



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:03 PM UTC

PDB ID : 2A42 / pdb_00002a42
Title : Actin-DNAse I Complex
Authors : Chereau, D.; Kerff, F.; Dominguez, R.
Deposited on : 2005-06-27
Resolution : 1.85 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

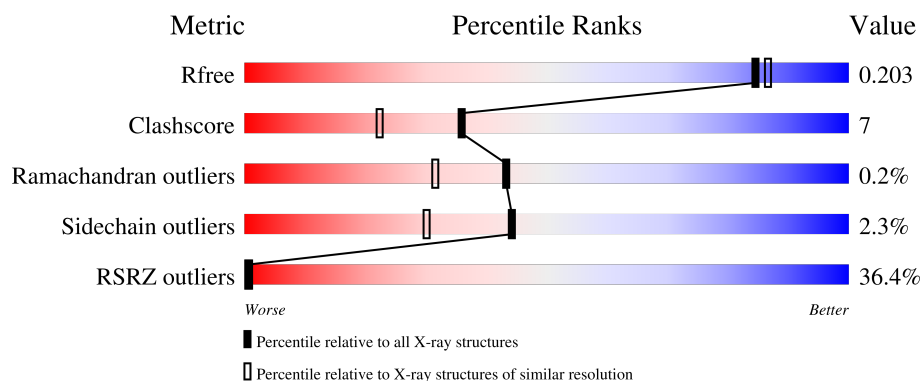
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	375	20% 78% 18% .
2	B	260	58% 90% 7% ..
3	C	2	100%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5546 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	22	0
			2939	1872	482	559	26			

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	255	Total	C	N	O	S	0	6	0
			2042	1299	338	399	6			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

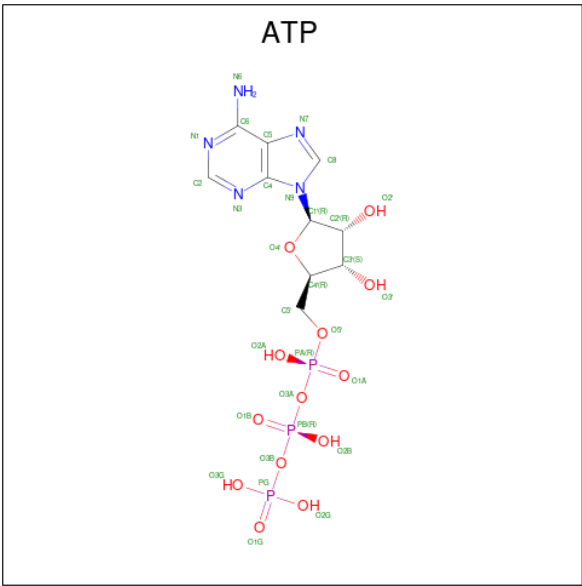


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

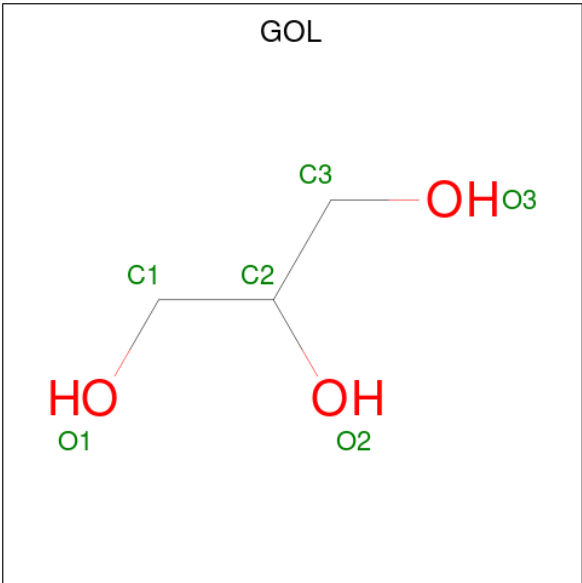
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

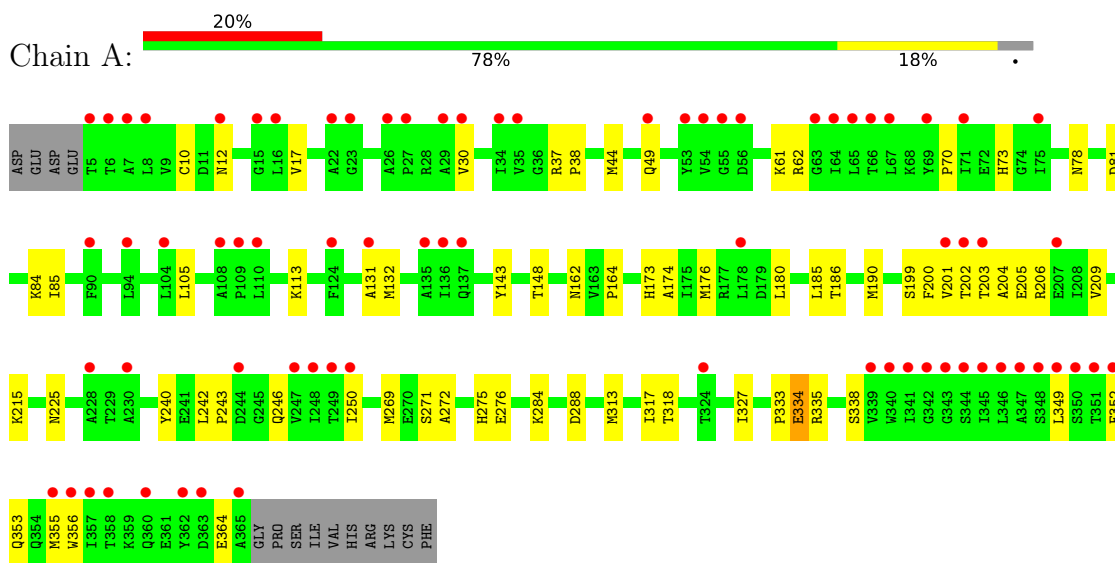
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	331	Total	O	0	1
			331	331		
8	B	154	Total	O	0	0
			154	154		

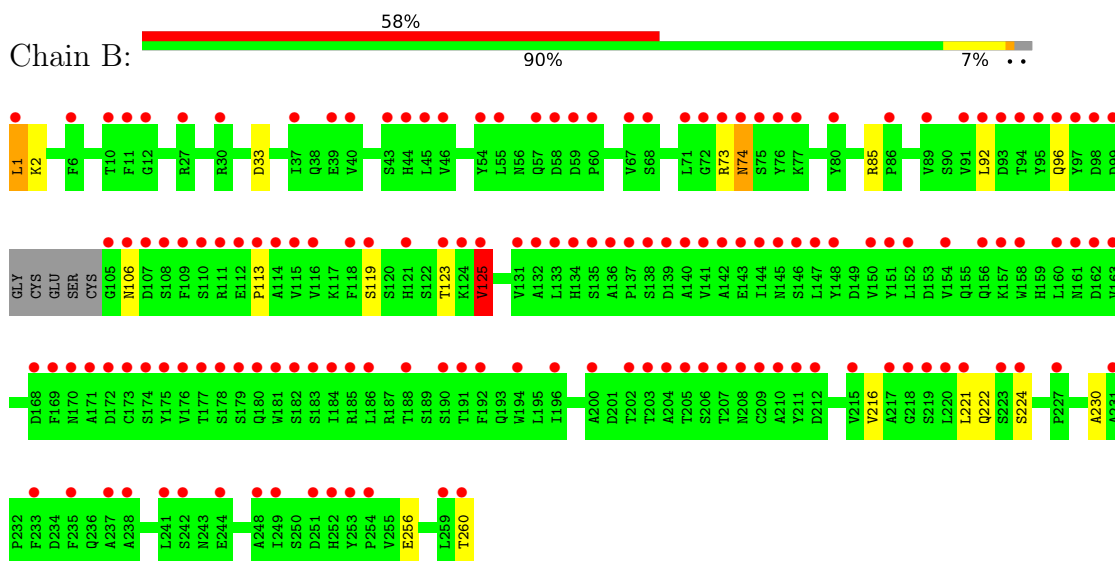
3 Residue-property plots [i](#)

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

Chain C:

100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	152.73Å 41.48Å 117.91Å 90.00° 109.28° 90.00°	Depositor
Resolution (Å)	38.70 – 1.85 38.70 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.4 (38.70-1.85) 97.5 (38.70-1.85)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.161 , 0.199 0.165 , 0.203	Depositor DCC
R_{free} test set	2973 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.6	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	0.92	EDS
Total number of atoms	5546	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MG, NAG, HIC, ATP, GOL

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	0.66	0/3035	0.93	0/4109
2	B	0.73	3/2105 (0.1%)	0.98	1/2864 (0.0%)
All	All	0.69	3/5140 (0.1%)	0.95	1/6973 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	123	THR	C-O	8.35	1.34	1.23
2	B	125	VAL	C-O	6.27	1.31	1.24
2	B	125	VAL	C-N	5.87	1.41	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	125	VAL	CB-CA-C	-7.16	100.38	111.26

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	2939	0	2954	57	0
2	B	2042	0	1999	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	28	0	25	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	31	0	12	0	0
6	A	18	0	24	5	0
7	B	1	0	0	0	0
8	A	331	0	0	10	0
8	B	154	0	0	1	0
All	All	5546	0	5014	74	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 7.

All (74) 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)
6:A:1384:GOL:H32	8:A:1702:HOH:O	1.58	1.03
1:A:173:HIS:ND1	8:A:1603:HOH:O	2.07	0.88
1:A:352:PHE:CD1	1:A:355:MET:HE3	2.10	0.87
1:A:12[B]:ASN:ND2	8:A:1556:HOH:O	2.12	0.82
1:A:162[B]:ASN:HD22	1:A:176:MET:HB2	1.49	0.77
1:A:352:PHE:HD1	1:A:355:MET:HE3	1.48	0.76
1:A:275:HIS:HA	1:A:313[B]:MET:HE1	1.71	0.71
1:A:148:THR:OG1	8:A:1659:HOH:O	2.10	0.69
1:A:276[B]:GLU:OE1	8:A:1672:HOH:O	2.11	0.67
1:A:313[B]:MET:HA	1:A:313[B]:MET:HE3	1.77	0.67
2:B:74:ASN:H	2:B:74:ASN:HD22	1.43	0.65
1:A:37:ARG:NH2	1:A:81:ASP:OD1	2.23	0.65
3:C:1:NAG:O3	3:C:2:NAG:H61	1.99	0.63
2:B:125:VAL:HG22	2:B:224:SER:OG	1.99	0.62
1:A:199:SER:OG	1:A:201[B]:VAL:HG23	2.01	0.61
1:A:333:PRO:HD2	1:A:334:GLU:OE2	2.02	0.60
1:A:190[B]:MET:SD	1:A:206:ARG:HG3	2.41	0.59
1:A:176:MET:HE1	1:A:284:LYS:NZ	2.17	0.59
1:A:180[A]:LEU:HD12	1:A:269[A]:MET:SD	2.41	0.59
1:A:349:LEU:O	1:A:353:GLN:NE2	2.27	0.58
1:A:202[B]:THR:N	1:A:205[B]:GLU:OE1	2.37	0.58
1:A:203[B]:THR:C	1:A:205[B]:GLU:H	2.11	0.58
2:B:74:ASN:HD22	2:B:74:ASN:N	2.01	0.58
6:A:1383:GOL:H12	8:A:1437:HOH:O	2.04	0.57
1:A:352:PHE:CE1	1:A:355:MET:HE3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:ARG:NH1	8:B:1389:HOH:O	2.22	0.55
1:A:318:THR:HA	1:A:327:ILE:HD13	1.89	0.55
1:A:78:ASN:ND2	1:A:81:ASP:OD2	2.40	0.54
6:A:1383:GOL:H31	8:A:1693:HOH:O	2.09	0.52
1:A:313[A]:MET:SD	1:A:317[A]:ILE:HD11	2.52	0.50
2:B:92:LEU:HD11	2:B:119:SER:HB3	1.94	0.49
1:A:10[B]:CYS:HB2	1:A:105:LEU:HD23	1.94	0.49
2:B:74:ASN:H	2:B:74:ASN:ND2	2.10	0.49
1:A:190[B]:MET:HG2	1:A:209:VAL:HG21	1.95	0.49
1:A:37:ARG:HH21	1:A:84:LYS:HE3	1.76	0.49
1:A:199:SER:OG	1:A:201[B]:VAL:CG2	2.61	0.49
1:A:62:ARG:HD3	1:A:203[A]:THR:CG2	2.44	0.48
1:A:201[B]:VAL:N	1:A:205[B]:GLU:OE1	2.46	0.48
2:B:1:LEU:HD22	2:B:33:ASP:CB	2.44	0.48
1:A:62:ARG:HD3	1:A:203[A]:THR:HG21	1.96	0.48
1:A:190[A]:MET:CG	1:A:200[A]:PHE:O	2.62	0.47
1:A:240:TYR:CE2	6:A:1384:GOL:H2	2.50	0.47
1:A:176:MET:HE1	1:A:284:LYS:CE	2.45	0.47
1:A:334:GLU:H	1:A:334:GLU:CD	2.23	0.47
2:B:230:ALA:HA	2:B:256:GLU:O	2.16	0.46
1:A:272:ALA:HB1	1:A:276[A]:GLU:HB2	1.97	0.46
1:A:190[A]:MET:HG3	1:A:200[A]:PHE:O	2.16	0.46
1:A:318:THR:HA	1:A:327:ILE:CD1	2.46	0.46
1:A:12[B]:ASN:CG	8:A:1432:HOH:O	2.59	0.45
1:A:242:LEU:HD12	1:A:246:GLN:CG	2.46	0.45
2:B:96[B]:GLN:HG3	2:B:113:PRO:O	2.17	0.45
1:A:203[B]:THR:C	1:A:205[B]:GLU:N	2.74	0.44
2:B:74:ASN:N	2:B:74:ASN:ND2	2.65	0.44
1:A:44:MET:HE2	1:A:61:LYS:HE3	2.00	0.44
2:B:73:ARG:NE	2:B:106:ASN:O	2.38	0.44
2:B:2:LYS:NZ	2:B:256:GLU:OE2	2.49	0.43
1:A:49:GLN:NE2	8:A:1552:HOH:O	2.26	0.43
1:A:70:PRO:HG2	1:A:85:ILE:HD12	2.00	0.42
1:A:352:PHE:HD1	1:A:355:MET:CE	2.26	0.42
2:B:216:VAL:HG23	2:B:222:GLN:HG2	2.02	0.42
1:A:242:LEU:HB3	1:A:243:PRO:HD2	2.00	0.42
1:A:186:THR:O	1:A:190[B]:MET:HG3	2.19	0.42
1:A:215:LYS:HE2	6:A:1384:GOL:O1	2.20	0.42
1:A:37:ARG:HA	1:A:38:PRO:HD3	1.92	0.42
1:A:132:MET:HE2	1:A:132:MET:HB2	1.95	0.41
1:A:269[B]:MET:HG2	1:A:271:SER:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203[B]:THR:O	1:A:205[B]:GLU:N	2.48	0.41
1:A:17:VAL:O	1:A:30:VAL:HA	2.20	0.41
1:A:313[A]:MET:HE3	8:A:1501:HOH:O	2.19	0.41
1:A:131:ALA:HB1	1:A:356:TRP:HB3	2.02	0.41
1:A:164:PRO:HG2	1:A:174:ALA:HB3	2.02	0.41
1:A:335:ARG:HA	1:A:338:SER:HB3	2.03	0.41
1:A:190[B]:MET:CG	1:A:209:VAL:HG11	2.51	0.40
1:A:143:TYR:OH	1:A:349:LEU:HD11	2.22	0.40

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	380/375 (101%)	368 (97%)	10 (3%)	2 (0%)	24	13
2	B	257/260 (99%)	250 (97%)	7 (3%)	0	100	100
All	All	637/635 (100%)	618 (97%)	17 (3%)	2 (0%)	43	25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	204[A]	ALA
1	A	204[B]	ALA

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	325/317 (102%)	318 (98%)	7 (2%)	45	32
2	B	231/229 (101%)	226 (98%)	5 (2%)	45	32
All	All	556/546 (102%)	544 (98%)	12 (2%)	44	32

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	LYS
1	A	185	LEU
1	A	225	ASN
1	A	250	ILE
1	A	288	ASP
1	A	334	GLU
1	A	364	GLU
2	B	1	LEU
2	B	74	ASN
2	B	125	VAL
2	B	221	LEU
2	B	260	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	137	GLN
1	A	280	ASN
2	B	74	ASN
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	10,11,12	1.07	1 (10%)	9,14,16	4.90	2 (22%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	HIC	CD2-CG	2.01	1.39	1.36

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	HIC	NE2-CE1-ND1	-12.56	107.85	112.66
1	A	73	HIC	CD2-NE2-CE1	6.72	109.36	106.71

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
3	NAG	C	1	3,2	14,14,15	0.53	0	17,19,21	1.13	1 (5%)
3	NAG	C	2	3	14,14,15	0.45	0	17,19,21	1.84	3 (17%)

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	NAG	C	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	NAG	C1-O5-C5	5.18	119.13	112.19
3	C	2	NAG	C4-C3-C2	-3.68	105.63	111.02
3	C	2	NAG	C2-N2-C7	-3.14	118.69	122.90
3	C	1	NAG	C2-N2-C7	-3.03	118.85	122.90

There are no chirality outliers.

All (2) torsion outliers are listed below:

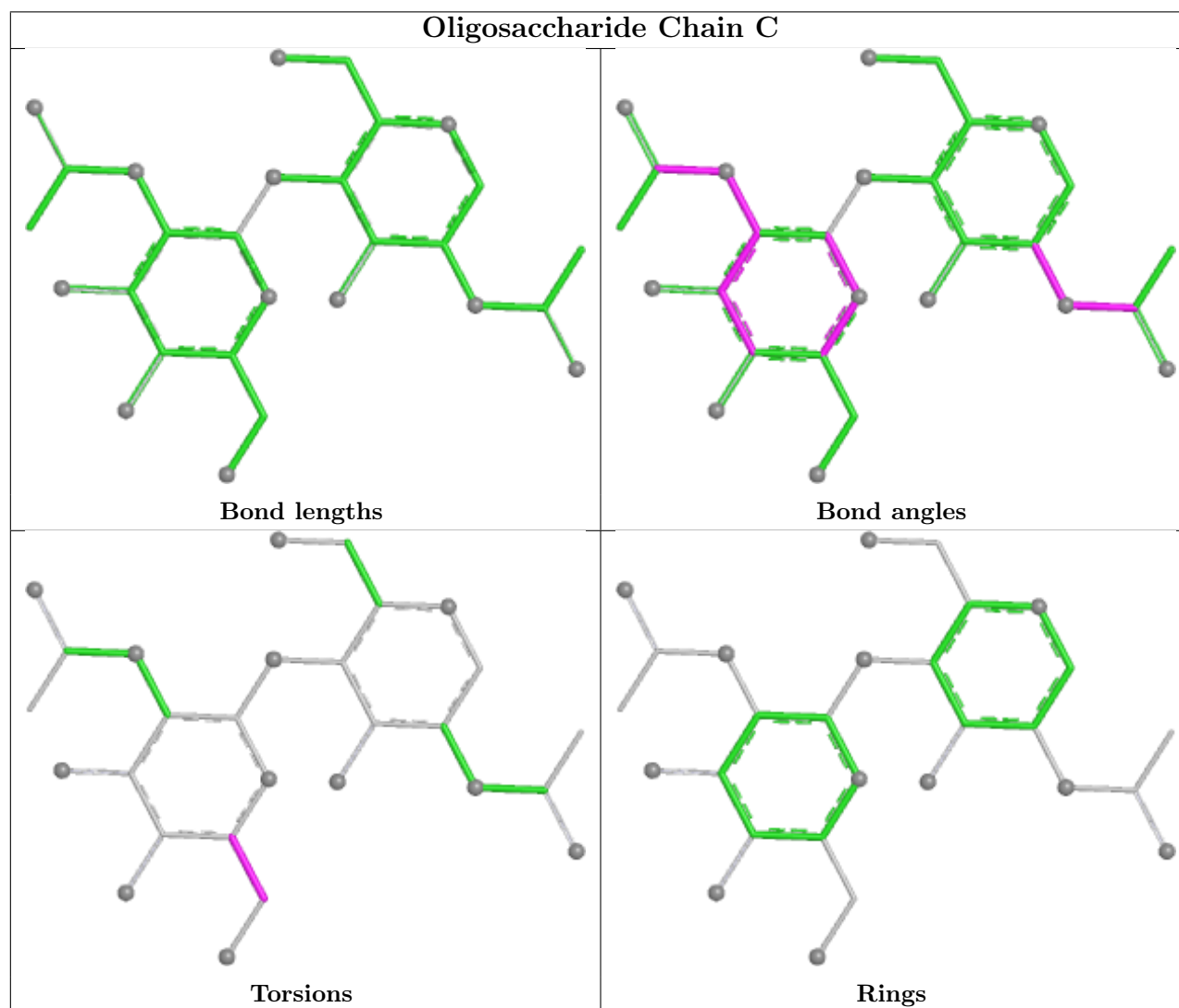
Mol	Chain	Res	Type	Atoms
3	C	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	NAG	1	0
3	C	2	NAG	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 oligosaccharide.



5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	$\# Z > 2$
6	GOL	A	1384	-	5,5,5	0.31	0	5,5,5	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	A	1383	-	5,5,5	0.35	0	5,5,5	0.25	0
5	ATP	A	1380	4	32,33,33	1.56	5 (15%)	48,52,52	1.84	13 (27%)
6	GOL	A	1382	-	5,5,5	0.40	0	5,5,5	0.68	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
6	GOL	A	1384	-	-	1/4/4/4	-
6	GOL	A	1383	-	-	1/4/4/4	-
5	ATP	A	1380	4	-	2/22/38/38	0/3/3/3
6	GOL	A	1382	-	-	0/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1380	ATP	C5-C4	5.10	1.48	1.39
5	A	1380	ATP	C8-N7	2.94	1.37	1.31
5	A	1380	ATP	PB-O3B	2.88	1.62	1.59
5	A	1380	ATP	C5-C6	2.28	1.47	1.41
5	A	1380	ATP	C5-N7	-2.12	1.35	1.39

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1380	ATP	N3-C4-N9	4.53	134.87	127.17
5	A	1380	ATP	C5-C4-N3	-4.48	120.55	126.72
5	A	1380	ATP	C4-N9-C8	4.42	110.38	105.74
5	A	1380	ATP	N3-C2-N1	-4.21	122.21	128.58
5	A	1380	ATP	C2-N1-C6	3.48	124.44	118.73
5	A	1380	ATP	C2-N3-C4	3.07	119.33	111.83
5	A	1380	ATP	N9-C8-N7	-2.76	110.02	113.94
5	A	1380	ATP	N6-C6-N1	2.38	123.67	118.38
5	A	1380	ATP	C4-C5-N7	-2.37	107.88	110.58
5	A	1380	ATP	C5-N7-C8	2.33	107.11	103.45
5	A	1380	ATP	O3G-PG-O2G	2.12	115.75	107.80
5	A	1380	ATP	O2'-C2'-C1'	2.10	117.34	110.10
5	A	1380	ATP	O3B-PG-O1G	-2.03	100.35	111.04

There are no chirality outliers.

All (4) torsion outliers are listed below:

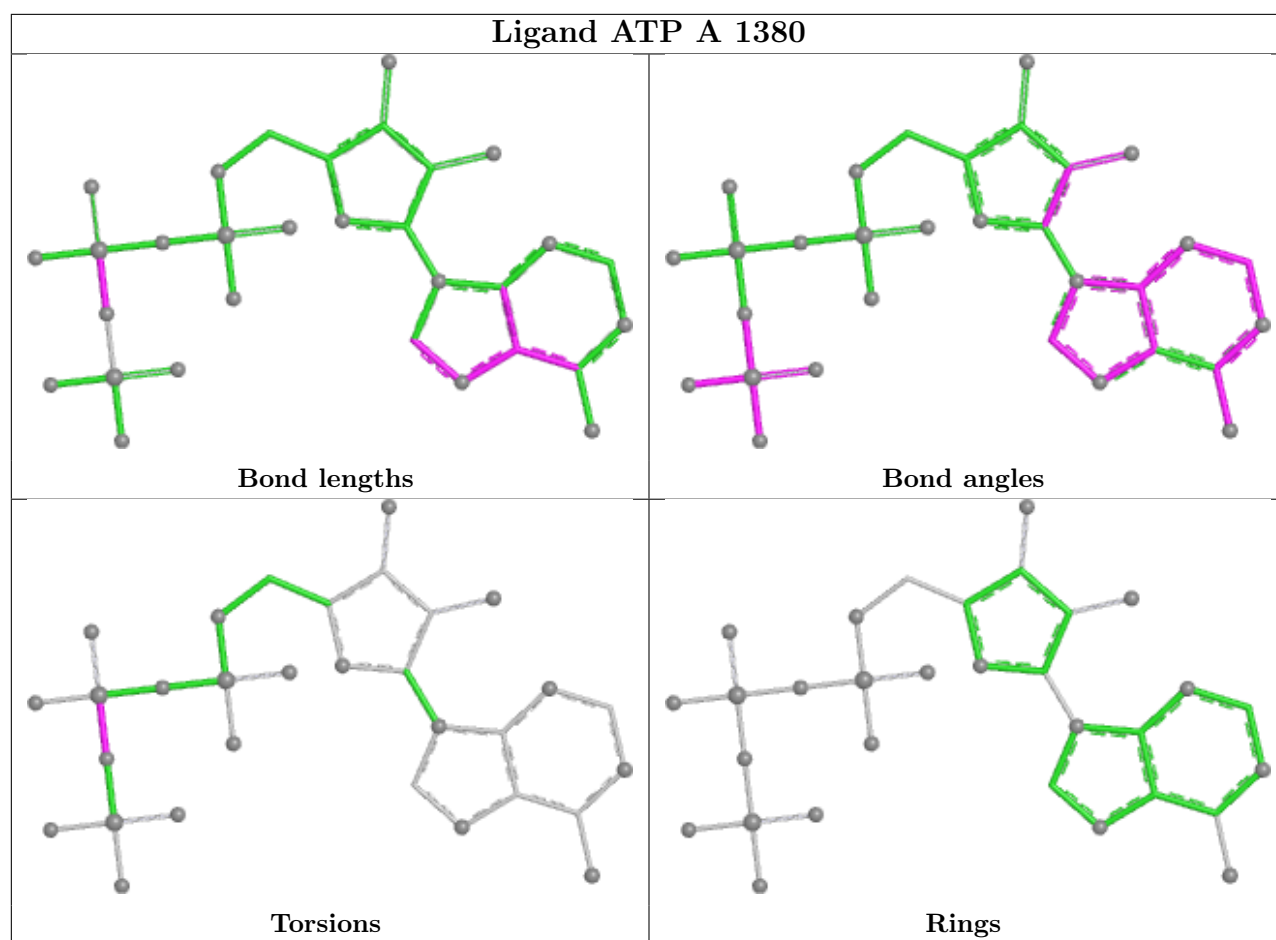
Mol	Chain	Res	Type	Atoms
6	A	1384	GOL	O2-C2-C3-O3
6	A	1383	GOL	O1-C1-C2-O2
5	A	1380	ATP	PG-O3B-PB-O1B
5	A	1380	ATP	PG-O3B-PB-O2B

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1384	GOL	3	0
6	A	1383	GOL	2	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	360/375 (96%)	1.44	74 (20%) 2 2	20, 42, 57, 73	22 (6%)
2	B	255/260 (98%)	2.29	150 (58%) 0 0	24, 42, 52, 72	6 (2%)
All	All	615/635 (96%)	1.79	224 (36%) 1 0	20, 42, 56, 73	28 (4%)

All (224) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	201[A]	VAL	5.2
2	B	181	TRP	4.9
2	B	260	THR	4.9
2	B	176	VAL	4.8
2	B	136	ALA	4.8
2	B	175	TYR	4.7
2	B	76	TYR	4.7
2	B	211	TYR	4.6
2	B	138	SER	4.6
2	B	209	CYS	4.6
1	A	349	LEU	4.5
1	A	5	THR	4.4
2	B	141	VAL	4.4
1	A	203[A]	THR	4.4
2	B	89	VAL	4.3
2	B	144	ILE	4.3
2	B	184	ILE	4.2
2	B	92	LEU	4.2
2	B	140	ALA	4.1
2	B	135	SER	4.0
2	B	173	CYS	4.0
1	A	341	ILE	4.0
2	B	137	PRO	4.0
2	B	72	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	106	ASN	3.9
2	B	109	PHE	3.9
2	B	177	THR	3.8
1	A	339	VAL	3.8
2	B	105	GLY	3.8
2	B	160	LEU	3.7
2	B	174	SER	3.6
2	B	121	HIS	3.6
1	A	350	SER	3.6
2	B	171	ALA	3.6
1	A	345	ILE	3.5
2	B	154	VAL	3.5
1	A	55	GLY	3.5
2	B	207	THR	3.5
2	B	147	LEU	3.5
2	B	183	SER	3.4
2	B	97	TYR	3.4
2	B	186	LEU	3.4
2	B	125	VAL	3.4
2	B	237	ALA	3.4
1	A	346	LEU	3.3
2	B	134	HIS	3.3
2	B	182	SER	3.3
1	A	347	ALA	3.3
2	B	142	ALA	3.3
2	B	71	LEU	3.3
2	B	152	LEU	3.3
2	B	74	ASN	3.3
2	B	179	SER	3.3
2	B	1	LEU	3.3
2	B	37	ILE	3.2
2	B	75	SER	3.2
1	A	356	TRP	3.2
1	A	34[A]	ILE	3.2
1	A	22	ALA	3.2
1	A	365	ALA	3.2
2	B	110[A]	SER	3.2
2	B	169	PHE	3.2
2	B	158	TRP	3.1
1	A	351	THR	3.1
2	B	202	THR	3.1
1	A	362	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	108	SER	3.1
2	B	143	GLU	3.1
2	B	220	LEU	3.1
1	A	69	TYR	3.0
2	B	148	TYR	3.0
2	B	150	VAL	3.0
2	B	170	ASN	3.0
2	B	178[A]	SER	3.0
2	B	200	ALA	3.0
2	B	40	VAL	3.0
1	A	23	GLY	3.0
2	B	203	THR	2.9
2	B	113	PRO	2.9
2	B	77	LYS	2.9
2	B	157	LYS	2.9
2	B	107	ASP	2.9
1	A	352	PHE	2.9
2	B	210	ALA	2.9
1	A	228	ALA	2.9
2	B	204	ALA	2.9
2	B	96[A]	GLN	2.8
1	A	108	ALA	2.8
1	A	136	ILE	2.8
1	A	6	THR	2.8
1	A	26	ALA	2.8
1	A	63	GLY	2.8
1	A	67	LEU	2.8
1	A	56	ASP	2.8
1	A	7	ALA	2.8
2	B	252	HIS	2.8
2	B	145	ASN	2.7
2	B	188	THR	2.7
2	B	80	TYR	2.7
2	B	133	LEU	2.7
2	B	253	TYR	2.7
2	B	99	ASP	2.7
2	B	168	ASP	2.7
1	A	202[A]	THR	2.7
2	B	259	LEU	2.7
2	B	98	ASP	2.6
1	A	249	THR	2.6
2	B	205	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	71	ILE	2.6
1	A	355	MET	2.6
2	B	111	ARG	2.6
2	B	172	ASP	2.6
2	B	248	ALA	2.6
2	B	57	GLN	2.6
1	A	340	TRP	2.6
1	A	348	SER	2.6
2	B	223	SER	2.6
2	B	227	PRO	2.6
1	A	65	LEU	2.6
2	B	123	THR	2.6
1	A	53	TYR	2.6
2	B	233	PHE	2.6
1	A	360	GLN	2.6
1	A	250	ILE	2.6
2	B	146	SER	2.6
2	B	192	PHE	2.5
2	B	93	ASP	2.5
2	B	139	ASP	2.5
2	B	208	ASN	2.5
1	A	363	ASP	2.5
1	A	66	THR	2.5
1	A	109	PRO	2.5
2	B	242	SER	2.5
2	B	249	ILE	2.5
1	A	54	VAL	2.5
2	B	91	VAL	2.5
2	B	251	ASP	2.5
1	A	110	LEU	2.4
2	B	206	SER	2.4
2	B	194	TRP	2.4
1	A	247	VAL	2.4
1	A	342	GLY	2.4
1	A	8	LEU	2.4
2	B	43	SER	2.4
2	B	6	PHE	2.4
1	A	64	ILE	2.4
1	A	135	ALA	2.4
1	A	30	VAL	2.4
2	B	54	TYR	2.4
2	B	191	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	248	ILE	2.4
2	B	190	SER	2.4
1	A	16	LEU	2.3
2	B	244	GLU	2.3
2	B	114	ALA	2.3
2	B	196	ILE	2.3
2	B	58	ASP	2.3
2	B	180	GLN	2.3
2	B	132	ALA	2.3
2	B	238	ALA	2.3
1	A	357	ILE	2.3
1	A	27	PRO	2.3
1	A	344	SER	2.3
2	B	231	ALA	2.3
2	B	254	PRO	2.3
1	A	15	GLY	2.3
2	B	73	ARG	2.3
1	A	49	GLN	2.3
2	B	131	VAL	2.3
1	A	358	THR	2.3
2	B	45	LEU	2.3
1	A	131	ALA	2.2
2	B	118	PHE	2.2
2	B	161	ASN	2.2
1	A	104	LEU	2.2
2	B	59	ASP	2.2
2	B	95	TYR	2.2
2	B	44	HIS	2.2
2	B	67	VAL	2.2
2	B	116	VAL	2.2
2	B	55	LEU	2.2
2	B	156	GLN	2.2
2	B	162	ASP	2.2
2	B	218	GLY	2.2
2	B	219	SER	2.2
1	A	124	PHE	2.2
2	B	119	SER	2.2
2	B	224	SER	2.2
1	A	178	LEU	2.2
2	B	12	GLY	2.2
2	B	60	PRO	2.2
1	A	230	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	124	LYS	2.2
2	B	185	ARG	2.2
1	A	207	GLU	2.1
1	A	137	GLN	2.1
1	A	94	LEU	2.1
1	A	29	ALA	2.1
2	B	217	ALA	2.1
2	B	11	PHE	2.1
2	B	30	ARG	2.1
2	B	112	GLU	2.1
2	B	221	LEU	2.1
1	A	90	PHE	2.1
1	A	244	ASP	2.1
1	A	324	THR	2.1
1	A	343	GLY	2.1
1	A	12[A]	ASN	2.1
2	B	215	VAL	2.1
2	B	212	ASP	2.1
1	A	75	ILE	2.0
2	B	39	GLU	2.0
2	B	151	TYR	2.0
2	B	10	THR	2.0
2	B	241	LEU	2.0
2	B	27	ARG	2.0
2	B	68	SER	2.0
2	B	235	PHE	2.0
2	B	94	THR	2.0
2	B	86	PRO	2.0
1	A	35	VAL	2.0
2	B	46	VAL	2.0
2	B	115	VAL	2.0
2	B	163	VAL	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.

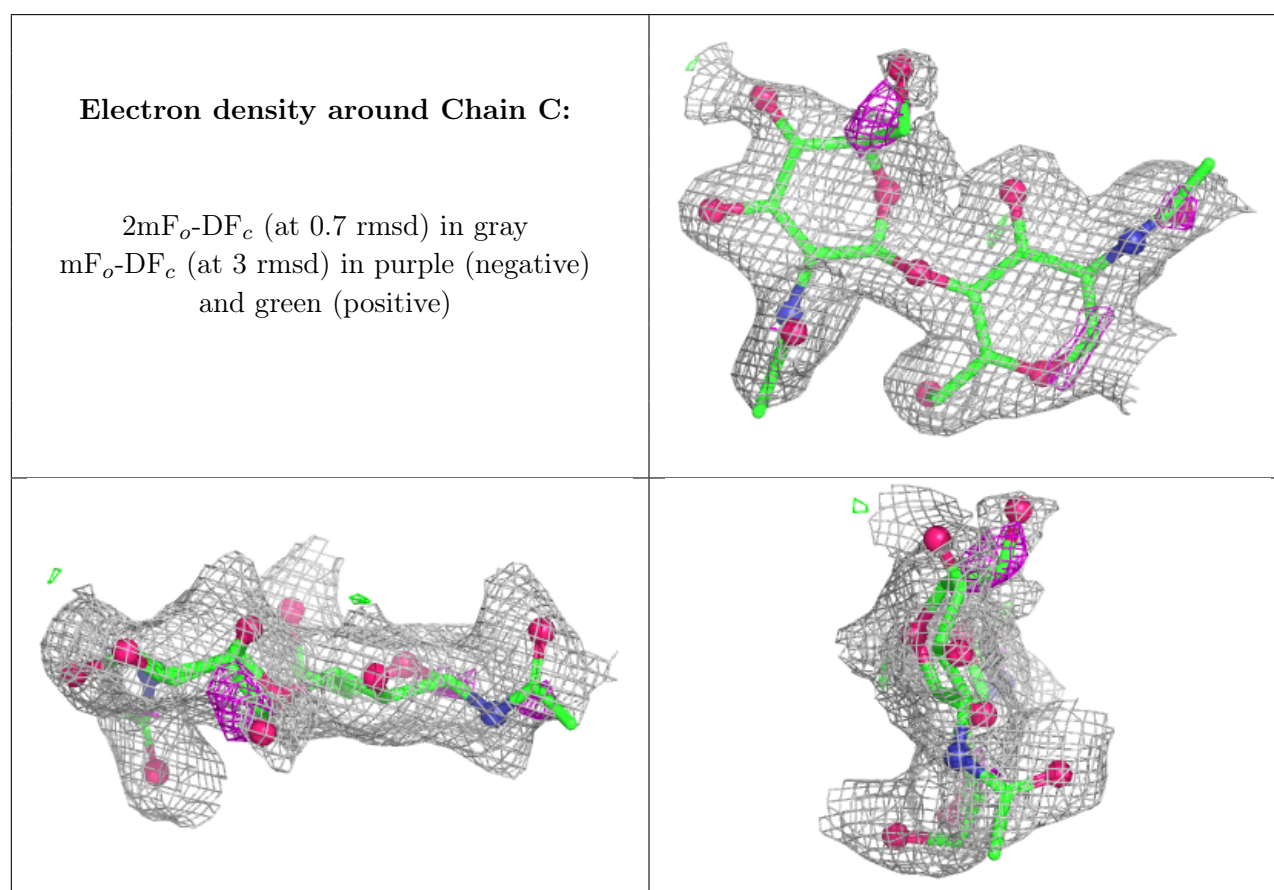
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	HIC	A	73	11/12	0.85	0.14	39,42,57,59	0

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
3	NAG	C	2	14/15	0.66	0.16	56,61,65,68	0
3	NAG	C	1	14/15	0.82	0.14	44,51,58,59	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.

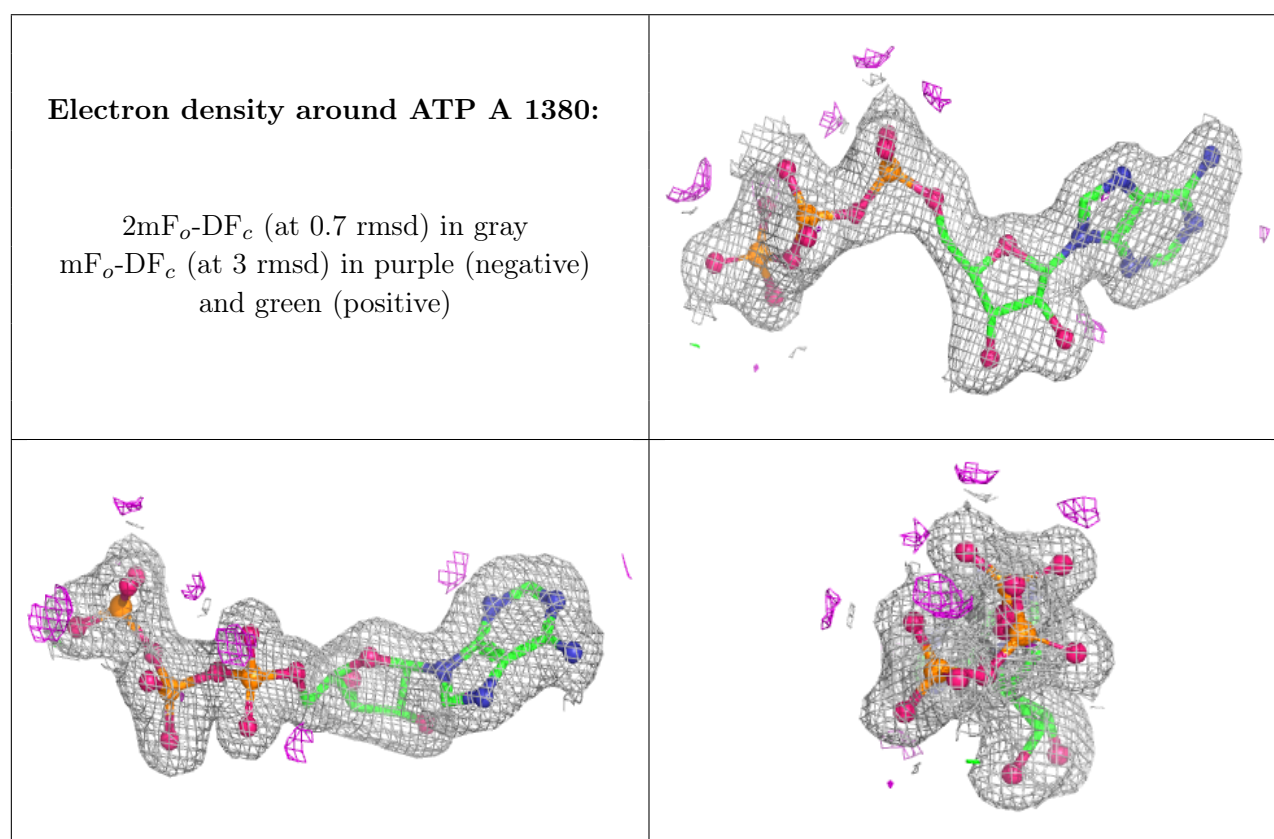


6.4 Ligands [i](#)

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
6	GOL	A	1382	6/6	0.75	0.21	51,60,62,63	0
6	GOL	A	1384	6/6	0.75	0.16	49,53,57,61	0
6	GOL	A	1383	6/6	0.78	0.16	56,58,59,61	0
7	MG	B	1273	1/1	0.96	0.12	46,46,46,46	0
4	CA	B	1272	1/1	0.98	0.11	37,37,37,37	0
5	ATP	A	1380	31/31	0.98	0.07	31,36,39,40	0
4	CA	A	1381	1/1	0.99	0.05	36,36,36,36	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.