2.1
2	B	260	GLY	2.1
2	B	29	ARG	2.1
1	A	82	ILE	2.1
2	B	180	ASP	2.1
2	B	173	VAL	2.1
1	A	238	THR	2.1
2	B	174	ALA	2.1
2	B	107	GLU	2.1
2	B	123	GLU	2.1
2	B	154	LEU	2.1
2	B	239	LEU	2.1
1	A	527	ASP	2.1
1	A	24	PRO	2.1
1	A	118	GLY	2.1
2	B	230	PHE	2.1
2	B	220	TRP	2.1
2	B	165	ALA	2.0
2	B	321	GLN	2.0
2	B	227	VAL	2.0
1	A	327	PHE	2.0
1	A	423	TRP	2.0
2	B	80	GLU	2.0
2	B	287	LEU	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 [i](#)

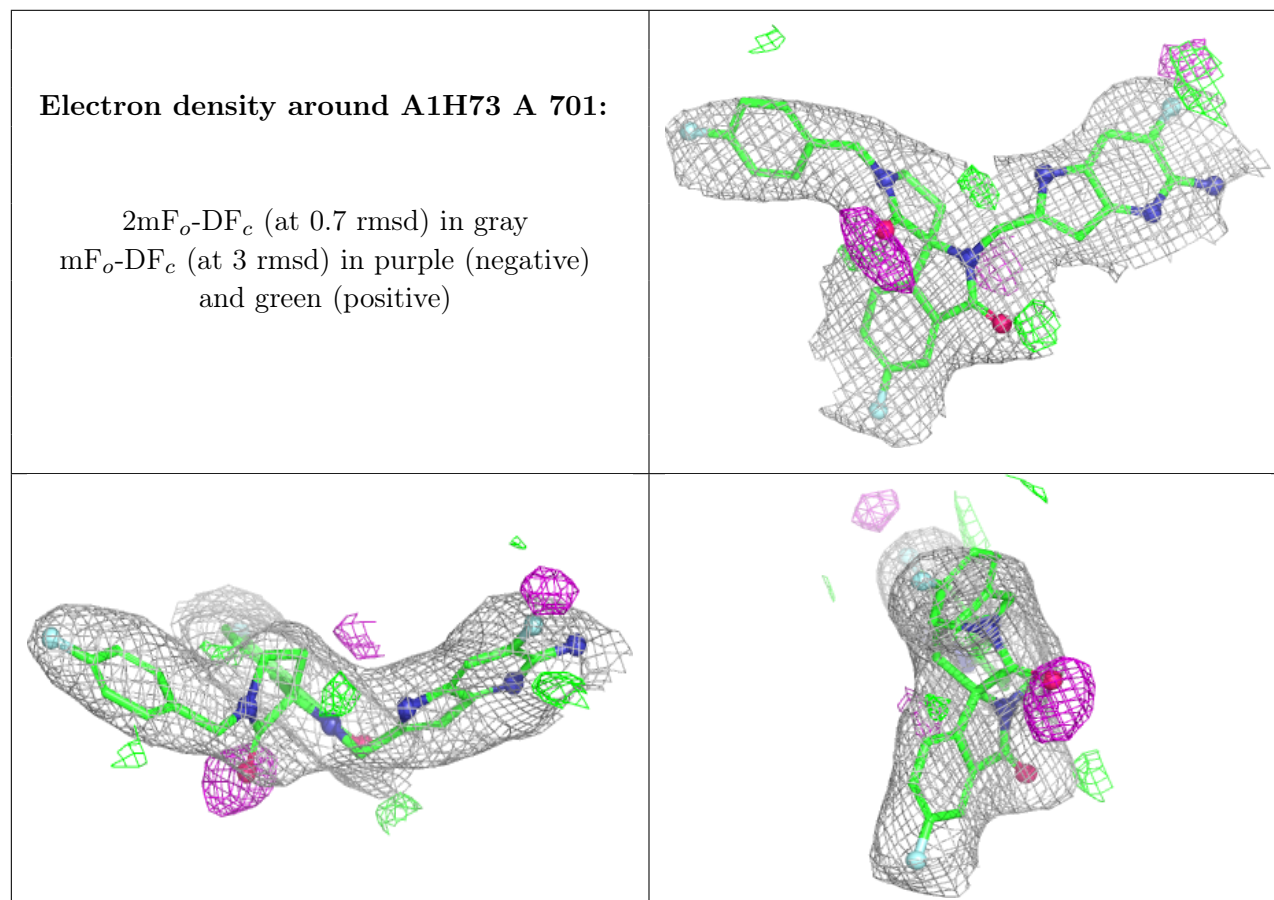
There are no oligosaccharides in this entry.

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
3	A1H73	A	701	36/36	0.88	0.11	40,46,54,56	0
4	MTA	A	702	20/20	0.89	0.11	26,27,31,31	0
5	SO4	A	703	5/5	0.89	0.20	80,81,81,81	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.