



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 05:20 PM BST

PDB ID : 6Y74
Title : X-ray crystal structure of human carbonic anhydrase IX catalytic domain.
Authors : Fisher, S.Z.; Koruza, K.
Deposited on : 2020-02-28
Resolution : 1.53 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

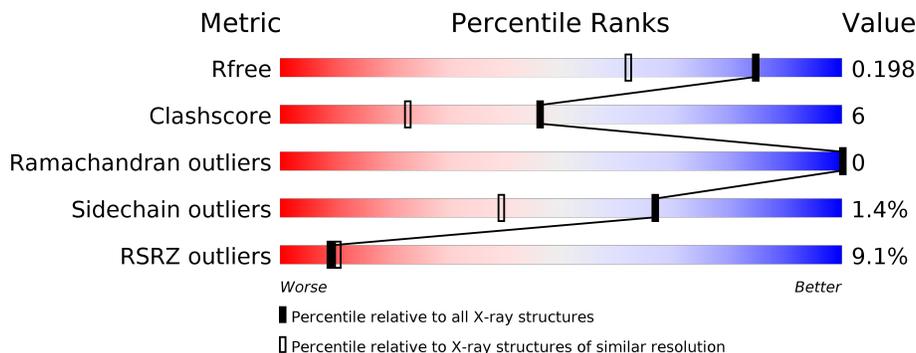
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.53 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	2556 (1.56-1.52)
Clashscore	141614	2634 (1.56-1.52)
Ramachandran outliers	138981	2580 (1.56-1.52)
Sidechain outliers	138945	2577 (1.56-1.52)
RSRZ outliers	127900	2524 (1.56-1.52)

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	258	 7% 88% 11% 5%
1	B	258	 11% 93% 5% 5%
2	C	3	 100%
3	D	2	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	ACT	A	507	-	-	X	-
6	ACT	B	505	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4815 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 Carbonic anhydrase 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	258	Total	C	N	O	S	0	17	0
			2085	1334	370	373	8			
1	B	258	Total	C	N	O	S	0	12	0
			2057	1311	361	379	6			

- Molecule 2 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
			Total	C	N	O			
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

- 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
			Total	C	N	O			
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

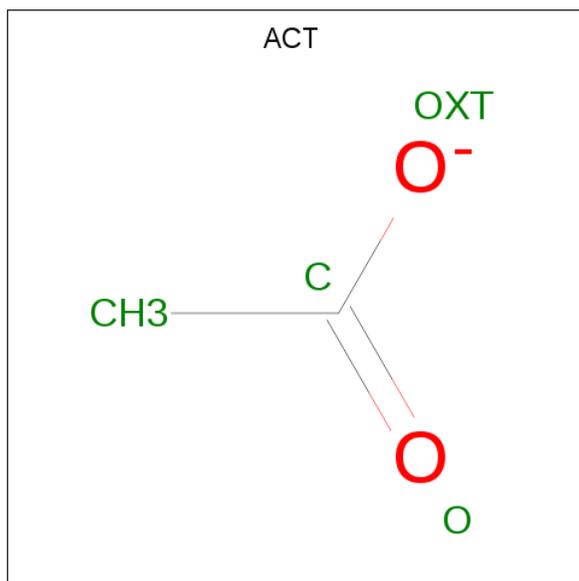
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by author).

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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		
5	A	2	Total	Cl	0	0
			2	2		

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	295	Total	O	0	10
			305	305		

Continued on next page...

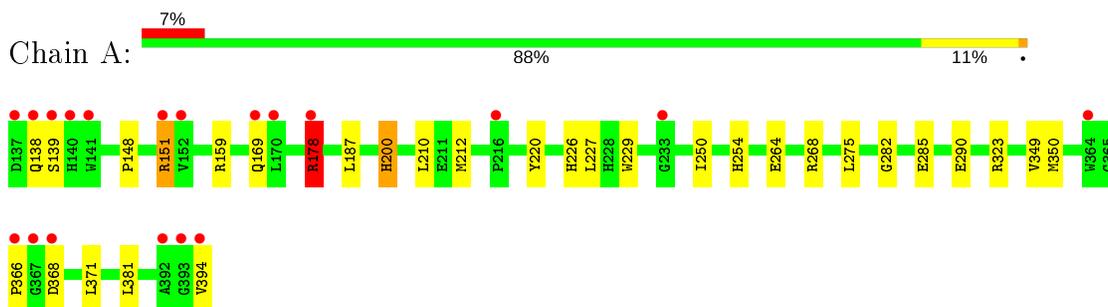
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	282	Total 288	O 288	0	6

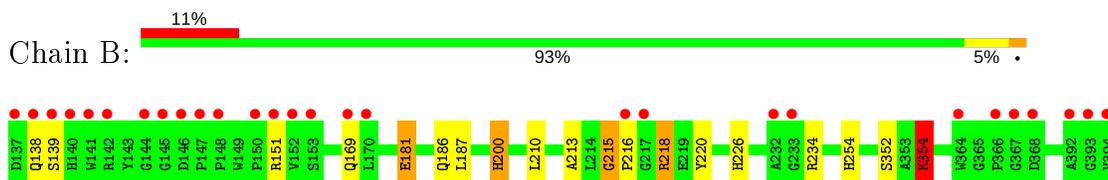
3 Residue-property plots [i](#)

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.

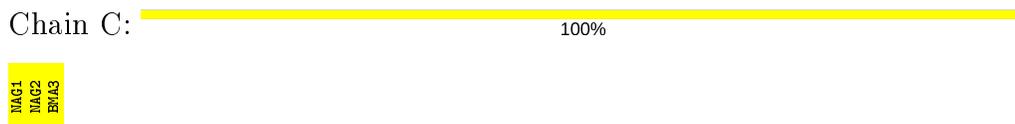
- Molecule 1: Carbonic anhydrase 9



- Molecule 1: Carbonic anhydrase 9



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



- Molecule 3: 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	113.93Å 78.34Å 74.32Å 90.00° 128.22° 90.00°	Depositor
Resolution (Å)	37.13 – 1.53 37.13 – 1.53	Depositor EDS
% Data completeness (in resolution range)	98.3 (37.13-1.53) 98.3 (37.13-1.53)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 1.53Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.174 , 0.198 0.174 , 0.198	Depositor DCC
R_{free} test set	3703 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	15.6	Xtrriage
Anisotropy	0.193	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.086 for -h-2*1,-k,l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4815	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.82% 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: ACT, ZN, BMA, NAG, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.74	0/2196	0.77	4/2997 (0.1%)
1	B	0.79	4/2147 (0.2%)	0.81	7/2932 (0.2%)
All	All	0.77	4/4343 (0.1%)	0.79	11/5929 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	215	GLY	C-N	-7.97	1.19	1.34
1	B	200[A]	HIS	CA-C	5.83	1.68	1.52
1	B	200[B]	HIS	CA-C	5.83	1.68	1.52
1	B	352	SER	CB-OG	-5.21	1.35	1.42

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	354[A]	LYS	CB-CA-C	-8.12	94.17	110.40
1	B	354[B]	LYS	CB-CA-C	-8.12	94.17	110.40
1	B	218	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	B	181[A]	GLU	N-CA-C	5.52	125.91	111.00
1	B	181[B]	GLU	N-CA-C	5.52	125.91	111.00
1	B	354[A]	LYS	CA-C-N	-5.44	105.23	117.20
1	B	354[B]	LYS	CA-C-N	-5.44	105.23	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200[A]	HIS	N-CA-C	5.43	125.65	111.00
1	A	200[B]	HIS	N-CA-C	5.43	125.65	111.00
1	A	178[A]	ARG	N-CA-C	5.25	125.19	111.00
1	A	178[B]	ARG	N-CA-C	5.25	125.19	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	354[A]	LYS	Mainchain
1	B	354[B]	LYS	Mainchain

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	2085	0	2089	35	0
1	B	2057	0	2021	18	0
2	C	39	0	34	0	0
3	D	28	0	25	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
6	A	4	0	3	2	0
6	B	4	0	3	3	0
7	A	305	0	0	13	0
7	B	288	0	0	8	0
All	All	4815	0	4175	53	0

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

All (53) 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:151:ARG:NH2	7:A:601:HOH:O	1.91	1.03
1:A:178[B]:ARG:HG3	1:A:178[B]:ARG:HH11	1.38	0.87
1:A:178[A]:ARG:HH11	1:A:178[A]:ARG:HG3	1.42	0.85
1:A:264:GLU:OE1	7:A:602:HOH:O	1.96	0.82
1:A:268[A]:ARG:NH1	7:A:604:HOH:O	2.15	0.75
1:A:159[B]:ARG:NH2	7:A:606:HOH:O	2.19	0.75
1:A:169:GLN:OE1	1:A:394:VAL:HG12	1.88	0.73
1:B:234:ARG:NH2	7:B:822[B]:HOH:O	2.22	0.72
1:B:186:GLN:OE1	7:B:841[B]:HOH:O	2.07	0.72
1:B:226:HIS:CE1	6:B:505:ACT:H1	2.25	0.71
1:A:226:HIS:CE1	6:A:507:ACT:H3	2.26	0.71
1:A:178[B]:ARG:HH11	1:A:178[B]:ARG:CG	2.02	0.71
1:A:200[B]:HIS:HD2	7:A:817:HOH:O	1.76	0.69
1:A:178[A]:ARG:NH1	1:A:178[A]:ARG:HG3	2.09	0.68
1:B:226:HIS:NE2	6:B:505:ACT:H1	2.08	0.67
1:A:148:PRO:HB2	1:A:151:ARG:HE	1.58	0.67
1:B:151:ARG:NH2	7:B:602:HOH:O	2.28	0.65
1:A:285:GLU:OE2	7:A:603:HOH:O	2.13	0.64
1:A:178[B]:ARG:HG3	1:A:178[B]:ARG:NH1	2.11	0.64
1:A:212[B]:MET:SD	1:A:275:LEU:HG	2.38	0.63
1:A:226:HIS:HE1	6:A:507:ACT:H3	1.63	0.61
1:B:187:LEU:HD21	1:B:210:LEU:HD11	1.83	0.61
1:A:200[B]:HIS:CD2	7:A:817:HOH:O	2.53	0.60
1:B:218:ARG:HG2	7:B:694:HOH:O	2.01	0.60
1:A:366:PRO:O	7:A:605:HOH:O	2.17	0.59
1:B:234:ARG:HG3	7:B:604:HOH:O	2.03	0.58
1:B:151:ARG:CZ	7:B:602:HOH:O	2.54	0.56
1:B:354[B]:LYS:HD2	7:B:781:HOH:O	2.04	0.56
1:A:151:ARG:NH1	7:A:608:HOH:O	2.26	0.55
1:B:181[A]:GLU:HB2	1:B:213:ALA:HB3	1.89	0.54
1:B:138:GLN:CD	1:B:138:GLN:H	2.10	0.54
1:A:220:TYR:HB3	1:A:254:HIS:HB3	1.90	0.54
1:A:323[A]:ARG:NE	7:A:616:HOH:O	2.39	0.53
1:A:282:GLY:HA3	1:A:350[B]:MET:HE2	1.91	0.52
1:A:178[B]:ARG:NH2	7:A:617:HOH:O	2.43	0.51
1:A:178[A]:ARG:NH1	1:A:178[A]:ARG:CG	2.72	0.50
1:A:148:PRO:CB	1:A:151:ARG:HH21	2.26	0.48
1:B:226:HIS:CE1	6:B:505:ACT:CH3	2.96	0.47
1:A:381:LEU:HA	1:A:381:LEU:HD23	1.81	0.47
1:A:187:LEU:HD21	1:A:210:LEU:HD11	1.98	0.44
1:A:159[A]:ARG:HD2	7:A:614:HOH:O	2.18	0.44
1:B:215:GLY:O	1:B:216:PRO:C	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212[B]:MET:SD	1:A:275:LEU:CG	3.05	0.43
1:B:200[B]:HIS:HD2	7:B:827:HOH:O	2.02	0.43
1:A:229:TRP:CZ2	1:A:371:LEU:HD22	2.54	0.42
1:A:148:PRO:HB2	1:A:151:ARG:HH21	1.83	0.42
1:B:220:TYR:HB3	1:B:254:HIS:HB3	2.01	0.42
1:A:227:LEU:HD23	1:A:250:ILE:HA	2.02	0.42
1:B:169:GLN:HG3	1:B:169:GLN:O	2.20	0.42
1:A:290:GLU:OE1	7:A:607:HOH:O	2.21	0.41
1:B:139:SER:OG	1:B:139:SER:O	2.36	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	273/258 (106%)	267 (98%)	6 (2%)	0	100	100
1	B	268/258 (104%)	259 (97%)	9 (3%)	0	100	100
All	All	541/516 (105%)	526 (97%)	15 (3%)	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	227/210 (108%)	219 (96%)	8 (4%)	36	8
1	B	222/210 (106%)	222 (100%)	0	100	100
All	All	449/420 (107%)	441 (98%)	8 (2%)	67	29

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	GLN
1	A	139	SER
1	A	151	ARG
1	A	178[A]	ARG
1	A	178[B]	ARG
1	A	349[A]	VAL
1	A	349[B]	VAL
1	A	368	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	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](#)

5 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
2	NAG	C	1	1,2	14,14,15	1.59	3 (21%)	17,19,21	1.83	4 (23%)
2	NAG	C	2	2	14,14,15	0.93	0	17,19,21	1.87	4 (23%)
2	BMA	C	3	2	11,11,12	0.54	0	15,15,17	1.69	4 (26%)
3	NAG	D	1	1,3	14,14,15	1.49	1 (7%)	17,19,21	1.54	5 (29%)
3	NAG	D	2	3	14,14,15	1.26	2 (14%)	17,19,21	2.78	7 (41%)

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
2	NAG	C	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	NAG	O7-C7	-4.04	1.14	1.23
3	D	1	NAG	O7-C7	-3.86	1.14	1.23
2	C	1	NAG	O5-C1	-2.61	1.39	1.43
3	D	2	NAG	O7-C7	-2.49	1.17	1.23
2	C	1	NAG	C2-N2	-2.15	1.42	1.46
3	D	2	NAG	O5-C1	-2.03	1.40	1.43

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	NAG	O4-C4-C3	-6.00	96.48	110.35
3	D	2	NAG	C4-C3-C2	5.35	118.85	111.02
2	C	2	NAG	C1-O5-C5	4.82	118.72	112.19
2	C	1	NAG	O5-C1-C2	-4.51	104.17	111.29
3	D	2	NAG	O5-C5-C6	4.14	113.70	107.20
3	D	2	NAG	C2-N2-C7	3.95	128.53	122.90
3	D	2	NAG	O5-C1-C2	-3.79	105.30	111.29
2	C	2	NAG	O5-C1-C2	-3.77	105.34	111.29
2	C	1	NAG	C1-O5-C5	3.26	116.61	112.19
2	C	3	BMA	O5-C5-C6	3.09	112.05	107.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	BMA	C1-C2-C3	2.96	113.31	109.67
2	C	2	NAG	C3-C4-C5	-2.75	105.33	110.24
2	C	3	BMA	C6-C5-C4	-2.49	107.17	113.00
3	D	1	NAG	C1-C2-N2	2.48	114.73	110.49
3	D	1	NAG	O7-C7-N2	2.47	126.49	121.95
3	D	1	NAG	O5-C1-C2	-2.47	107.39	111.29
2	C	1	NAG	C4-C3-C2	2.36	114.47	111.02
2	C	3	BMA	O3-C3-C2	2.33	114.46	109.99
3	D	1	NAG	C2-N2-C7	-2.28	119.65	122.90
3	D	2	NAG	C1-C2-N2	-2.23	106.69	110.49
2	C	2	NAG	O6-C6-C5	-2.20	103.74	111.29
3	D	1	NAG	O5-C5-C6	2.13	110.55	107.20
3	D	2	NAG	O7-C7-N2	2.11	125.83	121.95
2	C	1	NAG	C2-N2-C7	-2.05	119.99	122.90

There are no chirality outliers.

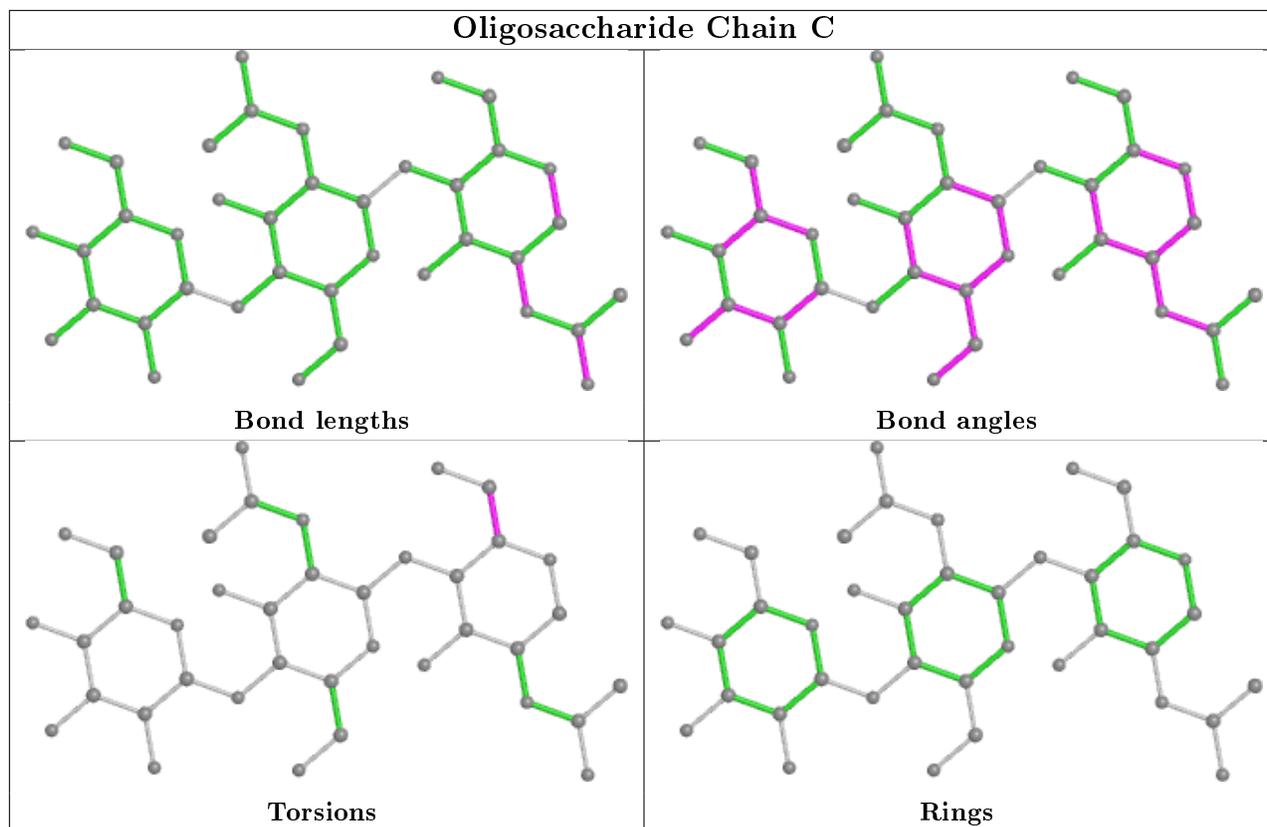
All (3) torsion outliers are listed below:

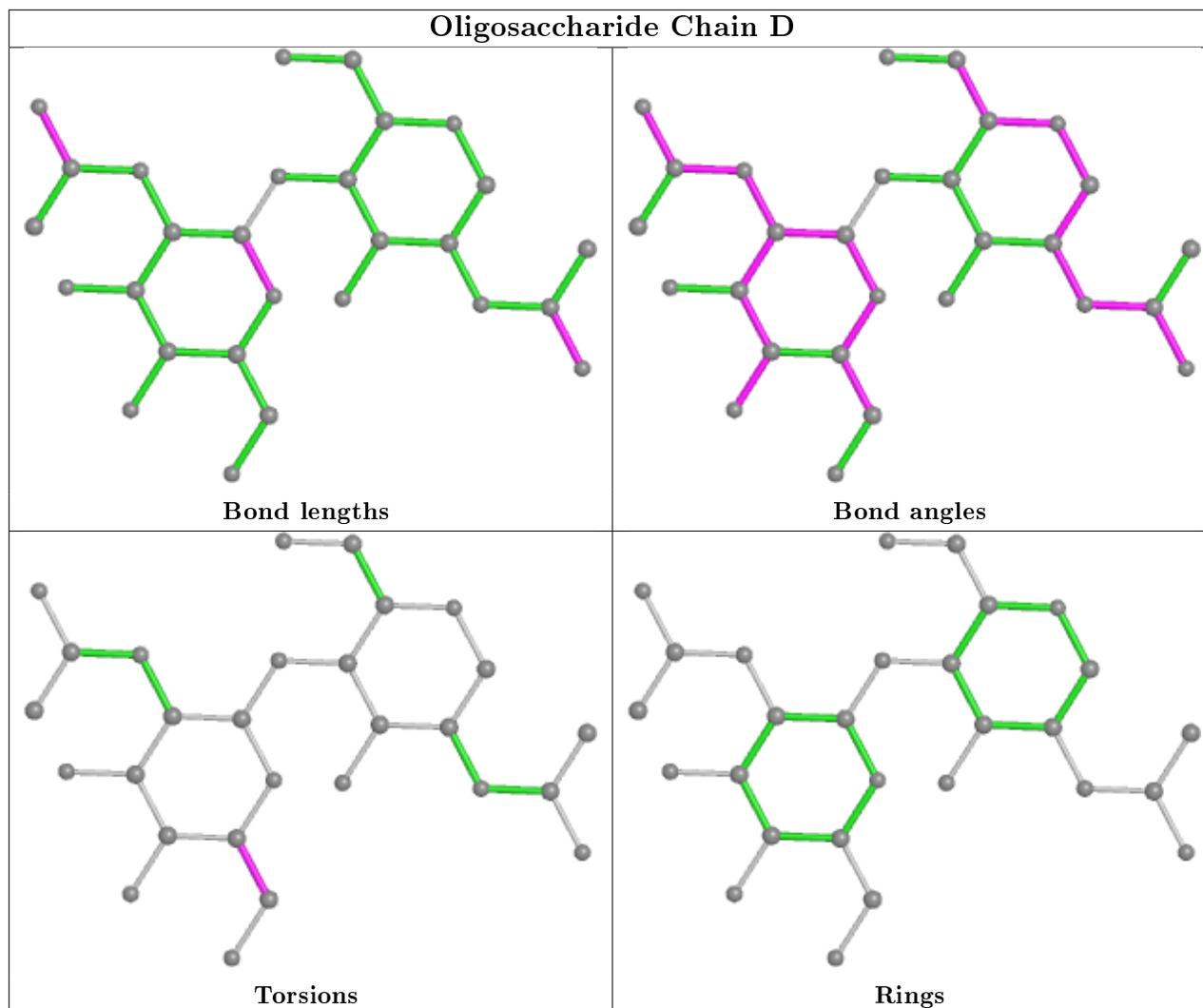
Mol	Chain	Res	Type	Atoms
3	D	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6

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 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 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	ACT	B	505	4	1,3,3	1.38	0	0,3,3	0.00	-
6	ACT	A	507	4	1,3,3	1.54	0	0,3,3	0.00	-

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.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	505	ACT	3	0
6	A	507	ACT	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	215:GLY	C	216:PRO	N	1.19

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	258/258 (100%)	0.76	19 (7%) 14 16	11, 17, 34, 104	0
1	B	258/258 (100%)	0.91	28 (10%) 5 5	10, 16, 47, 107	0
All	All	516/516 (100%)	0.83	47 (9%) 9 10	10, 17, 39, 107	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	138	GLN	21.8
1	B	137	ASP	19.9
1	A	137	ASP	18.8
1	A	138	GLN	18.5
1	B	140	HIS	14.0
1	B	139	SER	14.0
1	B	394	VAL	13.2
1	A	394	VAL	11.2
1	A	140	HIS	9.9
1	A	139	SER	9.3
1	B	147	PRO	8.2
1	B	146[A]	ASP	8.0
1	B	152	VAL	7.4
1	B	393	GLY	5.7
1	B	367	GLY	5.4
1	B	145	GLY	5.4
1	A	366	PRO	5.2
1	B	148	PRO	5.1
1	A	367	GLY	4.9
1	A	393	GLY	4.7
1	B	151	ARG	4.4
1	B	217	GLY	4.3
1	A	364	TRP	4.2
1	A	368	ASP	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	368	ASP	3.9
1	A	392	ALA	3.4
1	B	232	ALA	3.3
1	B	169	GLN	3.2
1	B	216	PRO	3.1
1	A	169	GLN	3.1
1	B	142	ARG	3.1
1	B	141	TRP	3.1
1	A	152	VAL	2.9
1	A	141	TRP	2.9
1	B	392	ALA	2.8
1	B	364	TRP	2.8
1	A	151	ARG	2.7
1	A	233	GLY	2.7
1	A	170	LEU	2.6
1	B	153	SER	2.6
1	A	216	PRO	2.5
1	B	170	LEU	2.5
1	B	233	GLY	2.5
1	A	178[A]	ARG	2.4
1	B	150	PRO	2.4
1	B	366	PRO	2.3
1	B	144	GLY	2.2

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

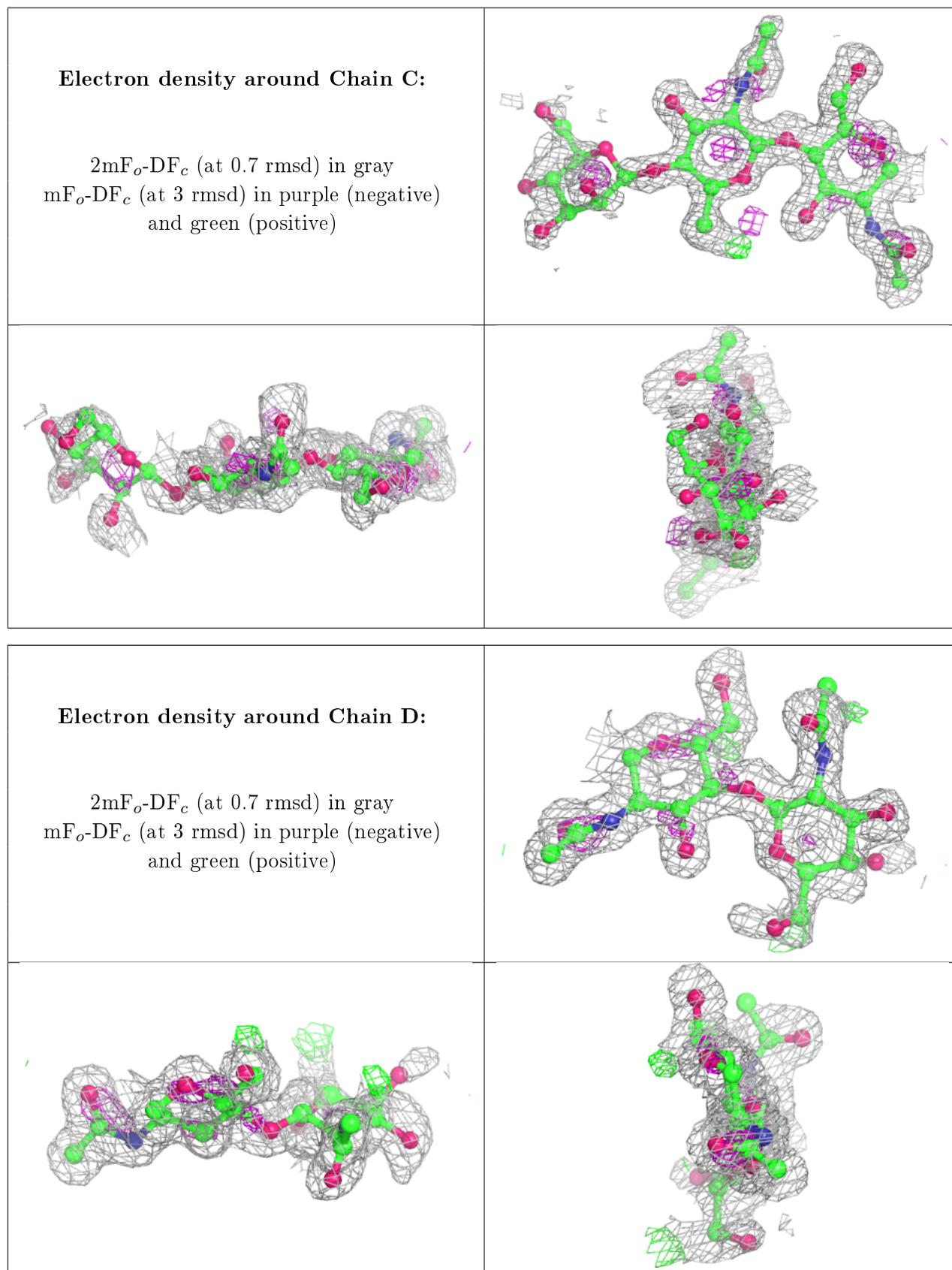
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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
2	BMA	C	3	11/12	0.37	0.40	55,69,84,84	0
2	NAG	C	2	14/15	0.67	0.27	32,37,45,49	0
3	NAG	D	2	14/15	0.78	0.28	30,42,57,64	0
2	NAG	C	1	14/15	0.89	0.14	17,21,25,30	0
3	NAG	D	1	14/15	0.89	0.15	16,19,23,31	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

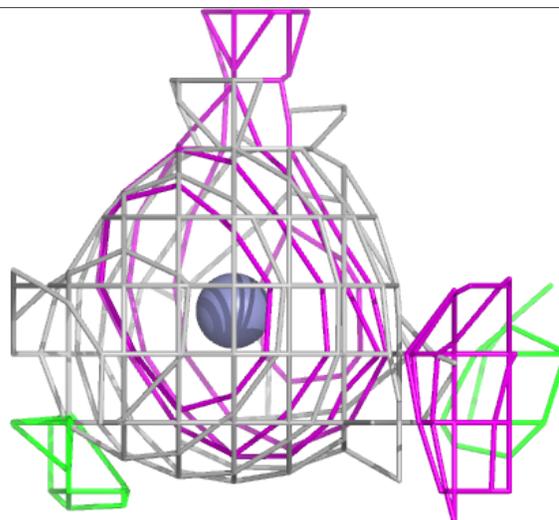
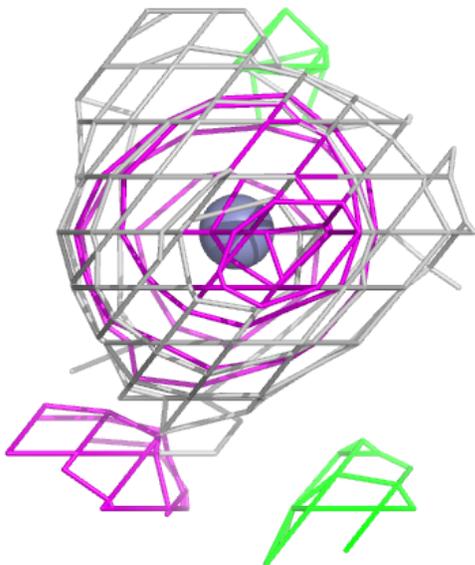
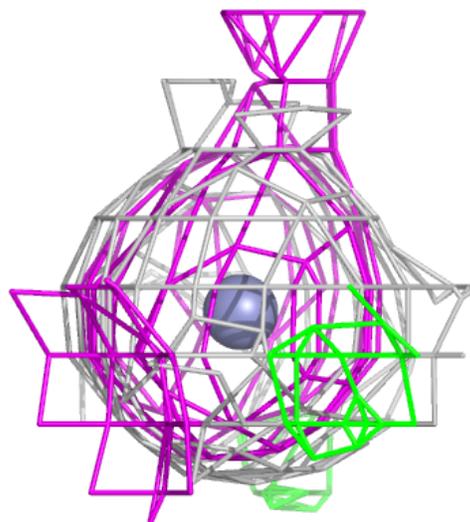
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

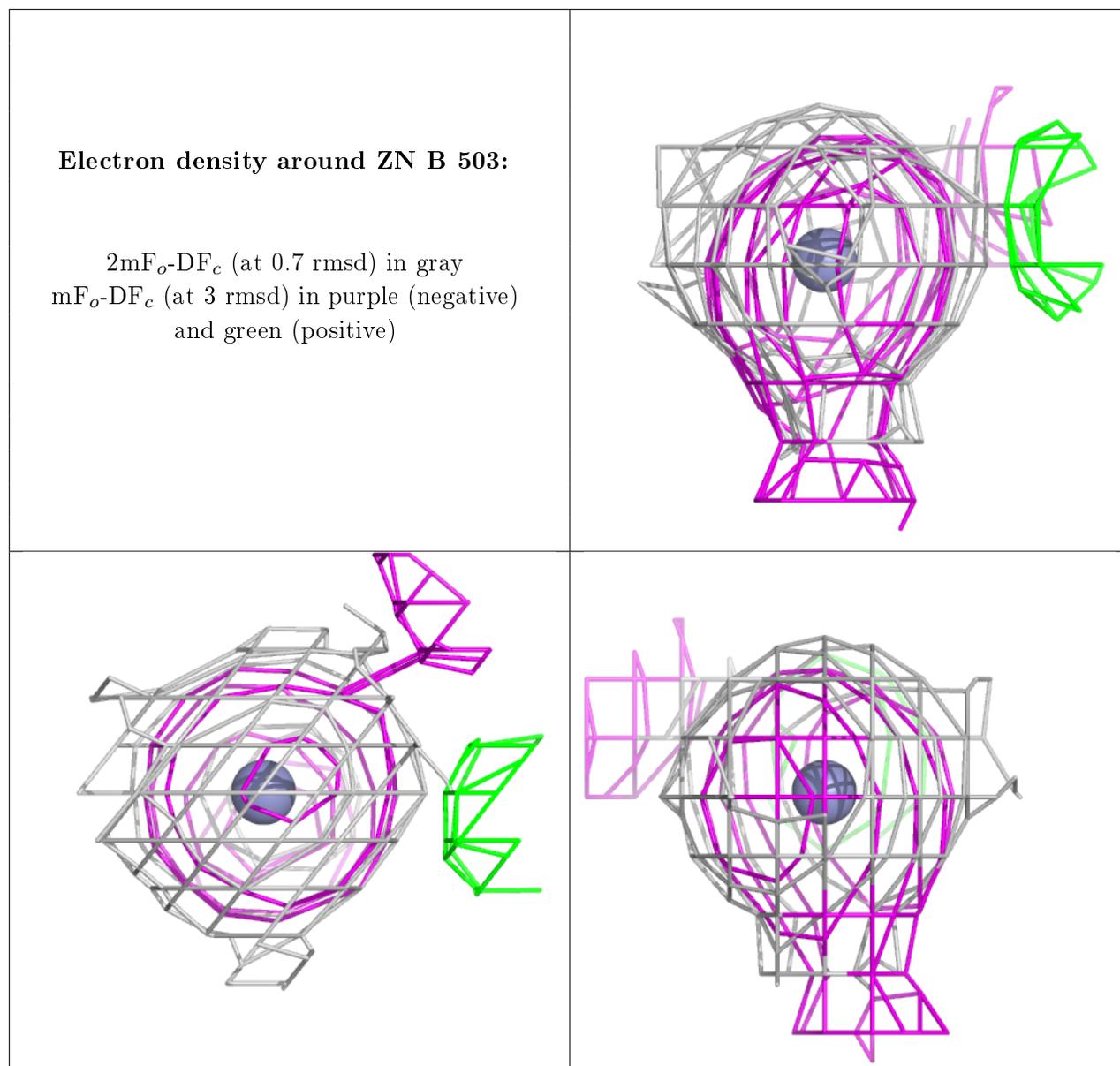
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	ACT	B	505	4/4	0.57	0.27	15,25,29,35	0
6	ACT	A	507	4/4	0.60	0.24	16,22,26,30	0
5	CL	A	506	1/1	0.99	0.05	21,21,21,21	0
5	CL	B	504	1/1	1.00	0.08	14,14,14,14	0
4	ZN	A	504	1/1	1.00	0.06	13,13,13,13	0
4	ZN	B	503	1/1	1.00	0.05	13,13,13,13	0
5	CL	A	505	1/1	1.00	0.09	12,12,12,12	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.

Electron density around ZN A 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.