



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:08 PM UTC

PDB ID : 6AEL / pdb_00006ael
Title : Crystal structure of ENPP1 in complex with 3'3'-cGAMP
Authors : Kato, K.; Nishimasu, H.; Hirano, S.; Hirano, H.; Ishitani, R.; Nureki, O.
Deposited on : 2018-08-05
Resolution : 1.90 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

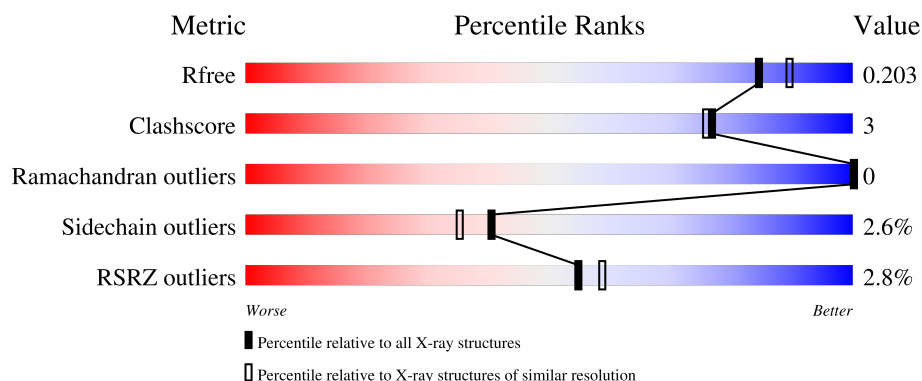
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	738	3% 90% 8% .
2	B	3	33% 33% 33%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	EDO	A	1019	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6373 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.

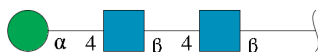
- Molecule 1 is a protein called Ectonucleotide pyrophosphatase/phosphodiesterase 1, isoform CRA_d.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	725	5850	3764	978	1079	29	0	6	0

There are 3 discrepancies between the modelled and reference sequences:

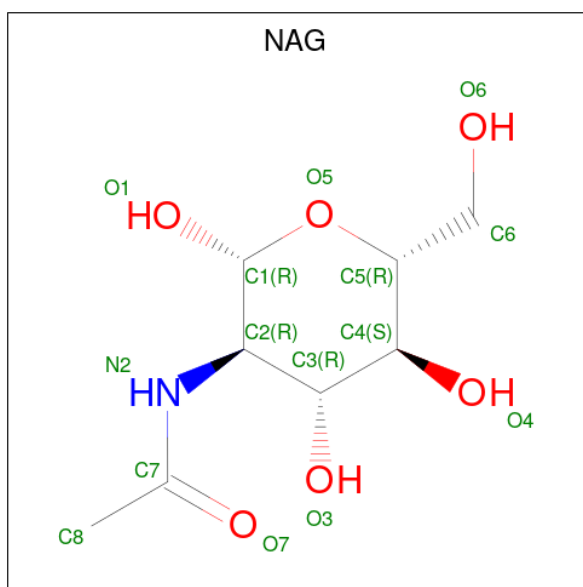
Chain	Residue	Modelled	Actual	Comment	Reference
A	168	GLY	-	See sequence details	UNP G3X9S2
A	169	PRO	-	See sequence details	UNP G3X9S2
A	238	ALA	THR	engineered mutation	UNP G3X9S2

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



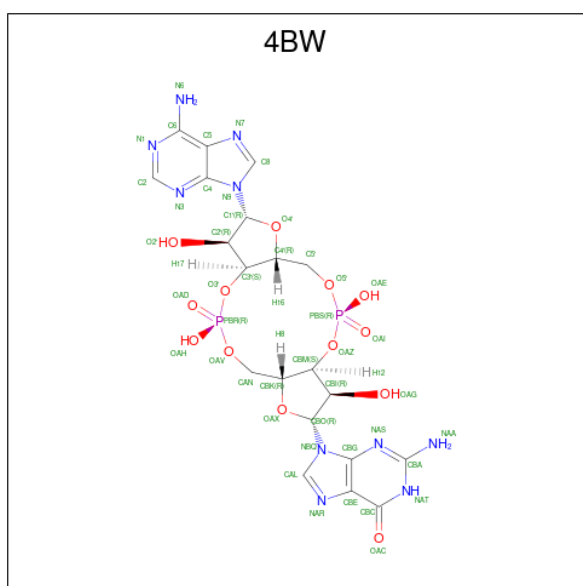
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	3	39	22	2	15	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is 2-amino-9-[(2R,3R,3aS,5R,7aR,9R,10R,10aS,12R,14aR)-9-(6-amino-9H-purin-9-yl)-3,5,10,12-tetrahydroxy-5,12-dioxidoctahydro-2H,7H-difuro[3,2-d:3',2'-j][1,3,7,9,2,8]tetraoxadiphosphacyclododecin-2-yl]-1,9-dihydro-6H-purin-6-one (CCD ID: 4BW) (formula: $C_{20}H_{24}N_{10}O_{13}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			45	20	10	13	2		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Zn	0	0
			2	2		

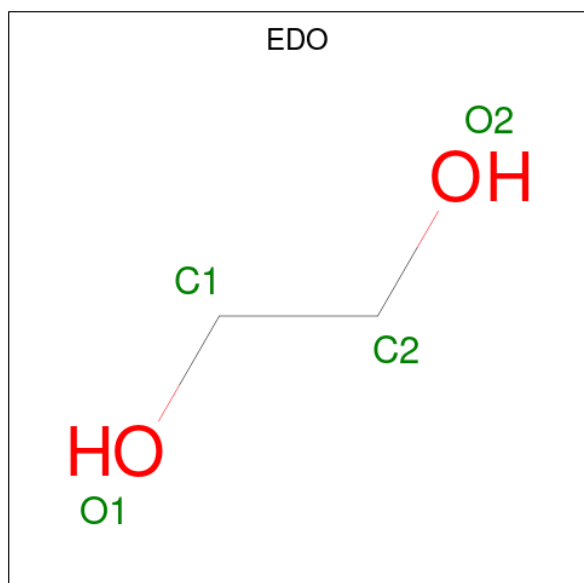
- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	6	Total	Cl	0	0
			6	6		

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

Continued on next page...

Continued from previous page...

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

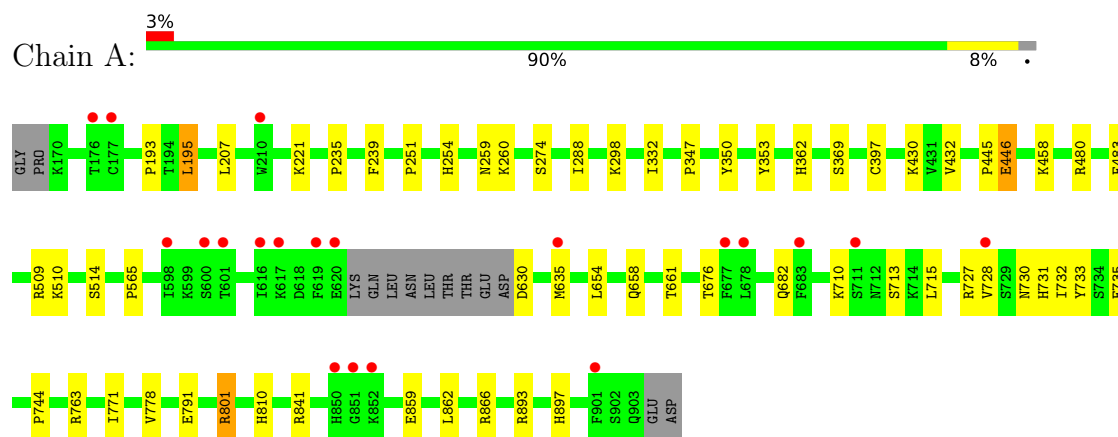
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	356	Total O 356 356	0	0

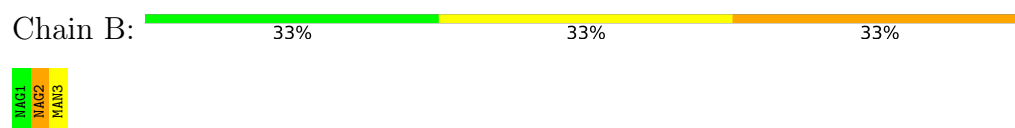
3 Residue-property plots [i](#)

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: Ectonucleotide pyrophosphatase/phosphodiesterase 1, isoform CRA_d



- Molecule 2: alpha-D-mannopyranose-(1-4)-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	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.17Å 94.06Å 74.27Å 90.00° 95.93° 90.00°	Depositor
Resolution (Å)	47.00 – 1.90 47.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.00-1.90) 100.0 (47.00-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 1.90Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.166 , 0.202 0.168 , 0.203	Depositor DCC
R_{free} test set	2894 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.9	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	0.96	EDS
Total number of atoms	6373	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, CA, ZN, NAG, 4BW, MAN, EDO

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	0.30	0/6042	0.47	0/8227

There are no bond length outliers.

There are no bond angle outliers.

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	5850	0	5653	32	0
2	B	39	0	34	1	0
3	A	42	0	39	1	0
4	A	45	0	22	1	0
5	A	2	0	0	0	0
6	A	1	0	0	0	0
7	A	6	0	0	1	0
8	A	32	0	48	6	0
9	A	356	0	0	4	0
All	All	6373	0	5796	34	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 3.

All (34) 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)
8:A:1020:EDO:H21	2:B:2:NAG:H3	1.64	0.80
7:A:1011:CL:CL	8:A:1019:EDO:O1	2.41	0.76
1:A:658:GLN:HB3	1:A:727:ARG:HH22	1.58	0.67
1:A:897:HIS:ND1	9:A:1104:HOH:O	2.28	0.66
1:A:565:PRO:HG2	8:A:1020:EDO:H12	1.80	0.63
1:A:710:LYS:O	1:A:801:ARG:NH2	2.33	0.60
1:A:432:VAL:HG13	8:A:1019:EDO:H21	1.82	0.60
1:A:251:PRO:HA	1:A:254:HIS:CE1	2.42	0.55
1:A:733:TYR:CZ	1:A:735:GLU:HB2	2.42	0.55
1:A:235:PRO:HD3	1:A:483:PHE:CE1	2.42	0.55
1:A:445:PRO:HD2	3:A:1001:NAG:H82	1.90	0.54
1:A:298:LYS:HB2	1:A:347:PRO:HA	1.93	0.51
1:A:195:LEU:HD23	1:A:350:TYR:HB2	1.93	0.51
1:A:658:GLN:HB3	1:A:727:ARG:NH2	2.25	0.51
1:A:430:LYS:HE3	8:A:1019:EDO:H12	1.92	0.51
1:A:676:THR:O	1:A:727:ARG:NH1	2.42	0.50
1:A:362:HIS:O	1:A:514:SER:HB2	2.12	0.50
1:A:763:ARG:NH1	1:A:859:GLU:OE2	2.43	0.48
1:A:207:LEU:HD21	1:A:221:LYS:HD3	1.95	0.48
1:A:509:ARG:HD2	1:A:510:LYS:O	2.15	0.46
1:A:778:VAL:HB	1:A:810:HIS:HB2	1.97	0.46
1:A:353:TYR:OH	4:A:1007:4BW:H21	2.17	0.45
1:A:446:GLU:HG2	9:A:1123:HOH:O	2.16	0.45
1:A:841[A]:ARG:NH1	9:A:1121:HOH:O	2.51	0.43
1:A:480:ARG:HD3	1:A:866:ARG:O	2.19	0.43
1:A:893:ARG:HD2	9:A:1101:HOH:O	2.19	0.42
1:A:193:PRO:HD2	1:A:397:CYS:O	2.19	0.41
1:A:195:LEU:HD23	1:A:350:TYR:CB	2.50	0.41
1:A:446:GLU:HG2	1:A:446:GLU:H	1.63	0.41
1:A:731:HIS:HD2	1:A:732:ILE:O	2.04	0.41
1:A:239:PHE:HB2	1:A:259:ASN:OD1	2.21	0.41
1:A:260:LYS:HD2	8:A:1019:EDO:H22	2.01	0.41
1:A:654:LEU:HB2	1:A:661:THR:HB	2.02	0.40
1:A:715:LEU:HD21	1:A:744:PRO: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	727/738 (98%)	700 (96%)	27 (4%)	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	655/675 (97%)	638 (97%)	17 (3%)	40	35

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	LEU
1	A	274	SER
1	A	288	ILE
1	A	332	ILE
1	A	369	SER
1	A	446	GLU
1	A	458	LYS
1	A	630	ASP
1	A	635	MET
1	A	682	GLN
1	A	713	SER
1	A	728	VAL
1	A	730	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	771	ILE
1	A	791	GLU
1	A	801	ARG
1	A	862	LEU

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

Mol	Chain	Res	Type
1	A	376	GLN
1	A	501	GLN
1	A	730	ASN
1	A	731	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	$\# Z > 2$
2	NAG	B	1	2,1	14,14,15	0.41	0	17,19,21	0.58	0
2	NAG	B	2	2	14,14,15	0.74	1 (7%)	17,19,21	0.66	0
2	MAN	B	3	2	11,11,12	1.13	2 (18%)	15,15,17	0.87	1 (6%)

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	B	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	MAN	B	3	2	-	1/2/19/22	1/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAG	O5-C1	-2.64	1.39	1.43
2	B	3	MAN	C1-C2	2.29	1.57	1.52
2	B	3	MAN	O5-C5	2.18	1.47	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	MAN	O2-C2-C3	-2.02	105.98	110.15

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	3	MAN	C4-C5-C6-O6

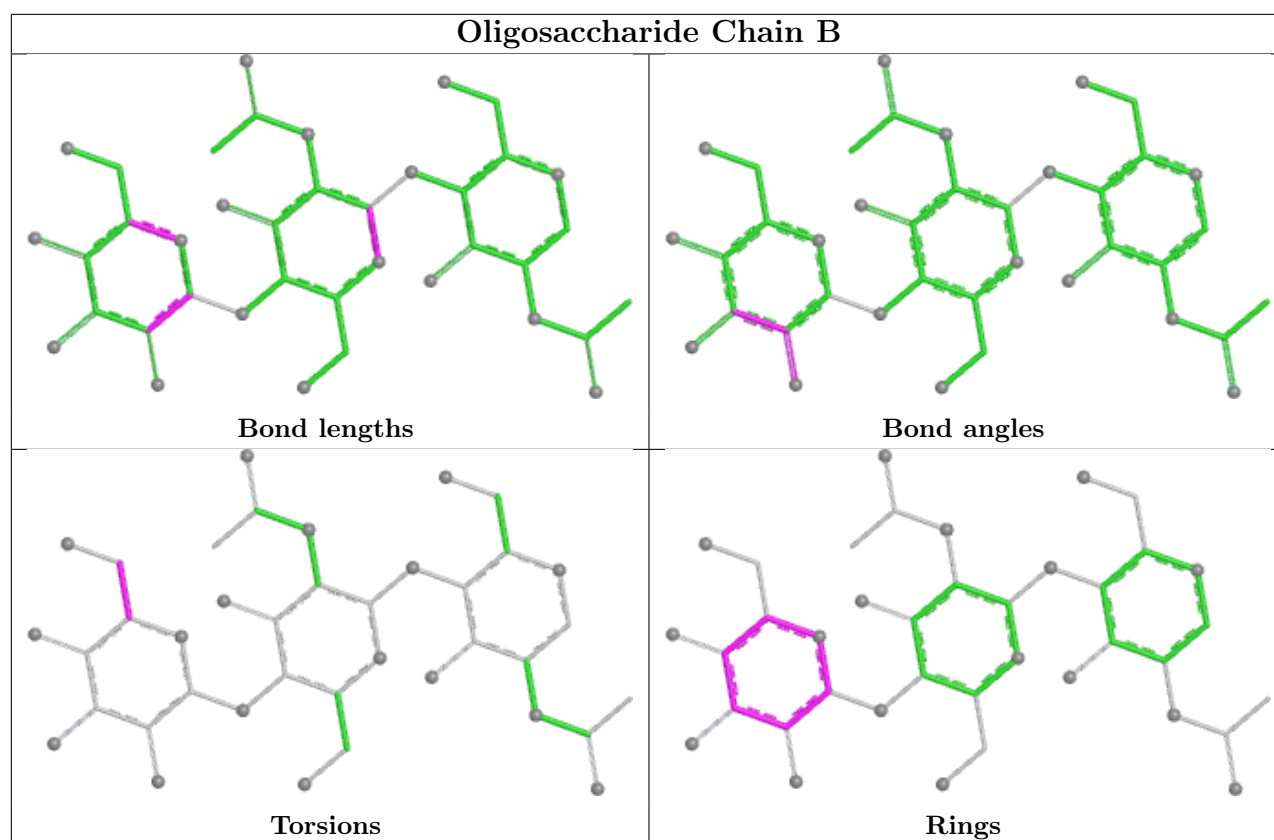
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	3	MAN	C1-C2-C3-C4-C5-O5

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	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 21 ligands modelled in this entry, 9 are monoatomic - leaving 12 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	$\# Z > 2$
4	4BW	A	1007	5	51,51,51	3.28	24 (47%)	76,80,80	2.04	25 (32%)
8	EDO	A	1018	-	3,3,3	0.42	0	2,2,2	0.37	0
8	EDO	A	1024	-	3,3,3	0.43	0	2,2,2	0.35	0
3	NAG	A	1001	1	14,14,15	0.32	0	17,19,21	0.67	1 (5%)
8	EDO	A	1020	-	3,3,3	0.47	0	2,2,2	0.08	0
3	NAG	A	1002	1	14,14,15	0.21	0	17,19,21	0.69	1 (5%)
8	EDO	A	1021	-	3,3,3	0.40	0	2,2,2	0.41	0
8	EDO	A	1019	-	3,3,3	0.27	0	2,2,2	0.53	0
8	EDO	A	1022	-	3,3,3	0.39	0	2,2,2	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	EDO	A	1023	-	3,3,3	0.47	0	2,2,2	0.25	0
3	NAG	A	1003	1	14,14,15	0.69	1 (7%)	17,19,21	0.72	1 (5%)
8	EDO	A	1017	-	3,3,3	0.51	0	2,2,2	0.38	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	4BW	A	1007	5	-	4/30/62/62	0/6/7/7
8	EDO	A	1018	-	-	0/1/1/1	-
8	EDO	A	1024	-	-	0/1/1/1	-
3	NAG	A	1001	1	-	3/6/23/26	0/1/1/1
8	EDO	A	1020	-	-	1/1/1/1	-
3	NAG	A	1002	1	-	0/6/23/26	0/1/1/1
8	EDO	A	1021	-	-	0/1/1/1	-
8	EDO	A	1019	-	-	0/1/1/1	-
8	EDO	A	1022	-	-	0/1/1/1	-
8	EDO	A	1023	-	-	0/1/1/1	-
3	NAG	A	1003	1	-	0/6/23/26	0/1/1/1
8	EDO	A	1017	-	-	0/1/1/1	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1007	4BW	OAX-CBO	8.67	1.62	1.42
4	A	1007	4BW	O4'-C1'	7.51	1.59	1.42
4	A	1007	4BW	CBI-CBO	-7.40	1.30	1.53
4	A	1007	4BW	CBG-NAS	7.20	1.50	1.34
4	A	1007	4BW	O4'-C4'	-6.62	1.30	1.45
4	A	1007	4BW	OAX-CBK	-5.90	1.31	1.45
4	A	1007	4BW	C2'-C1'	-5.85	1.35	1.53
4	A	1007	4BW	CBA-NAS	5.17	1.45	1.33
4	A	1007	4BW	C6-N6	4.79	1.46	1.34
4	A	1007	4BW	C5-C4	-3.70	1.32	1.39
4	A	1007	4BW	CBA-NAT	3.27	1.45	1.37
4	A	1007	4BW	CBA-NAA	3.22	1.41	1.34
4	A	1007	4BW	O3'-C3'	-3.10	1.33	1.44
4	A	1007	4BW	CBE-NAR	-3.05	1.32	1.39
4	A	1007	4BW	PBR-O3'	3.01	1.68	1.59
4	A	1007	4BW	C3'-C4'	2.88	1.60	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1007	4BW	CBC-NAT	2.86	1.44	1.38
4	A	1007	4BW	CBE-CBC	2.43	1.53	1.44
4	A	1007	4BW	PBS-OAZ	2.31	1.66	1.59
3	A	1003	NAG	C1-C2	2.31	1.55	1.52
4	A	1007	4BW	C8-N9	-2.26	1.33	1.37
4	A	1007	4BW	OAC-CBC	-2.07	1.19	1.23
4	A	1007	4BW	OAG-CBI	2.06	1.48	1.43
4	A	1007	4BW	PBS-O5'	2.02	1.67	1.59
4	A	1007	4BW	CAL-NAR	2.00	1.38	1.32

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1007	4BW	N1-C2-N3	-6.02	119.46	128.58
4	A	1007	4BW	C1'-N9-C8	-5.12	115.73	127.09
4	A	1007	4BW	CBE-CBG-NAS	-4.60	121.06	128.39
4	A	1007	4BW	N9-C8-N7	-4.57	107.45	113.94
4	A	1007	4BW	CBA-NAS-CBG	4.25	119.62	112.30
4	A	1007	4BW	C5-C4-N3	-3.96	121.27	126.72
4	A	1007	4BW	C4-N9-C1'	3.77	135.46	126.63
4	A	1007	4BW	C2-N3-C4	3.16	119.54	111.83
4	A	1007	4BW	CBM-CBI-CBO	3.15	106.83	99.89
4	A	1007	4BW	NBQ-CAL-NAR	-2.97	107.89	113.40
4	A	1007	4BW	C4-N9-C8	2.89	108.77	105.74
4	A	1007	4BW	C5-N7-C8	2.76	107.79	103.45
4	A	1007	4BW	NBQ-CBG-NAS	2.69	131.34	125.95
4	A	1007	4BW	CBA-NAT-CBC	-2.61	120.39	125.11
4	A	1007	4BW	OAC-CBC-CBE	-2.58	119.72	126.53
4	A	1007	4BW	CBE-CBC-NAT	2.47	119.55	113.25
4	A	1007	4BW	CBO-NBQ-CAL	-2.44	119.80	126.73
4	A	1007	4BW	C4'-O4'-C1'	-2.36	104.25	109.47
4	A	1007	4BW	N3-C4-N9	2.25	130.99	127.17
4	A	1007	4BW	O4'-C1'-C2'	-2.21	101.89	106.62
3	A	1001	NAG	C1-O5-C5	2.18	115.11	112.19
3	A	1003	NAG	C1-O5-C5	2.16	115.08	112.19
4	A	1007	4BW	PBS-O5'-C5'	-2.15	109.00	121.35
3	A	1002	NAG	C1-O5-C5	2.09	114.98	112.19
4	A	1007	4BW	OAH-PBR-O3'	2.06	115.07	106.70
4	A	1007	4BW	C4-C5-N7	-2.05	108.23	110.58
4	A	1007	4BW	PBR-OAV-CAN	-2.03	109.74	121.35
4	A	1007	4BW	CAL-NAR-CBE	2.01	107.84	104.26

There are no chirality outliers.

All (8) torsion outliers are listed below:

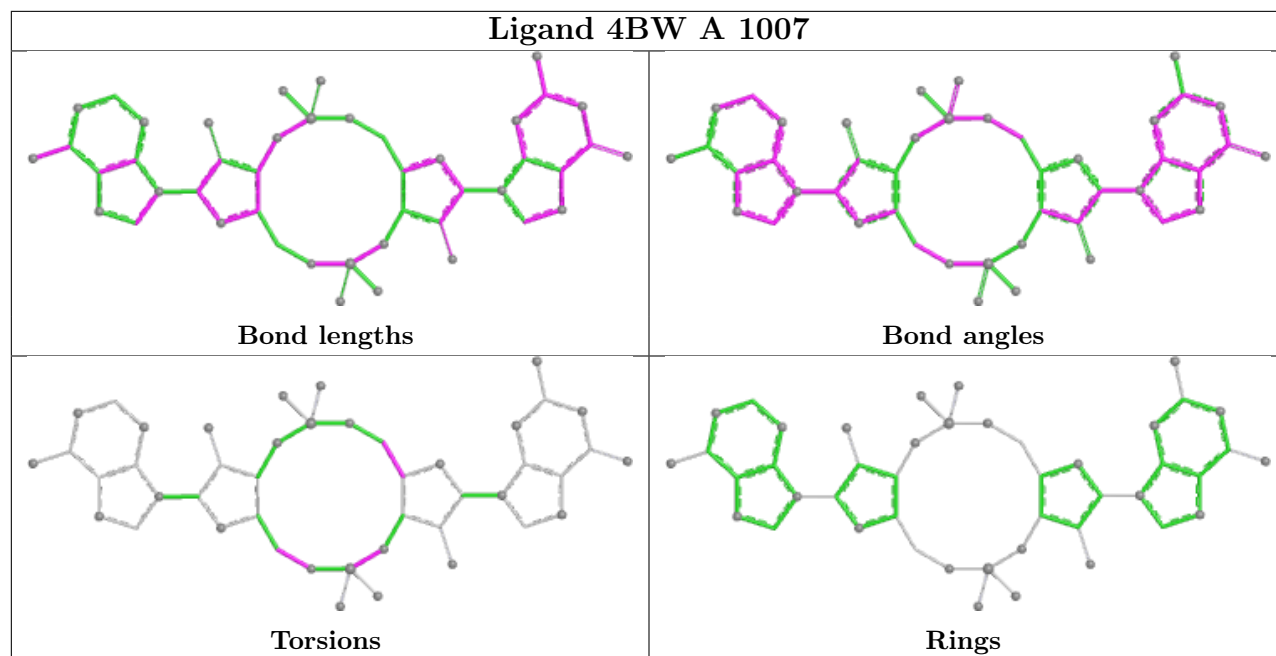
Mol	Chain	Res	Type	Atoms
3	A	1001	NAG	O5-C5-C6-O6
3	A	1001	NAG	C4-C5-C6-O6
4	A	1007	4BW	OAV-CAN-CBK-OAX
4	A	1007	4BW	OAV-CAN-CBK-CBM
3	A	1001	NAG	C1-C2-N2-C7
4	A	1007	4BW	C4'-C5'-O5'-PBS
8	A	1020	EDO	O1-C1-C2-O2
4	A	1007	4BW	CBM-OAZ-PBS-OAI

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1007	4BW	1	0
3	A	1001	NAG	1	0
8	A	1020	EDO	2	0
8	A	1019	EDO	4	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 [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	725/738 (98%)	-0.08	20 (2%) 55 59	13, 33, 63, 86	6 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	677	PHE	4.1
1	A	901	PHE	3.2
1	A	617	LYS	3.1
1	A	210	TRP	2.9
1	A	177	CYS	2.7
1	A	601	THR	2.6
1	A	678	LEU	2.5
1	A	600	SER	2.4
1	A	852	LYS	2.4
1	A	850	HIS	2.3
1	A	635	MET	2.3
1	A	711	SER	2.3
1	A	620	GLU	2.3
1	A	616	ILE	2.2
1	A	619	PHE	2.2
1	A	176	THR	2.2
1	A	598	ILE	2.2
1	A	851	GLY	2.2
1	A	683	PHE	2.1
1	A	728	VAL	2.0

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

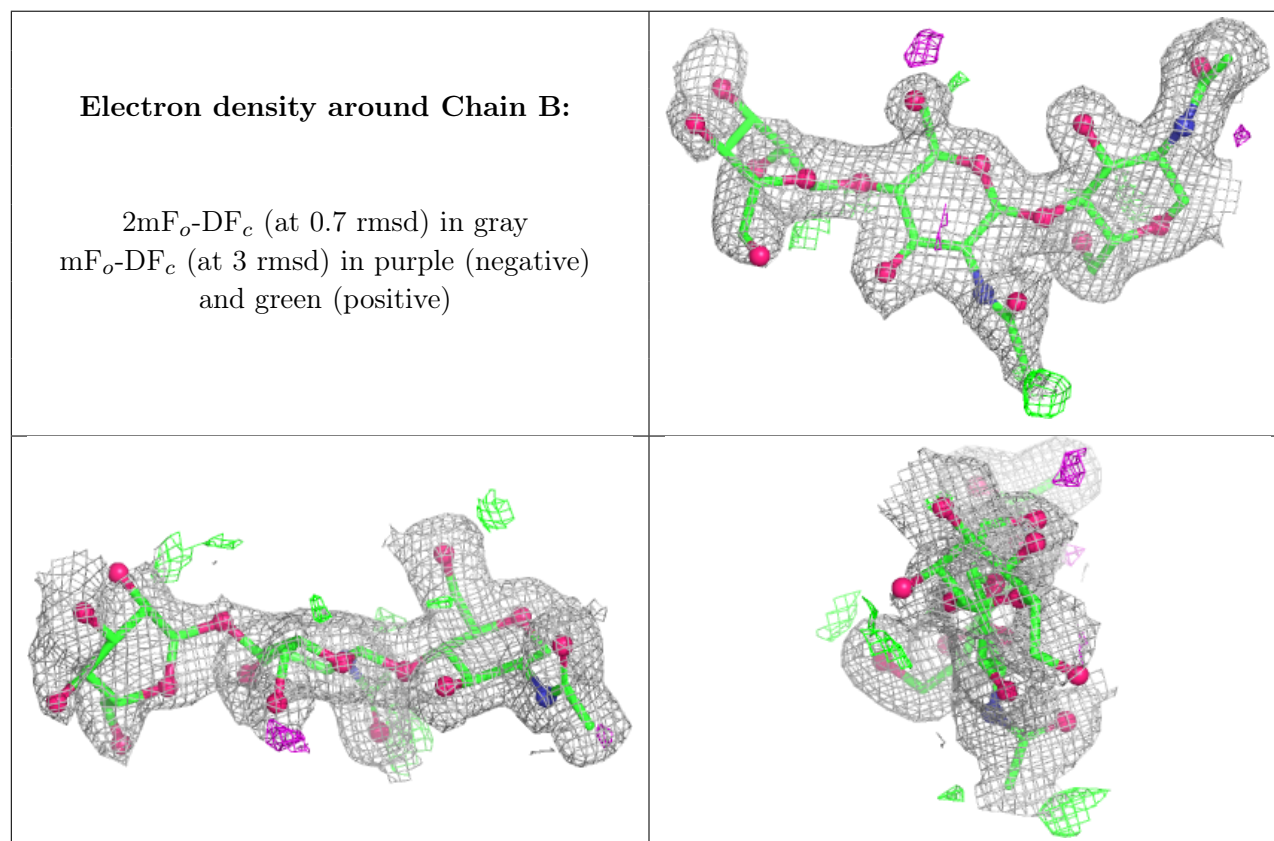
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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	MAN	B	3	11/12	0.61	0.13	71,76,80,81	0
2	NAG	B	2	14/15	0.91	0.10	29,37,49,62	0
2	NAG	B	1	14/15	0.97	0.04	12,17,22,24	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](#)

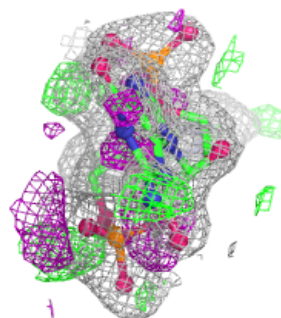
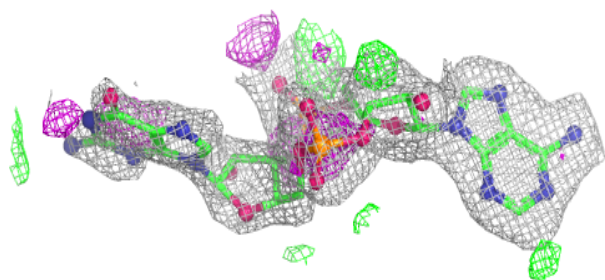
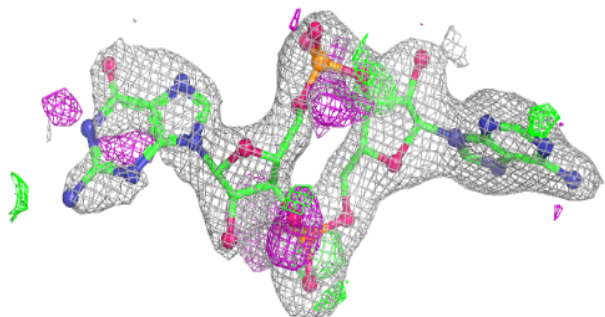
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists 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
3	NAG	A	1002	14/15	0.78	0.13	50,62,64,69	0
3	NAG	A	1001	14/15	0.80	0.13	43,52,60,61	0
8	EDO	A	1021	4/4	0.89	0.12	48,50,53,55	0
4	4BW	A	1007	45/45	0.91	0.12	25,53,71,73	0
8	EDO	A	1023	4/4	0.92	0.10	33,41,45,45	0
3	NAG	A	1003	14/15	0.93	0.07	15,22,30,40	0
7	CL	A	1016	1/1	0.93	0.07	37,37,37,37	0
8	EDO	A	1019	4/4	0.94	0.09	27,31,35,45	0
8	EDO	A	1020	4/4	0.94	0.09	35,35,40,41	0
8	EDO	A	1024	4/4	0.94	0.12	36,49,51,56	0
8	EDO	A	1018	4/4	0.96	0.07	26,28,30,30	0
8	EDO	A	1022	4/4	0.96	0.07	29,31,39,41	0
7	CL	A	1013	1/1	0.96	0.05	41,41,41,41	0
7	CL	A	1012	1/1	0.96	0.10	41,41,41,41	0
8	EDO	A	1017	4/4	0.97	0.06	24,25,26,30	0
5	ZN	A	1008	1/1	0.98	0.08	31,31,31,31	0
5	ZN	A	1009	1/1	0.98	0.10	40,40,40,40	0
7	CL	A	1015	1/1	0.98	0.07	30,30,30,30	0
7	CL	A	1011	1/1	0.99	0.04	40,40,40,40	0
7	CL	A	1014	1/1	0.99	0.05	27,27,27,27	0
6	CA	A	1010	1/1	1.00	0.05	24,24,24,24	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 4BW A 1007:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.