



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:35 PM UTC

PDB ID : 7MXC / pdb_00007mxc
Title : PRMT5:MEP50 complexed with adenosine
Authors : McTigue, M.; Deng, Y.L.; Liu, W.; Brooun, A.
Deposited on : 2021-05-18
Resolution : 2.41 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

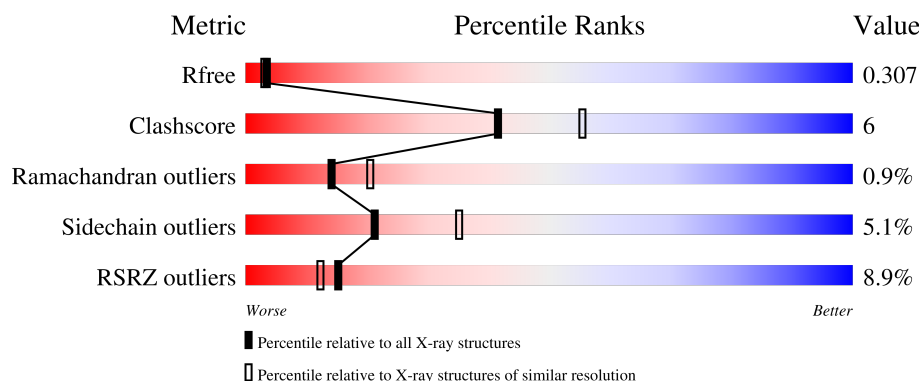
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	637	4% 79% 17% • •
2	B	366	16% 61% 19% • 19%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7531 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	621	Total	C	N	O	S	0	2	0
			5036	3220	866	925	25			

- Molecule 2 is a protein called Methylosome protein 50.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	298	Total	C	N	O	S	0	0	0
			2262	1422	387	441	12			

There are 25 discrepancies between the modelled and reference sequences:

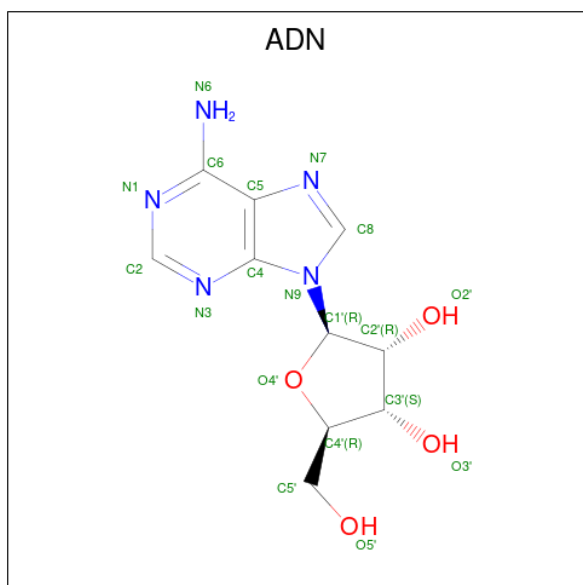
Chain	Residue	Modelled	Actual	Comment	Reference
B	-23	MET	-	expression tag	UNP Q9BQA1
B	-22	ALA	-	expression tag	UNP Q9BQA1
B	-21	SER	-	expression tag	UNP Q9BQA1
B	-20	HIS	-	expression tag	UNP Q9BQA1
B	-19	HIS	-	expression tag	UNP Q9BQA1
B	-18	HIS	-	expression tag	UNP Q9BQA1
B	-17	HIS	-	expression tag	UNP Q9BQA1
B	-16	HIS	-	expression tag	UNP Q9BQA1
B	-15	HIS	-	expression tag	UNP Q9BQA1
B	-14	ASP	-	expression tag	UNP Q9BQA1
B	-13	TYR	-	expression tag	UNP Q9BQA1
B	-12	ASP	-	expression tag	UNP Q9BQA1
B	-11	GLY	-	expression tag	UNP Q9BQA1
B	-10	ALA	-	expression tag	UNP Q9BQA1
B	-9	THR	-	expression tag	UNP Q9BQA1
B	-8	THR	-	expression tag	UNP Q9BQA1
B	-7	GLU	-	expression tag	UNP Q9BQA1
B	-6	ASN	-	expression tag	UNP Q9BQA1
B	-5	LEU	-	expression tag	UNP Q9BQA1
B	-4	TYR	-	expression tag	UNP Q9BQA1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	PHE	-	expression tag	UNP Q9BQA1
B	-2	GLN	-	expression tag	UNP Q9BQA1
B	-1	GLY	-	expression tag	UNP Q9BQA1
B	0	SER	-	expression tag	UNP Q9BQA1
B	1	LEU	-	expression tag	UNP Q9BQA1

- Molecule 3 is ADENOSINE (CCD ID: ADN) (formula: $C_{10}H_{13}N_5O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			19	10	5	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	174	Total	O	0	0
			174	174		
4	B	40	Total	O	0	0
			40	40		

GLU

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	99.92Å 137.96Å 177.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	109.03 – 2.41 109.03 – 2.41	Depositor EDS
% Data completeness (in resolution range)	99.3 (109.03-2.41) 99.4 (109.03-2.41)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.40Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.248 , 0.303 0.248 , 0.307	Depositor DCC
R_{free} test set	2392 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	48.3	Xtriage
Anisotropy	0.992	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7531	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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: ADN

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	0.74	0/5179	1.09	9/7045 (0.1%)
2	B	0.73	1/2314 (0.0%)	1.11	2/3156 (0.1%)
All	All	0.74	1/7493 (0.0%)	1.09	11/10201 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	168	ALA	CA-C	5.51	1.60	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	607	ASN	CA-CB-CG	5.72	118.32	112.60
1	A	341	ILE	CA-C-N	5.63	128.14	120.54
1	A	341	ILE	C-N-CA	5.63	128.14	120.54
1	A	456	PHE	CA-CB-CG	5.45	119.25	113.80
1	A	578	SER	N-CA-C	5.36	119.30	112.34
1	A	79	ASN	CA-CB-CG	5.13	117.73	112.60
2	B	240	VAL	N-CA-C	5.08	115.17	107.75
1	A	369	GLY	N-CA-C	5.05	122.63	112.34
1	A	586	ILE	CA-C-N	5.03	127.33	120.54
1	A	586	ILE	C-N-CA	5.03	127.33	120.54
2	B	277	ASP	CA-CB-CG	5.02	117.62	112.60

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	5036	0	4931	58	0
2	B	2262	0	2184	38	0
3	A	19	0	13	0	0
4	A	174	0	0	1	0
4	B	40	0	0	0	0
All	All	7531	0	7128	93	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (93) 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)
2:B:30:GLN:HB2	2:B:47:SER:O	1.91	0.69
1:A:525:ASN:HB3	1:A:530:ILE:HG21	1.79	0.65
1:A:141:HIS:O	1:A:147:HIS:CE1	2.52	0.63
1:A:30:LEU:HD11	1:A:82:ILE:HD11	1.81	0.62
1:A:629:THR:HG22	1:A:629:THR:O	2.00	0.61
2:B:322:VAL:HG12	2:B:322:VAL:O	1.99	0.61
1:A:149:SER:HB2	4:A:918:HOH:O	2.01	0.61
1:A:586:ILE:HA	1:A:626:HIS:NE2	2.16	0.61
1:A:468:TYR:CE1	1:A:521:PHE:HB2	2.37	0.60
1:A:527:ASP:HB3	1:A:530:ILE:HG22	1.83	0.60
2:B:102:ALA:HB2	2:B:122:TYR:CD2	2.37	0.60
1:A:32:ALA:HA	1:A:35:LYS:HZ1	1.67	0.59
2:B:27:MET:HE2	2:B:59:TRP:CD1	2.37	0.59
2:B:176:SER:HA	2:B:220:TRP:NE1	2.17	0.59
1:A:553:GLY:HA3	1:A:582:ILE:HG22	1.84	0.58
1:A:50:PHE:CE1	1:A:62:ARG:NH1	2.72	0.57
1:A:567:ILE:HA	1:A:572:HIS:CD2	2.39	0.57
1:A:364:LEU:HB3	1:A:420:MET:HE2	1.86	0.56
1:A:129:GLU:HB2	1:A:187[B]:MET:HE1	1.87	0.56
2:B:58:LEU:HB2	2:B:77:VAL:HG12	1.87	0.56
1:A:609:LYS:O	1:A:637:LEU:HB2	2.06	0.56
2:B:282:VAL:HG12	2:B:290:LEU:HD12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:GLU:HA	1:A:188:TRP:CD1	2.43	0.54
1:A:212:LEU:HG	1:A:250:HIS:CE1	2.43	0.54
1:A:405:GLN:HA	1:A:409:TRP:HB2	1.90	0.53
1:A:285:GLU:O	1:A:289:GLN:HG2	2.09	0.52
2:B:134:LEU:HD23	2:B:175:ALA:HB1	1.91	0.52
1:A:493:ASP:HB3	1:A:496:ALA:HB2	1.91	0.52
1:A:421:ARG:HG2	1:A:452:GLY:HA3	1.92	0.51
1:A:441:ALA:HB2	1:A:555:PHE:HB2	1.93	0.51
1:A:599:CYS:HB3	1:A:619:ALA:HB3	1.93	0.51
1:A:301:ALA:HB1	1:A:505:ARG:HG2	1.92	0.51
2:B:69:ASN:HB3	2:B:72:PHE:HB2	1.92	0.51
1:A:271:HIS:NE2	2:B:125:ASP:OD1	2.29	0.50
1:A:68:ARG:NH2	2:B:54:TRP:CZ3	2.79	0.50
1:A:187[B]:MET:CE	1:A:188:TRP:HD1	2.26	0.48
2:B:27:MET:HG2	2:B:70:GLU:HG3	1.95	0.48
2:B:177:PRO:HD3	2:B:220:TRP:CG	2.48	0.48
2:B:280:LEU:HD22	2:B:315:THR:HG21	1.95	0.48
2:B:284:ASP:HB3	2:B:290:LEU:HD21	1.96	0.48
1:A:476:SER:HB2	1:A:512:LEU:HD21	1.96	0.47
1:A:484:VAL:O	1:A:497:GLN:HG3	2.15	0.47
2:B:289:GLU:OE2	2:B:292:ARG:HB2	2.14	0.47
1:A:45:VAL:HG23	1:A:46:PHE:HD1	1.80	0.47
1:A:368:ARG:HB3	1:A:400:THR:HG21	1.96	0.47
1:A:512:LEU:HD13	1:A:546:THR:HG21	1.96	0.47
2:B:28:GLU:HB3	2:B:48:SER:HB3	1.96	0.47
1:A:319:LEU:HD22	1:A:323:THR:HG21	1.97	0.47
2:B:265:PRO:HD3	2:B:305:TRP:HB2	1.97	0.47
2:B:66:ALA:HB1	2:B:72:PHE:HB3	1.97	0.46
1:A:19:ASP:HB3	1:A:267:THR:HB	1.96	0.46
1:A:147:HIS:HB3	1:A:201:ARG:NH1	2.29	0.46
1:A:350:PRO:HG2	1:A:353:GLU:HG3	1.97	0.46
2:B:77:VAL:HB	2:B:115:ILE:HB	1.98	0.46
2:B:135:SER:OG	2:B:177:PRO:O	2.34	0.46
2:B:110:GLU:H	2:B:110:GLU:CD	2.24	0.45
1:A:73:LEU:HB2	1:A:78:TRP:CE2	2.51	0.45
1:A:434:SER:HB2	1:A:436:LEU:HG	1.98	0.45
2:B:144:SER:HB3	2:B:146:ASP:OD1	2.16	0.45
2:B:93:GLY:HA2	2:B:107:GLU:HA	1.98	0.45
2:B:306:SER:HB3	2:B:309:ASN:O	2.17	0.45
1:A:342:TYR:HD1	1:A:382:ALA:HB2	1.82	0.45
1:A:362:MET:SD	1:A:429:ALA:HB2	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:LEU:HD13	1:A:433:VAL:HG12	1.99	0.45
1:A:179:TYR:O	1:A:216:HIS:HE1	2.00	0.44
2:B:70:GLU:H	2:B:70:GLU:CD	2.25	0.44
1:A:416:VAL:HG21	1:A:423:TRP:CZ2	2.53	0.44
2:B:265:PRO:HD3	2:B:305:TRP:CB	2.47	0.44
2:B:134:LEU:HD12	2:B:139:GLN:HB3	2.00	0.44
1:A:361:LEU:HD11	1:A:431:ILE:HD12	2.00	0.44
1:A:32:ALA:HA	1:A:35:LYS:NZ	2.32	0.44
1:A:23:VAL:HG22	1:A:29:THR:HG21	1.99	0.44
2:B:261:LEU:HD22	2:B:271:LEU:HD21	2.00	0.43
2:B:303:ALA:HB1	2:B:313:LEU:HD11	2.01	0.43
1:A:592:VAL:HG21	1:A:598:ILE:HD11	2.01	0.43
1:A:362:MET:HG2	1:A:389:TYR:HB2	2.01	0.42
2:B:194:LEU:HB2	2:B:206:ILE:HD11	2.01	0.42
1:A:371:LEU:HD11	1:A:435:GLU:HB2	2.01	0.42
1:A:349:VAL:O	1:A:384:ARG:NH1	2.49	0.42
1:A:68:ARG:NH2	2:B:54:TRP:CH2	2.88	0.42
1:A:315:LEU:HD11	1:A:421:ARG:NH2	2.35	0.42
2:B:28:GLU:HG2	2:B:48:SER:HB3	2.00	0.42
1:A:567:ILE:HG21	1:A:579:TRP:HB2	2.01	0.41
2:B:31:LEU:HD23	2:B:46:ALA:HB2	2.02	0.41
1:A:420:MET:HE1	1:A:436:LEU:HD11	2.02	0.41
2:B:254:HIS:HD2	2:B:258:VAL:HG22	1.85	0.41
1:A:362:MET:SD	1:A:456:PHE:CE1	3.15	0.40
1:A:599:CYS:HG	1:A:618:THR:HG1	1.69	0.40
2:B:60:LEU:HD22	2:B:108:LEU:HD11	2.03	0.40
2:B:171:THR:HG21	2:B:216:THR:HA	2.03	0.40
2:B:179:LYS:HB2	2:B:182:VAL:HB	2.04	0.40
1:A:238:THR:HA	1:A:272:HIS:HE1	1.87	0.40
1:A:248:LYS:O	1:A:252:ARG:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	619/637 (97%)	589 (95%)	25 (4%)	5 (1%)	16	23
2	B	292/366 (80%)	267 (91%)	22 (8%)	3 (1%)	12	18
All	All	911/1003 (91%)	856 (94%)	47 (5%)	8 (1%)	14	20

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	147	ILE
1	A	147	HIS
2	B	135	SER
1	A	148	SER
1	A	441	ALA
1	A	531	ASP
1	A	530	ILE
2	B	127	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	556/562 (99%)	531 (96%)	25 (4%)	24	40
2	B	253/310 (82%)	237 (94%)	16 (6%)	16	27
All	All	809/872 (93%)	768 (95%)	41 (5%)	21	35

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	14	VAL
1	A	102	ASN
1	A	127	ASN
1	A	149	SER

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Mol	Chain	Res	Type
1	A	155	VAL
1	A	208	ILE
1	A	227	LYS
1	A	240	LYS
1	A	248	LYS
1	A	281	LEU
1	A	299	LEU
1	A	326	VAL
1	A	339	GLN
1	A	351	GLU
1	A	355	ASP
1	A	393	LYS
1	A	405	GLN
1	A	475	ILE
1	A	525	ASN
1	A	526	ARG
1	A	548	LEU
1	A	578	SER
1	A	582	ILE
1	A	594	GLU
2	B	65	CYS
2	B	77	VAL
2	B	96	VAL
2	B	114	LEU
2	B	131	VAL
2	B	135	SER
2	B	141	VAL
2	B	206	ILE
2	B	225	SER
2	B	243	LYS
2	B	283	LEU
2	B	290	LEU
2	B	294	GLN
2	B	300	VAL
2	B	320	HIS
2	B	326	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	66	GLN

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Mol	Chain	Res	Type
1	A	131	ASN
1	A	272	HIS
1	A	396	ASN
1	A	455	HIS
1	A	572	HIS
1	A	588	GLN
2	B	69	ASN
2	B	111	ASN
2	B	254	HIS

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](#)

1 ligand is 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	ADN	A	701	-	21,21,21	0.19	0	31,31,31	0.61	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	ADN	A	701	-	-	0/6/22/22	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

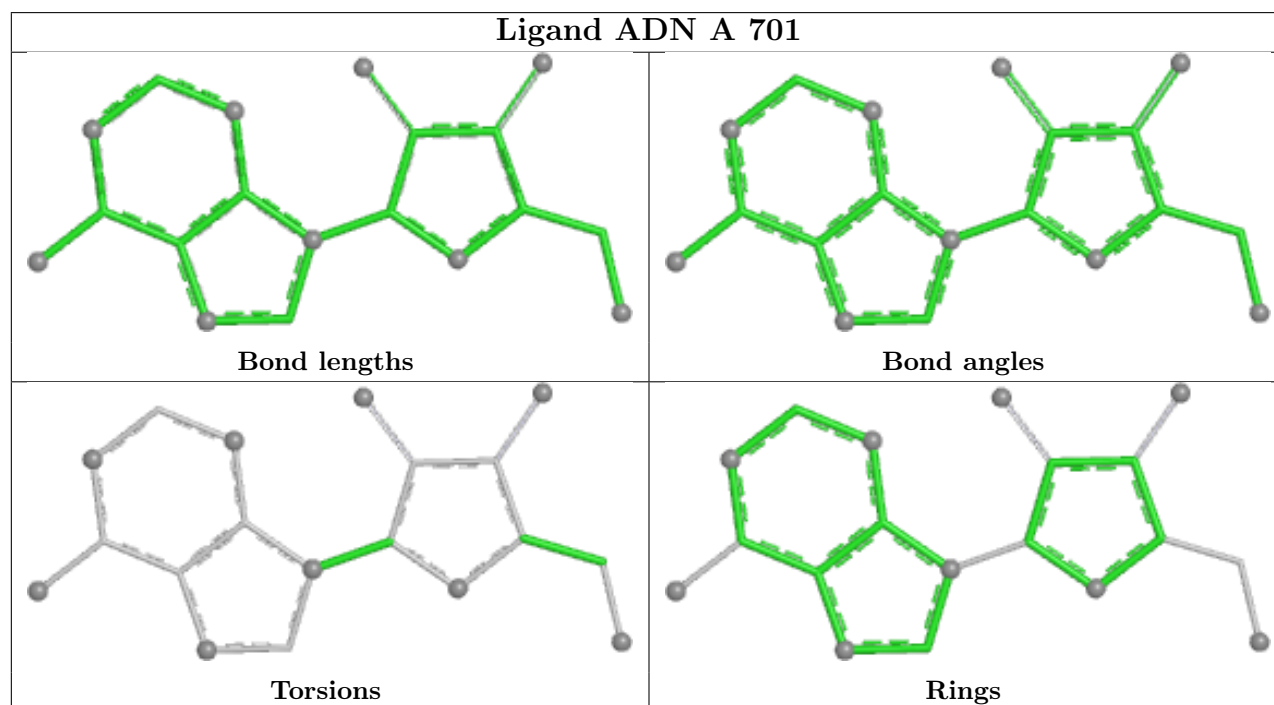
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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.



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	621/637 (97%)	0.74	23 (3%) 45 41	22, 58, 88, 103	2 (0%)
2	B	298/366 (81%)	1.37	59 (19%) 3 2	54, 76, 96, 105	0
All	All	919/1003 (91%)	0.94	82 (8%) 15 12	22, 65, 93, 105	2 (0%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	248	VAL	5.9
2	B	207	GLY	4.4
2	B	249	LEU	3.9
1	A	45	VAL	3.3
2	B	31	LEU	3.1
2	B	41	ALA	3.1
2	B	329	THR	3.1
2	B	218	LEU	3.1
2	B	313	LEU	3.0
1	A	530	ILE	2.9
2	B	303	ALA	2.9
2	B	43	LEU	2.9
2	B	261	LEU	2.9
2	B	327	VAL	2.8
2	B	114	LEU	2.8
1	A	278	CYS	2.8
1	A	249	MET	2.8
2	B	49	LEU	2.7
2	B	87	THR	2.7
1	A	208	ILE	2.7
2	B	322	VAL	2.6
2	B	103	VAL	2.6
2	B	44	LEU	2.6
2	B	271	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	108	LEU	2.6
2	B	312	LEU	2.5
2	B	106	TRP	2.5
2	B	105	LEU	2.5
2	B	77	VAL	2.5
2	B	104	GLU	2.5
2	B	62	LYS	2.5
2	B	179	LYS	2.5
1	A	462	VAL	2.5
2	B	300	VAL	2.5
2	B	225	SER	2.5
1	A	299	LEU	2.4
2	B	283	LEU	2.4
2	B	97	ALA	2.4
1	A	361	LEU	2.4
2	B	60	LEU	2.4
2	B	58	LEU	2.4
1	A	560	TYR	2.4
2	B	323	VAL	2.4
1	A	409	TRP	2.4
2	B	34	ALA	2.4
1	A	65	PRO	2.4
1	A	59	ALA	2.4
2	B	291	PHE	2.3
2	B	318	TRP	2.3
1	A	231	LEU	2.3
2	B	243	LYS	2.3
2	B	219	ALA	2.3
2	B	274	LEU	2.3
2	B	45	GLY	2.2
1	A	529	MET	2.2
1	A	147	HIS	2.2
2	B	88	TRP	2.2
2	B	134	LEU	2.2
1	A	20	LEU	2.2
2	B	282	VAL	2.1
2	B	25	ALA	2.1
2	B	86	LEU	2.1
2	B	26	CYS	2.1
2	B	24	PRO	2.1
2	B	316	VAL	2.1
2	B	42	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	98	SER	2.1
2	B	177	PRO	2.1
1	A	243	PHE	2.1
1	A	281	LEU	2.1
1	A	287	LEU	2.1
2	B	95	LEU	2.1
2	B	143	GLY	2.1
1	A	175	HIS	2.1
2	B	116	VAL	2.0
2	B	290	LEU	2.0
1	A	293	PRO	2.0
1	A	91	ARG	2.0
2	B	29	ARG	2.0
2	B	137	GLY	2.0
1	A	29	THR	2.0
2	B	302	ASP	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](#)

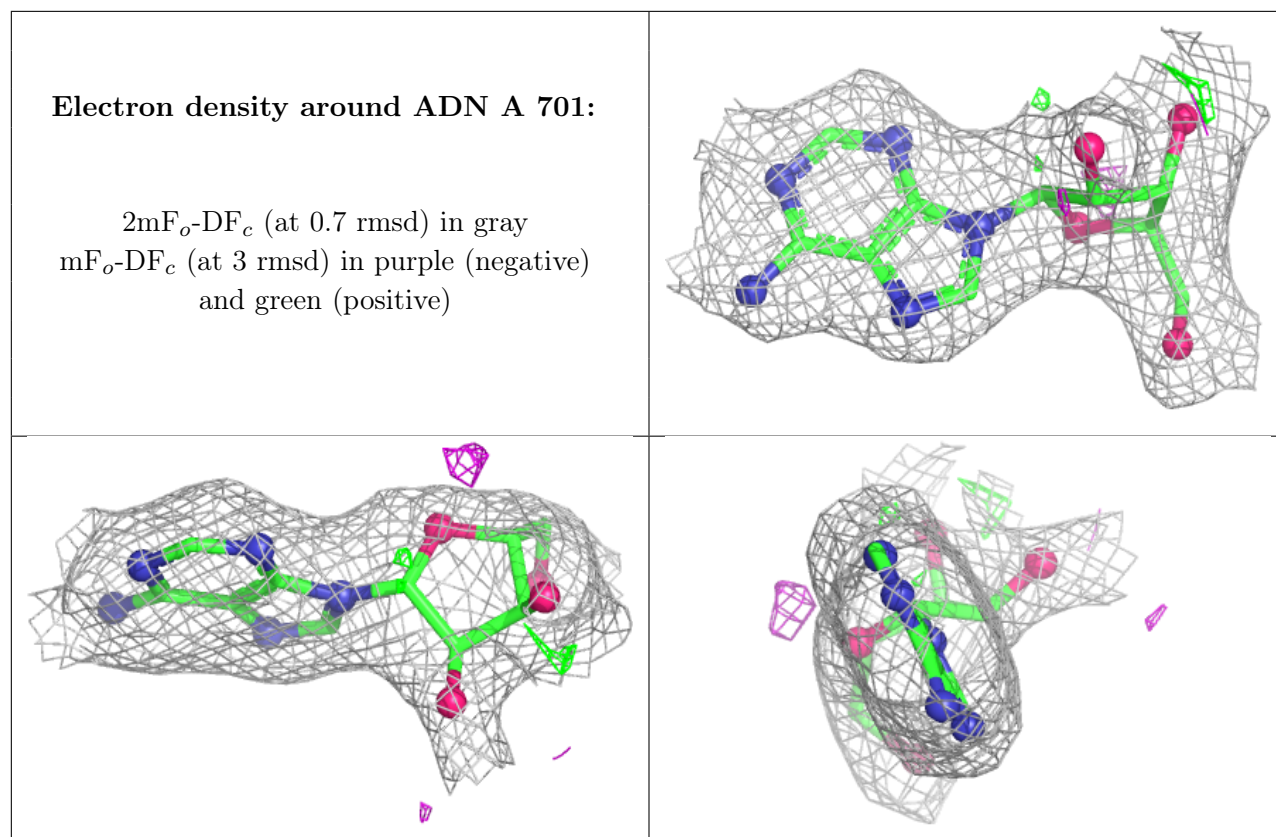
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
3	ADN	A	701	19/19	0.90	0.10	38,40,45,45	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.