wwPDB X-ray Structure Validation Summary Report (i)

Dec 16, 2023 – 08:39 pm GMT

PDB ID	:	4BTY
Title	:	Crystal structure of human vascular adhesion protein-1 in complex with pyridazinone inhibitors
Authors	:	Bligt-Linden, E.; Pihlavisto, M.; Szatmari, I.; Otwinowski, Z.; Smith, D.J.; Lazar, L.; Fulop, F.; Salminen, T.A.
Deposited on	:	2013-06-19
Resolution	:	3.10 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:

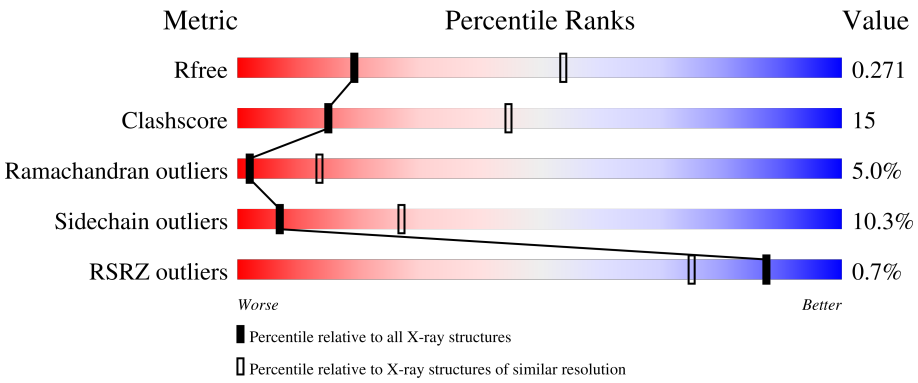
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 chain
1	A	737	62% 28% 6% •
1	B	737	% 61% 29% 5% • •
2	C	2	50% 50%
2	E	2	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	D	5	60% 40%

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	NAG	E	2	X	-	-	-
3	NAG	D	1	X	-	-	-
3	BMA	D	3	-	-	X	-
3	MAN	D	4	X	-	-	-
3	MAN	D	5	X	-	X	-
6	NAG	A	1768	X	-	-	-
6	NAG	A	1769	-	-	-	X
6	NAG	A	1770	-	-	-	X
6	NAG	B	1773	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 11484 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.

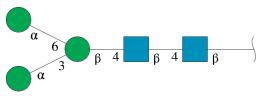
- Molecule 1 is a protein called MEMBRANE PRIMARY AMINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	711	5604	3595	968	1021	20	0	0	0
1	B	707	5567	3574	957	1016	20	0	0	0

- Molecule 2 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			
2	C	2	28	16	2	10	0	0	0
2	E	2	28	16	2	10	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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			
3	D	5	61	34	2	25	0	0	0

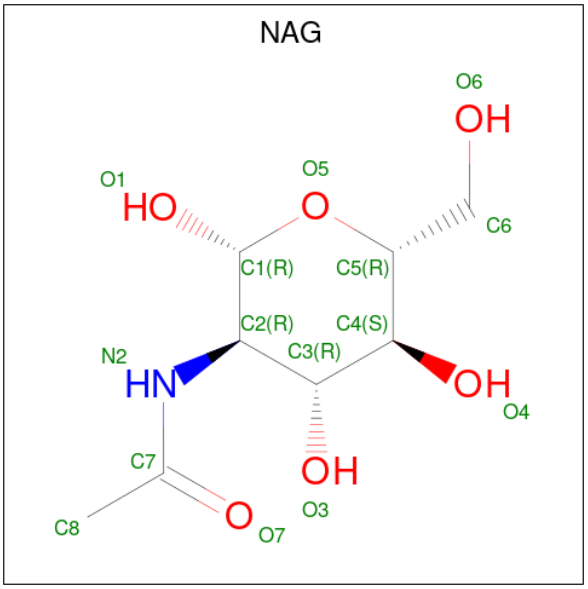
- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



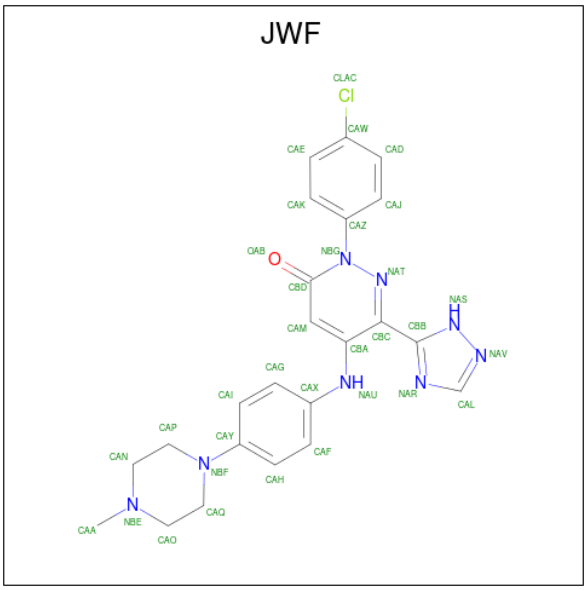
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 14 8 1 5	0	0
6	A	1	Total C N O 14 8 1 5	0	0
6	A	1	Total C N O 14 8 1 5	0	0
6	A	1	Total C N O 14 8 1 5	0	0
6	B	1	Total C N O 14 8 1 5	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 7 is 5-[4-(4-methylpiperazin-1-yl)phenylamino]-2-(4-chlorophenyl)-6-(1H-1,2,4-triazol-5-yl)-3(2H)-pyridazinone (three-letter code: JWF) (formula: $C_{23}H_{23}ClN_8O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
7	A	1	33	23	1	8	1	0	0
			Total	C	Cl	N	O		
7	B	1	33	23	1	8	1	0	0

- Molecule 8 is water.

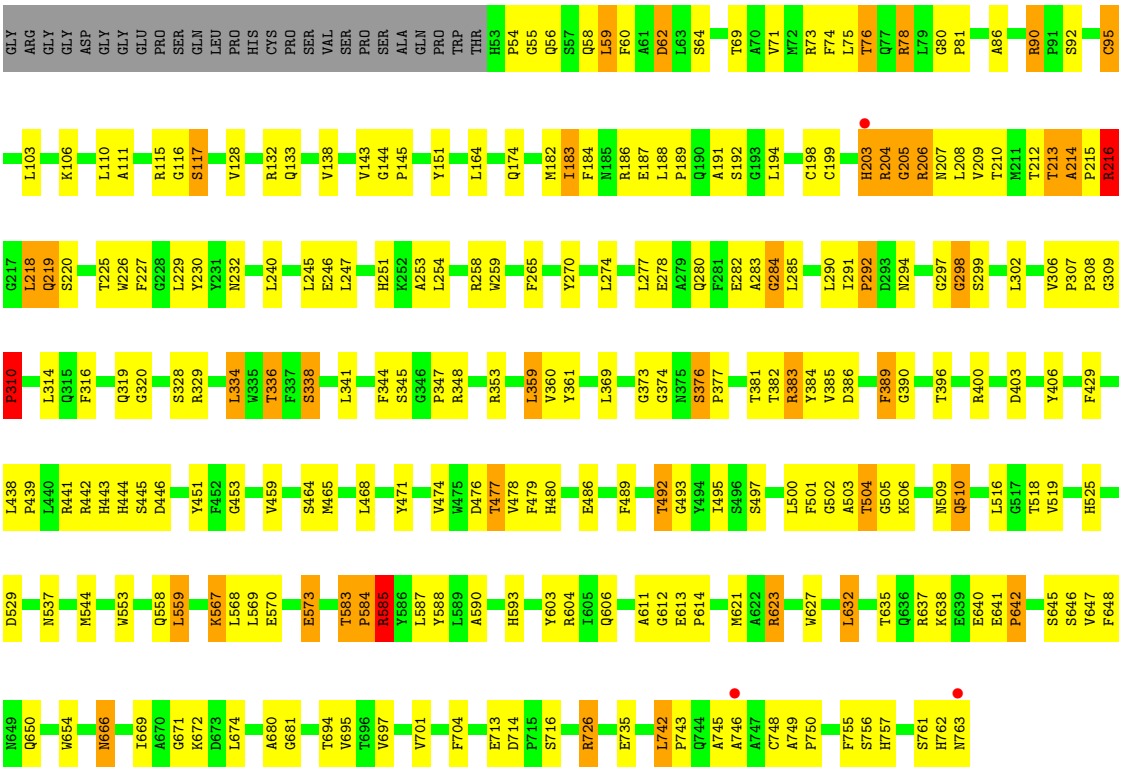
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	26	26	26	0	0
			Total	O		
8	B	14	14	14	0	0

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.

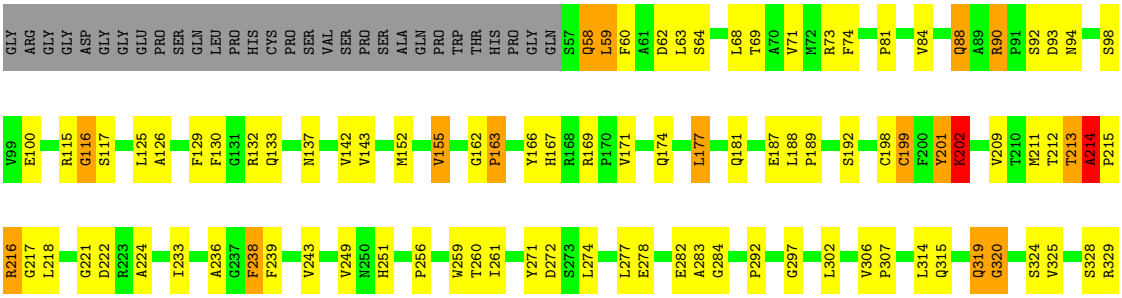
• Molecule 1: MEMBRANE PRIMARY AMINE OXIDASE

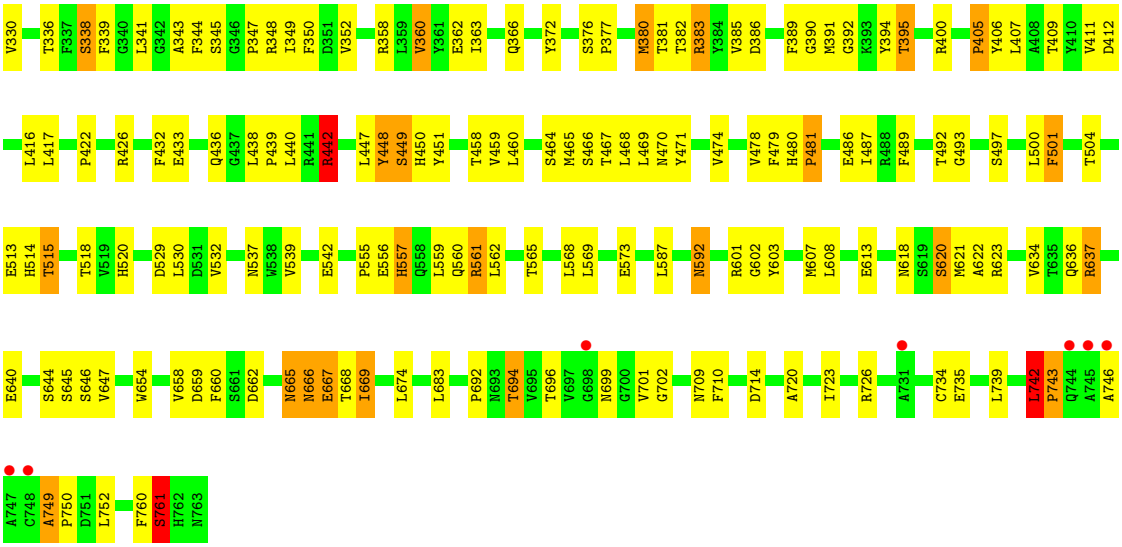
Chain A: 62% 28% 6% •



• Molecule 1: MEMBRANE PRIMARY AMINE OXIDASE

Chain B: % 61% 29% 5% • •





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

Chain C: 50% 50%

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

Chain E: 100%

• Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 60% 40%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	226.74Å 226.74Å 218.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.20 – 3.10 49.15 – 3.10	Depositor EDS
% Data completeness (in resolution range)	76.2 (49.20-3.10) 76.2 (49.15-3.10)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.184 , 0.246 0.217 , 0.271	Depositor DCC
R_{free} test set	2314 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	88.2	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 78.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11484	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical 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.

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: BMA, NAG, MAN, JWF, TPQ, CA, CU

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	0.67	1/5769 (0.0%)	0.89	5/7867 (0.1%)
1	B	0.66	1/5730 (0.0%)	0.88	1/7815 (0.0%)
All	All	0.66	2/11499 (0.0%)	0.88	6/15682 (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	A	0	2
1	B	0	7
All	All	0	9

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	666	ASN	CG-ND2	6.88	1.50	1.32
1	B	592	ASN	CG-ND2	5.50	1.46	1.32

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	585	ARG	NE-CZ-NH1	8.69	124.65	120.30
1	A	529	ASP	CB-CG-OD2	-7.20	111.82	118.30
1	B	529	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	A	258	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	A	585	ARG	NE-CZ-NH2	-5.69	117.46	120.30

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	292	PRO	Peptide
1	A	438	LEU	Peptide
1	B	162	GLY	Peptide
1	B	202	LYS	Peptide
1	B	213	THR	Peptide

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	5604	0	5335	169	0
1	B	5567	0	5299	182	0
2	C	28	0	25	1	0
2	E	28	0	25	1	0
3	D	61	0	52	9	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	56	0	52	1	0
6	B	28	0	26	4	0
7	A	33	0	23	5	0
7	B	33	0	23	3	0
8	A	26	0	0	2	0
8	B	14	0	0	4	0
All	All	11484	0	10860	337	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 15.

The worst 5 of 337 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:B:592:ASN:ND2	6:B:1772:NAG:C1	1.90	1.35
1:B:592:ASN:ND2	6:B:1772:NAG:O5	1.62	1.32

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3:BMA:O4	3:D:5:MAN:H2	1.33	1.25
3:D:3:BMA:C4	3:D:5:MAN:H2	1.79	1.13
1:B:592:ASN:HD22	6:B:1772:NAG:C1	1.59	1.00

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	708/737 (96%)	596 (84%)	73 (10%)	39 (6%)	2 11
1	B	704/737 (96%)	593 (84%)	79 (11%)	32 (4%)	2 15
All	All	1412/1474 (96%)	1189 (84%)	152 (11%)	71 (5%)	2 13

5 of 71 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	LEU
1	A	116	GLY
1	A	203	HIS
1	A	204	ARG
1	A	206	ARG

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	588/610 (96%)	527 (90%)	61 (10%)	7 27
1	B	584/610 (96%)	524 (90%)	60 (10%)	7 27
All	All	1172/1220 (96%)	1051 (90%)	121 (10%)	7 27

5 of 121 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	726	ARG
1	B	621	MET
1	B	192	SER
1	B	620	SER
1	B	701	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	592	ASN
1	B	593	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	TPQ	A	471	1	13,14,15	1.38	4 (30%)	15,19,21	1.53	3 (20%)
1	TPQ	B	471	1	13,14,15	1.37	2 (15%)	15,19,21	1.77	3 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPQ	A	471	1	-	1/5/22/24	0/1/1/1
1	TPQ	B	471	1	-	2/5/22/24	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	471	TPQ	C3-C4	2.84	1.40	1.35
1	A	471	TPQ	C3-C4	2.53	1.39	1.35
1	A	471	TPQ	C6-C5	-2.45	1.38	1.44
1	A	471	TPQ	C3-C2	-2.17	1.38	1.44
1	B	471	TPQ	C3-C2	-2.11	1.39	1.44

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	471	TPQ	CB-CA-C	-4.28	103.45	111.47
1	B	471	TPQ	C6-C1-C2	4.08	121.78	118.64
1	A	471	TPQ	C6-C1-C2	3.49	121.32	118.64
1	A	471	TPQ	CB-CA-C	-3.11	105.64	111.47
1	A	471	TPQ	O5-C5-C4	2.58	123.60	119.38

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	471	TPQ	N-CA-CB-C1
1	B	471	TPQ	C-CA-CB-C1
1	A	471	TPQ	N-CA-CB-C1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

9 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	0.58	0	17,19,21	1.39	2 (11%)
2	NAG	C	2	2	14,14,15	0.70	0	17,19,21	1.24	2 (11%)
3	NAG	D	1	1,3	14,14,15	0.69	0	17,19,21	2.01	4 (23%)
3	NAG	D	2	3	14,14,15	0.52	0	17,19,21	1.69	1 (5%)
3	BMA	D	3	3	11,11,12	1.31	2 (18%)	15,15,17	2.45	7 (46%)
3	MAN	D	4	3	11,11,12	1.69	3 (27%)	15,15,17	1.87	5 (33%)
3	MAN	D	5	3	11,11,12	0.26	0	15,15,17	0.64	0
2	NAG	E	1	2,1	14,14,15	0.81	0	17,19,21	1.57	4 (23%)
2	NAG	E	2	2	14,14,15	0.71	0	17,19,21	2.76	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	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	2/2/19/22	0/1/1/1
3	MAN	D	4	3	1/1/4/5	0/2/19/22	0/1/1/1
3	MAN	D	5	3	1/1/4/5	0/2/19/22	0/1/1/1
2	NAG	E	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	E	2	2	1/1/5/7	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4	MAN	C1-C2	3.46	1.60	1.52
3	D	4	MAN	C2-C3	3.27	1.57	1.52
3	D	3	BMA	O3-C3	2.80	1.49	1.43
3	D	4	MAN	C4-C3	2.41	1.58	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3	BMA	O6-C6	2.11	1.51	1.42

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2	NAG	O5-C1-C2	6.19	121.06	111.29
3	D	3	BMA	O3-C3-C2	5.82	121.15	109.99
2	E	2	NAG	C1-O5-C5	5.60	119.78	112.19
3	D	2	NAG	C1-O5-C5	5.27	119.33	112.19
3	D	1	NAG	O4-C4-C3	-4.56	99.80	110.35

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	E	2	NAG	C1
3	D	1	NAG	C1
3	D	4	MAN	C1
3	D	5	MAN	C1

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C3-C2-N2-C7
2	E	1	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6

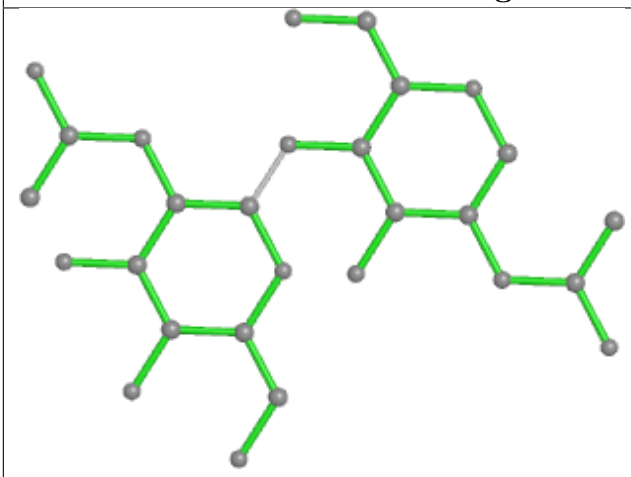
There are no ring outliers.

6 monomers are involved in 11 short contacts:

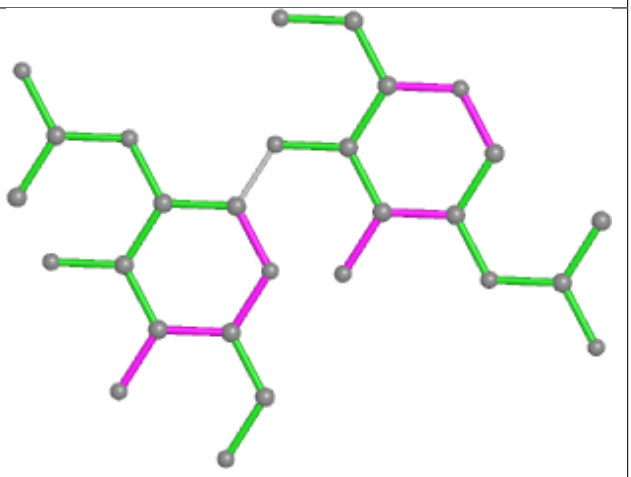
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	NAG	1	0
2	C	1	NAG	1	0
3	D	5	MAN	8	0
3	D	3	BMA	8	0
2	E	1	NAG	1	0
2	E	2	NAG	1	0

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

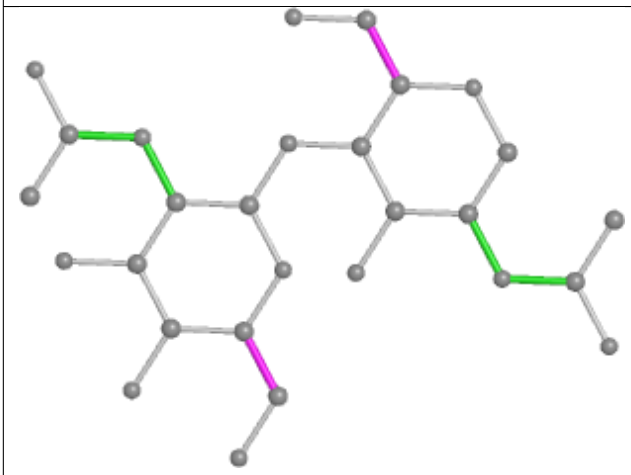
Oligosaccharide Chain C



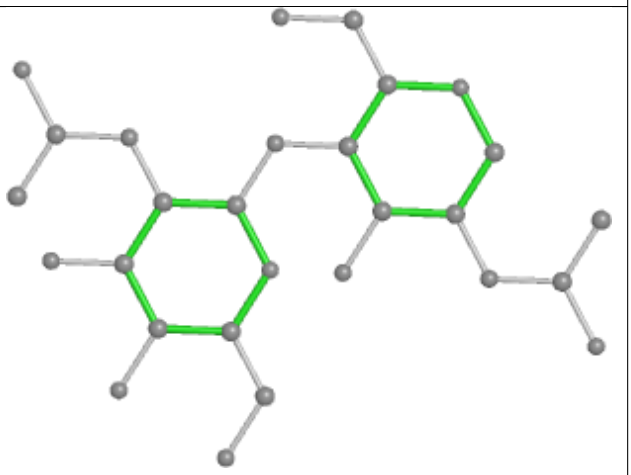
Bond lengths



Bond angles

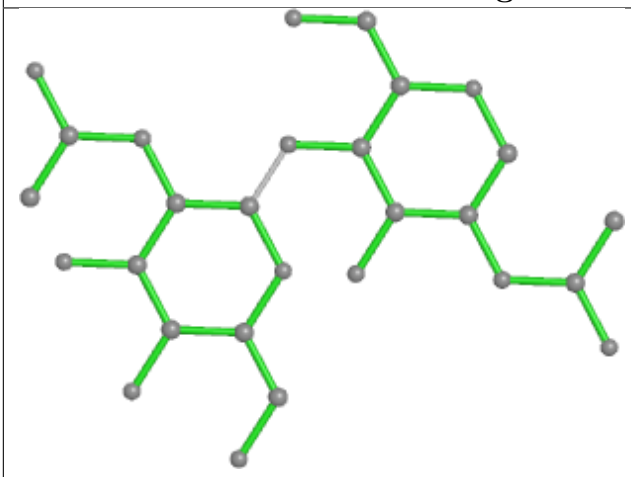


Torsions

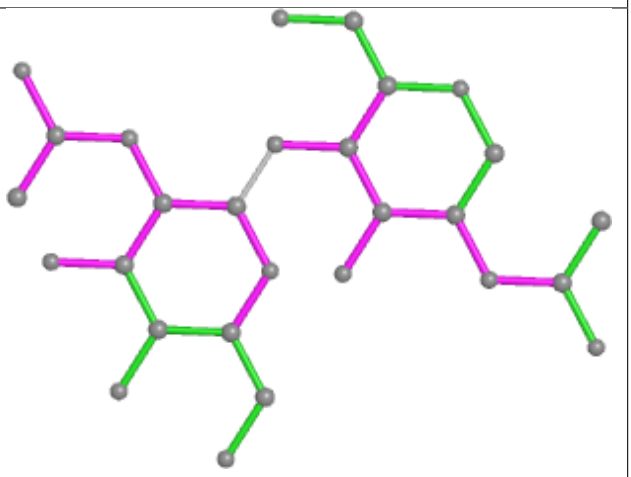


Rings

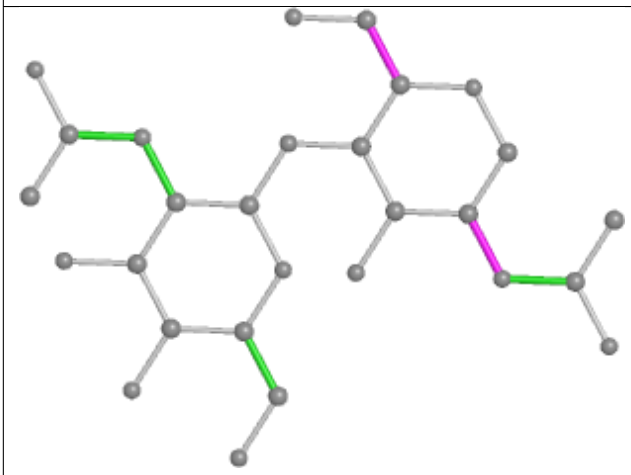
Oligosaccharide Chain E



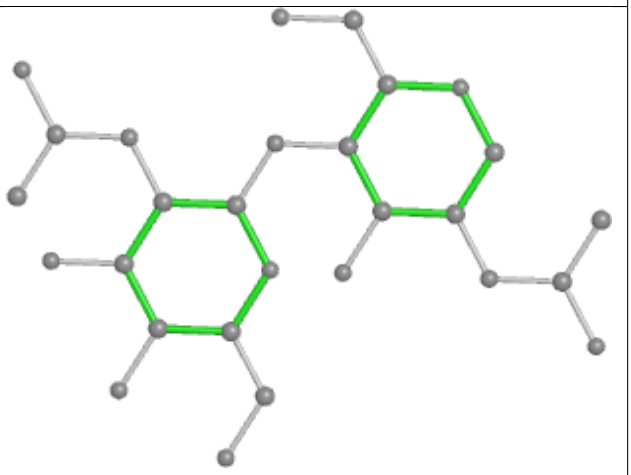
Bond lengths



Bond angles

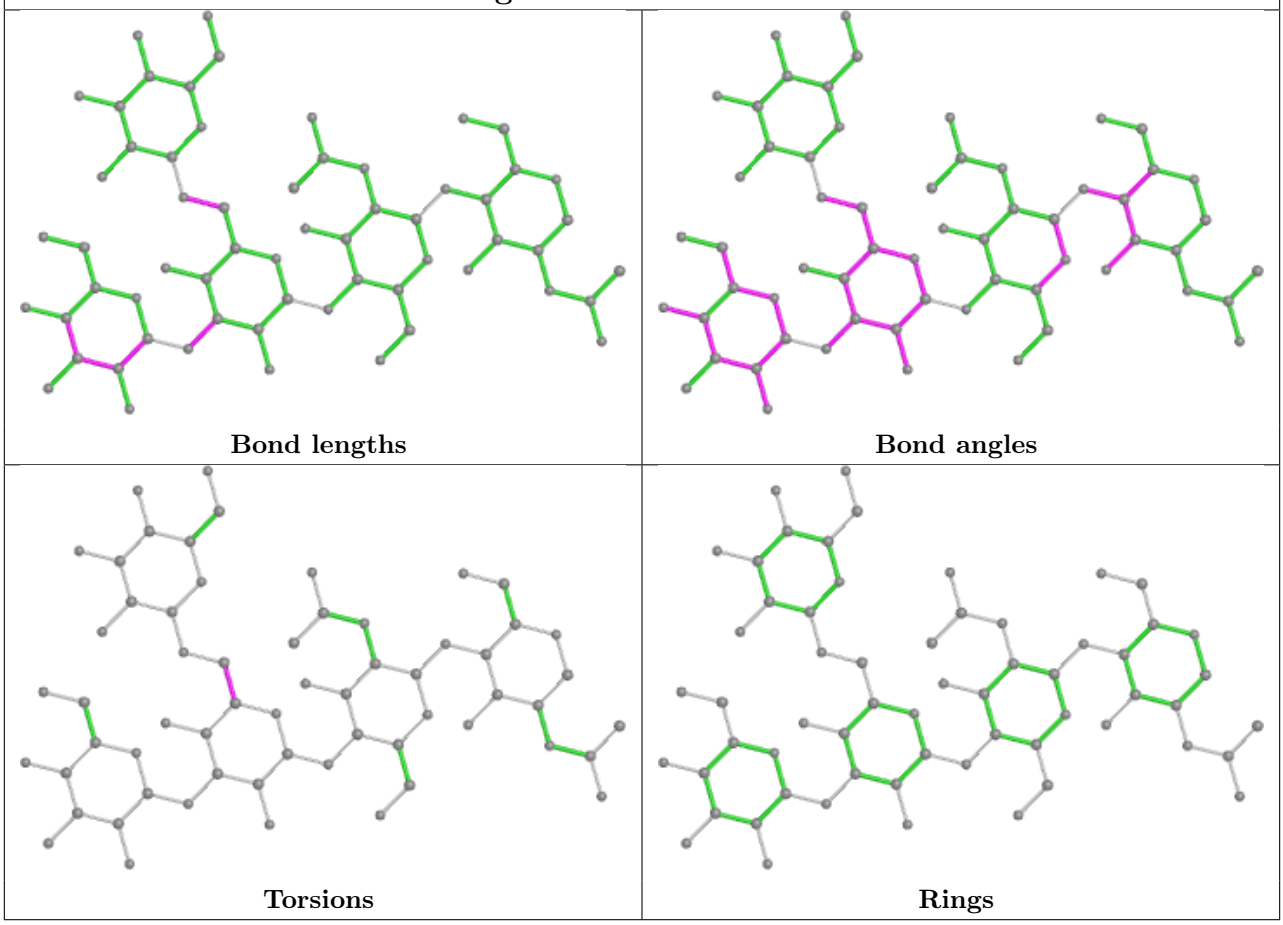


Torsions



Rings

Oligosaccharide Chain D



5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 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	NAG	B	1772	-	14,14,15	0.28	0	17,19,21	0.62	0
6	NAG	A	1770	1	14,14,15	2.67	3 (21%)	17,19,21	3.97	9 (52%)
7	JWF	B	2000	-	34,37,37	2.16	6 (17%)	44,52,52	2.51	14 (31%)
6	NAG	A	1768	1	14,14,15	1.00	1 (7%)	17,19,21	2.65	6 (35%)
6	NAG	A	1767	1	14,14,15	0.83	0	17,19,21	2.28	7 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	JWF	A	2000	-	34,37,37	2.51	8 (23%)	44,52,52	2.30	17 (38%)
6	NAG	B	1773	1	14,14,15	1.62	2 (14%)	17,19,21	2.69	4 (23%)
6	NAG	A	1769	1	14,14,15	0.79	0	17,19,21	1.98	4 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	1772	-	-	2/6/23/26	0/1/1/1
6	NAG	A	1770	1	-	2/6/23/26	0/1/1/1
7	JWF	B	2000	-	-	2/12/26/26	0/5/5/5
6	NAG	A	1768	1	1/1/5/7	2/6/23/26	0/1/1/1
6	NAG	A	1767	1	-	3/6/23/26	0/1/1/1
7	JWF	A	2000	-	-	2/12/26/26	0/5/5/5
6	NAG	B	1773	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1769	1	-	2/6/23/26	0/1/1/1

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2000	JWF	NAV-NAS	-8.93	1.18	1.37
6	A	1770	NAG	C1-C2	7.85	1.64	1.52
7	B	2000	JWF	NAV-NAS	-7.46	1.21	1.37
7	A	2000	JWF	NBG-NAT	-6.75	1.19	1.38
7	B	2000	JWF	NBG-NAT	-6.21	1.21	1.38

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1770	NAG	O5-C1-C2	-9.25	96.69	111.29
7	A	2000	JWF	NAR-CBB-NAS	-9.08	107.20	114.72
6	B	1773	NAG	C1-O5-C5	9.02	124.41	112.19
6	A	1770	NAG	C2-N2-C7	8.46	134.96	122.90
7	B	2000	JWF	NAR-CBB-NAS	-7.99	108.09	114.72

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	1768	NAG	C1

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1767	NAG	C3-C2-N2-C7
6	A	1768	NAG	C3-C2-N2-C7
6	A	1770	NAG	C3-C2-N2-C7
6	B	1773	NAG	O5-C5-C6-O6
6	B	1773	NAG	C4-C5-C6-O6

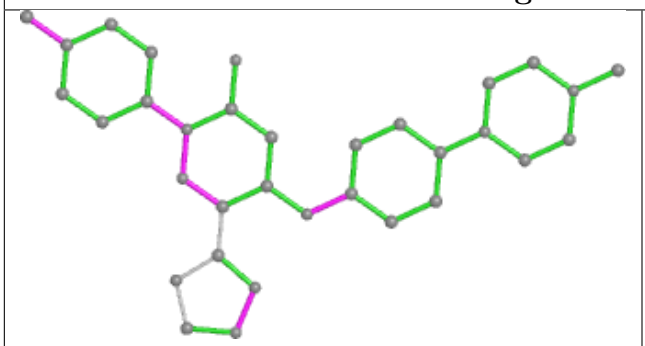
There are no ring outliers.

4 monomers are involved in 13 short contacts:

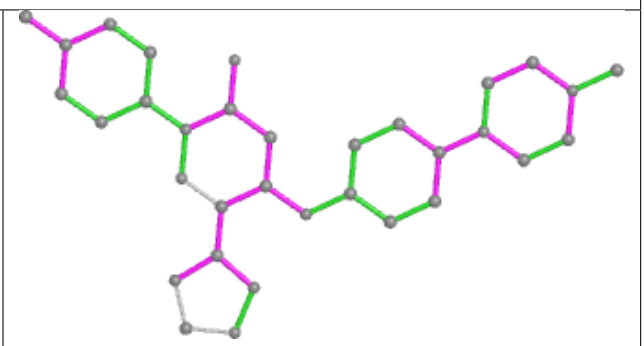
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1772	NAG	4	0
7	B	2000	JWF	3	0
6	A	1768	NAG	1	0
7	A	2000	JWF	5	0

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.

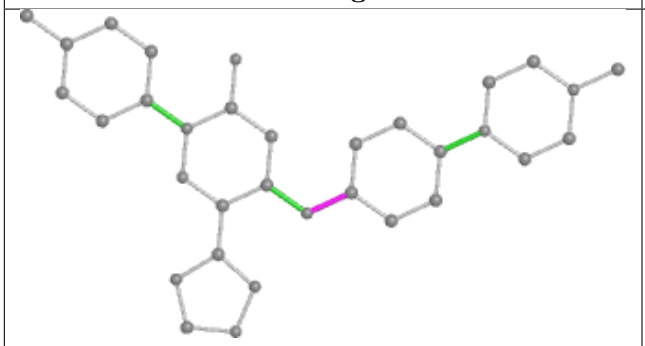
Ligand JWF B 2000



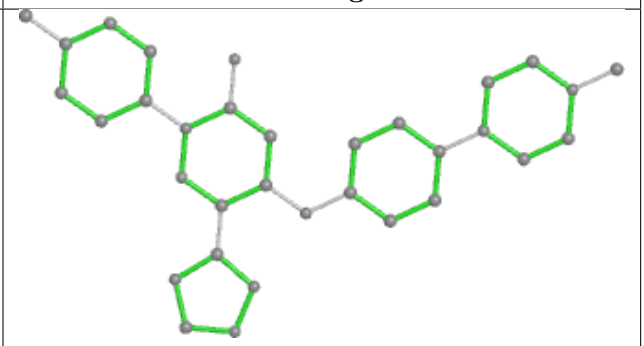
Bond lengths



Bond angles

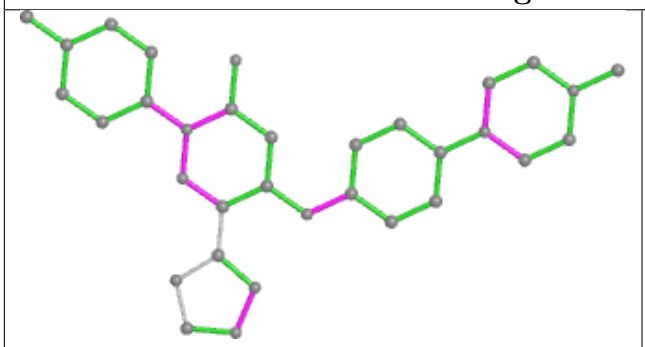


Torsions

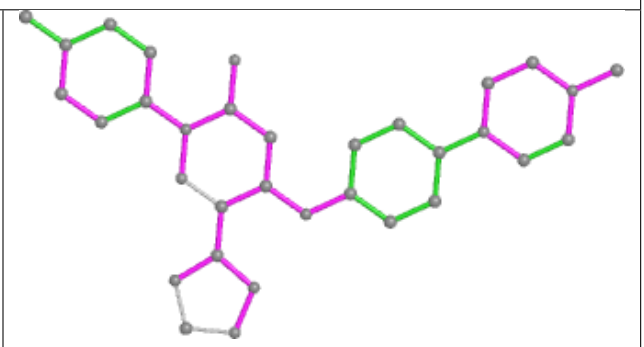


Rings

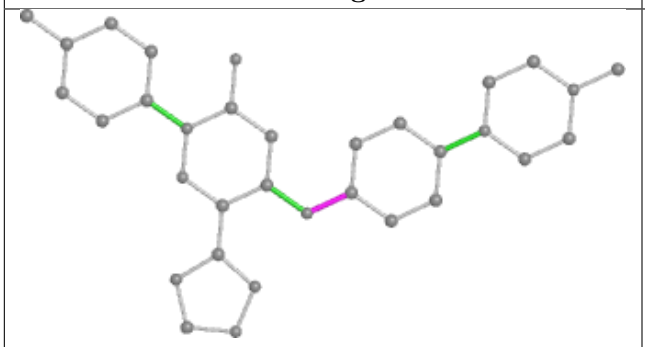
Ligand JWF A 2000



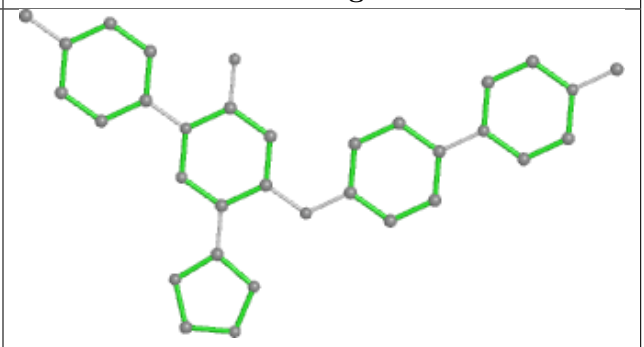
Bond lengths



Bond angles



Torsions



Rings

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	710/737 (96%)	-0.26	3 (0%)	92	84	58, 83, 112, 163	0
1	B	706/737 (95%)	-0.16	7 (0%)	82	67	63, 84, 115, 180	0
All	All	1416/1474 (96%)	-0.21	10 (0%)	87	75	58, 83, 115, 180	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	746	ALA	4.0
1	B	744	GLN	3.9
1	B	745	ALA	3.9
1	A	203	HIS	3.4
1	A	763	ASN	3.2

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
1	TPQ	A	471	14/15	0.94	0.24	68,74,80,80	0
1	TPQ	B	471	14/15	0.97	0.31	68,76,90,94	0

6.3 Carbohydrates (i)

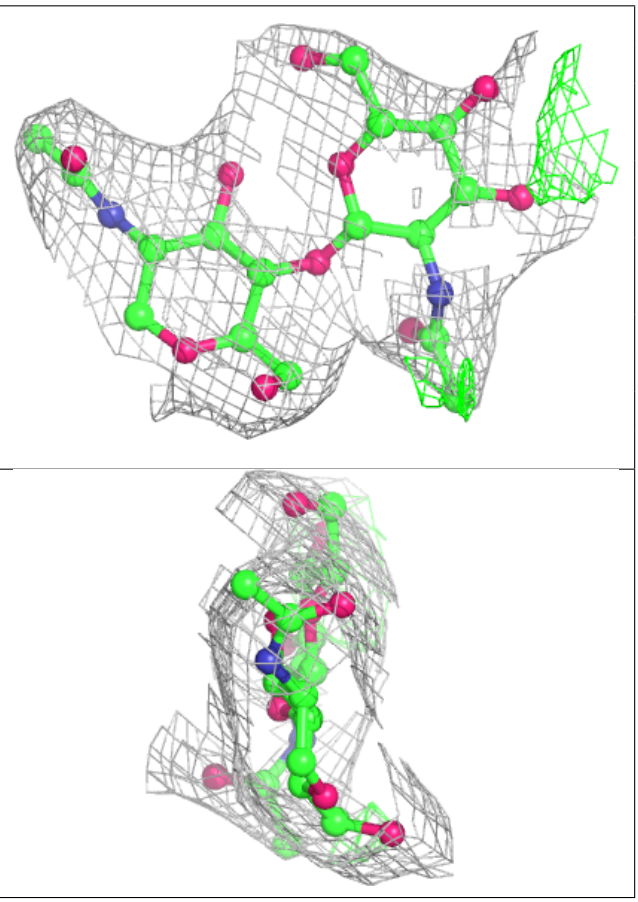
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MAN	D	5	11/12	0.56	0.36	89,129,154,162	0
3	BMA	D	3	11/12	0.80	0.30	113,133,158,163	0
3	MAN	D	4	11/12	0.81	0.49	87,119,138,139	0
2	NAG	C	2	14/15	0.85	0.24	101,123,145,157	0
3	NAG	D	1	14/15	0.90	0.16	74,82,91,94	0
2	NAG	E	2	14/15	0.90	0.23	106,130,141,143	0
3	NAG	D	2	14/15	0.94	0.17	100,110,119,123	0
2	NAG	E	1	14/15	0.94	0.14	97,105,126,137	0
2	NAG	C	1	14/15	0.96	0.17	78,83,93,101	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.

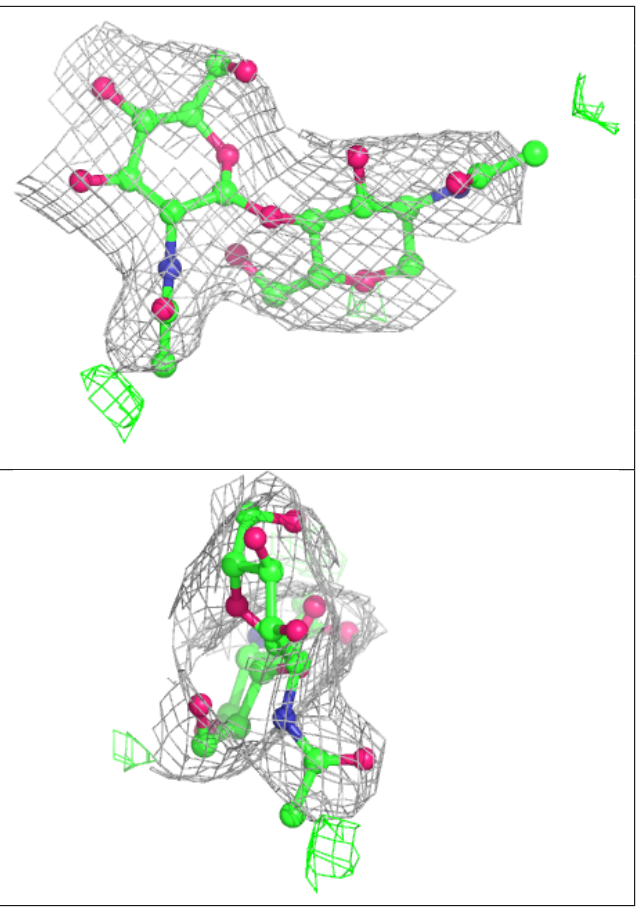
Electron density around Chain C:

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



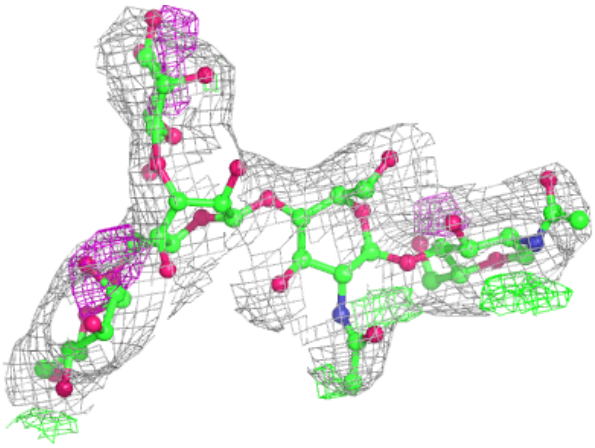
Electron density around Chain E:

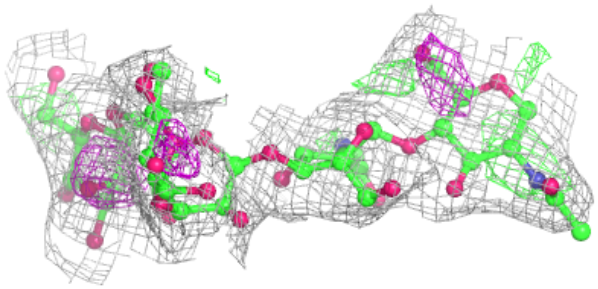
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

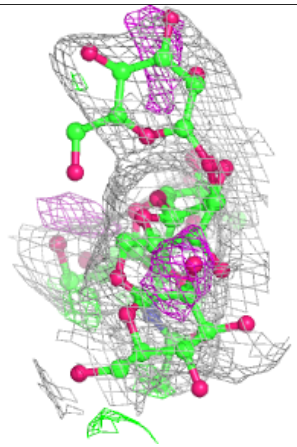


Electron density around Chain D:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-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, 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	NAG	A	1770	14/15	0.54	0.61	114,149,166,170	0
6	NAG	A	1769	14/15	0.63	0.56	127,148,167,183	0
6	NAG	B	1772	14/15	0.64	0.21	98,134,157,157	0
6	NAG	A	1768	14/15	0.67	0.28	121,169,177,179	0
6	NAG	B	1773	14/15	0.76	0.46	118,149,156,156	0
5	CA	A	1764	1/1	0.77	0.13	94,94,94,94	0
6	NAG	A	1767	14/15	0.87	0.20	93,104,130,130	0
4	CU	A	1762	1/1	0.89	0.20	85,85,85,85	0
4	CU	B	1762	1/1	0.90	0.24	74,74,74,74	0
7	JWF	B	2000	33/33	0.91	0.21	71,78,101,108	0
5	CA	B	1764	1/1	0.93	0.11	81,81,81,81	0
5	CA	B	1763	1/1	0.95	0.05	72,72,72,72	0

Continued on next page...

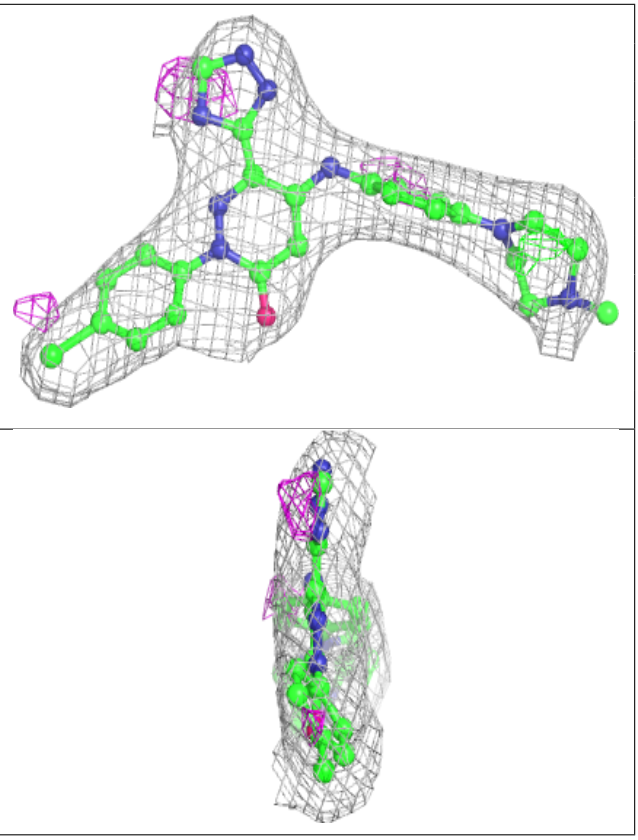
Continued from previous page...

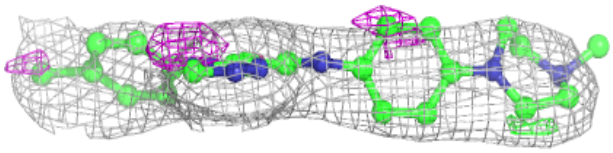
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	JWF	A	2000	33/33	0.96	0.18	71,90,120,127	0
5	CA	A	1763	1/1	0.96	0.05	71,71,71,71	0

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 JWF B 2000:

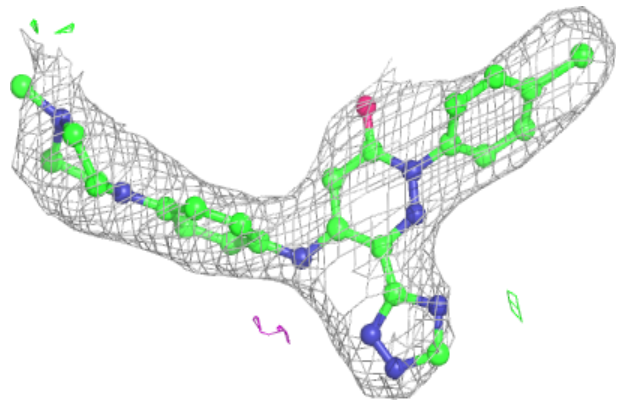
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

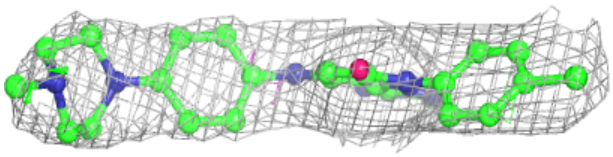


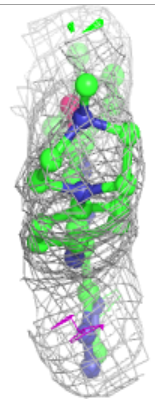


Electron density around JWF A 2000:

$2mF_o$-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.