



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:08 AM UTC

PDB ID : 4LCA / pdb_00004lca
Title : Crystal structure of probable sugar kinase protein from Rhizobium Etli CFN 42 complexed with thymidine
Authors : Malashkevich, V.N.; Bhosle, R.; Toro, R.; Hillerich, B.; Gizzi, A.; Garforth, S.; Kar, A.; Chan, M.K.; Laffuer, J.; Patel, H.; Matikainen, B.; Chamala, S.; Lim, S.; Celikgil, A.; Villegas, G.; Evans, B.; Love, J.; Fiser, A.; Khafizov, K.; Seidel, R.; Bonanno, J.B.; Almo, S.C.; New York Structural Genomics Research Consortium (NYSGRC)
Deposited on : 2013-06-21
Resolution : 1.50 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

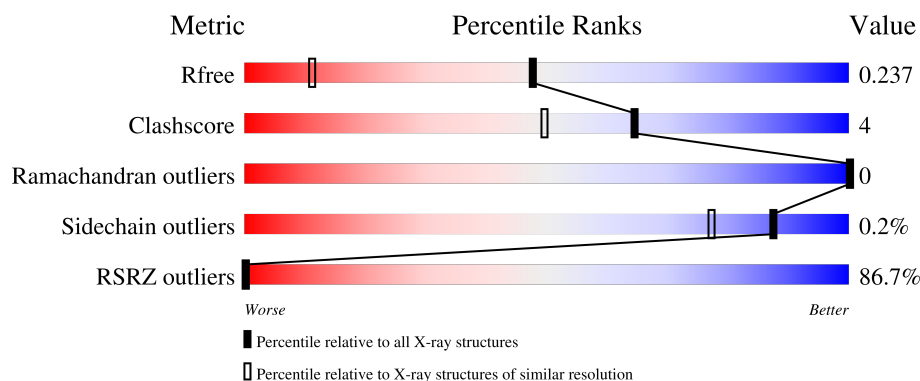
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	352	82% 89% 6%
1	B	352	75% 87% 7% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

Ideal geometry (proteins)	: Engh & Huber (2001)
Ideal geometry (DNA, RNA)	: Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: 2.49

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	K	B	406	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5997 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 Probable sugar kinase protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	Se	0	11	0
			2565	1607	450	490	8	10			
1	B	330	Total	C	N	O	S	Se	0	10	0
			2557	1599	445	495	8	10			

There are 44 discrepancies between the modelled and reference sequences:

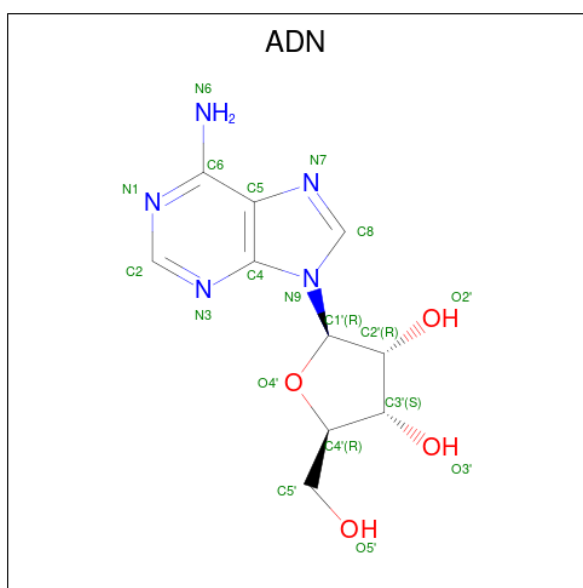
Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MSE	-	expression tag	UNP Q2KDX6
A	-22	HIS	-	expression tag	UNP Q2KDX6
A	-21	HIS	-	expression tag	UNP Q2KDX6
A	-20	HIS	-	expression tag	UNP Q2KDX6
A	-19	HIS	-	expression tag	UNP Q2KDX6
A	-18	HIS	-	expression tag	UNP Q2KDX6
A	-17	HIS	-	expression tag	UNP Q2KDX6
A	-16	SER	-	expression tag	UNP Q2KDX6
A	-15	SER	-	expression tag	UNP Q2KDX6
A	-14	GLY	-	expression tag	UNP Q2KDX6
A	-13	VAL	-	expression tag	UNP Q2KDX6
A	-12	ASP	-	expression tag	UNP Q2KDX6
A	-11	LEU	-	expression tag	UNP Q2KDX6
A	-10	GLY	-	expression tag	UNP Q2KDX6
A	-9	THR	-	expression tag	UNP Q2KDX6
A	-8	GLU	-	expression tag	UNP Q2KDX6
A	-7	ASN	-	expression tag	UNP Q2KDX6
A	-6	LEU	-	expression tag	UNP Q2KDX6
A	-5	TYR	-	expression tag	UNP Q2KDX6
A	-4	PHE	-	expression tag	UNP Q2KDX6
A	-3	GLN	-	expression tag	UNP Q2KDX6
A	-2	SER	-	expression tag	UNP Q2KDX6
B	-23	MSE	-	expression tag	UNP Q2KDX6
B	-22	HIS	-	expression tag	UNP Q2KDX6
B	-21	HIS	-	expression tag	UNP Q2KDX6

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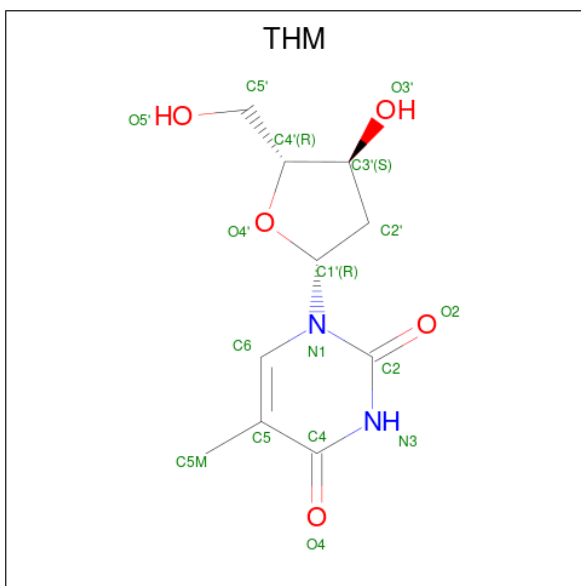
Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	HIS	-	expression tag	UNP Q2KDX6
B	-19	HIS	-	expression tag	UNP Q2KDX6
B	-18	HIS	-	expression tag	UNP Q2KDX6
B	-17	HIS	-	expression tag	UNP Q2KDX6
B	-16	SER	-	expression tag	UNP Q2KDX6
B	-15	SER	-	expression tag	UNP Q2KDX6
B	-14	GLY	-	expression tag	UNP Q2KDX6
B	-13	VAL	-	expression tag	UNP Q2KDX6
B	-12	ASP	-	expression tag	UNP Q2KDX6
B	-11	LEU	-	expression tag	UNP Q2KDX6
B	-10	GLY	-	expression tag	UNP Q2KDX6
B	-9	THR	-	expression tag	UNP Q2KDX6
B	-8	GLU	-	expression tag	UNP Q2KDX6
B	-7	ASN	-	expression tag	UNP Q2KDX6
B	-6	LEU	-	expression tag	UNP Q2KDX6
B	-5	TYR	-	expression tag	UNP Q2KDX6
B	-4	PHE	-	expression tag	UNP Q2KDX6
B	-3	GLN	-	expression tag	UNP Q2KDX6
B	-2	SER	-	expression tag	UNP Q2KDX6

- Molecule 2 is ADENOSINE (CCD ID: ADN) (formula: $C_{10}H_{13}N_5O_4$).



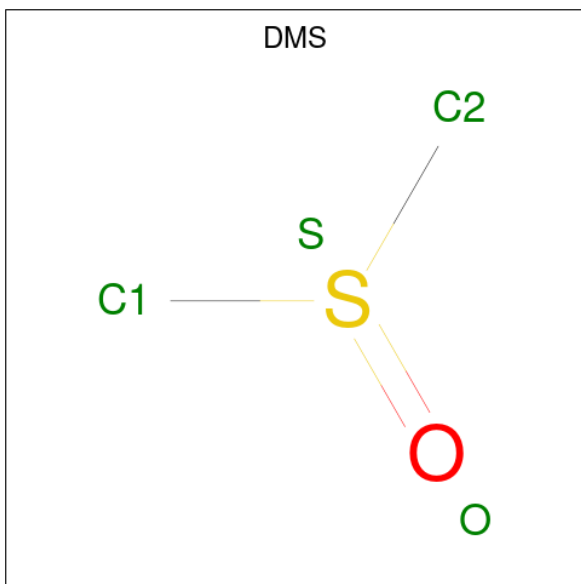
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			19	10	5	4		
2	B	1	Total	C	N	O	0	0
			19	10	5	4		

- Molecule 3 is THYMIDINE (CCD ID: THM) (formula: $C_{10}H_{14}N_2O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	17	1
			34	20	4	10		
3	B	1	Total	C	N	O	16	1
			34	20	4	10		
3	B	1	Total	C	N	O	0	0
			17	10	2	5		

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O S 4 2 1 1	0	0
4	A	1	Total C O S 4 2 1 1	0	0
4	B	1	Total C O S 4 2 1 1	0	0
4	B	1	Total C O S 4 2 1 1	0	0

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total K 1 1	0	0
5	B	1	Total K 1 1	0	0

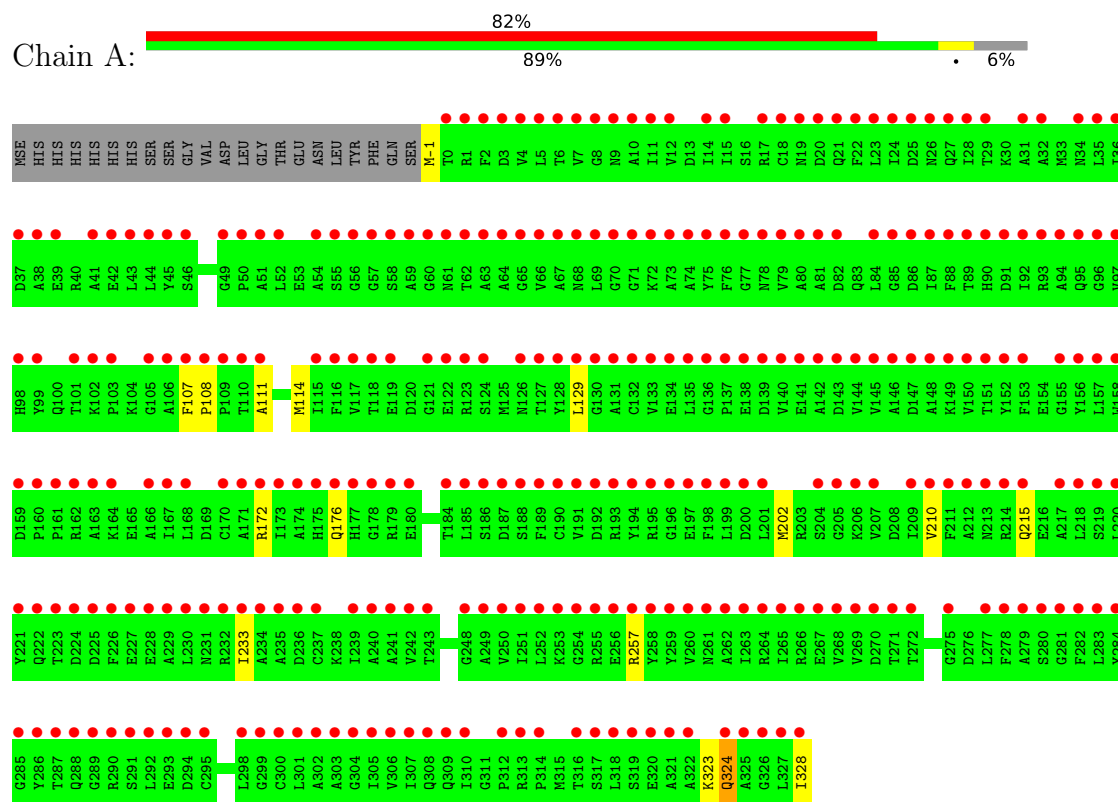
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	331	Total O 331 331	0	0
6	B	401	Total O 403 403	0	2

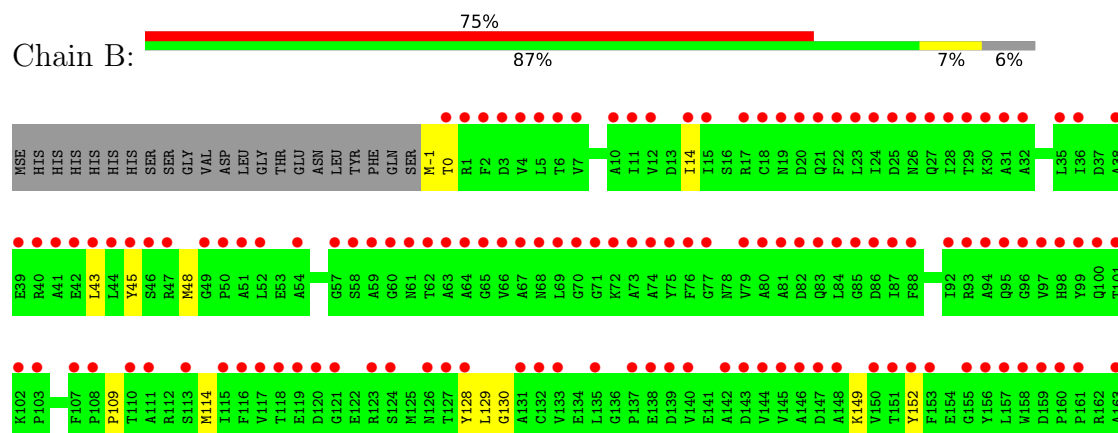
3 Residue-property plots

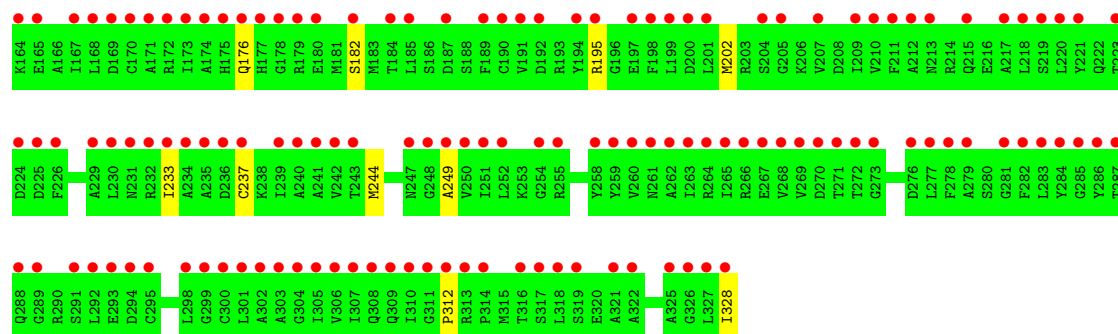
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Probable sugar kinase protein



• Molecule 1: Probable sugar kinase protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.52Å 80.78Å 82.66Å 90.00° 98.09° 90.00°	Depositor
Resolution (Å)	40.18 – 1.50 40.18 – 1.50	Depositor EDS
% Data completeness (in resolution range)	95.2 (40.18-1.50) 95.2 (40.18-1.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 1.49Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.200 , 0.248 0.192 , 0.237	Depositor DCC
R_{free} test set	5181 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å ²)	18.2	Xtrriage
Anisotropy	0.385	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 100.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	5997	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.38 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5659e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: K, DMS, ADN, THM

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	0.57	0/2625	0.83	1/3531 (0.0%)
1	B	0.66	0/2614	0.87	1/3517 (0.0%)
All	All	0.62	0/5239	0.85	2/7048 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	114	MSE	CA-CB-CG	-5.37	103.36	114.10
1	A	114	MSE	CA-CB-CG	-5.23	103.63	114.10

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	2565	0	2565	16	0
1	B	2557	0	2537	25	0
2	A	19	0	13	0	0
2	B	19	0	13	0	0
3	A	34	0	28	0	0
3	B	51	0	42	0	0
4	A	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	8	0	12	4	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	331	0	0	5	0
6	B	403	0	0	6	0
All	All	5997	0	5222	41	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 4.

All (41) 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:257[B]:ARG:HH11	1:A:257[B]:ARG:HG3	1.17	1.06
1:B:195[B]:ARG:HG2	1:B:195[B]:ARG:NH1	1.56	1.06
1:B:195[B]:ARG:HH11	1:B:195[B]:ARG:CG	1.69	1.04
1:A:257[B]:ARG:HH11	1:A:257[B]:ARG:CG	1.86	0.88
1:B:195[B]:ARG:HG2	1:B:195[B]:ARG:HH11	0.75	0.75
1:A:215:GLN:HG2	6:A:802:HOH:O	1.86	0.74
1:B:0:THR:HG21	1:B:149:LYS:HG3	1.72	0.71
1:B:195[B]:ARG:NH1	1:B:195[B]:ARG:CG	2.41	0.61
1:A:172:ARG:NH2	6:A:811:HOH:O	2.34	0.60
1:B:328:ILE:HG13	6:B:865:HOH:O	2.04	0.58
1:B:-1:MSE:N	6:B:667:HOH:O	2.34	0.57
1:A:257[B]:ARG:HG3	1:A:257[B]:ARG:NH1	2.00	0.57
1:A:257[B]:ARG:CG	1:A:257[B]:ARG:NH1	2.54	0.56
1:A:-1:MSE:N	6:A:675:HOH:O	2.40	0.53
1:B:176:GLN:HG3	6:B:671:HOH:O	2.11	0.51
1:B:128:TYR:CE2	4:B:404:DMS:H11	2.47	0.50
1:B:0:THR:CG2	1:B:149:LYS:HE3	2.42	0.49
1:B:195[B]:ARG:CZ	6:B:815:HOH:O	2.60	0.49
1:B:312:PRO:HD3	6:B:781:HOH:O	2.13	0.49
1:A:323:LYS:HA	1:A:328:ILE:HD13	1.97	0.46
1:A:107:PHE:HA	1:A:108:PRO:C	2.40	0.45
1:A:176:GLN:HG3	6:A:664:HOH:O	2.17	0.45
1:B:45:TYR:CG	4:B:403:DMS:H11	2.52	0.44
1:B:-1:MSE:N	6:B:814:HOH:O	2.51	0.44
1:B:202:MSE:HE3	1:B:237[B]:CYS:HB2	1.98	0.44
1:A:202:MSE:HE1	1:A:233:ILE:HG13	1.99	0.44
1:A:111:ALA:HB2	1:A:129:LEU:O	2.18	0.43
1:B:202:MSE:HE1	1:B:233:ILE:HG13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:PRO:CG	4:B:404:DMS:H13	2.49	0.42
1:A:202:MSE:HE3	1:A:210[A]:VAL:HG21	2.01	0.42
1:B:43:LEU:C	1:B:43:LEU:HD13	2.44	0.42
1:A:257[B]:ARG:NH1	6:A:652:HOH:O	2.53	0.42
1:B:244:MSE:HE2	1:B:249:ALA:C	2.45	0.41
1:B:109:PRO:HG3	4:B:404:DMS:H13	2.01	0.41
1:B:14:ILE:O	1:B:48:MSE:HE1	2.21	0.41
1:A:-1:MSE:HE3	1:A:-1:MSE:HB2	2.00	0.41
1:A:324:GLN:HE21	1:A:324:GLN:HB2	1.56	0.41
1:B:0:THR:HG21	1:B:149:LYS:HE3	2.03	0.41
1:B:0:THR:HG22	1:B:149:LYS:HE3	2.03	0.41
1:B:129:LEU:O	1:B:130:GLY:C	2.63	0.41
1:B:152:TYR:HA	1:B:182:SER:O	2.21	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	339/352 (96%)	335 (99%)	4 (1%)	0	100	100
1	B	338/352 (96%)	333 (98%)	5 (2%)	0	100	100
All	All	677/704 (96%)	668 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	268/266 (101%)	267 (100%)	1 (0%)	84	71
1	B	267/266 (100%)	267 (100%)	0	100	100
All	All	535/532 (101%)	534 (100%)	1 (0%)	87	77

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	324	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	177	HIS
1	A	324	GLN
1	B	21	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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
3	THM	B	405	-	18,18,18	1.38	3 (16%)	26,26,26	2.23	8 (30%)
2	ADN	A	401	-	21,21,21	1.71	4 (19%)	31,31,31	1.88	8 (25%)
4	DMS	B	404	-	3,3,3	0.67	0	3,3,3	0.58	0
4	DMS	B	403	-	3,3,3	0.59	0	3,3,3	0.48	0
2	ADN	B	401	-	21,21,21	1.60	3 (14%)	31,31,31	2.21	8 (25%)
3	THM	B	402[A]	-	18,18,18	1.61	3 (16%)	26,26,26	3.51	12 (46%)
3	THM	A	402[A]	-	18,18,18	2.38	7 (38%)	26,26,26	4.17	10 (38%)
3	THM	B	402[B]	-	18,18,18	1.48	6 (33%)	26,26,26	2.29	7 (26%)
4	DMS	A	403	-	3,3,3	0.56	0	3,3,3	0.87	0
3	THM	A	402[B]	-	18,18,18	1.31	4 (22%)	26,26,26	2.38	9 (34%)
4	DMS	A	404	-	3,3,3	0.60	0	3,3,3	0.58	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	THM	B	405	-	-	0/6/18/18	0/2/2/2
2	ADN	A	401	-	-	1/6/22/22	0/3/3/3
2	ADN	B	401	-	-	1/6/22/22	0/3/3/3
3	THM	B	402[A]	-	-	2/6/18/18	0/2/2/2
3	THM	A	402[A]	-	-	0/6/18/18	0/2/2/2
3	THM	B	402[B]	-	-	0/6/18/18	0/2/2/2
3	THM	A	402[B]	-	-	2/6/18/18	0/2/2/2

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402[A]	THM	C4-N3	-6.31	1.27	1.38
2	B	401	ADN	C5-C4	5.27	1.48	1.39
2	A	401	ADN	C5-C4	4.80	1.47	1.39
3	A	402[A]	THM	C2-N3	-4.08	1.30	1.38
3	B	402[A]	THM	C4-N3	-3.73	1.31	1.38
3	B	402[A]	THM	C6-C5	3.66	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402[A]	THM	C6-N1	-3.39	1.32	1.38
2	A	401	ADN	C8-N7	2.98	1.37	1.31
2	B	401	ADN	C5-C6	2.93	1.49	1.41
3	A	402[A]	THM	C4-C5	2.87	1.49	1.44
2	A	401	ADN	C5-C6	2.84	1.48	1.41
3	B	402[B]	THM	C6-C5	2.84	1.39	1.34
2	A	401	ADN	C5-N7	-2.83	1.33	1.39
3	B	405	THM	C4-C5	2.78	1.49	1.44
3	B	402[B]	THM	C4-N3	-2.75	1.33	1.38
3	B	402[A]	THM	C2-N3	-2.56	1.33	1.38
3	B	405	THM	C6-C5	2.52	1.38	1.34
3	A	402[A]	THM	O2-C2	-2.50	1.18	1.23
3	A	402[A]	THM	C6-C5	2.49	1.38	1.34
3	A	402[B]	THM	C4-N3	-2.49	1.34	1.38
3	B	405	THM	C2-N1	2.49	1.42	1.38
3	B	402[B]	THM	C4-C5	2.43	1.48	1.44
3	A	402[B]	THM	C6-C5	2.28	1.38	1.34
3	B	402[B]	THM	C6-N1	-2.28	1.34	1.38
3	A	402[B]	THM	C6-N1	-2.25	1.34	1.38
3	B	402[B]	THM	C2-N1	2.24	1.42	1.38
3	A	402[A]	THM	C2-N1	2.24	1.42	1.38
3	A	402[B]	THM	C2-N3	-2.21	1.34	1.38
3	B	402[B]	THM	C2-N3	-2.14	1.34	1.38
2	B	401	ADN	C5-N7	-2.02	1.35	1.39

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402[A]	THM	O4-C4-C5	-11.75	111.48	124.92
3	A	402[A]	THM	N3-C2-N1	11.63	130.03	114.89
3	A	402[A]	THM	O2-C2-N3	-8.54	105.74	121.49
3	A	402[A]	THM	C4-N3-C2	-7.32	117.75	127.34
3	A	402[A]	THM	C6-C5-C4	6.53	123.40	118.02
3	A	402[A]	THM	C6-N1-C2	-6.26	115.07	121.30
2	B	401	ADN	C2-N1-C6	6.14	128.81	118.73
3	A	402[A]	THM	C5-C6-N1	-5.73	117.09	123.31
3	B	402[A]	THM	O4-C4-N3	5.72	130.87	120.11
3	B	402[B]	THM	N3-C2-N1	5.54	122.10	114.89
3	B	402[B]	THM	C4-N3-C2	-5.44	120.21	127.34
2	B	401	ADN	N3-C2-N1	-5.37	120.45	128.58
3	B	402[A]	THM	N3-C2-N1	5.36	121.86	114.89
3	A	402[B]	THM	N3-C2-N1	5.28	121.76	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	405	THM	C4-N3-C2	-5.20	120.53	127.34
3	A	402[B]	THM	C4-N3-C2	-5.13	120.62	127.34
3	A	402[A]	THM	O4'-C1'-N1	4.98	116.71	107.86
3	B	405	THM	C5-C4-N3	4.87	119.56	115.32
3	A	402[B]	THM	O4-C4-C5	-4.69	119.55	124.92
3	B	405	THM	O4-C4-C5	-4.56	119.71	124.92
3	B	402[A]	THM	C5M-C5-C4	-4.51	113.97	118.78
3	B	405	THM	N3-C2-N1	4.48	120.72	114.89
3	B	402[A]	THM	O4'-C1'-N1	4.33	115.55	107.86
2	B	401	ADN	C4'-O4'-C1'	-4.20	100.19	109.47
3	B	402[B]	THM	C5-C4-N3	4.16	118.94	115.32
3	B	402[A]	THM	C5-C6-N1	-4.15	118.80	123.31
3	B	402[B]	THM	C5-C6-N1	-4.12	118.84	123.31
2	A	401	ADN	C5-C4-N3	-4.12	121.04	126.72
3	A	402[B]	THM	C5-C4-N3	3.96	118.77	115.32
3	B	402[A]	THM	O2-C2-N3	-3.69	114.68	121.49
2	A	401	ADN	N3-C2-N1	-3.64	123.08	128.58
2	A	401	ADN	N3-C4-N9	3.60	133.29	127.17
3	B	402[B]	THM	O4-C4-C5	-3.57	120.83	124.92
2	B	401	ADN	N3-C4-N9	3.54	133.19	127.17
2	B	401	ADN	N6-C6-N1	3.49	126.15	118.38
3	A	402[A]	THM	O4-C4-C5	3.49	128.91	124.92
2	A	401	ADN	C4'-O4'-C1'	-3.38	102.00	109.47
3	A	402[B]	THM	O4'-C1'-N1	3.34	113.79	107.86
3	A	402[A]	THM	C5M-C5-C6	-3.32	118.36	122.85
3	B	402[A]	THM	C4-N3-C2	-3.25	123.08	127.34
3	A	402[B]	THM	C5-C6-N1	-3.16	119.88	123.31
3	B	405	THM	C5-C6-N1	-3.06	119.99	123.31
3	B	402[B]	THM	O2-C2-N1	-3.04	118.84	122.80
3	B	405	THM	C5M-C5-C4	3.02	122.01	118.78
3	A	402[A]	THM	O4-C4-N3	-3.02	114.44	120.11
2	A	401	ADN	C2-N3-C4	2.95	119.04	111.83
3	A	402[B]	THM	O2-C2-N1	-2.93	118.98	122.80
2	A	401	ADN	C2-N1-C6	2.93	123.54	118.73
3	B	405	THM	O2-C2-N1	-2.82	119.12	122.80
2	B	401	ADN	C5-C4-N3	-2.79	122.87	126.72
3	B	402[A]	THM	C6-N1-C2	-2.77	118.54	121.30
2	B	401	ADN	C2-N3-C4	2.75	118.55	111.83
2	B	401	ADN	C4-N9-C8	2.69	108.56	105.74
2	A	401	ADN	N6-C6-N1	2.69	124.36	118.38
3	B	402[A]	THM	C6-C5-C4	2.58	120.14	118.02
3	A	402[B]	THM	C2'-C1'-N1	-2.55	107.43	113.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402[A]	THM	C5-C4-N3	2.48	117.48	115.32
2	A	401	ADN	C4-N9-C8	2.38	108.24	105.74
3	B	402[A]	THM	C5M-C5-C6	2.23	125.87	122.85
3	A	402[B]	THM	C1'-N1-C2	2.15	121.87	117.66
3	B	405	THM	C5M-C5-C6	-2.06	120.06	122.85
3	B	402[B]	THM	C2'-C1'-N1	-2.03	108.75	113.81

There are no chirality outliers.

All (6) torsion outliers are listed below:

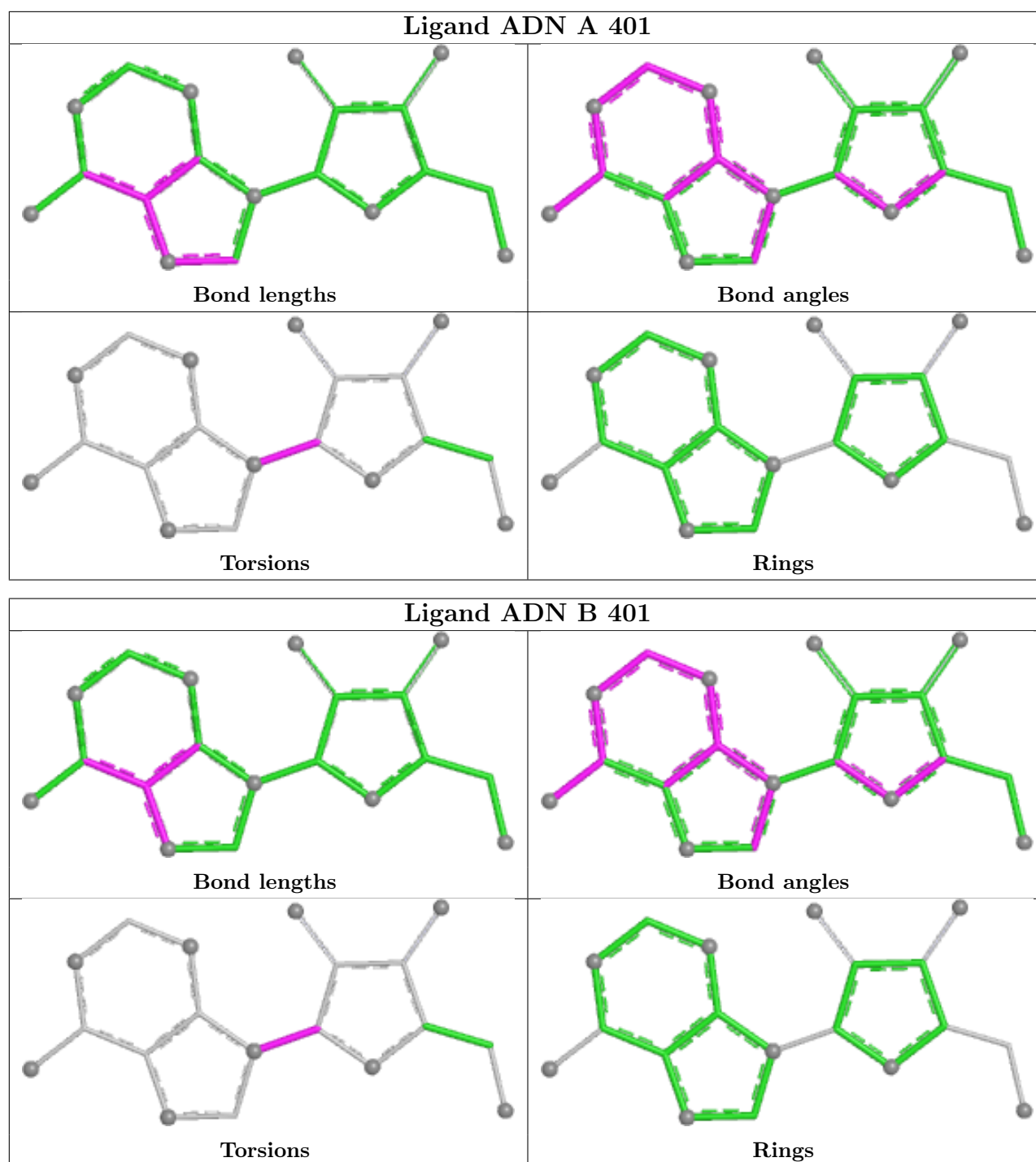
Mol	Chain	Res	Type	Atoms
3	A	402[B]	THM	O4'-C1'-N1-C2
3	A	402[B]	THM	O4'-C1'-N1-C6
3	B	402[A]	THM	O4'-C1'-N1-C2
3	B	402[A]	THM	O4'-C1'-N1-C6
2	B	401	ADN	C2'-C1'-N9-C8
2	A	401	ADN	C2'-C1'-N9-C8

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	404	DMS	3	0
4	B	403	DMS	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 [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	320/352 (90%)	3.31	290 (90%) 0 0	10, 21, 34, 53	11 (3%)
1	B	320/352 (90%)	3.03	265 (82%) 0 0	9, 18, 30, 67	10 (3%)
All	All	640/704 (90%)	3.17	555 (86%) 0 0	9, 20, 33, 67	21 (3%)

All (555) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	263	ILE	10.0
1	A	97	VAL	7.4
1	B	266	ARG	7.2
1	A	264	ARG	6.8
1	A	168	LEU	6.7
1	A	24	ILE	6.4
1	B	24	ILE	6.1
1	A	325	ALA	6.0
1	A	321	ALA	5.8
1	B	265	ILE	5.8
1	B	264	ARG	5.7
1	A	64	ALA	5.6
1	A	210[A]	VAL	5.6
1	B	140	VAL	5.5
1	B	31	ALA	5.5
1	A	2	PHE	5.4
1	B	310	ILE	5.3
1	B	0	THR	5.3
1	A	282	PHE	5.3
1	B	2	PHE	5.3
1	B	28	ILE	5.2
1	A	41	ALA	5.2
1	A	242	VAL	5.2
1	A	135	LEU	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	239	ILE	5.2
1	A	71	GLY	5.1
1	A	191	VAL	5.1
1	B	97	VAL	5.1
1	A	31	ALA	5.1
1	A	158	TRP	5.0
1	A	0	THR	5.0
1	A	241	ALA	5.0
1	A	116	PHE	5.0
1	A	266	ARG	5.0
1	B	116	PHE	4.9
1	B	321	ALA	4.9
1	A	218	LEU	4.8
1	B	252	LEU	4.8
1	A	28	ILE	4.8
1	B	328	ILE	4.8
1	B	51	ALA	4.8
1	A	43	LEU	4.8
1	B	199	LEU	4.8
1	A	143	ASP	4.8
1	A	259	TYR	4.8
1	A	76	PHE	4.8
1	A	79	VAL	4.7
1	A	207[A]	VAL	4.7
1	A	52[A]	LEU	4.7
1	B	44	LEU	4.7
1	B	84	LEU	4.7
1	A	221	TYR	4.7
1	A	211	PHE	4.7
1	B	224	ASP	4.7
1	B	302	ALA	4.7
1	A	15	ILE	4.7
1	A	22	PHE	4.7
1	A	234	ALA	4.7
1	B	191	VAL	4.7
1	A	5	LEU	4.7
1	B	279	ALA	4.7
1	A	49	GLY	4.6
1	B	207[A]	VAL	4.6
1	A	23	LEU	4.6
1	B	43	LEU	4.6
1	A	146	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	41	ALA	4.6
1	A	190	CYS	4.6
1	A	103	PRO	4.6
1	B	283	LEU	4.6
1	A	150	VAL	4.6
1	B	268	VAL	4.6
1	B	189	PHE	4.5
1	A	328	ILE	4.5
1	A	201	LEU	4.5
1	B	74	ALA	4.5
1	A	263	ILE	4.5
1	A	217	ALA	4.5
1	A	220	LEU	4.5
1	B	85	GLY	4.4
1	A	199	LEU	4.4
1	A	140	VAL	4.4
1	B	210[A]	VAL	4.4
1	B	259	TYR	4.4
1	A	265	ILE	4.4
1	A	85	GLY	4.4
1	B	278	PHE	4.4
1	A	44	LEU	4.4
1	A	283	LEU	4.4
1	B	190	CYS	4.4
1	A	194	TYR	4.4
1	A	6	THR	4.4
1	A	302	ALA	4.4
1	A	223	THR	4.3
1	A	279	ALA	4.3
1	B	145	VAL	4.3
1	B	67	ALA	4.3
1	A	18	CYS	4.3
1	B	220	LEU	4.3
1	B	211	PHE	4.3
1	B	239	ILE	4.3
1	A	153	PHE	4.2
1	A	4	VAL	4.2
1	A	226	PHE	4.2
1	B	197	GLU	4.2
1	A	66	VAL	4.2
1	A	67	ALA	4.2
1	A	94	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	212	ALA	4.2
1	B	241	ALA	4.2
1	B	262	ALA	4.2
1	A	11	ILE	4.2
1	A	173	ILE	4.2
1	B	18	CYS	4.2
1	A	252	LEU	4.2
1	B	15	ILE	4.1
1	B	170	CYS	4.1
1	A	171	ALA	4.1
1	B	217	ALA	4.1
1	A	70	GLY	4.1
1	A	301	LEU	4.1
1	B	23	LEU	4.1
1	B	218	LEU	4.1
1	B	229	ALA	4.1
1	B	322	ALA	4.1
1	B	258	TYR	4.1
1	A	189	PHE	4.0
1	A	92	ILE	4.0
1	A	80	ALA	4.0
1	A	258	TYR	4.0
1	A	147	ASP	4.0
1	A	88	PHE	4.0
1	A	278	PHE	4.0
1	A	268	VAL	4.0
1	B	11	ILE	4.0
1	B	36	ILE	4.0
1	A	35	LEU	4.0
1	A	157	LEU	4.0
1	A	272	THR	4.0
1	B	194	TYR	4.0
1	B	226	PHE	4.0
1	B	79	VAL	4.0
1	A	236	ASP	4.0
1	B	49	GLY	3.9
1	B	223	THR	4.0
1	A	317	SER	3.9
1	A	284	TYR	3.9
1	B	261	ASN	3.9
1	A	14	ILE	3.9
1	A	115	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	310	ILE	3.9
1	A	180	GLU	3.9
1	B	22	PHE	3.9
1	A	36	ILE	3.9
1	A	54	ALA	3.9
1	A	84	LEU	3.9
1	B	35	LEU	3.9
1	B	142	ALA	3.9
1	B	107	PHE	3.9
1	B	158	TRP	3.9
1	B	200	ASP	3.9
1	A	303	ALA	3.9
1	A	102	LYS	3.8
1	A	300	CYS	3.8
1	B	284	TYR	3.8
1	B	215	GLN	3.8
1	A	107	PHE	3.8
1	A	131	ALA	3.8
1	A	240	ALA	3.8
1	A	167	ILE	3.8
1	A	292	LEU	3.8
1	A	132	CYS	3.8
1	A	99	TYR	3.8
1	A	184	THR	3.8
1	B	146	ALA	3.8
1	A	209	ILE	3.8
1	B	173	ILE	3.8
1	B	242	VAL	3.8
1	A	289	GLY	3.8
1	B	205	GLY	3.8
1	A	286	TYR	3.8
1	A	215	GLN	3.8
1	A	291	SER	3.8
1	B	317	SER	3.8
1	A	51	ALA	3.8
1	A	63	ALA	3.8
1	A	305	ILE	3.7
1	B	209	ILE	3.7
1	A	161	PRO	3.7
1	B	156	TYR	3.7
1	A	196	GLY	3.7
1	A	281	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	76	PHE	3.7
1	B	92	ILE	3.7
1	B	6	THR	3.7
1	B	42	GLU	3.7
1	B	64	ALA	3.7
1	B	174	ALA	3.7
1	A	230	LEU	3.7
1	B	168	LEU	3.7
1	A	224	ASP	3.7
1	B	287	THR	3.7
1	A	73	ALA	3.7
1	A	142	ALA	3.7
1	B	240	ALA	3.7
1	A	50	PRO	3.6
1	A	200	ASP	3.6
1	A	287	THR	3.6
1	B	69	LEU	3.6
1	B	153	PHE	3.6
1	A	243	THR	3.6
1	B	127	THR	3.6
1	B	14	ILE	3.6
1	A	145	VAL	3.6
1	A	250	VAL	3.6
1	B	250	VAL	3.6
1	A	235	ALA	3.6
1	B	80	ALA	3.6
1	B	303	ALA	3.6
1	B	75	TYR	3.6
1	B	327	LEU	3.6
1	A	198	PHE	3.6
1	B	54	ALA	3.6
1	B	286	TYR	3.5
1	B	219[A]	SER	3.5
1	B	198	PHE	3.5
1	A	322	ALA	3.5
1	A	160	PRO	3.5
1	B	312	PRO	3.5
1	A	75	TYR	3.5
1	A	124	SER	3.5
1	A	121	GLY	3.5
1	A	304	GLY	3.5
1	A	42	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	295	CYS	3.5
1	B	115	ILE	3.5
1	B	66	VAL	3.5
1	A	212	ALA	3.5
1	B	281	GLY	3.5
1	A	152	TYR	3.5
1	A	237[A]	CYS	3.5
1	A	69	LEU	3.5
1	A	27	GLN	3.5
1	A	59	ALA	3.5
1	A	74	ALA	3.5
1	B	32	ALA	3.5
1	A	285	GLY	3.4
1	B	282	PHE	3.4
1	A	156	TYR	3.4
1	A	318	LEU	3.4
1	B	301	LEU	3.4
1	A	251	ILE	3.4
1	A	254	GLY	3.4
1	B	144	VAL	3.4
1	A	195[A]	ARG	3.4
1	B	5	LEU	3.4
1	B	52	LEU	3.4
1	B	318	LEU	3.4
1	A	32	ALA	3.4
1	A	174	ALA	3.4
1	B	81	ALA	3.4
1	B	167	ILE	3.4
1	B	305	ILE	3.4
1	B	124	SER	3.4
1	A	148	ALA	3.4
1	B	163	ALA	3.4
1	A	72	LYS	3.3
1	A	205	GLY	3.3
1	B	60	GLY	3.3
1	A	151	THR	3.3
1	B	172[A]	ARG	3.3
1	A	134	GLU	3.3
1	B	249	ALA	3.3
1	A	294	ASP	3.3
1	B	143[A]	ASP	3.3
1	B	307	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	178	GLY	3.3
1	B	289	GLY	3.3
1	B	319	SER	3.3
1	A	170	CYS	3.3
1	A	128	TYR	3.3
1	B	100[A]	GLN	3.3
1	A	175	HIS	3.2
1	A	219[A]	SER	3.2
1	B	117	VAL	3.2
1	B	221	TYR	3.2
1	B	171	ALA	3.2
1	A	1	ARG	3.2
1	B	232	ARG	3.2
1	A	87	ILE	3.2
1	A	187	ASP	3.2
1	B	147	ASP	3.2
1	A	186	SER	3.2
1	A	62	THR	3.2
1	B	251	ILE	3.2
1	A	12	VAL	3.2
1	B	247	ASN	3.2
1	B	45	TYR	3.2
1	B	63	ALA	3.2
1	B	131	ALA	3.2
1	B	316	THR	3.1
1	A	137	PRO	3.1
1	A	319	SER	3.1
1	B	300	CYS	3.1
1	A	60	GLY	3.1
1	B	267	GLU	3.1
1	A	192	ASP	3.1
1	B	102	LYS	3.1
1	A	127	THR	3.1
1	A	316	THR	3.1
1	B	157	LEU	3.1
1	A	299	GLY	3.1
1	A	3	ASP	3.1
1	A	229	ALA	3.1
1	B	59	ALA	3.1
1	B	73	ALA	3.1
1	A	306	VAL	3.1
1	B	133	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	98	HIS	3.1
1	B	71	GLY	3.1
1	B	25	ASP	3.1
1	A	106	ALA	3.1
1	A	19	ASN	3.0
1	A	133	VAL	3.0
1	B	128	TYR	3.0
1	A	312	PRO	3.0
1	B	292	LEU	3.0
1	B	180	GLU	3.0
1	A	7	VAL	3.0
1	B	150	VAL	3.0
1	A	162[A]	ARG	3.0
1	A	188	SER	3.0
1	B	237[A]	CYS	3.0
1	A	271	THR	3.0
1	B	325	ALA	3.0
1	A	139	ASP	3.0
1	A	225	ASP	3.0
1	B	236	ASP	3.0
1	B	1	ARG	3.0
1	B	269	VAL	3.0
1	B	185	LEU	3.0
1	B	201	LEU	3.0
1	A	58[A]	SER	3.0
1	B	118	THR	3.0
1	A	197	GLU	2.9
1	A	108	PRO	2.9
1	A	95	GLN	2.9
1	B	7	VAL	2.9
1	B	195[A]	ARG	2.9
1	A	130	GLY	2.9
1	A	233	ILE	2.9
1	A	270	ASP	2.9
1	A	117	VAL	2.9
1	B	272	THR	2.9
1	A	213	ASN	2.9
1	B	234	ALA	2.9
1	A	119	GLU	2.9
1	B	99	TYR	2.9
1	A	298	LEU	2.9
1	A	56	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	105	GLY	2.9
1	B	70	GLY	2.9
1	B	248	GLY	2.9
1	B	46	SER	2.9
1	B	82	ASP	2.8
1	B	235	ALA	2.8
1	A	307	ILE	2.8
1	A	267	GLU	2.8
1	A	101	THR	2.8
1	B	121	GLY	2.8
1	B	135	LEU	2.8
1	B	260	VAL	2.8
1	A	109	PRO	2.8
1	B	50	PRO	2.8
1	B	27	GLN	2.8
1	B	231	ASN	2.8
1	A	172	ARG	2.8
1	A	118	THR	2.8
1	A	77	GLY	2.8
1	A	129	LEU	2.8
1	B	298	LEU	2.8
1	B	306	VAL	2.8
1	B	26	ASN	2.8
1	A	232	ARG	2.8
1	B	169	ASP	2.8
1	B	182	SER	2.8
1	A	29	THR	2.8
1	A	89	THR	2.8
1	B	271	THR	2.8
1	B	299	GLY	2.8
1	B	176	GLN	2.8
1	A	111	ALA	2.7
1	A	177	HIS	2.8
1	A	269	VAL	2.7
1	B	270	ASP	2.7
1	A	110	THR	2.7
1	A	45	TYR	2.7
1	B	314	PRO	2.7
1	A	81	ALA	2.7
1	A	96	GLY	2.7
1	A	136	GLY	2.7
1	A	123[A]	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	313	ARG	2.7
1	B	255	ARG	2.7
1	B	192	ASP	2.7
1	A	293	GLU	2.7
1	B	62	THR	2.7
1	B	204	SER	2.7
1	B	160	PRO	2.7
1	A	255	ARG	2.7
1	B	123	ARG	2.7
1	A	166	ALA	2.6
1	A	262	ALA	2.6
1	B	148	ALA	2.6
1	B	178	GLY	2.6
1	B	326	GLY	2.6
1	B	243	THR	2.6
1	B	161	PRO	2.6
1	A	57	GLY	2.6
1	B	132	CYS	2.6
1	A	163	ALA	2.6
1	A	122	GLU	2.6
1	B	254	GLY	2.6
1	B	98	HIS	2.6
1	B	175	HIS	2.6
1	B	20	ASP	2.6
1	A	204	SER	2.6
1	B	88	PHE	2.6
1	B	277	LEU	2.6
1	B	12	VAL	2.6
1	B	311	GLY	2.6
1	A	179	ARG	2.6
1	B	58[A]	SER	2.6
1	B	291	SER	2.6
1	B	21	GLN	2.5
1	A	86	ASP	2.5
1	B	313	ARG	2.5
1	B	57	GLY	2.5
1	A	144	VAL	2.5
1	A	164	LYS	2.5
1	A	10	ALA	2.5
1	B	95	GLN	2.5
1	A	277	LEU	2.5
1	B	152	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	55	SER	2.5
1	A	260[A]	VAL	2.5
1	B	30	LYS	2.5
1	A	38	ALA	2.5
1	A	159	ASP	2.5
1	B	233	ILE	2.5
1	A	326	GLY	2.5
1	B	230	LEU	2.5
1	A	68	ASN	2.5
1	B	47	ARG	2.5
1	B	184	THR	2.5
1	B	86	ASP	2.5
1	B	225	ASP	2.5
1	A	248	GLY	2.4
1	B	179	ARG	2.4
1	B	103	PRO	2.4
1	A	26	ASN	2.4
1	B	3	ASP	2.4
1	B	120	ASP	2.4
1	B	139	ASP	2.4
1	A	46	SER	2.4
1	B	10	ALA	2.4
1	A	222	GLN	2.4
1	B	65	GLY	2.4
1	B	285	GLY	2.4
1	A	185	LEU	2.4
1	B	165	GLU	2.4
1	B	17	ARG	2.4
1	A	65	GLY	2.4
1	A	138	GLU	2.4
1	A	256	GLU	2.4
1	A	37	ASP	2.4
1	A	324	GLN	2.4
1	B	77	GLY	2.4
1	B	94	ALA	2.3
1	A	25	ASP	2.3
1	A	288	GLN	2.3
1	A	309	GLN	2.3
1	B	151	THR	2.3
1	A	90	HIS	2.3
1	B	38	ALA	2.3
1	B	288	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	308	GLN	2.3
1	A	214	ARG	2.3
1	B	113	SER	2.3
1	B	39	GLU	2.3
1	B	101	THR	2.3
1	A	34	ASN	2.3
1	B	61	ASN	2.3
1	A	8	GLY	2.3
1	A	176	GLN	2.3
1	A	149	LYS	2.3
1	A	280	SER	2.3
1	B	293	GLU	2.3
1	B	29	THR	2.3
1	B	93	ARG	2.3
1	A	39	GLU	2.3
1	B	87	ILE	2.3
1	B	119	GLU	2.3
1	B	111	ALA	2.2
1	B	126	ASN	2.2
1	A	20	ASP	2.2
1	B	187	ASP	2.2
1	B	110	THR	2.2
1	B	273	GLY	2.2
1	B	4	VAL	2.2
1	B	138	GLU	2.2
1	A	78	ASN	2.2
1	B	68	ASN	2.2
1	A	21	GLN	2.2
1	A	320	GLU	2.2
1	B	72	LYS	2.2
1	B	19	ASN	2.2
1	A	82	ASP	2.2
1	B	276	ASP	2.2
1	A	141	GLU	2.2
1	A	314	PRO	2.2
1	A	155	GLY	2.2
1	B	96	GLY	2.2
1	A	126	ASN	2.2
1	B	213	ASN	2.2
1	A	206	LYS	2.2
1	A	327	LEU	2.1
1	B	137	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	93	ARG	2.1
1	B	295	CYS	2.1
1	A	231	ASN	2.1
1	A	227	GLU	2.1
1	A	253	LYS	2.1
1	A	290	ARG	2.1
1	A	249	ALA	2.1
1	A	308	GLN	2.1
1	A	275	GLY	2.1
1	B	155	GLY	2.1
1	B	304	GLY	2.1
1	A	61	ASN	2.1
1	B	164	LYS	2.1
1	B	177	HIS	2.1
1	B	309	GLN	2.1
1	B	159	ASP	2.1
1	B	294	ASP	2.1
1	B	108	PRO	2.1
1	A	17	ARG	2.0
1	B	40	ARG	2.0
1	A	261	ASN	2.0
1	A	193	ARG	2.0
1	A	257[A]	ARG	2.0
1	A	228	GLU	2.0
1	B	83	GLN	2.0
1	A	9	ASN	2.0
1	A	91	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.

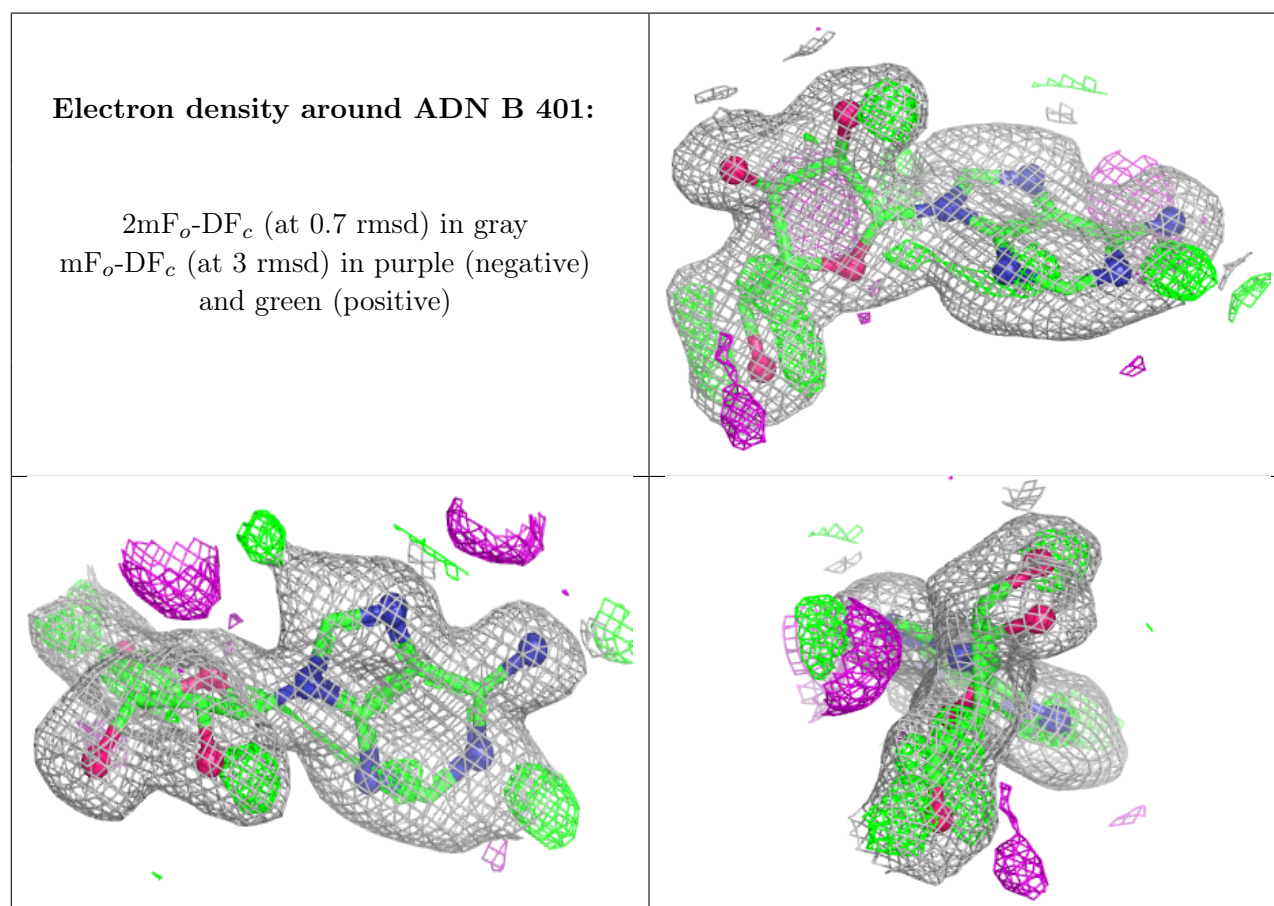
6.4 Ligands [i](#)

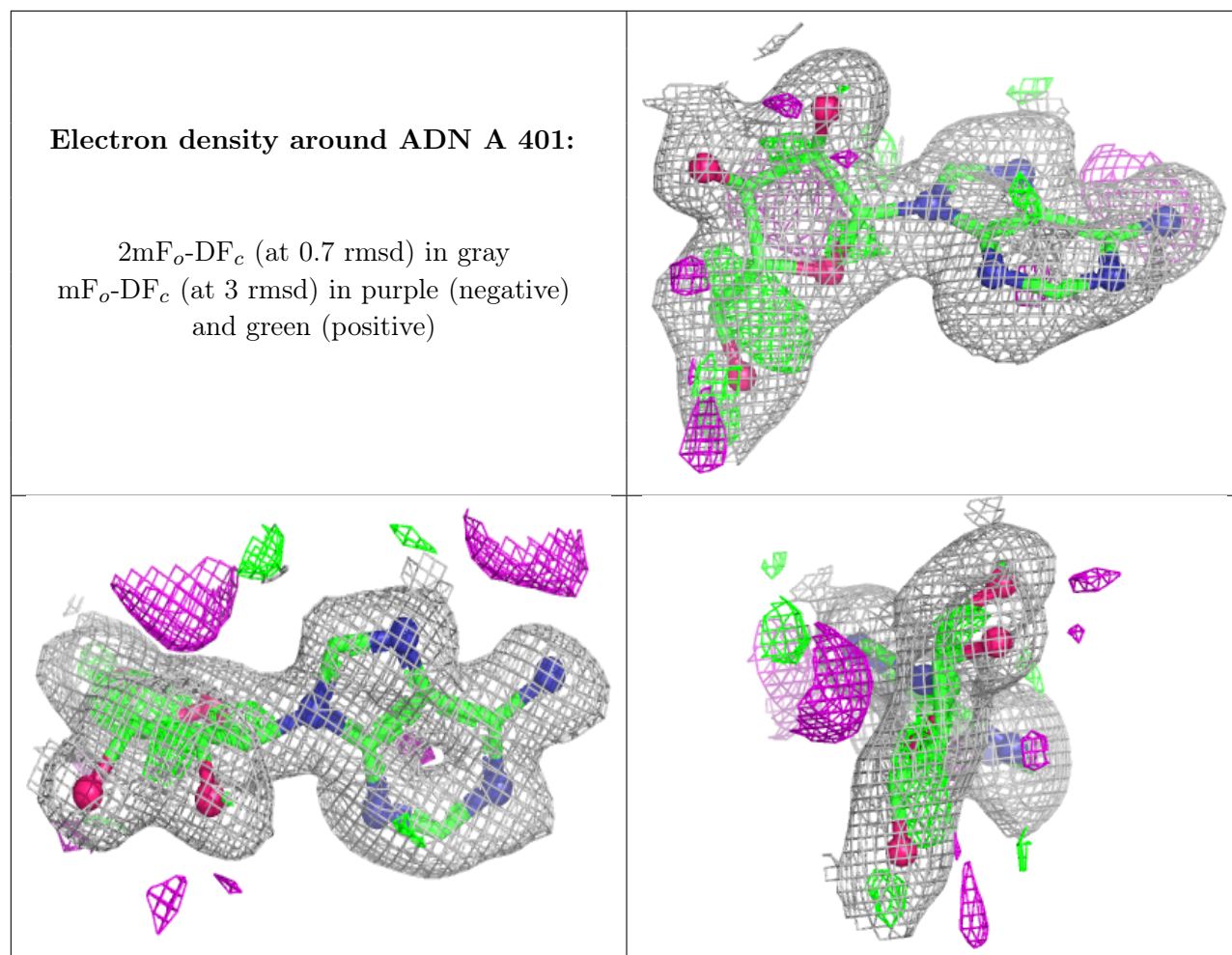
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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(Å ²)	Q<0.9
5	K	B	406	1/1	0.53	0.47	44,44,44,44	0
4	DMS	B	404	4/4	0.70	0.25	31,43,43,44	0
3	THM	A	402[A]	17/17	-	-	25,33,36,36	17
3	THM	A	402[B]	17/17	-	-	25,34,38,39	17
3	THM	B	405	17/17	0.71	0.18	24,29,35,40	17
3	THM	B	402[A]	17/17	0.71	0.34	27,38,45,46	17
3	THM	B	402[B]	17/17	0.71	0.34	27,39,47,47	17
2	ADN	B	401	19/19	0.74	0.14	11,14,15,16	0
4	DMS	A	404	4/4	0.74	0.21	37,39,42,45	0
2	ADN	A	401	19/19	0.75	0.14	13,15,17,18	0
4	DMS	B	403	4/4	0.82	0.19	24,24,28,29	0
5	K	A	405	1/1	0.83	0.29	45,45,45,45	0
4	DMS	A	403	4/4	0.84	0.18	23,24,26,28	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 ⓘ

There are no such residues in this entry.