



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 11:40 AM BST

PDB ID : 2A3Z
Title : Ternary complex of the WH2 domain of WASP with Actin-DNAse I
Authors : Chereau, D.; Kerff, F.; Dominguez, R.
Deposited on : 2005-06-27
Resolution : 2.08 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 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 : 2.13.1
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) : 2.13.1

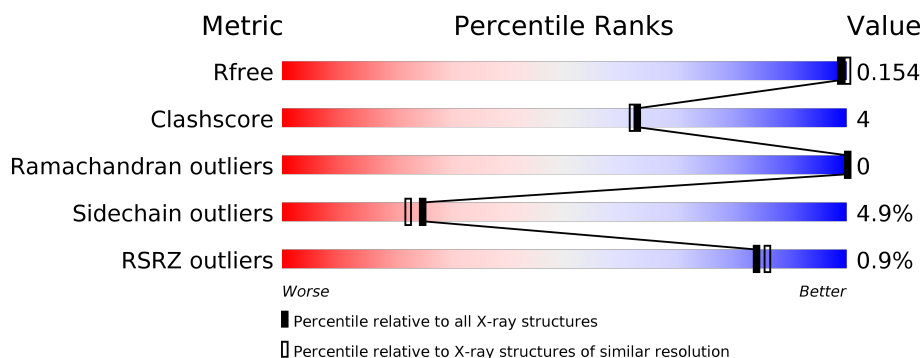
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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 on 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	375	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 13%, green 82%, grey 4%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 82% 13% • • </div> </div>
2	B	260	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 90%, yellow 9%, orange 1%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 90% 9% • </div> </div>
3	C	29	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 45%, yellow 7%, orange 7%, grey 41%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 45% 7% 7% 41% </div> </div>
4	D	2	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 100% </div> </div>

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 5584 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 Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	17	0
			2903	1844	481	557	21			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	HIC	HIS	modified residue	UNP P68135

- Molecule 2 is a protein called Deoxyribonuclease-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	260	Total	C	N	O	S	0	4	0
			2069	1311	345	405	8			

- Molecule 3 is a protein called Wiskott-Aldrich syndrome protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	17	Total	C	N	O	0	0	0
			134	82	28	24			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

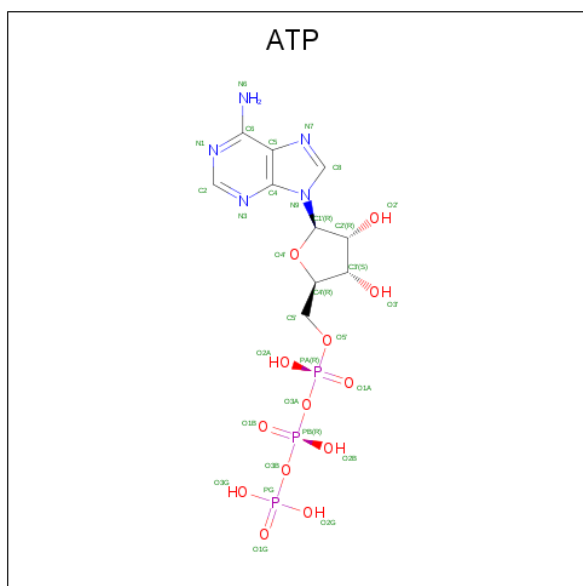


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).

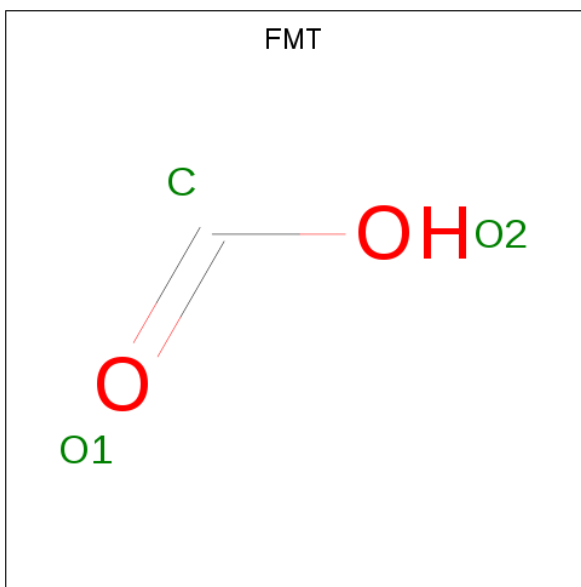


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 9 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			3	1	2		

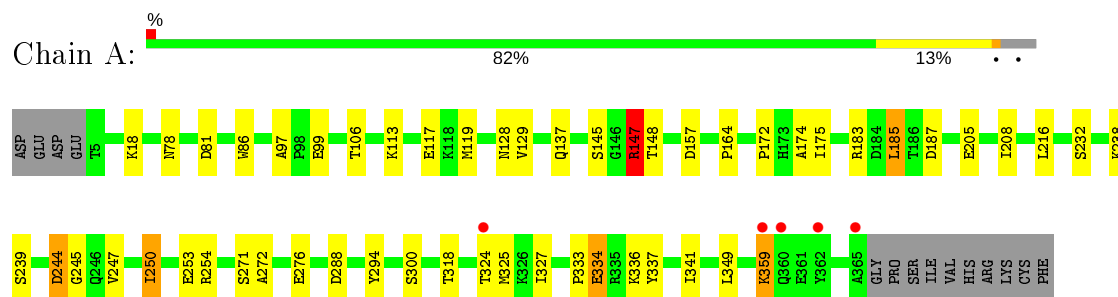
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	235	Total	O	0	0
			235	235		
10	B	156	Total	O	0	0
			156	156		
10	C	4	Total	O	0	0
			4	4		

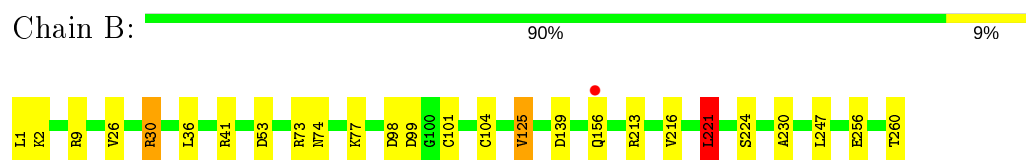
3 Residue-property plots [i](#)

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.

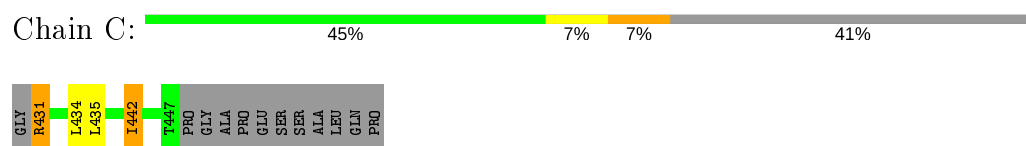
- Molecule 1: Actin, alpha skeletal muscle



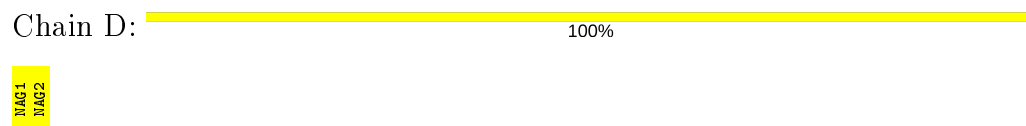
- Molecule 2: Deoxyribonuclease-1



- Molecule 3: Wiskott-Aldrich syndrome protein



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	153.27Å 41.80Å 119.42Å 90.00° 108.68° 90.00°	Depositor
Resolution (Å)	40.10 – 2.08 40.17 – 2.08	Depositor EDS
% Data completeness (in resolution range)	95.8 (40.10-2.08) 95.8 (40.17-2.08)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.55 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.153 , 0.210 0.161 , 0.154	Depositor DCC
R_{free} test set	4135 reflections (9.84%)	wwPDB-VP
Wilson B-factor (Å ²)	29.4	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5584	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% 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: GOL, MG, NAG, FMT, HIC, ATP, CA

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	0.71	0/3001	0.86	3/4061 (0.1%)
2	B	0.71	0/2127	0.95	5/2895 (0.2%)
3	C	0.47	0/133	0.80	0/176
All	All	0.71	0/5261	0.89	8/7132 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	30[A]	ARG	NE-CZ-NH1	7.14	123.87	120.30
2	B	30[B]	ARG	NE-CZ-NH1	7.14	123.87	120.30
2	B	53	ASP	CB-CG-OD1	6.12	123.81	118.30
1	A	147	ARG	NE-CZ-NH2	5.87	123.23	120.30
2	B	213	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	A	185	LEU	CB-CG-CD1	5.22	119.87	111.00
1	A	187	ASP	CB-CG-OD1	5.18	122.96	118.30
2	B	221	LEU	CB-CG-CD2	5.14	119.75	111.00

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	2903	0	2914	34	0
2	B	2069	0	2011	8	0
3	C	134	0	145	3	0
4	D	28	0	25	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	31	0	12	0	0
7	A	12	0	16	3	0
7	B	6	0	8	0	0
8	B	1	0	0	0	0
9	B	3	0	1	0	0
10	A	235	0	0	4	0
10	B	156	0	0	1	0
10	C	4	0	0	2	0
All	All	5584	0	5132	44	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 (44) 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:216:LEU:HD22	1:A:238[A]:LYS:HG2	1.60	0.83
3:C:431:ARG:NH2	10:C:381:HOH:O	2.19	0.70
1:A:238[A]:LYS:HE2	10:A:1618:HOH:O	1.93	0.69
2:B:125:VAL:HG22	2:B:224:SER:OG	1.92	0.69
1:A:172:PRO:HA	1:A:175:ILE:HD12	1.77	0.66
1:A:324:THR:O	1:A:324:THR:HG22	1.94	0.66
1:A:205:GLU:HA	1:A:208:ILE:HD12	1.83	0.60
1:A:254:ARG:HH22	7:A:1383:GOL:H31	1.70	0.56
1:A:86:TRP:CH2	1:A:119[B]:MET:HG3	2.40	0.56
1:A:97:ALA:HB1	1:A:99:GLU:OE2	2.06	0.55
1:A:333:PRO:HD2	1:A:334:GLU:OE2	2.07	0.55
2:B:73:ARG:HH11	2:B:73:ARG:HG3	1.73	0.52
1:A:238[A]:LYS:CE	10:A:1618:HOH:O	2.53	0.52
2:B:74:ASN:ND2	10:B:1509:HOH:O	2.43	0.51
1:A:336:LYS:HE2	10:A:1601:HOH:O	2.10	0.50
1:A:18:LYS:HD3	1:A:18:LYS:N	2.27	0.50
1:A:324:THR:O	1:A:324:THR:CG2	2.61	0.49
1:A:244[B]:ASP:CG	1:A:245:GLY:N	2.65	0.48
2:B:230:ALA:HA	2:B:256:GLU:O	2.12	0.48
1:A:86:TRP:HH2	1:A:119[B]:MET:HG3	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ARG:HH12	7:A:1383:GOL:H31	1.78	0.47
1:A:129:VAL:O	1:A:359:LYS:HG3	2.15	0.47
2:B:26:VAL:O	2:B:30[B]:ARG:HG3	2.15	0.46
1:A:349:LEU:HD23	3:C:442:ILE:HG13	1.98	0.46
1:A:318:THR:HA	1:A:327:ILE:HD13	1.98	0.46
2:B:216:VAL:HB	2:B:221:LEU:HD13	1.99	0.44
1:A:250:ILE:HD12	1:A:253:GLU:HB2	1.99	0.44
1:A:294:TYR:CD2	1:A:325:MET:HG2	2.53	0.44
1:A:164:PRO:HG2	1:A:174:ALA:HB3	2.00	0.43
2:B:99:ASP:HB3	2:B:104:CYS:HB3	2.00	0.43
1:A:157:ASP:O	1:A:183:ARG:HB2	2.19	0.43
2:B:41:ARG:HD2	2:B:77:LYS:O	2.19	0.42
1:A:272:ALA:HB1	1:A:276[A]:GLU:HB2	2.01	0.42
1:A:337:TYR:O	1:A:341:ILE:HG13	2.19	0.42
1:A:359:LYS:HB2	1:A:359:LYS:HE2	1.75	0.42
1:A:239:SER:HB3	1:A:247:VAL:CG1	2.49	0.42
1:A:254:ARG:HH12	7:A:1383:GOL:C3	2.33	0.42
1:A:145:SER:OG	1:A:147:ARG:HD2	2.20	0.42
1:A:148:THR:OG1	10:A:1471:HOH:O	2.21	0.41
1:A:106:THR:HB	1:A:137:GLN:HG3	2.03	0.41
3:C:431:ARG:NH1	10:C:381:HOH:O	2.53	0.41
1:A:78:ASN:ND2	1:A:81:ASP:OD2	2.54	0.41
1:A:113[A]:LYS:NZ	1:A:117:GLU:OE2	2.43	0.41
1:A:318:THR:HA	1:A:327:ILE:CD1	2.50	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	375/375 (100%)	369 (98%)	6 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	262/260 (101%)	256 (98%)	6 (2%)	0	100	100
3	C	15/29 (52%)	15 (100%)	0	0	100	100
All	All	652/664 (98%)	640 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	321/317 (101%)	306 (95%)	15 (5%)	26	24
2	B	233/229 (102%)	221 (95%)	12 (5%)	23	20
3	C	14/22 (64%)	10 (71%)	4 (29%)	0	0
All	All	568/568 (100%)	537 (94%)	31 (6%)	25	18

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128[A]	ASN
1	A	128[B]	ASN
1	A	147	ARG
1	A	185	LEU
1	A	232	SER
1	A	244[A]	ASP
1	A	244[B]	ASP
1	A	250	ILE
1	A	271	SER
1	A	288[A]	ASP
1	A	288[B]	ASP
1	A	300[A]	SER
1	A	300[B]	SER
1	A	334	GLU
1	A	359	LYS
2	B	1	LEU

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Mol	Chain	Res	Type
2	B	2	LYS
2	B	9	ARG
2	B	36	LEU
2	B	98	ASP
2	B	101	CYS
2	B	125	VAL
2	B	139	ASP
2	B	156	GLN
2	B	221	LEU
2	B	247	LEU
2	B	260	THR
3	C	431	ARG
3	C	434	LEU
3	C	435	LEU
3	C	442	ILE

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

Mol	Chain	Res	Type
1	A	92	ASN
1	A	137	GLN
2	B	155	GLN
2	B	161	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue 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	$\# Z > 2$
1	HIC	A	73	1	8,11,12	1.01	0	6,14,16	0.51	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
1	HIC	A	73	1	-	0/5/6/8	0/1/1/1

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.

5.5 Carbohydrates ⓘ

2 monosaccharides 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	$\# Z > 2$
4	NAG	D	1	2,4	14,14,15	0.67	0	17,19,21	1.47	4 (23%)
4	NAG	D	2	4	14,14,15	0.50	0	17,19,21	2.68	4 (23%)

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	NAG	D	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2	NAG	C1-O5-C5	7.32	122.11	112.19
4	D	2	NAG	O5-C1-C2	5.68	120.26	111.29
4	D	2	NAG	C4-C3-C2	3.22	115.73	111.02
4	D	1	NAG	C1-O5-C5	3.12	116.42	112.19
4	D	2	NAG	C3-C4-C5	2.93	115.46	110.24
4	D	1	NAG	O4-C4-C3	-2.63	104.28	110.35
4	D	1	NAG	O5-C1-C2	-2.16	107.89	111.29
4	D	1	NAG	C2-N2-C7	-2.01	120.05	122.90

There are no chirality outliers.

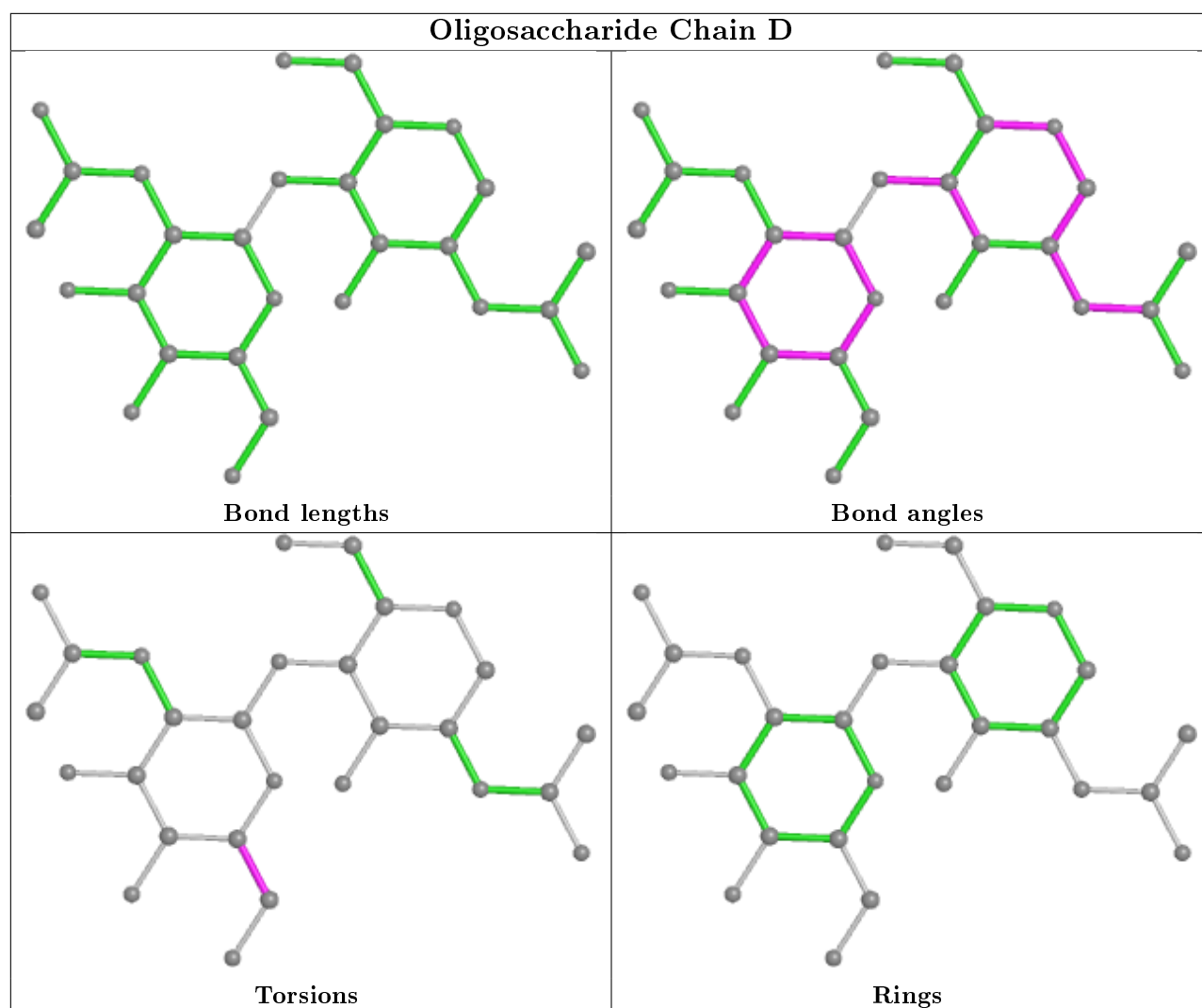
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	2	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6

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 oligosaccharide.



5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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	$\# Z > 2$
7	GOL	A	1383	-	5,5,5	0.42	0	5,5,5	0.88	0
7	GOL	B	1384	-	5,5,5	0.37	0	5,5,5	1.20	0
6	ATP	A	1380	5	26,33,33	0.95	1 (3%)	31,52,52	1.36	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	A	1382	-	5,5,5	0.36	0	5,5,5	0.98	0
9	FMT	B	1275	-	0,2,2	0.00	-	0,1,1	0.00	-

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
7	GOL	A	1383	-	-	3/4/4/4	-
6	ATP	A	1380	5	-	0/18/38/38	0/3/3/3
7	GOL	A	1382	-	-	3/4/4/4	-
7	GOL	B	1384	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1380	ATP	C5-C4	2.48	1.47	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1380	ATP	O4'-C1'-C2'	-3.36	102.02	106.93
6	A	1380	ATP	N3-C2-N1	-3.06	123.89	128.68
6	A	1380	ATP	O2B-PB-O1B	2.55	124.85	112.24
6	A	1380	ATP	C2-N1-C6	2.54	123.09	118.75
6	A	1380	ATP	O3G-PG-O2G	2.20	116.04	107.64

There are no chirality outliers.

All (6) torsion outliers are listed below:

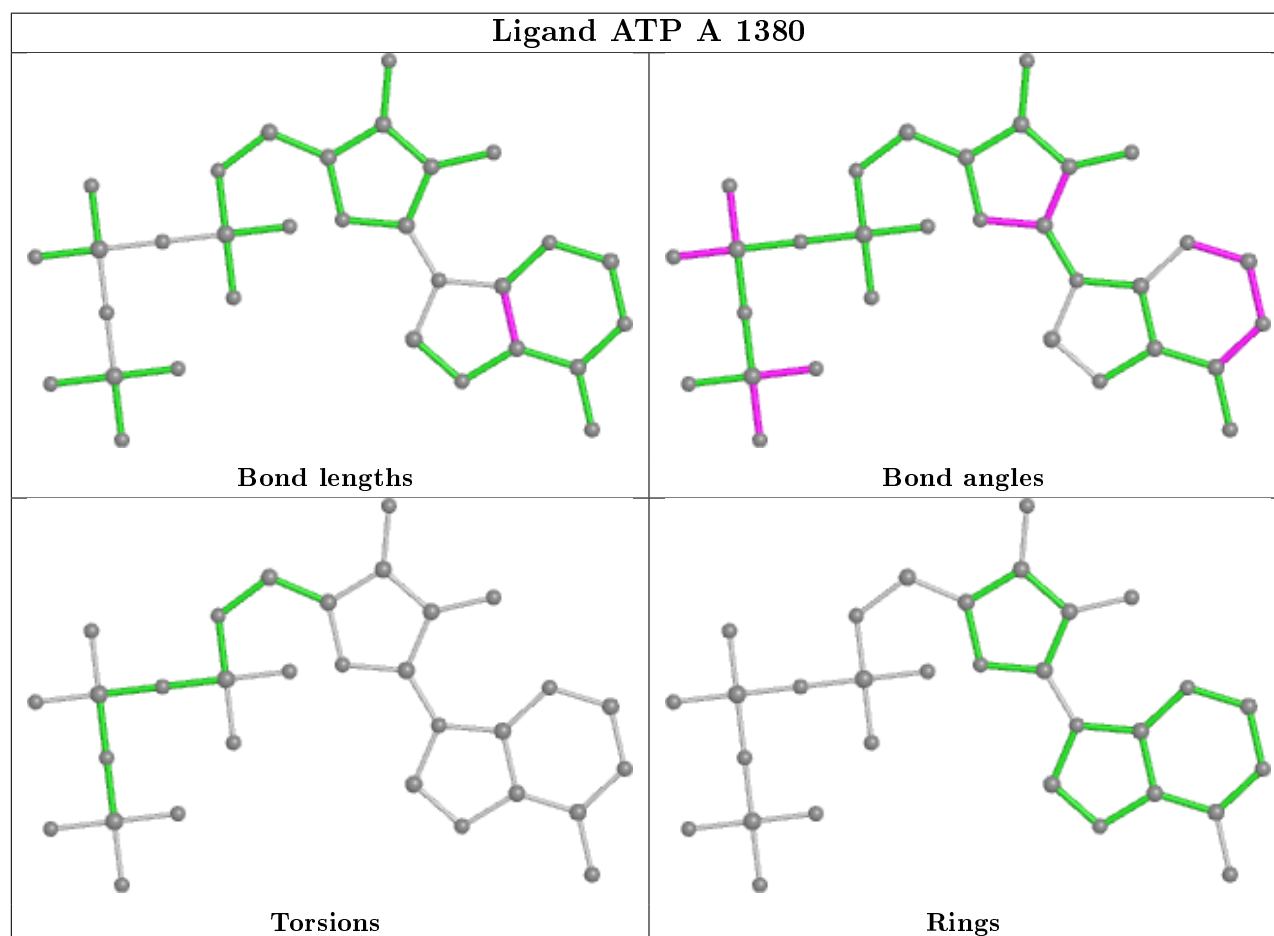
Mol	Chain	Res	Type	Atoms
7	A	1382	GOL	C1-C2-C3-O3
7	A	1383	GOL	C1-C2-C3-O3
7	A	1382	GOL	O2-C2-C3-O3
7	A	1383	GOL	O1-C1-C2-O2
7	A	1383	GOL	O2-C2-C3-O3
7	A	1382	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1383	GOL	3	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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	360/375 (96%)	-0.29	5 (1%) 75 78	20, 30, 45, 61	0
2	B	260/260 (100%)	-0.47	1 (0%) 92 93	25, 31, 43, 50	0
3	C	17/29 (58%)	0.35	0 100 100	44, 47, 55, 55	0
All	All	637/664 (95%)	-0.34	6 (0%) 84 86	20, 31, 46, 61	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	365	ALA	5.3
1	A	360	GLN	2.6
1	A	359	LYS	2.6
1	A	324	THR	2.5
2	B	156	GLN	2.1
1	A	362	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	HIC	A	73	11/12	0.97	0.09	28,30,40,41	0

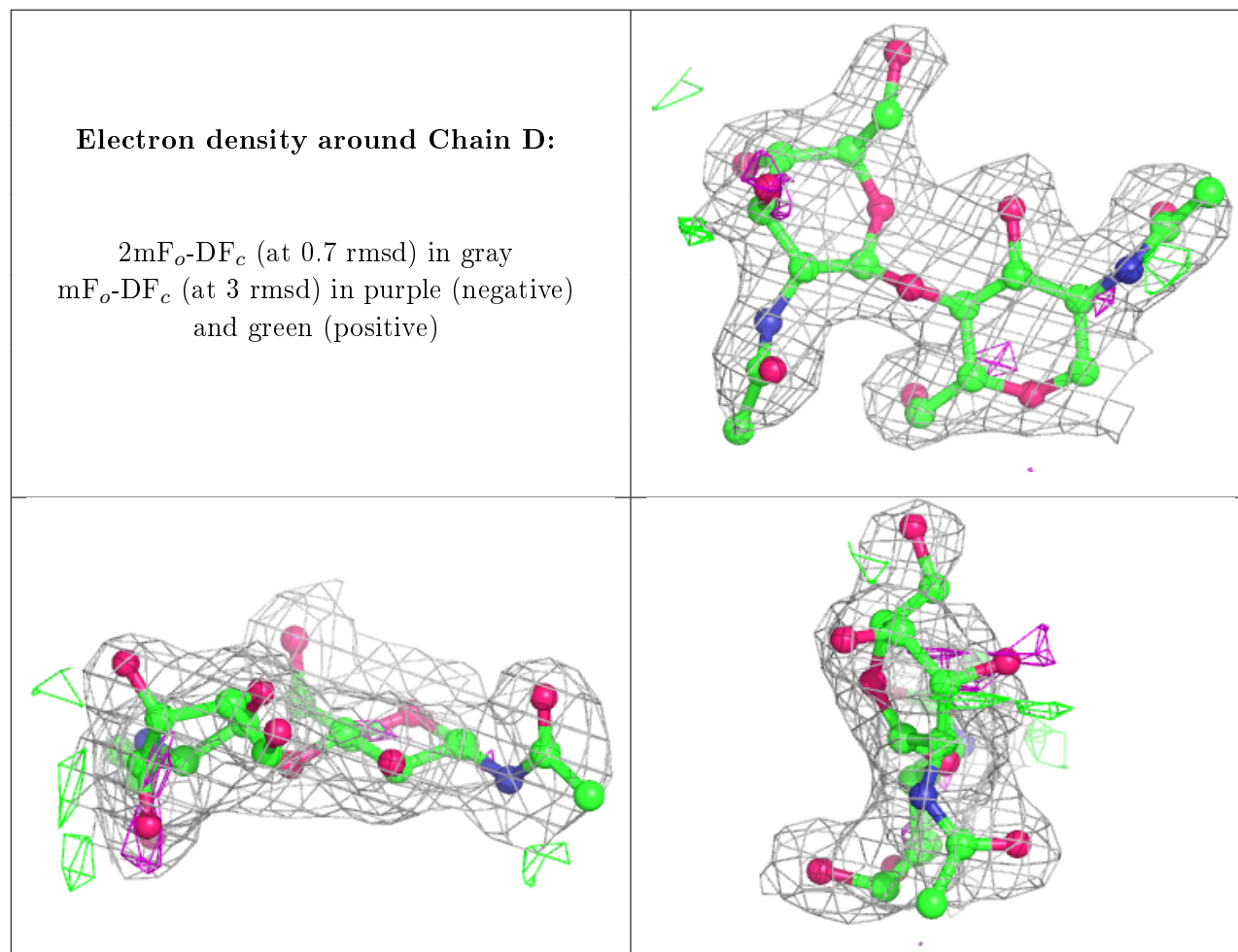
6.3 Carbohydrates [i](#)

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
4	NAG	D	2	14/15	0.91	0.28	54,59,64,64	0
4	NAG	D	1	14/15	0.94	0.20	37,43,50,53	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



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.

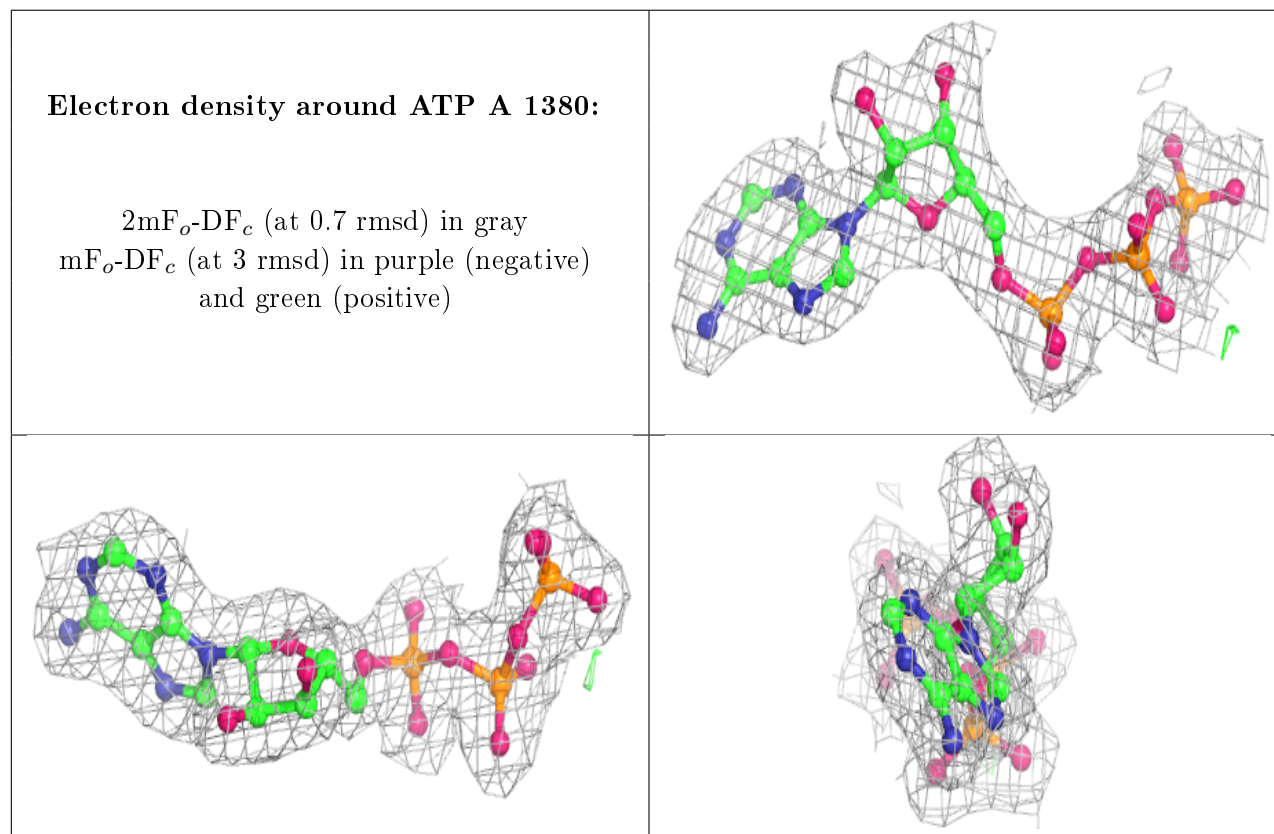
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	GOL	A	1383	6/6	0.79	0.18	58,60,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	GOL	B	1384	6/6	0.90	0.27	34,39,41,43	0
9	FMT	B	1275	3/3	0.90	0.17	44,44,47,48	0
7	GOL	A	1382	6/6	0.90	0.18	57,62,64,68	0
8	MG	B	1274	1/1	0.96	0.05	28,28,28,28	0
6	ATP	A	1380	31/31	0.99	0.10	22,25,27,28	0
5	CA	A	1381	1/1	0.99	0.10	24,24,24,24	0
5	CA	B	1273	1/1	1.00	0.02	26,26,26,26	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.