

wwPDB X-ray Structure Validation Summary Report (i)

Sep 17, 2023 – 12:06 AM EDT

PDB ID : 4RRY

Title: Crystal Structure of Apo Murine H90W Cyclooxygenase-2

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Deposited on : 2014-11-06

Resolution : 2.43 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) 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 : 2.35.1

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)

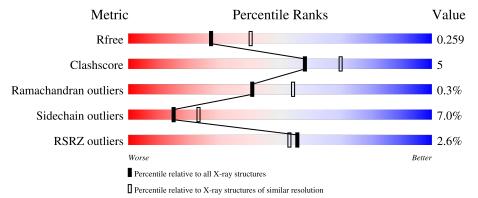
Validation Pipeline (wwPDB-VP) : 2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\mathring{A})}) \end{array}$
R_{free}	130704	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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 <=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 o	chain
1	A	587	79%	13% • 6%
1	В		2%	
1		587	80% 4%	12% • 6%
1	С	587	78% 2%	14% • 6%
1	D	587	80%	12% • 6%
2	Е	2	50%	50%



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Mol	Chain	Length	Quality of chain
2	F	2	100%
2	G	2	100%
2	Н	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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BOG	A	706	-	-	-	X
4	BOG	С	706	-	-	=	X
4	BOG	D	705	-	-	=	X



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 18993 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 Prostaglandin G/H synthase 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	552	Total	С	N	О	S	0	0	0
1	A	352	4478	2890	749	814	25	0	0	0
1	В	552	Total	С	N	О	S	0	0	0
1	Б	352	4478	2890	749	814	25	0	U	
1	C	552	Total	С	N	О	S	0	0	0
1		352	4478	2890	749	814	25	0	U	
1	D	559	Total	С	N	О	S	0	0	0
1		552	4478	2890	749	814	25		U	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	90	TRP	HIS	engineered mutation	UNP Q05769
В	90	TRP	HIS	engineered mutation	UNP Q05769
С	90	TRP	HIS	engineered mutation	UNP Q05769
D	90	TRP	HIS	engineered mutation	UNP Q05769

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



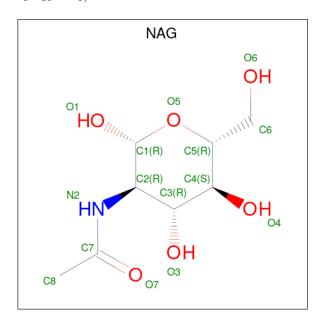
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	E	2	Total C N O 28 16 2 10	0	0	0
2	F	2	Total C N O 28 16 2 10	0	0	0
2	G	2	Total C N O 28 16 2 10	0	0	0



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

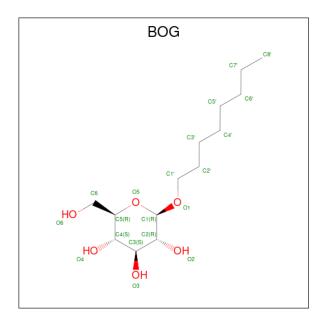
 \bullet Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $\rm C_8H_{15}NO_6).$



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

 \bullet Molecule 4 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $\mathrm{C}_{14}\mathrm{H}_{28}\mathrm{O}_6).$





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O	0	0
4	Λ	1	20 14 6	U	U
4	A	1	Total C O	0	0
4	11	1	20 14 6	U	0
4	В	1	Total C O	0	0
4		1	20 14 6		0
4	\mathbf{C}	1	Total C O	0	0
4	C	1	20 14 6	U	U
4	\mathbf{C}	1	Total C O	0	0
	C	1	20 14 6	Ů	0
4	D	1	Total C O	0	0
T	D	1	20 14 6		

• Molecule 5 is water.

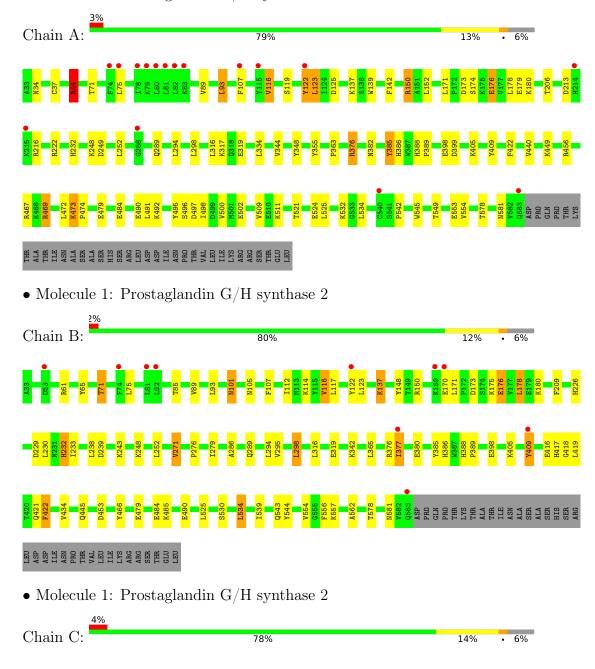
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	214	Total O 214 214	0	0
5	В	212	Total O 212 212	0	0
5	С	145	Total O 145 145	0	0
5	D	166	Total O 166 166	0	0



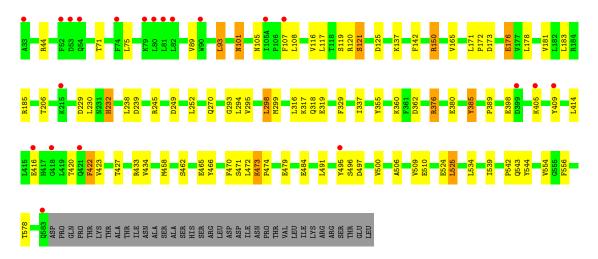
3 Residue-property plots (i)

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.

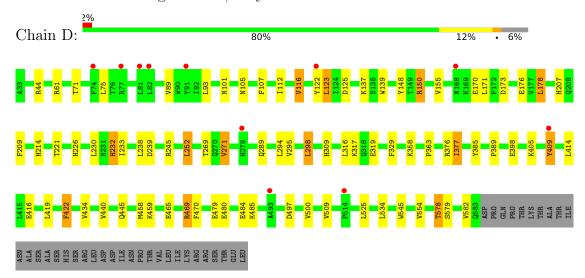
• Molecule 1: Prostaglandin G/H synthase 2







• Molecule 1: Prostaglandin G/H synthase 2



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

Chain E: 50% 50%

NAG1 NAG2

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

Chain F:

NAG1 NAG2

 $\bullet \ \, \text{Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2$



Chain G:	100%	
NAG1 NAG2		
• Molecule 2: opyranose	2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2	2-deoxy-beta-D-gluc
Chain H:	100%	



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	181.19Å 134.47Å 121.89Å	Donositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.36 - 2.43	Depositor
resolution (A)	49.36 - 2.43	EDS
% Data completeness	99.6 (49.36-2.43)	Depositor
(in resolution range)	87.3 (49.36-2.43)	EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.99 (at 2.42Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
D D.	0.209 , 0.259	Depositor
R, R_{free}	0.212 , 0.259	DCC
R_{free} test set	3370 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	33.9	Xtriage
Anisotropy	0.646	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.31 , 41.6	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18993	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 48.99 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.9529e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: NAG, BOG

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	Bo	ond angles
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.31	0/4606	0.46	1/6247~(0.0%)
1	В	0.30	0/4606	0.45	0/6247
1	С	0.33	0/4606	0.46	0/6247
1	D	0.30	0/4606	0.46	0/6247
All	All	0.31	0/18424	0.46	1/24988 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	44	ARG	NE-CZ-NH1	5.69	123.14	120.30

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	4478	0	4376	46	0
1	В	4478	0	4376	42	0
1	С	4478	0	4376	52	0
1	D	4478	0	4376	41	0
2	Е	28	0	25	1	0
2	F	28	0	25	0	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	28	0	25	0	0
2	Н	28	0	25	0	0
3	Α	28	0	26	0	0
3	В	28	0	26	0	0
3	С	28	0	26	0	0
3	D	28	0	26	0	0
4	A	40	0	56	3	0
4	В	20	0	28	2	0
4	С	40	0	56	5	0
4	D	20	0	28	1	0
5	A	214	0	0	5	0
5	В	212	0	0	5	0
5	С	145	0	0	0	0
5	D	166	0	0	6	0
All	All	18993	0	17876	173	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 5.

The worst 5 of 173 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:C:120:ARG:HD3	4:C:706:BOG:O2	1.73	0.88
1:A:44:ARG:HH11	1:A:44:ARG:HG2	1.46	0.80
1:B:150:ARG:HD3	5:B:939:HOH:O	1.82	0.79
1:B:294:LEU:HD22	1:B:409:TYR:HD1	1.49	0.76
1:A:123:LEU:O	1:A:469:ARG:NH2	2.20	0.74

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	Perce	ntiles
1	A	550/587 (94%)	528 (96%)	21 (4%)	1 (0%)	47	61
1	В	550/587 (94%)	534 (97%)	14 (2%)	2 (0%)	34	47
1	C	550/587 (94%)	523 (95%)	24 (4%)	3 (0%)	29	40
1	D	550/587 (94%)	533 (97%)	16 (3%)	1 (0%)	47	61
All	All	2200/2348~(94%)	2118 (96%)	75 (3%)	7 (0%)	41	54

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	С	416	GLU
1	A	398	GLU
1	D	398	GLU
1	С	398	GLU
1	В	398	GLU

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	493/525~(94%)	460 (93%)	33 (7%)	16 25
1	В	493/525 (94%)	457 (93%)	36 (7%)	14 21
1	С	493/525 (94%)	460 (93%)	33 (7%)	16 25
1	D	493/525 (94%)	457 (93%)	36 (7%)	14 21
All	All	1972/2100 (94%)	1834 (93%)	138 (7%)	15 23

5 of 138 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	238	LEU
1	D	289	GLN
1	D	419	LEU
1	В	238	LEU
1	В	232	HIS



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

8 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	Mol Type Cha		Chain Res L		Res Link		Во	Bond lengths			Bond angles		
MIOI	Mol Type Chain	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2			
2	NAG	Е	1	2,1	14,14,15	0.19	0	17,19,21	0.59	0			
2	NAG	Е	2	2	14,14,15	0.24	0	17,19,21	0.47	0			
2	NAG	F	1	2,1	14,14,15	0.35	0	17,19,21	0.47	0			
2	NAG	F	2	2	14,14,15	0.25	0	17,19,21	0.44	0			
2	NAG	G	1	2,1	14,14,15	0.24	0	17,19,21	0.52	0			
2	NAG	G	2	2	14,14,15	0.29	0	17,19,21	0.48	0			
2	NAG	Н	1	2,1	14,14,15	0.32	0	17,19,21	0.56	0			
2	NAG	Н	2	2	14,14,15	0.32	0	17,19,21	0.42	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
2	NAG	Е	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	Е	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	Н	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	Н	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Н	2	NAG	C4-C5-C6-O6
2	Н	2	NAG	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6

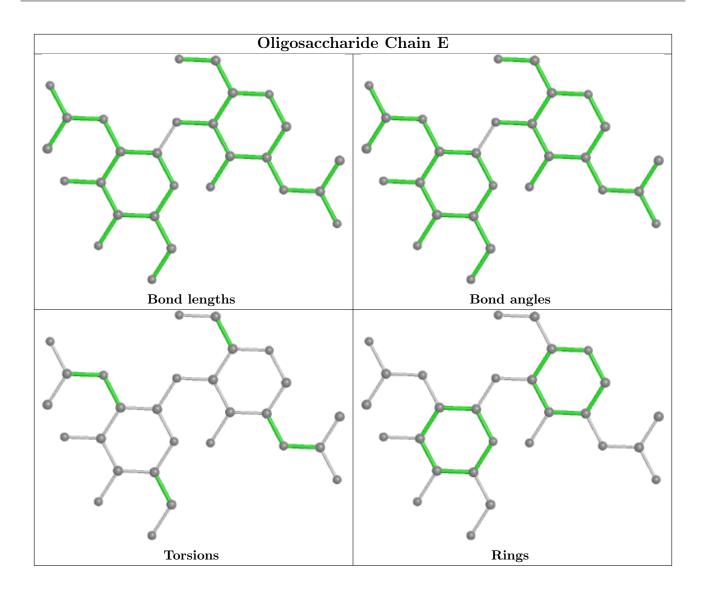
There are no ring outliers.

1 monomer is involved in 1 short contact:

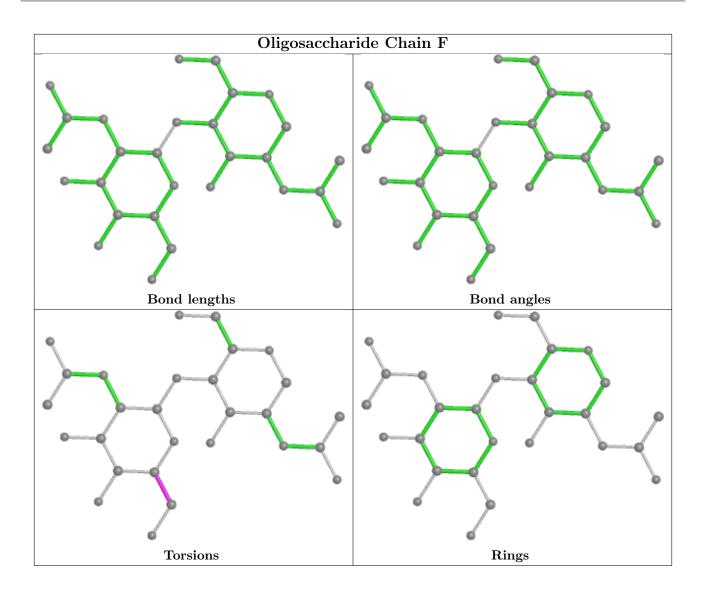
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Е	2	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

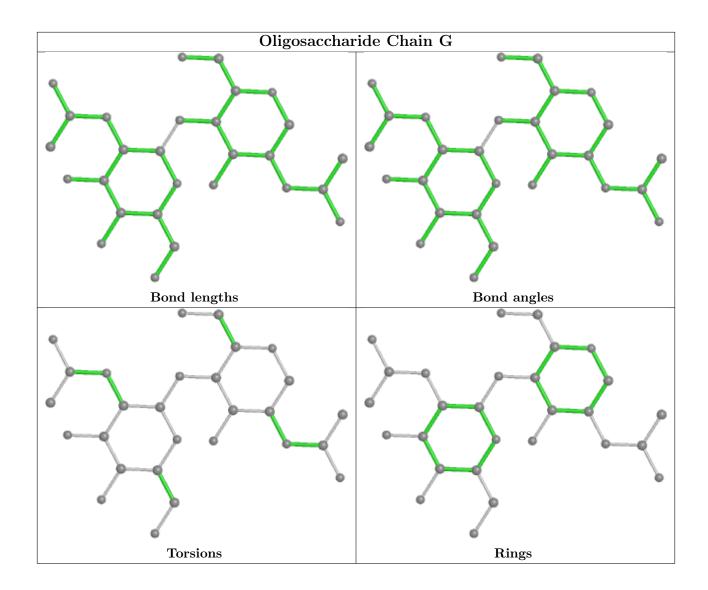




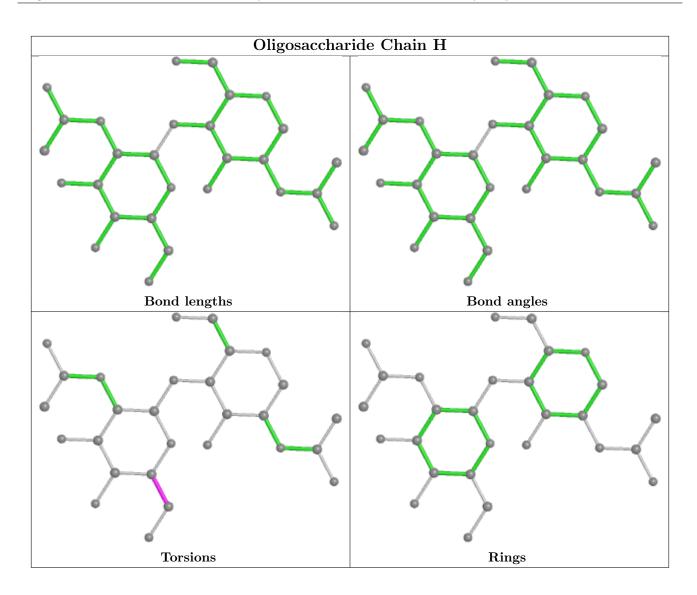












5.6 Ligand geometry (i)

14 ligands 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	Tuno	Chain	Res Link		Во	ths	Bond angles			
IVIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BOG	С	705	-	20,20,20	1.04	1 (5%)	25,25,25	1.16	2 (8%)
3	NAG	A	704	1	14,14,15	0.25	0	17,19,21	0.33	0
3	NAG	A	701	1	14,14,15	0.35	0	17,19,21	0.53	0



Mol	Trmo	Chain	Res	Link	Bo	ond leng	ths	Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	В	704	1	14,14,15	0.45	0	17,19,21	0.48	0
3	NAG	D	704	1	14,14,15	0.30	0	17,19,21	0.45	0
4	BOG	A	706	-	20,20,20	1.09	1 (5%)	25,25,25	1.15	2 (8%)
4	BOG	A	705	-	20,20,20	1.08	1 (5%)	25,25,25	1.12	3 (12%)
4	BOG	D	705	-	20,20,20	1.07	1 (5%)	25,25,25	1.11	2 (8%)
3	NAG	С	704	1	14,14,15	0.36	0	17,19,21	0.29	0
3	NAG	В	701	1	14,14,15	0.23	0	17,19,21	0.52	0
4	BOG	В	705	-	20,20,20	1.07	1 (5%)	25,25,25	1.15	2 (8%)
3	NAG	С	701	1	14,14,15	0.23	0	17,19,21	0.46	0
4	BOG	С	706	-	20,20,20	1.07	1 (5%)	25,25,25	1.14	2 (8%)
3	NAG	D	701	1	14,14,15	0.47	0	17,19,21	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
4	BOG	С	705	-	-	7/11/31/31	0/1/1/1
3	NAG	A	704	1	-	2/6/23/26	0/1/1/1
3	NAG	A	701	1	-	2/6/23/26	0/1/1/1
3	NAG	В	704	1	-	1/6/23/26	0/1/1/1
3	NAG	D	704	1	-	1/6/23/26	0/1/1/1
4	BOG	A	706	-	-	4/11/31/31	0/1/1/1
4	BOG	A	705	-	-	3/11/31/31	0/1/1/1
4	BOG	D	705	-	-	2/11/31/31	0/1/1/1
3	NAG	С	704	1	-	2/6/23/26	0/1/1/1
3	NAG	В	701	1	-	2/6/23/26	0/1/1/1
4	BOG	В	705	-	-	3/11/31/31	0/1/1/1
3	NAG	С	701	1	-	2/6/23/26	0/1/1/1
4	BOG	С	706	-	-	5/11/31/31	0/1/1/1
3	NAG	D	701	1	-	2/6/23/26	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
4	С	705	BOG	O2-C2	-2.58	1.36	1.43
4	A	705	BOG	O2-C2	-2.57	1.36	1.43



Continued	trom	mmoninonic	maaa
COHABABACA		DIEUIUU	DUIUE
0 0 1000100000			

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
4	A	706	BOG	O2-C2	-2.57	1.36	1.43
4	С	706	BOG	O2-C2	-2.55	1.37	1.43
4	D	705	BOG	O2-C2	-2.51	1.37	1.43

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
4	С	705	BOG	C1'-O1-C1	3.71	119.99	113.84
4	В	705	BOG	C1'-O1-C1	3.54	119.71	113.84
4	D	705	BOG	C1'-O1-C1	3.53	119.69	113.84
4	С	706	BOG	C1'-O1-C1	3.46	119.58	113.84
4	A	706	BOG	C1'-O1-C1	3.42	119.51	113.84

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	С	705	BOG	C2'-C1'-O1-C1
3	С	701	NAG	O5-C5-C6-O6
3	С	701	NAG	C4-C5-C6-O6
3	D	701	NAG	O5-C5-C6-O6
3	D	701	NAG	C4-C5-C6-O6

There are no ring outliers.

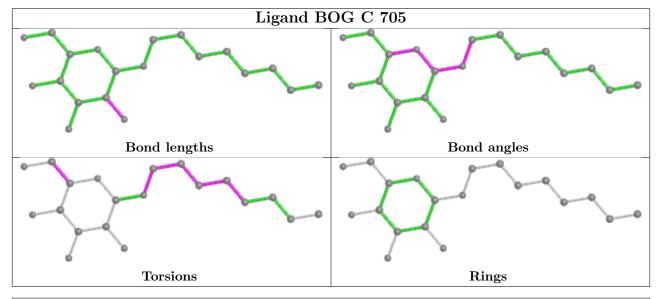
5 monomers are involved in 11 short contacts:

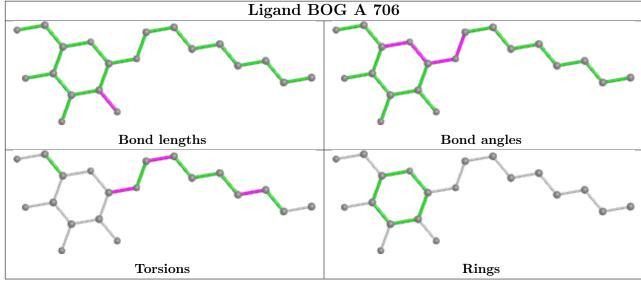
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	С	705	BOG	2	0
4	A	706	BOG	3	0
4	D	705	BOG	1	0
4	В	705	BOG	2	0
4	С	706	BOG	3	0

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 then 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

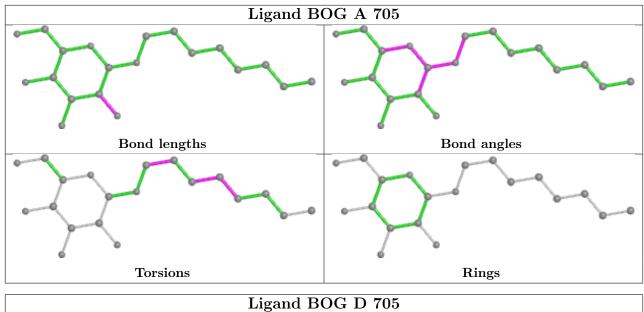


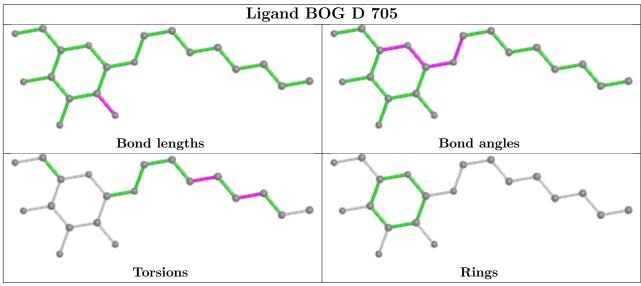
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

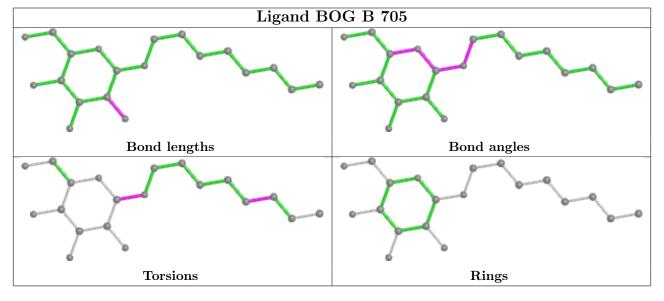




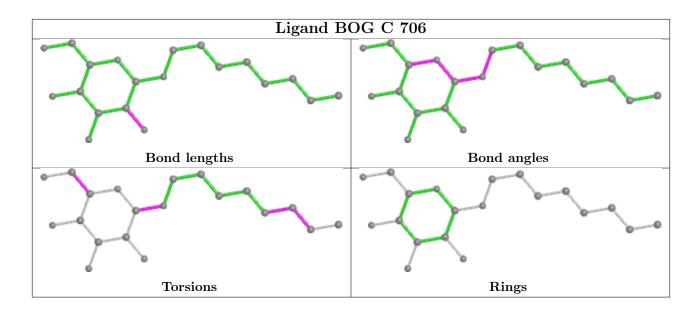












5.7 Other polymers (i)

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, 95^{th} 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>	$\# \mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	552/587 (94%)	-0.21	16 (2%) 51 49	26, 41, 69, 98	0
1	В	552/587 (94%)	-0.15	10 (1%) 68 65	25, 40, 69, 90	0
1	С	552/587 (94%)	-0.06	21 (3%) 40 38	28, 53, 83, 106	0
1	D	552/587 (94%)	-0.03	11 (1%) 65 62	27, 48, 77, 95	0
All	All	2208/2348 (94%)	-0.12	58 (2%) 56 53	25, 45, 77, 106	0

The worst 5 of 58 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	583	GLN	6.7
1	С	409	TYR	4.7
1	С	81	LEU	4.2
1	С	82	LEU	3.8
1	A	75	LEU	3.7

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, 95^{th} 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.

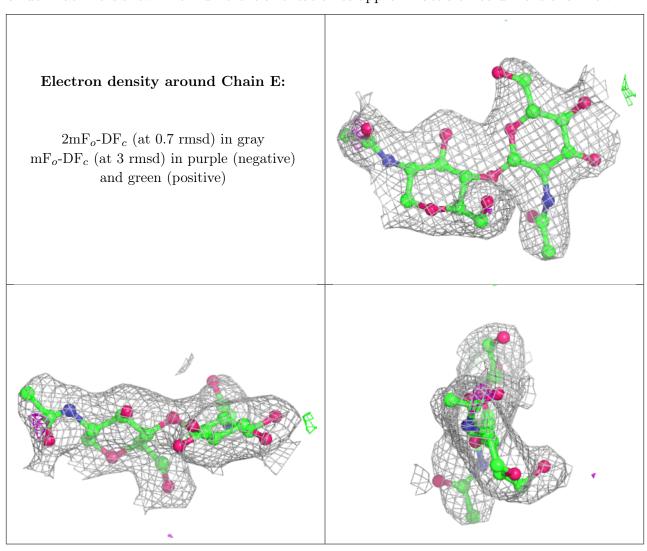
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	NAG	Ε	2	14/15	0.90	0.20	56,66,73,76	0
2	NAG	F	2	14/15	0.92	0.13	48,66,73,78	0



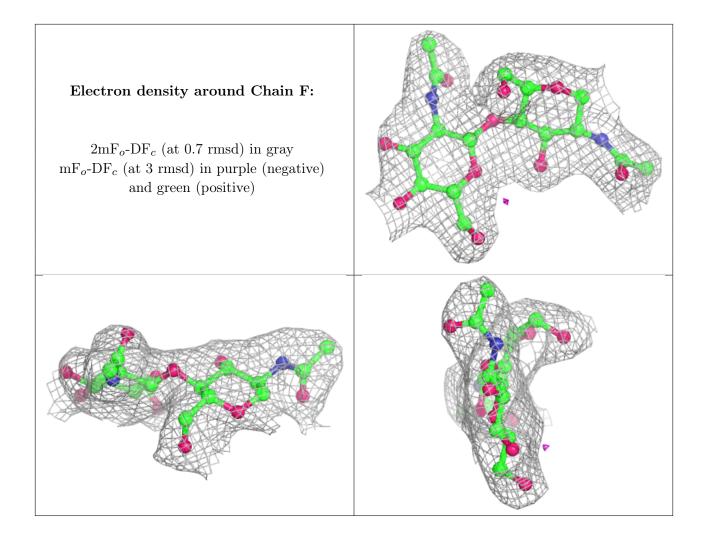
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	NAG	Н	2	14/15	0.92	0.16	52,60,69,71	0
2	NAG	G	2	14/15	0.93	0.21	54,59,69,72	0
2	NAG	Н	1	14/15	0.95	0.10	27,38,45,55	0
2	NAG	Е	1	14/15	0.95	0.11	28,36,42,53	0
2	NAG	G	1	14/15	0.96	0.10	31,44,49,51	0
2	NAG	F	1	14/15	0.96	0.12	30,39,47,59	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



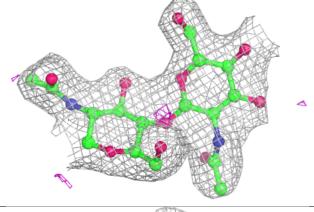


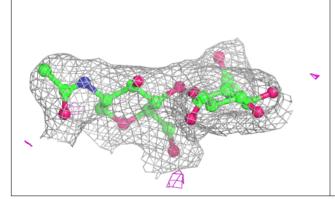


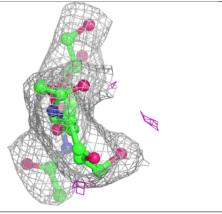


Electron density around Chain G: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${ m mF}_o{ m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive) Electron density around Chain H: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray

 ${
m mF}_o{
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)









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, 95^{th} 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.

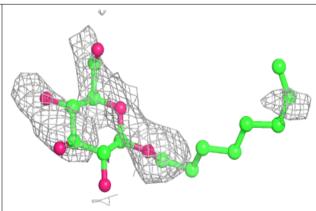
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
4	BOG	A	706	20/20	0.47	0.57	134,147,150,153	0
4	BOG	D	705	20/20	0.58	0.54	139,147,151,151	0
4	BOG	С	706	20/20	0.59	0.46	133,145,148,150	0
4	BOG	В	705	20/20	0.69	0.40	137,142,147,147	0
3	NAG	В	701	14/15	0.72	0.29	68,79,86,91	0
3	NAG	D	701	14/15	0.75	0.17	63,74,82,85	0
3	NAG	С	704	14/15	0.78	0.24	63,72,85,92	0
3	NAG	D	704	14/15	0.82	0.16	56,62,73,75	0
3	NAG	A	701	14/15	0.83	0.18	61,72,88,90	0
4	BOG	С	705	20/20	0.83	0.27	59,72,86,87	0
3	NAG	С	701	14/15	0.86	0.25	63,80,87,88	0
4	BOG	A	705	20/20	0.88	0.21	44,58,97,99	0
3	NAG	A	704	14/15	0.89	0.23	58,68,76,77	0
3	NAG	В	704	14/15	0.91	0.13	46,55,62,68	0

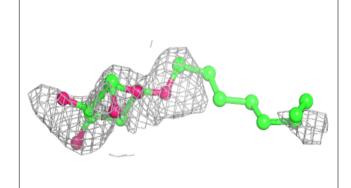
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

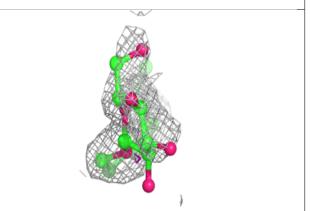


Electron density around BOG A 706:

 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

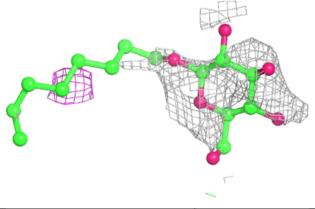


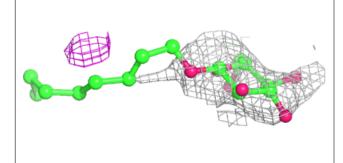


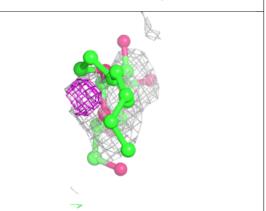


Electron density around BOG D 705:

 $2 \text{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray $\text{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



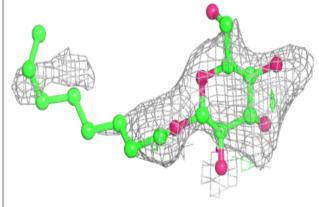


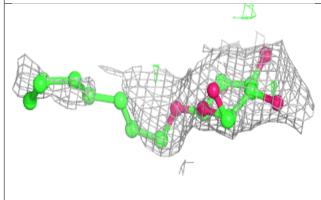


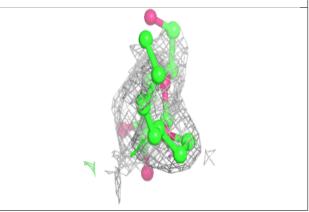


Electron density around BOG C 706:

 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

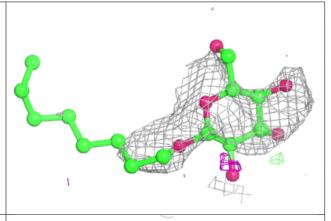


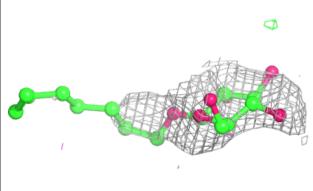


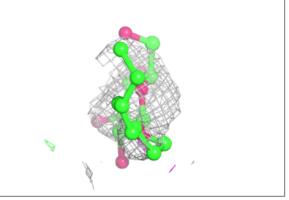


Electron density around BOG B 705:

 $2 \mathrm{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



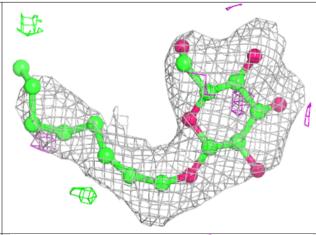


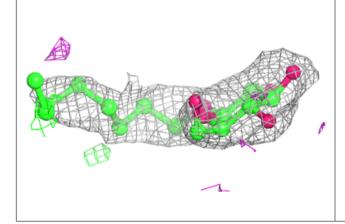


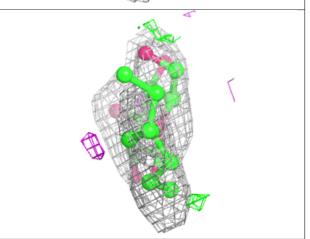


Electron density around BOG C 705:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

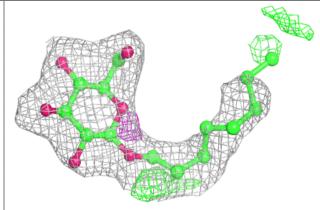


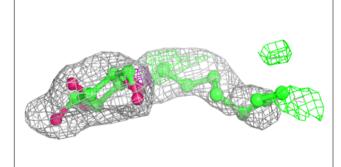


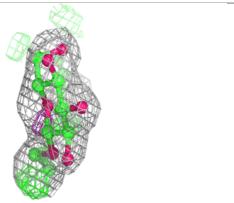


Electron density around BOG A 705:

 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)









6.5 Other polymers (i)

There are no such residues in this entry.

