



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 07:26 PM UTC

PDB ID : 2HA0 / pdb_00002ha0
Title : Crystal structure of mouse acetylcholinesterase complexed with 4-ketoamyltri methylammonium
Authors : Bourne, Y.; Radic, Z.; Sulzenbacher, G.; Kim, E.; Taylor, P.; Marchot, P.
Deposited on : 2006-06-12
Resolution : 2.20 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

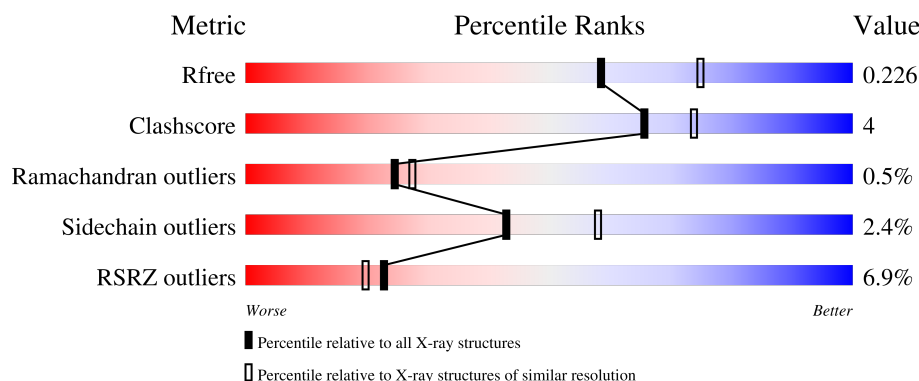
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

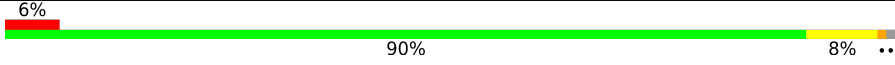
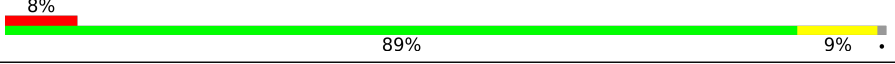
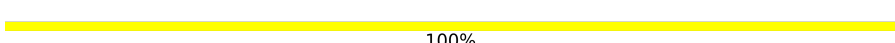
The reported resolution of this entry is 2.20 Å.

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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	543	
1	B	543	
2	C	2	

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
2	FUC	C	2	X	-	-	-
4	IOD	A	702	-	-	X	-
4	IOD	A	705	-	-	X	-
4	IOD	B	1602	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 9175 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 Acetylcholinesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	0	8	0
			4222	2708	739	760	15			
1	B	536	Total	C	N	O	S	0	3	0
			4196	2693	728	761	14			

- Molecule 2 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			24	14	1	9			

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

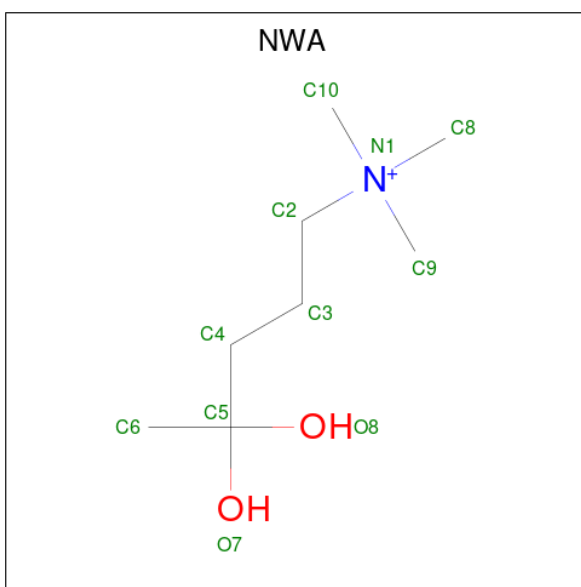


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is IODIDE ION (CCD ID: IOD) (formula: I).

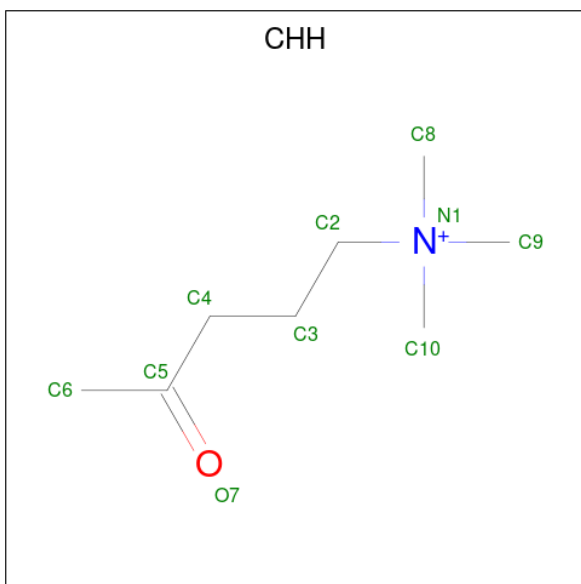
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total	I	0	0
			7	7		
4	B	7	Total	I	0	0
			7	7		

- Molecule 5 is 4,4-DIHYDROXY-N,N,N-TRIMETHYLPENTAN-1-AMINIUM (CCD ID: NWA) (formula: C₈H₂₀NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			10	8	1	1		
5	B	1	Total	C	N	O	0	0
			10	8	1	1		

- Molecule 6 is N,N,N-TRIMETHYL-4-OXOPENTAN-1-AMINIUM (CCD ID: CHH) (formula: C₈H₁₈NO).



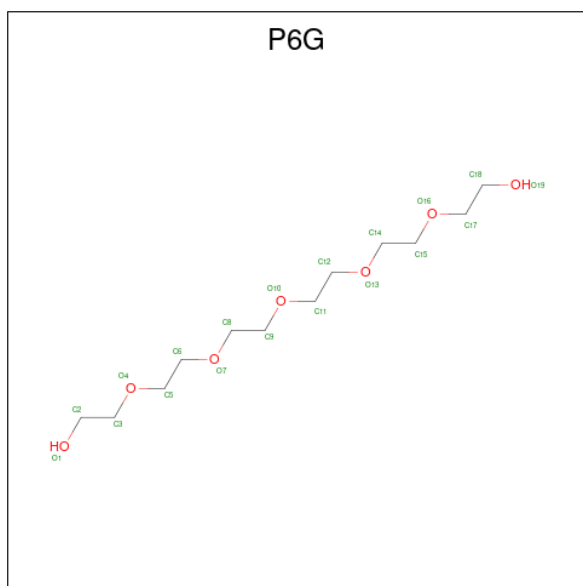
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			10	8	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			10	8	1	1		

- Molecule 7 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			19	12	7		

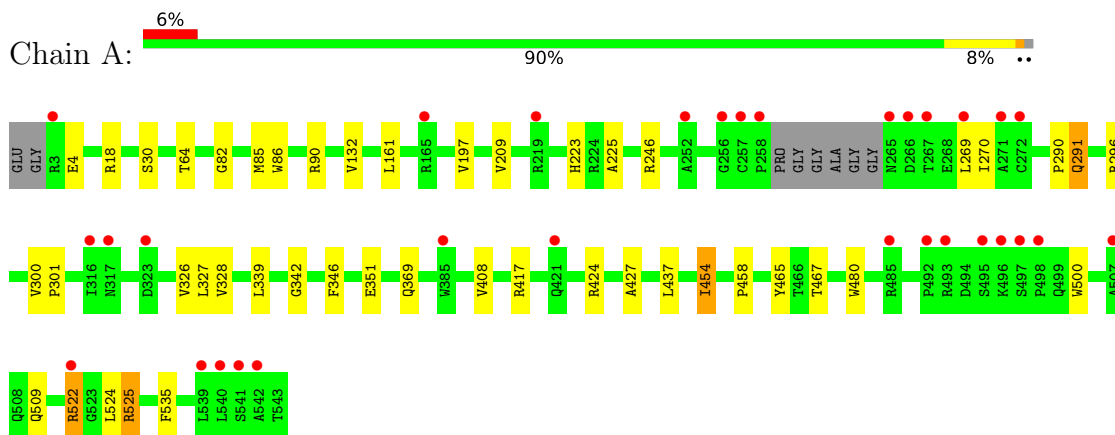
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	333	Total	O	0	0
			333	333		
8	B	299	Total	O	0	0
			299	299		

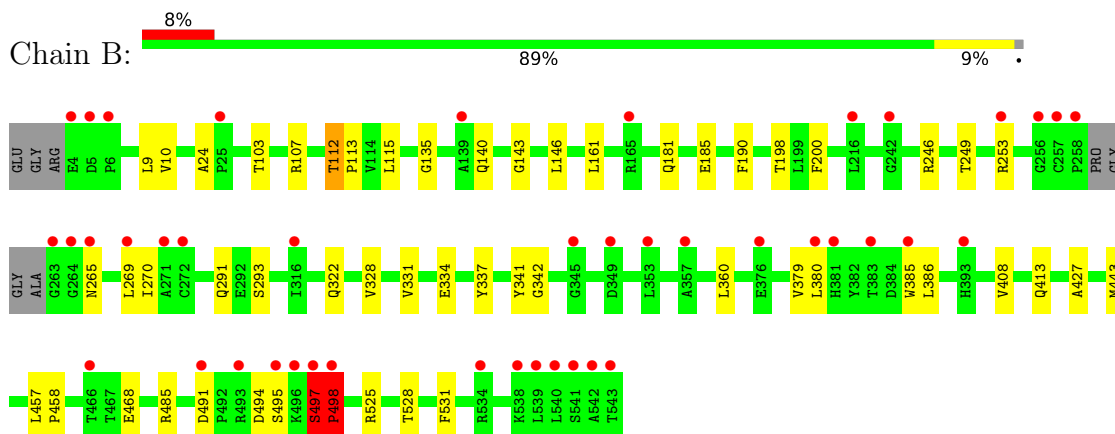
3 Residue-property plots [i](#)

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: Acetylcholinesterase



- Molecule 1: Acetylcholinesterase



- Molecule 2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.23Å 111.80Å 226.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 30.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.00-2.20) 98.0 (30.00-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.83 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.182 , 0.219 0.196 , 0.226	Depositor DCC
R_{free} test set	2019 reflections (1.92%)	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.759	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9175	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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: NAG, NWA, CHH, FUC, IOD, P6G

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	0/4381	0.79	2/5983 (0.0%)
1	B	0.62	0/4332	0.80	0/5918
All	All	0.64	0/8713	0.80	2/11901 (0.0%)

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	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	342	GLY	CA-C-N	-5.78	118.67	122.60
1	A	342	GLY	C-N-CA	-5.78	118.67	122.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	497	SER	Peptide

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	4222	0	4111	30	0
1	B	4196	0	4089	31	0
2	C	24	0	22	0	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
4	A	7	0	0	5	0
4	B	7	0	0	4	0
5	A	10	0	18	0	0
5	B	10	0	18	0	0
6	A	10	0	18	2	0
6	B	10	0	18	1	0
7	A	19	0	26	2	0
8	A	333	0	0	5	0
8	B	299	0	0	5	0
All	All	9175	0	8346	65	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (65) 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)
4:B:1604:IOD:I	8:B:1915:HOH:O	2.26	1.20
4:B:1602:IOD:I	8:B:1929:HOH:O	2.48	1.01
1:B:161:LEU:HD11	1:B:269:LEU:HD22	1.48	0.95
4:A:705:IOD:I	6:A:710:CHH:O7	2.63	0.86
1:A:161:LEU:HD11	1:A:269:LEU:HD22	1.59	0.83
1:A:296:ARG:HE	1:A:369:GLN:HE22	1.27	0.82
1:B:112:THR:HG21	1:B:143:GLY:O	1.82	0.79
4:B:1603:IOD:I	8:B:1706:HOH:O	2.84	0.65
1:A:85[B]:MET:HE1	8:A:923:HOH:O	2.00	0.60
1:B:181[A]:GLN:OE1	8:B:1701:HOH:O	2.17	0.59
4:A:704:IOD:I	8:A:810:HOH:O	2.88	0.57
1:A:4:GLU:OE1	1:A:18:ARG:HD3	2.05	0.57
1:A:197:VAL:H	1:A:223:HIS:HD2	1.55	0.53
1:A:327:LEU:HD11	1:A:500:TRP:CH2	2.44	0.53
1:B:491:ASP:HB3	1:B:494:ASP:HB3	1.91	0.53
1:A:197:VAL:H	1:A:223:HIS:CD2	2.28	0.51
1:A:291:GLN:NE2	8:A:805:HOH:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:VAL:HG12	1:A:328:VAL:HG13	1.94	0.50
1:A:85[B]:MET:CE	8:A:923:HOH:O	2.59	0.49
1:B:112:THR:HG22	1:B:113:PRO:HD2	1.95	0.49
1:A:290:PRO:HD2	4:A:702:IOD:I	2.83	0.48
1:A:458:PRO:HA	1:A:465:TYR:CD2	2.48	0.48
1:B:103:THR:HG21	1:B:190:PHE:HB3	1.94	0.48
1:B:380:LEU:HD22	1:B:385:TRP:CZ2	2.49	0.48
1:A:64:THR:HB	1:A:90[B]:ARG:NH1	2.29	0.47
1:B:24:ALA:HB3	1:B:140:GLN:HG3	1.96	0.47
1:A:85[A]:MET:HE2	1:A:86:TRP:CZ2	2.50	0.47
1:B:181[A]:GLN:CD	8:B:1701:HOH:O	2.58	0.47
1:B:135:GLY:HA3	1:B:146:LEU:HD22	1.96	0.47
1:A:509:GLN:HE21	1:A:522[A]:ARG:NH2	2.13	0.47
1:A:454:ILE:CD1	1:A:480:TRP:CZ2	2.98	0.45
1:A:209:VAL:CG1	1:A:225:ALA:HB1	2.47	0.45
1:B:113:PRO:HG2	1:B:485:ARG:HG2	1.97	0.45
1:B:249:THR:HG22	1:B:253[A]:ARG:NH2	2.31	0.45
1:A:351:GLU:OE1	8:A:801:HOH:O	2.21	0.45
1:B:408:VAL:HG11	1:B:525:ARG:HG3	1.99	0.45
4:A:705:IOD:I	6:A:710:CHH:C5	3.35	0.45
1:A:296:ARG:HE	1:A:369:GLN:NE2	2.05	0.44
1:A:535:PHE:CE2	7:A:711:P6G:H112	2.53	0.43
1:B:360:LEU:HD22	1:B:379:VAL:HG21	1.99	0.43
1:A:291:GLN:HB2	4:A:702:IOD:I	2.89	0.43
1:B:115:LEU:HD23	1:B:198:THR:HB	1.99	0.43
1:B:337:TYR:HA	1:B:443:MET:CE	2.48	0.43
1:B:161:LEU:HD12	1:B:270:ILE:HD11	2.00	0.43
1:B:328:VAL:O	1:B:427:ALA:HA	2.17	0.43
1:B:181[B]:GLN:HE21	1:B:185:GLU:HG3	1.84	0.43
1:B:341:TYR:CZ	6:B:1610:CHH:H63	2.54	0.43
7:A:711:P6G:H61	1:B:380:LEU:HB3	2.01	0.43
1:B:331:VAL:HG22	1:B:334:GLU:CD	2.44	0.42
1:A:339:LEU:HD13	1:A:346:PHE:CE2	2.54	0.42
1:A:326:VAL:HG12	1:A:328:VAL:CG1	2.50	0.42
1:B:528:THR:O	1:B:531:PHE:HB3	2.20	0.42
1:B:10:VAL:HG22	1:B:107:ARG:NH1	2.35	0.42
1:B:161:LEU:HD12	1:B:270:ILE:CG1	2.50	0.42
1:B:380:LEU:HD22	1:B:385:TRP:HZ2	1.85	0.42
1:A:82:GLY:HA2	1:A:85[B]:MET:HE3	2.01	0.41
1:A:522[B]:ARG:CZ	1:B:386:LEU:HD22	2.50	0.41
1:A:161:LEU:HD12	1:A:270:ILE:CG1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:VAL:O	1:A:427:ALA:HA	2.20	0.41
1:B:457:LEU:N	1:B:458:PRO:CD	2.84	0.41
1:A:300:VAL:HB	1:A:301:PRO:HD2	2.03	0.41
1:B:293:SER:OG	4:B:1602:IOD:I	3.07	0.41
1:B:497:SER:C	1:B:498:PRO:O	2.64	0.41
1:A:408:VAL:HG11	1:A:525:ARG:HG3	2.03	0.41
1:A:522[B]:ARG:NH2	1:B:386:LEU:HD22	2.36	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	539/543 (99%)	523 (97%)	16 (3%)	0	100	100
1	B	535/543 (98%)	515 (96%)	15 (3%)	5 (1%)	14	14
All	All	1074/1086 (99%)	1038 (97%)	31 (3%)	5 (0%)	24	27

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	265	ASN
1	B	498	PRO
1	B	495	SER
1	B	497	SER
1	B	342	GLY

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	448/443 (101%)	435 (97%)	13 (3%)	37	51
1	B	443/443 (100%)	434 (98%)	9 (2%)	48	64
All	All	891/886 (101%)	869 (98%)	22 (2%)	43	56

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	SER
1	A	132	VAL
1	A	246	ARG
1	A	291	GLN
1	A	417	ARG
1	A	424	ARG
1	A	437	LEU
1	A	454	ILE
1	A	467	THR
1	A	522[A]	ARG
1	A	522[B]	ARG
1	A	524	LEU
1	A	525	ARG
1	B	9	LEU
1	B	112	THR
1	B	200	PHE
1	B	246	ARG
1	B	291	GLN
1	B	322	GLN
1	B	413	GLN
1	B	468	GLU
1	B	498	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	181	GLN
1	A	184	GLN
1	A	223	HIS
1	A	291	GLN

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Mol	Chain	Res	Type
1	A	322	GLN
1	A	369	GLN
1	A	381	HIS
1	A	474	GLN
1	A	499	GLN
1	A	509	GLN
1	B	291	GLN
1	B	381	HIS
1	B	474	GLN

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 ⓘ

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	$\# Z > 2$
2	NAG	C	1	2,1	14,14,15	0.64	0	17,19,21	1.33	2 (11%)
2	FUC	C	2	2	10,10,11	0.69	0	14,14,16	1.86	2 (14%)

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	2,1	-	2/6/23/26	0/1/1/1
2	FUC	C	2	2	1/1/4/5	-	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(°)
2	C	2	FUC	C1-C2-C3	-5.14	102.16	109.64
2	C	1	NAG	C1-O5-C5	3.19	116.45	112.19
2	C	2	FUC	O5-C5-C4	2.52	114.08	109.55
2	C	1	NAG	O5-C1-C2	-2.19	107.90	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	2	FUC	C1

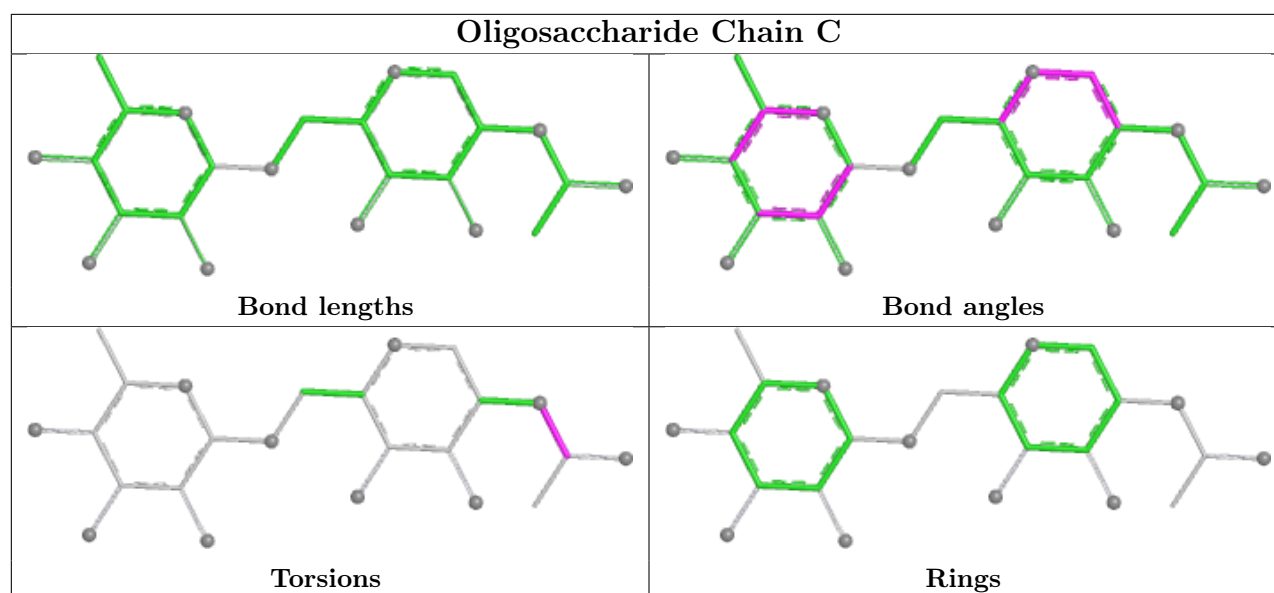
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	O7-C7-N2-C2
2	C	1	NAG	C8-C7-N2-C2

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 21 ligands modelled in this entry, 14 are monoatomic - leaving 7 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	$\# Z > 2$
3	NAG	A	701	1	14,14,15	0.53	0	17,19,21	1.11	1 (5%)
6	CHH	B	1610	-	9,9,9	0.78	0	11,12,12	0.66	0
5	NWA	B	1609	1	9,9,10	0.74	0	11,12,15	0.34	0
7	P6G	A	711	-	18,18,18	2.21	6 (33%)	17,17,17	1.36	1 (5%)
3	NAG	B	1601	1	14,14,15	0.53	0	17,19,21	1.73	1 (5%)
6	CHH	A	710	-	9,9,9	0.79	0	11,12,12	0.65	0
5	NWA	A	709	1	9,9,10	0.74	0	11,12,15	0.43	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
3	NAG	A	701	1	-	2/6/23/26	0/1/1/1
6	CHH	B	1610	-	-	3/7/7/7	-
5	NWA	B	1609	1	-	0/7/7/8	-
7	P6G	A	711	-	-	7/16/16/16	-
3	NAG	B	1601	1	-	4/6/23/26	0/1/1/1
6	CHH	A	710	-	-	2/7/7/7	-
5	NWA	A	709	1	-	0/7/7/8	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	711	P6G	O10-C9	4.40	1.61	1.42
7	A	711	P6G	O13-C12	4.04	1.59	1.42
7	A	711	P6G	O19-C18	3.65	1.60	1.42
7	A	711	P6G	O4-C3	3.42	1.56	1.42
7	A	711	P6G	O16-C15	3.36	1.56	1.42
7	A	711	P6G	O7-C6	2.43	1.52	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1601	NAG	C1-O5-C5	6.40	120.76	112.19
7	A	711	P6G	O1-C2-C3	3.16	130.41	111.82
3	A	701	NAG	O5-C5-C6	2.22	111.97	107.66

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1601	NAG	C8-C7-N2-C2
3	B	1601	NAG	O7-C7-N2-C2
6	B	1610	CHH	C3-C4-C5-O7
6	B	1610	CHH	C3-C4-C5-C6
3	B	1601	NAG	O5-C5-C6-O6
3	B	1601	NAG	C4-C5-C6-O6
7	A	711	P6G	O16-C17-C18-O19
6	B	1610	CHH	N1-C2-C3-C4
7	A	711	P6G	O1-C2-C3-O4
3	A	701	NAG	C8-C7-N2-C2
7	A	711	P6G	O4-C5-C6-O7
6	A	710	CHH	C3-C4-C5-O7

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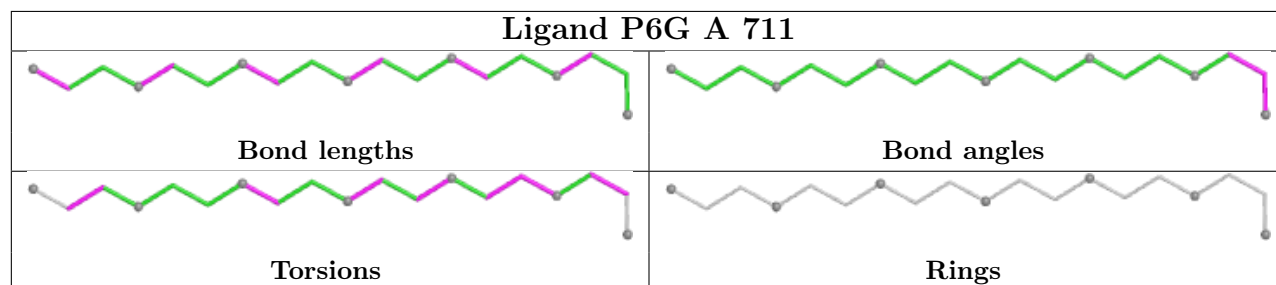
Mol	Chain	Res	Type	Atoms
6	A	710	CHH	C3-C4-C5-C6
3	A	701	NAG	O7-C7-N2-C2
7	A	711	P6G	C11-C12-O13-C14
7	A	711	P6G	C8-C9-O10-C11
7	A	711	P6G	C9-C8-O7-C6
7	A	711	P6G	C6-C5-O4-C3

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1610	CHH	1	0
7	A	711	P6G	2	0
6	A	710	CHH	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 ⓘ

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	535/543 (98%)	0.52	31 (5%)	29 25	30, 53, 74, 105	8 (1%)
1	B	536/543 (98%)	0.68	43 (8%)	18 16	32, 58, 79, 106	3 (0%)
All	All	1071/1086 (98%)	0.60	74 (6%)	23 20	30, 55, 78, 106	11 (1%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	497	SER	7.3
1	A	541	SER	6.0
1	A	3	ARG	5.7
1	B	258	PRO	5.5
1	B	495	SER	5.5
1	B	498	PRO	4.8
1	A	323	ASP	4.5
1	B	542	ALA	4.4
1	A	317	ASN	4.4
1	A	258	PRO	4.3
1	A	316	ILE	4.1
1	B	496	LYS	4.0
1	B	272	CYS	4.0
1	B	263	GLY	4.0
1	B	4	GLU	4.0
1	B	253[A]	ARG	3.9
1	A	272	CYS	3.8
1	B	540	LEU	3.8
1	B	539	LEU	3.7
1	A	496	LYS	3.7
1	A	522[A]	ARG	3.6
1	A	542	ALA	3.6
1	A	495	SER	3.6
1	A	265	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	257	CYS	3.2
1	B	357	ALA	3.2
1	A	492	PRO	3.2
1	B	543	THR	3.2
1	B	165	ARG	3.1
1	A	257	CYS	3.0
1	A	497	SER	3.0
1	A	539	LEU	2.9
1	B	538	LYS	2.9
1	A	267	THR	2.8
1	A	498	PRO	2.7
1	B	256	GLY	2.7
1	B	376	GLU	2.7
1	A	269	LEU	2.7
1	B	353	LEU	2.7
1	A	165	ARG	2.7
1	B	269	LEU	2.7
1	A	540	LEU	2.7
1	B	380	LEU	2.6
1	B	271	ALA	2.6
1	B	493	ARG	2.6
1	A	256	GLY	2.6
1	B	316	ILE	2.6
1	A	421	GLN	2.5
1	B	25	PRO	2.5
1	A	252	ALA	2.5
1	B	385	TRP	2.4
1	A	493	ARG	2.4
1	B	383	THR	2.4
1	B	264	GLY	2.4
1	B	265	ASN	2.4
1	A	385	TRP	2.3
1	A	271	ALA	2.3
1	A	219[A]	ARG	2.3
1	B	381	HIS	2.3
1	B	349	ASP	2.2
1	B	491	ASP	2.2
1	A	507	ALA	2.2
1	B	541	SER	2.2
1	B	466	THR	2.2
1	B	6	PRO	2.1
1	A	485	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	393	HIS	2.1
1	B	139	ALA	2.1
1	B	5	ASP	2.1
1	B	242	GLY	2.1
1	B	345	GLY	2.1
1	A	266	ASP	2.0
1	B	216[A]	LEU	2.0
1	B	534	ARG	2.0

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

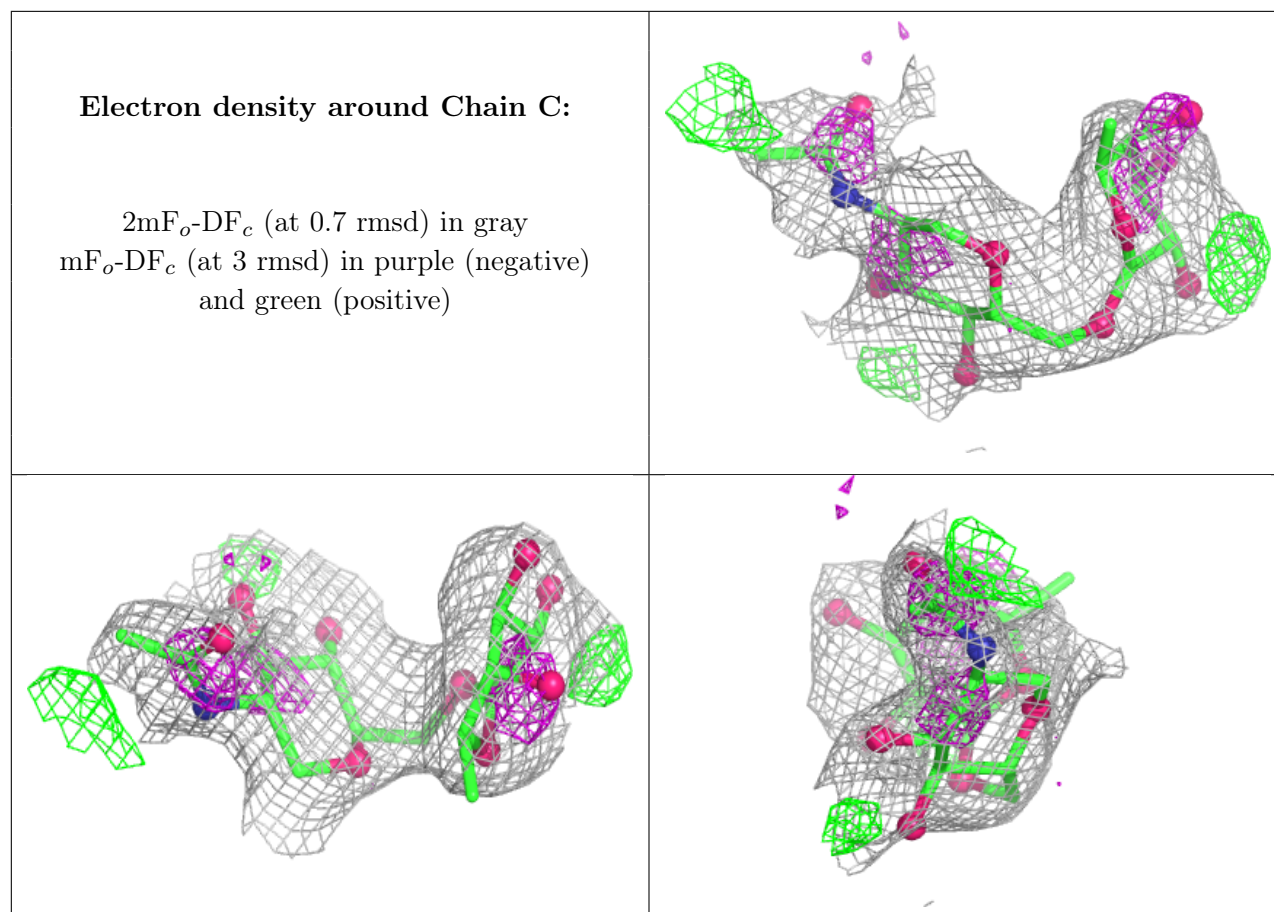
There are no non-standard protein/DNA/RNA residues in this entry.

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($\text{\AA}^2$)	Q<0.9
2	FUC	C	2	10/11	0.70	0.16	92,94,94,95	0
2	NAG	C	1	14/15	0.78	0.17	79,84,87,90	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	B	1601	14/15	0.52	0.26	86,90,94,94	0
3	NAG	A	701	14/15	0.57	0.18	82,87,88,89	0
6	CHH	B	1610	10/10	0.83	0.33	76,76,77,77	10
6	CHH	A	710	10/10	0.85	0.27	71,73,74,75	10
7	P6G	A	711	19/19	0.85	0.18	47,64,73,74	0
4	IOD	B	1608	1/1	0.92	0.12	72,72,72,72	1
4	IOD	B	1604	1/1	0.93	0.09	88,88,88,88	1
4	IOD	B	1607	1/1	0.93	0.13	79,79,79,79	1
4	IOD	A	706	1/1	0.93	0.09	70,70,70,70	1
5	NWA	B	1609	10/11	0.96	0.12	45,52,54,54	0
5	NWA	A	709	10/11	0.96	0.10	42,46,47,48	0
4	IOD	A	703	1/1	0.97	0.06	55,55,55,55	1

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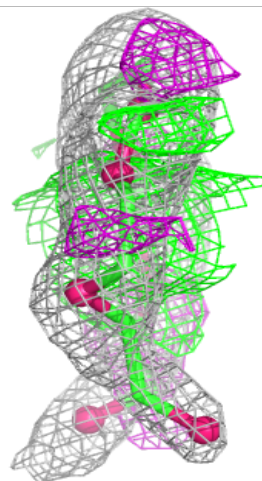
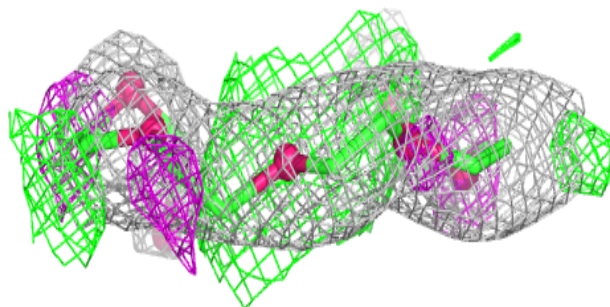
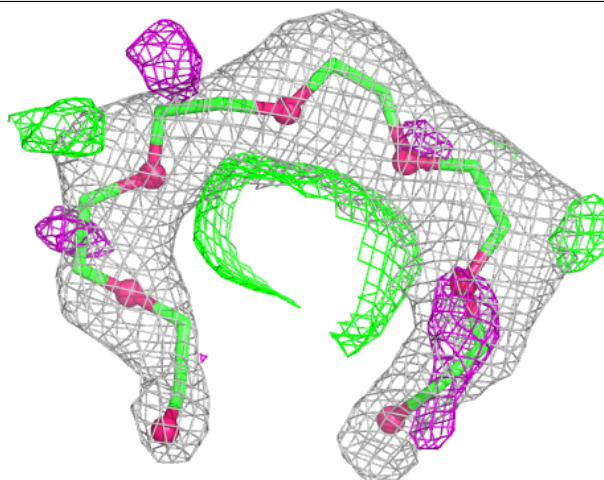
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	IOD	A	707	1/1	0.98	0.09	64,64,64,64	1
4	IOD	B	1605	1/1	0.98	0.06	47,47,47,47	1
4	IOD	B	1606	1/1	0.98	0.08	71,71,71,71	1
4	IOD	A	708	1/1	0.98	0.05	53,53,53,53	1
4	IOD	B	1603	1/1	0.98	0.09	57,57,57,57	1
4	IOD	B	1602	1/1	0.99	0.07	54,54,54,54	1
4	IOD	A	705	1/1	0.99	0.07	55,55,55,55	1
4	IOD	A	704	1/1	0.99	0.06	52,52,52,52	1
4	IOD	A	702	1/1	1.00	0.07	49,49,49,49	1

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 P6G A 711:

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.