



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 11:46 PM BST

PDB ID : 2D1K  
Title : Ternary complex of the WH2 domain of mim with actin-dnase I  
Authors : Chereau, D.; Kerff, F.; Dominguez, R.  
Deposited on : 2005-08-26  
Resolution : 2.50 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](mailto: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.

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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

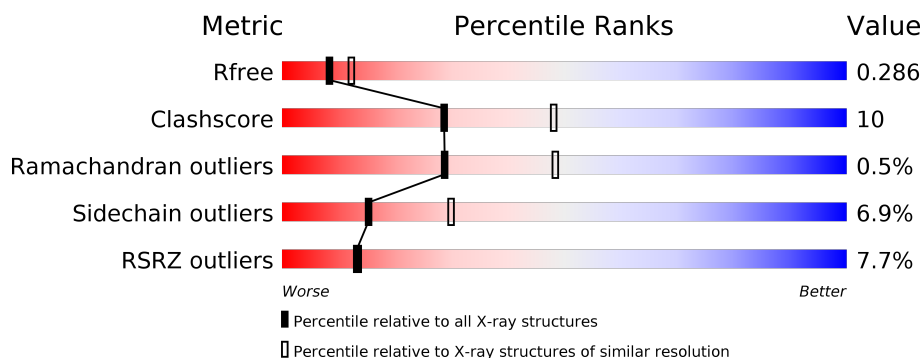
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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>9%</div> <div>68%</div> <div>29%</div> <div>..</div> </div>
2	B	260	<div> <div>%</div> <div>82%</div> <div>16%</div> <div>.</div> </div>
3	C	32	<div> <div>53%</div> <div>53%</div> <div>31%</div> <div>6%</div> <div>9%</div> </div>
4	D	3	<div> <div>33%</div> <div>33%</div> <div>33%</div> </div>

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5355 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	371	Total	C	N	O	S	0	0	0
			2897	1833	489	554	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	1	0
			2056	1303	344	401	8			

- Molecule 3 is a protein called Metastasis suppressor protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	29	Total	C	N	O	S	0	0	0
			226	135	47	43	1			

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

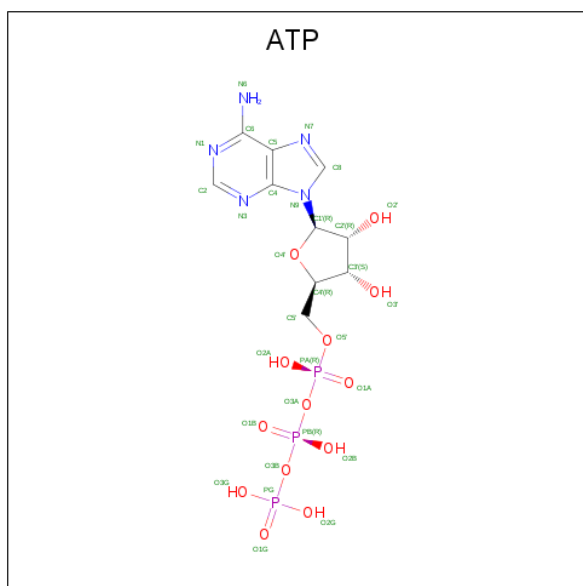


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	3	Total	C	N	O		0	0	0
			39	22	2	15				

- 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: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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

- Molecule 7 is MAGNESIUM ION (three-letter code: 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	34	Total	O	0	0
			34	34		
8	B	68	Total	O	0	0
			68	68		

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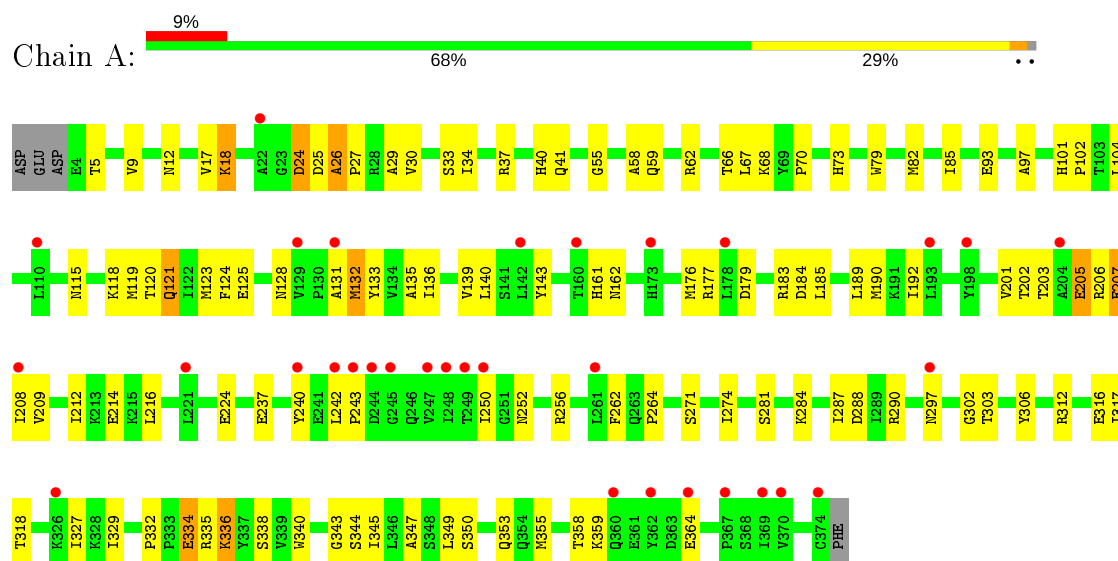
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total	O	0	0
			1	1		

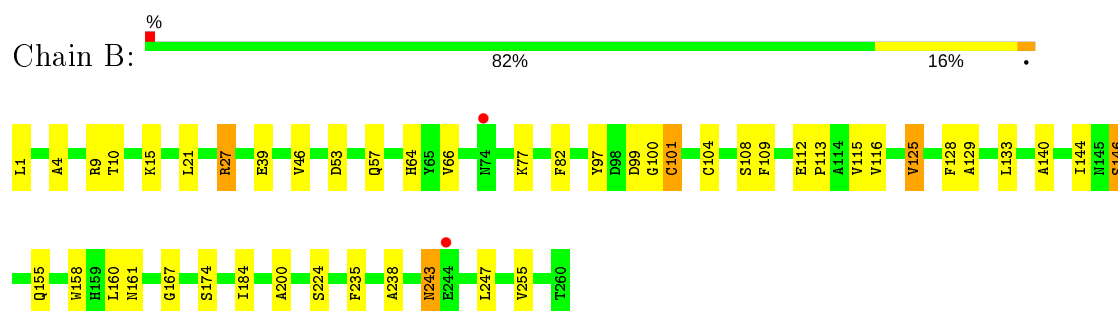
### 3 Residue-property plots [i](#)

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.

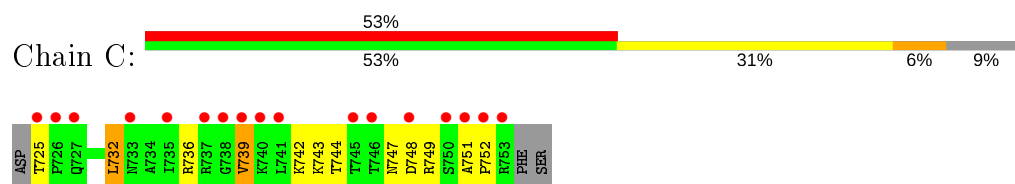
- Molecule 1: Actin, alpha skeletal muscle



- Molecule 2: Deoxyribonuclease-1



- Molecule 3: Metastasis suppressor protein 1



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

Chain D: 33% 33% 33%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.09 Å   75.49 Å   228.99 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	41.40 – 2.50 41.40 – 2.50	Depositor EDS
% Data completeness (in resolution range)	89.6 (41.40-2.50) 89.6 (41.40-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.80 (at 2.51 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.217   ,   0.284 0.218   ,   0.286	Depositor DCC
$R_{free}$ test set	1165 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.5	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 54.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5355	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MG, BMA, NAG, CA, HIC, ATP

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	0.47	0/2946	0.64	0/3990
2	B	0.70	0/2105	0.73	0/2867
3	C	0.60	1/227 (0.4%)	0.72	0/303
All	All	0.58	1/5278 (0.0%)	0.68	0/7160

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	749	ARG	CZ-NH2	5.25	1.39	1.33

There are no bond angle outliers.

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	2897	0	2869	74	0
2	B	2056	0	1993	27	0
3	C	226	0	238	8	0
4	D	39	0	34	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	31	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	1	0	0	0	0
8	A	34	0	0	2	0
8	B	68	0	0	2	0
8	C	1	0	0	0	0
All	All	5355	0	5146	101	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 10.

All (101) 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:25:ASP:N	1:A:26:ALA:HB3	1.77	1.00
1:A:25:ASP:H	1:A:26:ALA:HB3	1.38	0.85
1:A:242:LEU:HB3	1:A:243:PRO:HD2	1.70	0.73
1:A:120:THR:HA	1:A:132:MET:CE	2.20	0.72
1:A:345:ILE:HG23	3:C:739:VAL:HG21	1.71	0.71
1:A:26:ALA:HB1	3:C:744:THR:HB	1.72	0.70
1:A:207:GLU:O	3:C:752:PRO:HB2	1.93	0.68
1:A:59:GLN:O	1:A:62:ARG:HG3	1.94	0.67
1:A:216:LEU:HD13	1:A:250:ILE:HG21	1.74	0.67
1:A:202:THR:OG1	1:A:205:GLU:HB2	1.93	0.67
1:A:25:ASP:N	1:A:26:ALA:CB	2.56	0.65
2:B:9:ARG:HA	2:B:39:GLU:OE1	1.98	0.63
1:A:120:THR:HA	1:A:132:MET:HE3	1.82	0.62
1:A:185:LEU:HD23	1:A:306:TYR:OH	2.00	0.62
1:A:120:THR:HA	1:A:132:MET:HE1	1.82	0.61
1:A:121:GLN:O	1:A:125:GLU:HB2	1.99	0.61
1:A:335:ARG:HA	1:A:338:SER:HB2	1.82	0.61
2:B:125:VAL:HG22	2:B:224:SER:OG	2.01	0.60
1:A:25:ASP:H	1:A:26:ALA:CB	2.10	0.59
1:A:288:ASP:HB3	8:A:1407:HOH:O	2.02	0.58
1:A:136:ILE:HD12	1:A:136:ILE:H	1.69	0.57
1:A:162:ASN:HB2	1:A:176:MET:HB2	1.86	0.56
1:A:18:LYS:N	1:A:18:LYS:HD3	2.20	0.56
1:A:30:VAL:HB	3:C:748:ASP:HA	1.88	0.56
3:C:742:LYS:HD3	3:C:743:LYS:H	1.71	0.56
1:A:37:ARG:HH11	1:A:68:LYS:HD2	1.72	0.55
2:B:99:ASP:HB3	2:B:104:CYS:HB3	1.89	0.55
1:A:302:GLY:HA3	6:A:1380:ATP:O4'	2.07	0.54
1:A:177:ARG:NH1	1:A:179:ASP:CG	2.61	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ILE:HG21	1:A:67:LEU:HD22	1.90	0.54
1:A:297:ASN:HB3	1:A:329:ILE:HG13	1.90	0.54
1:A:9:VAL:HG21	1:A:344:SER:HA	1.91	0.53
2:B:100:GLY:O	2:B:101:CYS:HB3	2.08	0.53
1:A:262:PHE:CE1	1:A:274:ILE:HD11	2.43	0.53
1:A:123:MET:HG3	1:A:132:MET:HE2	1.89	0.53
1:A:242:LEU:HB3	1:A:243:PRO:CD	2.37	0.53
1:A:70:PRO:HG2	1:A:85:ILE:HD12	1.90	0.52
1:A:176:MET:HG3	1:A:281:SER:HB2	1.92	0.52
1:A:26:ALA:H	1:A:27:PRO:HD3	1.75	0.52
1:A:34:ILE:CG2	1:A:67:LEU:HD22	2.40	0.51
2:B:155:GLN:NE2	2:B:161:ASN:OD1	2.43	0.51
1:A:124:PHE:O	1:A:128:ASN:HA	2.10	0.50
2:B:128:PHE:HA	2:B:160:LEU:HD21	1.93	0.50
1:A:79:TRP:CZ3	1:A:118:LYS:HB3	2.46	0.50
1:A:177:ARG:HH12	1:A:179:ASP:CG	2.15	0.49
1:A:40:HIS:NE2	2:B:53:ASP:OD1	2.38	0.49
3:C:732:LEU:HB3	3:C:736:ARG:HH21	1.77	0.49
1:A:202:THR:HG1	1:A:205:GLU:HB2	1.77	0.48
1:A:205:GLU:HA	1:A:208:ILE:HD12	1.96	0.48
1:A:97:ALA:O	1:A:101:HIS:HD2	1.97	0.48
2:B:200:ALA:O	8:B:1276:HOH:O	2.20	0.48
2:B:144:ILE:HG22	2:B:184:ILE:CG2	2.44	0.47
1:A:25:ASP:OD1	1:A:26:ALA:HB2	2.15	0.47
2:B:109:PHE:CZ	2:B:146:SER:HB3	2.49	0.47
1:A:55:GLY:O	1:A:58:ALA:HB3	2.15	0.47
1:A:24:ASP:OD1	1:A:24:ASP:N	2.48	0.46
1:A:161:HIS:CE1	1:A:177:ARG:HG3	2.51	0.46
2:B:115:VAL:HG12	2:B:158:TRP:CZ3	2.51	0.45
2:B:133:LEU:O	2:B:167:GLY:HA3	2.17	0.45
1:A:190:MET:HG2	1:A:209:VAL:HG21	1.99	0.45
1:A:29:ALA:CB	1:A:93:GLU:HG3	2.47	0.45
2:B:116:VAL:O	2:B:129:ALA:HA	2.16	0.45
1:A:214:GLU:HG2	6:A:1380:ATP:C5	2.52	0.45
1:A:216:LEU:HD11	1:A:240:TYR:HB2	1.99	0.45
1:A:345:ILE:HG23	3:C:739:VAL:CG2	2.44	0.45
2:B:9:ARG:O	2:B:10:THR:C	2.55	0.45
1:A:102:PRO:HA	1:A:131:ALA:O	2.17	0.45
2:B:97:TYR:HB3	2:B:113:PRO:HD2	1.99	0.45
1:A:190:MET:HG2	1:A:209:VAL:HG11	2.00	0.44
2:B:243:ASN:O	2:B:247:LEU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:751:ALA:HA	3:C:752:PRO:HD3	1.85	0.44
2:B:66:VAL:HB	2:B:82:PHE:HB2	2.00	0.43
1:A:104:LEU:HD22	1:A:347:ALA:HB2	2.00	0.43
1:A:104:LEU:HD12	1:A:133:TYR:HB3	2.00	0.43
2:B:144:ILE:HG22	2:B:184:ILE:HG21	2.01	0.43
1:A:41:GLN:HB3	2:B:64:HIS:CD2	2.53	0.43
2:B:4:ALA:HA	2:B:255:VAL:O	2.18	0.43
1:A:318:THR:HA	1:A:327:ILE:HD11	2.00	0.43
1:A:203:THR:OG1	2:B:46:VAL:HG21	2.18	0.43
1:A:336:LYS:HE2	6:A:1380:ATP:C8	2.54	0.43
1:A:189:LEU:HA	1:A:192:ILE:HG12	2.01	0.42
1:A:317:ILE:HG13	1:A:317:ILE:H	1.58	0.42
1:A:297:ASN:HB3	1:A:329:ILE:CG1	2.49	0.42
1:A:139:VAL:HG12	1:A:143:TYR:CZ	2.54	0.42
1:A:252:ASN:O	1:A:256:ARG:HG3	2.19	0.42
2:B:27:ARG:HG2	8:B:1293:HOH:O	2.18	0.42
1:A:201:VAL:HB	8:A:1403:HOH:O	2.19	0.41
1:A:208:ILE:HD13	1:A:243:PRO:HD3	2.02	0.41
2:B:140:ALA:O	2:B:144:ILE:HG13	2.20	0.41
1:A:264:PRO:HG2	1:A:271:SER:O	2.21	0.41
1:A:332:PRO:HB2	1:A:334:GLU:OE2	2.19	0.41
1:A:115:ASN:O	1:A:119:MET:HG3	2.20	0.41
2:B:235:PHE:HA	2:B:238:ALA:HB3	2.03	0.41
1:A:312:ARG:HD2	1:A:316:GLU:HG2	2.03	0.41
1:A:287:ILE:HA	1:A:290:ARG:HD2	2.03	0.41
2:B:112:GLU:HA	2:B:113:PRO:HD3	1.91	0.41
1:A:340:TRP:O	1:A:343:GLY:N	2.54	0.40
2:B:53:ASP:O	2:B:57:GLN:HB3	2.21	0.40
2:B:21:LEU:HD21	4:D:1:NAG:H62	2.03	0.40
1:A:135:ALA:HB3	1:A:140:LEU:HD11	2.04	0.40
1:A:17:VAL:HG23	1:A:33:SER:HB3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	368/375 (98%)	339 (92%)	26 (7%)	3 (1%)	19	35
2	B	259/260 (100%)	239 (92%)	20 (8%)	0	100	100
3	C	27/32 (84%)	22 (82%)	5 (18%)	0	100	100
All	All	654/667 (98%)	600 (92%)	51 (8%)	3 (0%)	29	48

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	ALA
1	A	353	GLN
1	A	350	SER

### 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	313/317 (99%)	288 (92%)	25 (8%)	12	23
2	B	230/229 (100%)	220 (96%)	10 (4%)	29	53
3	C	25/28 (89%)	21 (84%)	4 (16%)	2	4
All	All	568/574 (99%)	529 (93%)	39 (7%)	15	30

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	12	ASN
1	A	18	LYS
1	A	24	ASP
1	A	66	THR
1	A	82	MET
1	A	121	GLN

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Mol	Chain	Res	Type
1	A	132	MET
1	A	183	ARG
1	A	184	ASP
1	A	205	GLU
1	A	206	ARG
1	A	207	GLU
1	A	212	ILE
1	A	224	GLU
1	A	237	GLU
1	A	284	LYS
1	A	303	THR
1	A	334	GLU
1	A	336	LYS
1	A	349	LEU
1	A	355	MET
1	A	358	THR
1	A	359	LYS
1	A	364	GLU
2	B	1	LEU
2	B	15	LYS
2	B	27	ARG
2	B	77	LYS
2	B	101	CYS
2	B	108	SER
2	B	125	VAL
2	B	146	SER
2	B	174	SER
2	B	243	ASN
3	C	725	THR
3	C	732	LEU
3	C	739	VAL
3	C	747	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	121	GLN
1	A	128	ASN
1	A	280	ASN
2	B	44	HIS
3	C	727	GLN

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Mol	Chain	Res	Type
3	C	747	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	1.20	2 (25%)	6,14,16	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
1	HIC	A	73	1	-	1/5/6/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	HIC	CD2-NE2	-2.36	1.34	1.38
1	A	73	HIC	CD2-CG	2.23	1.39	1.36

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	73	HIC	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

3 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	0.61	0	17,19,21	2.02	5 (29%)
4	NAG	D	2	4	14,14,15	0.39	0	17,19,21	2.18	5 (29%)
4	BMA	D	3	4	11,11,12	0.62	0	15,15,17	0.69	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
4	NAG	D	1	2,4	-	3/6/23/26	0/1/1/1
4	NAG	D	2	4	-	5/6/23/26	0/1/1/1
4	BMA	D	3	4	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2	NAG	C1-O5-C5	5.52	119.68	112.19
4	D	1	NAG	C2-N2-C7	4.50	129.31	122.90
4	D	1	NAG	C1-C2-N2	4.19	117.64	110.49
4	D	2	NAG	C2-N2-C7	4.10	128.74	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2	NAG	C8-C7-N2	3.05	121.27	116.10
4	D	2	NAG	O5-C5-C6	2.97	111.86	107.20
4	D	1	NAG	O5-C1-C2	-2.88	106.74	111.29
4	D	2	NAG	C4-C3-C2	-2.34	107.59	111.02
4	D	1	NAG	C8-C7-N2	2.24	119.90	116.10
4	D	1	NAG	O4-C4-C3	-2.16	105.36	110.35

There are no chirality outliers.

All (10) torsion outliers are listed below:

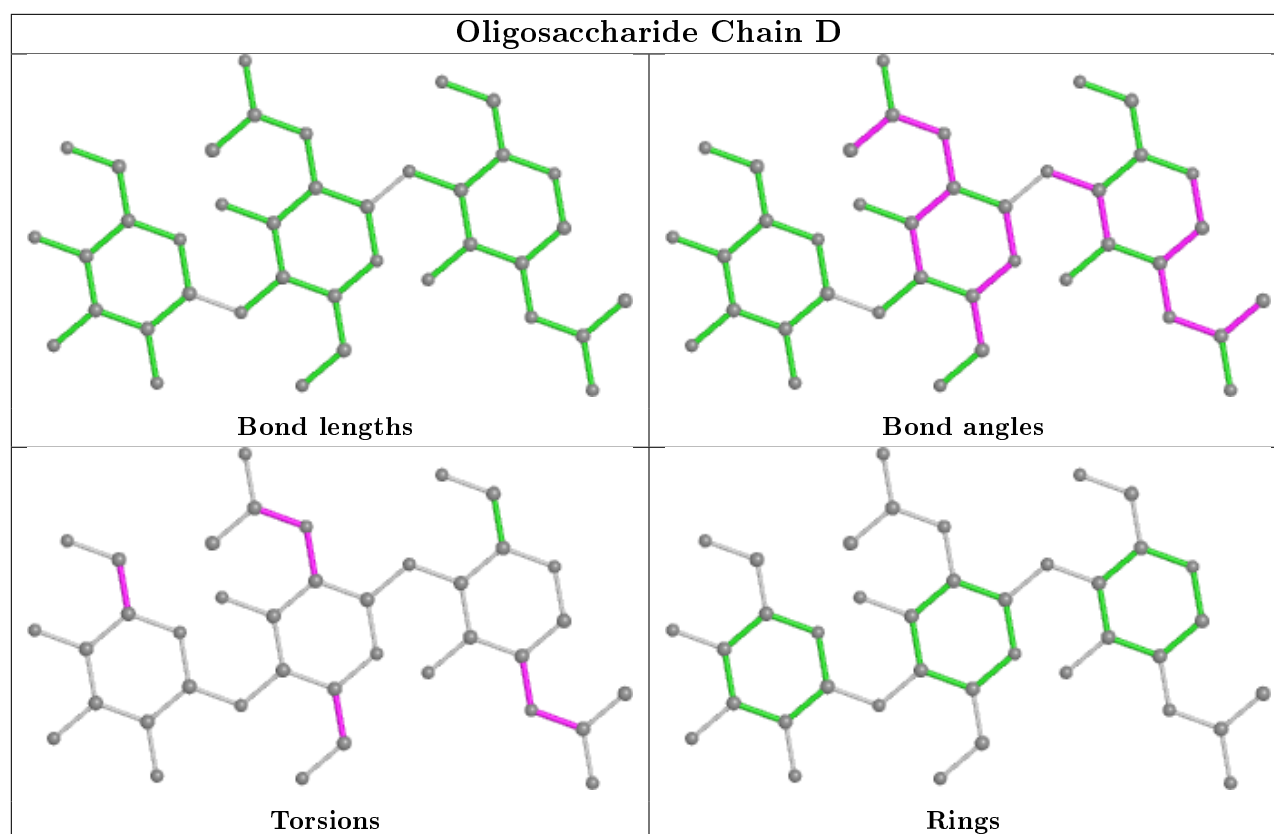
Mol	Chain	Res	Type	Atoms
4	D	1	NAG	C1-C2-N2-C7
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
4	D	3	BMA	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
4	D	3	BMA	C4-C5-C6-O6
4	D	2	NAG	C3-C2-N2-C7
4	D	2	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	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 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	ATP	A	1380	5	26,33,33	0.97	1 (3%)	31,52,52	1.76	6 (19%)

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	ATP	A	1380	5	-	3/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1380	ATP	C5-C4	2.55	1.47	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1380	ATP	PA-O3A-PB	-5.38	114.37	132.83
6	A	1380	ATP	PB-O3B-PG	-3.61	120.44	132.83
6	A	1380	ATP	N3-C2-N1	-3.47	123.26	128.68
6	A	1380	ATP	C4-C5-N7	-2.56	106.73	109.40
6	A	1380	ATP	C1'-N9-C4	-2.09	122.98	126.64
6	A	1380	ATP	C2-N1-C6	2.06	122.28	118.75

There are no chirality outliers.

All (3) torsion outliers are listed below:

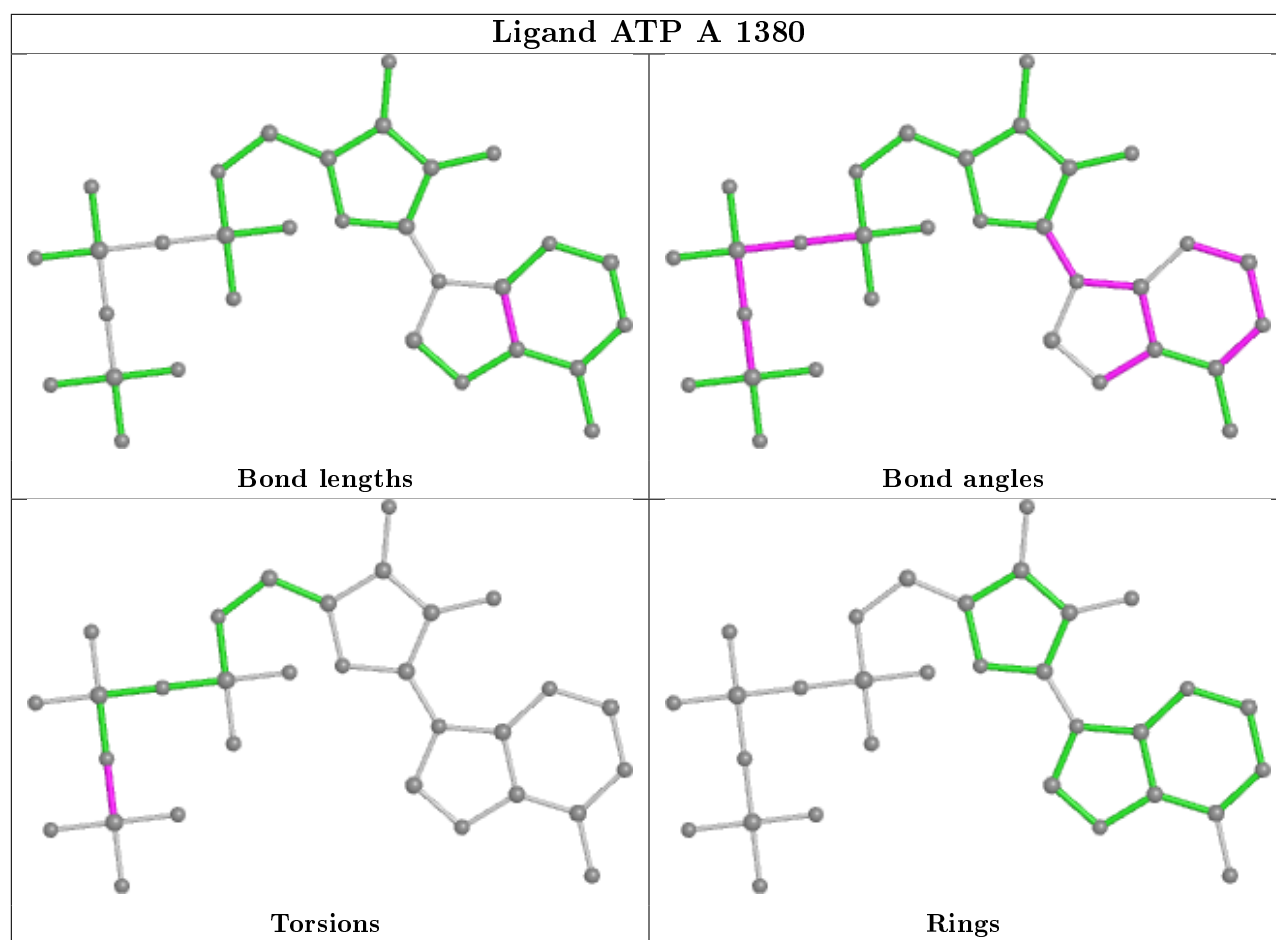
Mol	Chain	Res	Type	Atoms
6	A	1380	ATP	PB-O3B-PG-O2G
6	A	1380	ATP	PB-O3B-PG-O1G
6	A	1380	ATP	PB-O3B-PG-O3G

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1380	ATP	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	370/375 (98%)	0.54	32 (8%) 10 10	44, 71, 86, 99	2 (0%)
2	B	260/260 (100%)	0.00	2 (0%) 86 87	26, 40, 53, 77	2 (0%)
3	C	29/32 (90%)	3.07	17 (58%) 0 0	75, 88, 108, 112	0
All	All	659/667 (98%)	0.44	51 (7%) 13 13	26, 57, 87, 112	4 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	752	PRO	7.9
3	C	751	ALA	6.8
3	C	726	PRO	6.6
1	A	242	LEU	6.3
3	C	748	ASP	6.3
3	C	753	ARG	6.0
3	C	725	THR	5.4
1	A	245	GLY	4.8
1	A	173	HIS	4.5
1	A	243	PRO	4.4
3	C	746	THR	4.2
3	C	738	GLY	4.1
1	A	244	ASP	3.9
3	C	727	GLN	3.8
1	A	110	LEU	3.6
1	A	367	PRO	3.6
2	B	74	ASN	3.5
3	C	737	ARG	3.4
1	A	247	VAL	3.4
1	A	364	GLU	3.1
1	A	297	ASN	3.1
3	C	745	THR	3.0
1	A	370	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
3	C	741	LEU	3.0
1	A	250	ILE	3.0
1	A	374	CYS	2.8
1	A	198	TYR	2.7
1	A	362	TYR	2.7
3	C	739	VAL	2.7
1	A	193	LEU	2.7
1	A	326	LYS	2.7
1	A	208	ILE	2.6
1	A	240	TYR	2.6
1	A	261	LEU	2.6
2	B	244	GLU	2.6
1	A	178	LEU	2.5
1	A	131	ALA	2.5
1	A	369	ILE	2.5
3	C	735	ILE	2.4
3	C	733	ASN	2.4
1	A	249	THR	2.3
3	C	750	SER	2.3
3	C	740	LYS	2.2
1	A	360	GLN	2.2
1	A	221	LEU	2.2
1	A	204	ALA	2.2
1	A	22	ALA	2.2
1	A	248	ILE	2.1
1	A	142	LEU	2.1
1	A	160	THR	2.0
1	A	129	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, 95<sup>th</sup> 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.

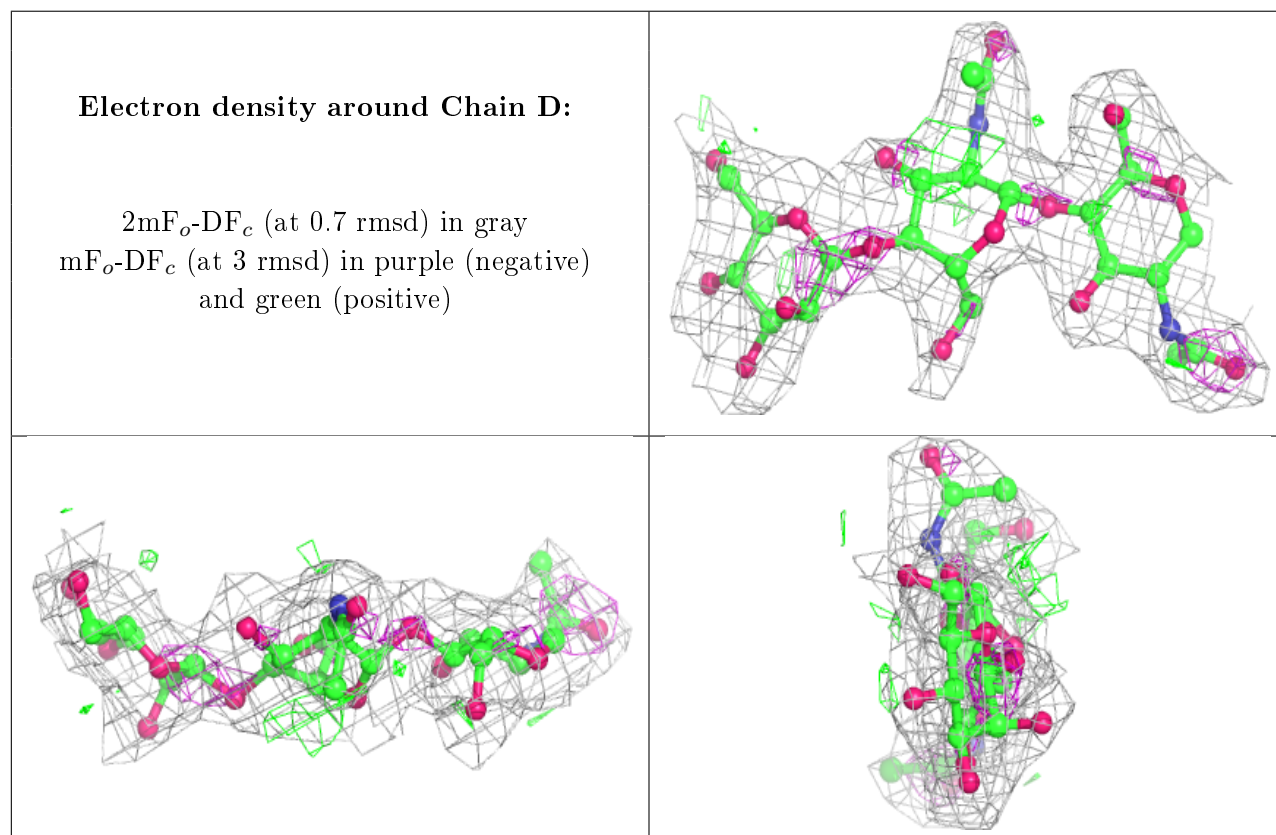
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	HIC	A	73	11/12	0.89	0.17	48,49,53,58	0

### 6.3 Carbohydrates ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	BMA	D	3	11/12	0.80	0.35	79,80,82,82	0
4	NAG	D	2	14/15	0.83	0.27	70,72,76,78	0
4	NAG	D	1	14/15	0.91	0.19	54,58,61,66	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.

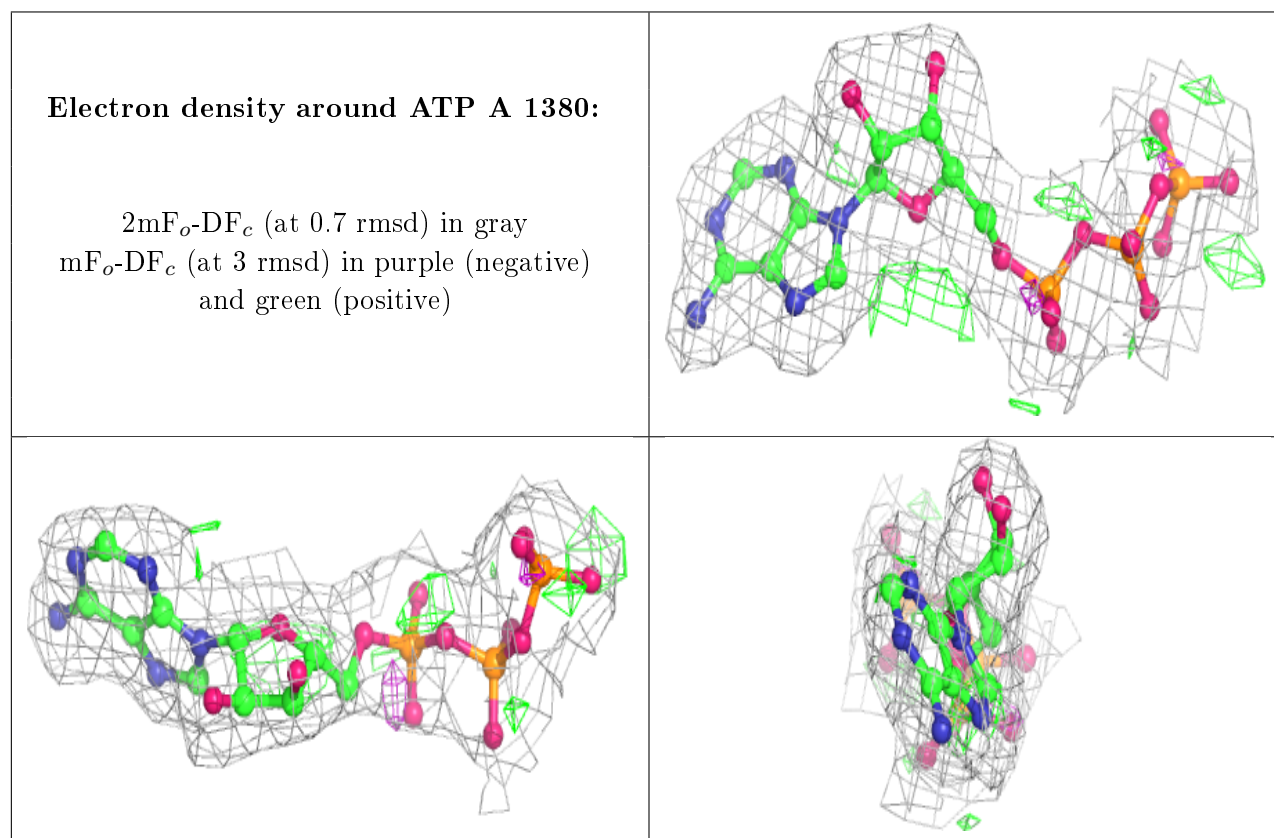


### 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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
7	MG	B	1274	1/1	0.92	0.17	42,42,42,42	0
5	CA	B	1273	1/1	0.96	0.05	36,36,36,36	0
6	ATP	A	1380	31/31	0.96	0.10	59,65,67,68	0
5	CA	A	1381	1/1	0.97	0.13	64,64,64,64	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.