



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 03:14 AM BST

PDB ID : 5EHQ
Title : mAChE-anti TZ2PA5 complex
Authors : Bourne, Y.; Marchot, P.
Deposited on : 2015-10-28
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

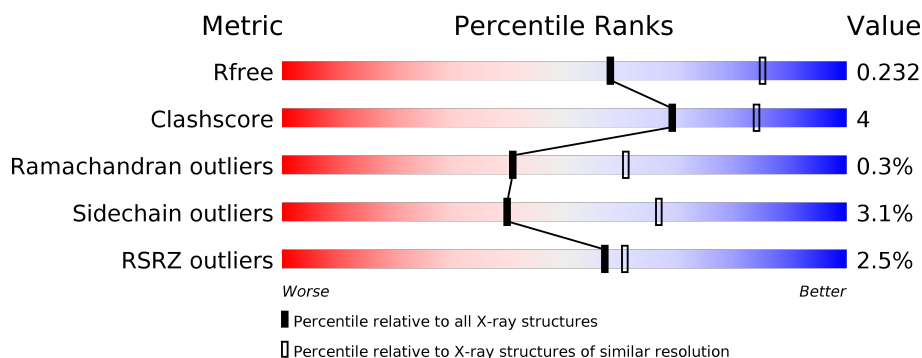
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	543	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>12%</div> <div></div> </div> </div>
1	B	543	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>11%</div> <div></div> </div> </div>
2	C	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>
3	D	3	<div> <div></div> <div> <div>33%</div> <div>67%</div> </div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8756 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.

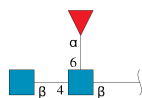
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	538	Total	C	N	O	S	0	2	0
			4213	2702	733	764	14			
1	B	537	Total	C	N	O	S	0	3	0
			4198	2695	724	765	14			

- 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 an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



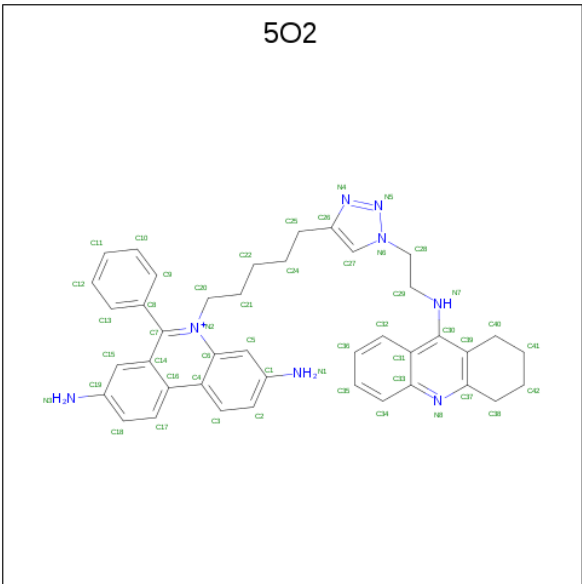
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is 6-phenyl-5-[5-[1-[2-(1,2,3,4-tetrahydroacridin-9-ylamino)ethyl]-1,2,3-triazol-4-yl]pentyl]phenanthridin-5-ium-3,8-diamine (three-letter code: 5O2) (formula: C₄₁H₄₃N₈).



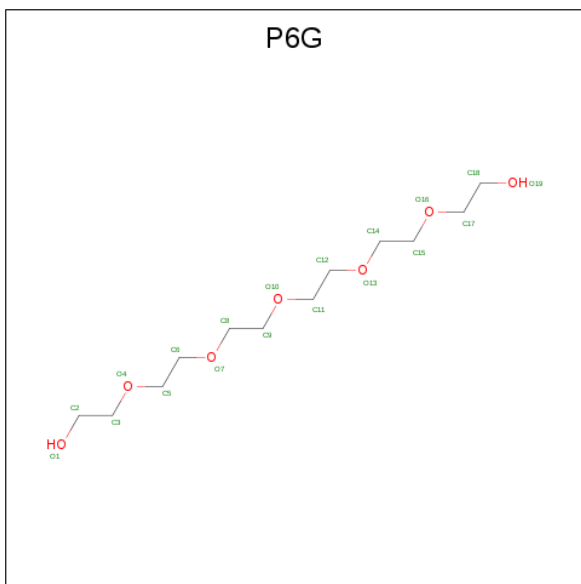
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N		0	0
			49	41	8			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	N	0	0
			49	41	8		

- Molecule 6 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C₁₂H₂₆O₇).



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

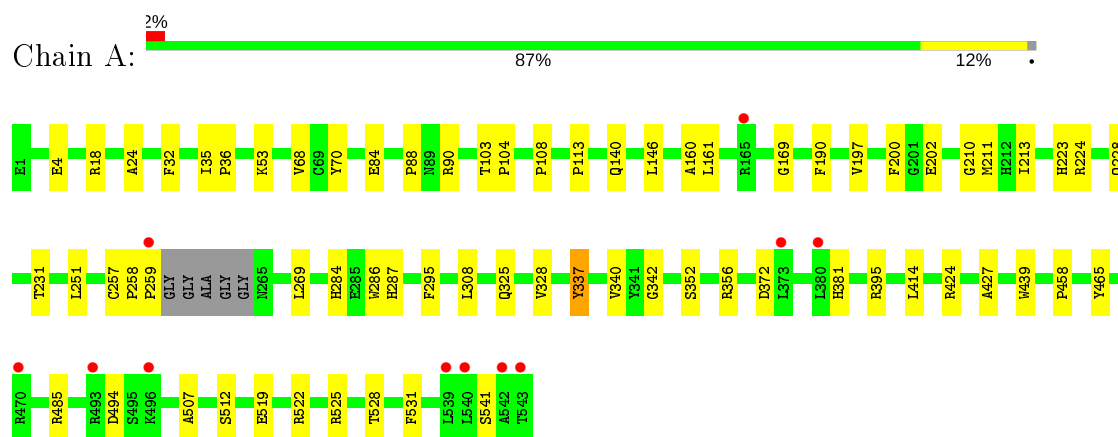
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	83	Total	O	0	0
			83	83		
7	B	55	Total	O	0	0
			55	55		

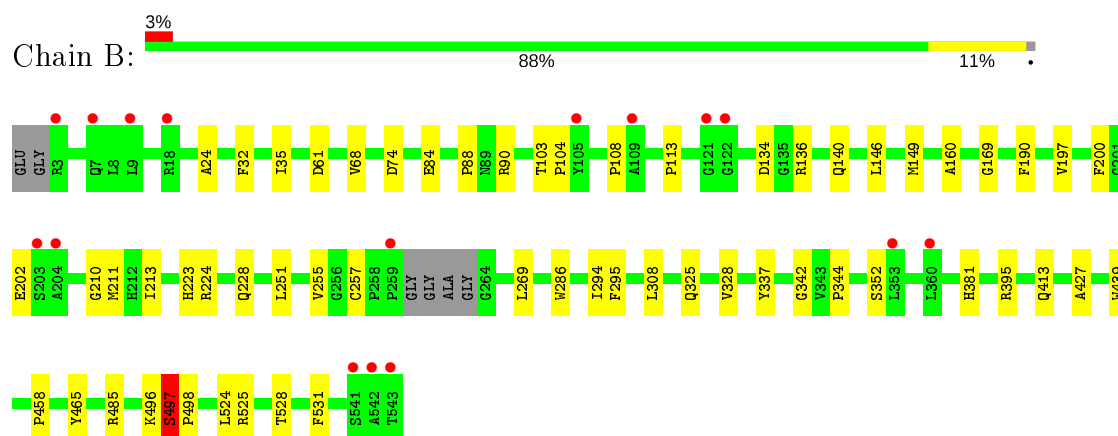
3 Residue-property plots [i](#)

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



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

Chain D:

33%

67%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.82Å 113.16Å 225.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.16 – 2.50 46.16 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (46.16-2.50) 99.2 (46.16-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.191 , 0.215 0.202 , 0.232	Depositor DCC
R_{free} test set	1421 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	50.4	Xtriage
Anisotropy	0.932	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8756	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: 5O2, NAG, P6G, FUC

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	0.53	0/4341	0.68	0/5932
1	B	0.51	0/4334	0.69	0/5924
All	All	0.52	0/8675	0.69	0/11856

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4213	0	4099	32	0
1	B	4198	0	4078	31	0
2	C	24	0	22	0	0
3	D	38	0	34	1	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
5	A	49	0	43	2	0
5	B	49	0	43	4	0
6	B	19	0	26	2	0
7	A	83	0	0	0	0
7	B	55	0	0	1	0
All	All	8756	0	8371	63	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 (63) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:VAL:H	1:A:223:HIS:HD2	1.25	0.83
1:B:197:VAL:H	1:B:223:HIS:HD2	1.24	0.82
1:B:497:SER:HB2	1:B:498:PRO:C	2.05	0.76
1:B:197:VAL:H	1:B:223:HIS:CD2	2.04	0.76
1:A:197:VAL:H	1:A:223:HIS:CD2	2.03	0.75
1:B:381:HIS:CE1	6:B:606:P6G:H31	2.26	0.70
1:A:259:PRO:HB3	1:A:269:LEU:HD12	1.76	0.66
1:B:286:TRP:CZ2	5:B:605:5O2:H11	2.36	0.60
1:B:286:TRP:CE2	5:B:605:5O2:H11	2.37	0.59
1:A:113:PRO:HG2	1:A:485:ARG:HG2	1.84	0.59
1:B:113:PRO:HG2	1:B:485:ARG:HG2	1.86	0.57
1:B:68:VAL:HG23	1:B:90:ARG:HB2	1.87	0.56
1:B:344:PRO:HA	3:D:2:NAG:H81	1.87	0.56
1:A:68:VAL:HG23	1:A:90:ARG:HB2	1.88	0.55
1:B:328:VAL:O	1:B:427:ALA:HA	2.08	0.54
1:A:4:GLU:OE2	1:A:18:ARG:HD3	2.09	0.53
1:B:224:ARG:HG2	1:B:325:GLN:HB2	1.91	0.52
1:B:211:MET:HG2	1:B:308:LEU:HD21	1.92	0.52
1:A:507:ALA:O	1:A:522[B]:ARG:HG3	2.11	0.51
1:A:328:VAL:O	1:A:427:ALA:HA	2.09	0.51
1:A:211:MET:HG2	1:A:308:LEU:HD21	1.92	0.50
1:A:224:ARG:HG2	1:A:325:GLN:HB2	1.93	0.50
1:A:439:TRP:CZ2	5:A:1504:5O2:H35	2.47	0.49
1:A:104:PRO:HD2	1:A:108:PRO:HD3	1.94	0.49
1:A:284:HIS:HA	1:A:287:HIS:HD2	1.78	0.48
1:A:202:GLU:HA	1:A:228:GLN:O	2.13	0.48
1:B:439:TRP:CZ2	5:B:605:5O2:H35	2.48	0.48
1:B:160:ALA:HB2	1:B:169:GLY:HA3	1.95	0.48
1:B:294:ILE:HA	5:B:605:5O2:H21	1.95	0.48
1:B:104:PRO:HD2	1:B:108:PRO:HD3	1.95	0.47
1:A:284:HIS:HA	1:A:287:HIS:CD2	2.50	0.47
1:A:68:VAL:HG11	1:A:88:PRO:HB3	1.96	0.47
1:B:202:GLU:HA	1:B:228:GLN:O	2.14	0.47
1:A:160:ALA:HB2	1:A:169:GLY:HA3	1.95	0.46
1:A:337:TYR:O	1:A:340:VAL:HG22	2.15	0.46
1:A:528:THR:O	1:A:531:PHE:HB3	2.16	0.45
1:A:381:HIS:HA	6:B:606:P6G:H182	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:VAL:HG11	1:B:88:PRO:HB3	1.98	0.45
1:B:134:ASP:OD1	1:B:136:ARG:HB2	2.17	0.44
1:B:255:VAL:HG23	1:B:257:CYS:HB2	1.98	0.44
1:A:103:THR:HG21	1:A:190:PHE:HB3	1.99	0.44
1:A:231:THR:HG22	1:A:414:LEU:HD22	2.00	0.43
1:B:103:THR:HG21	1:B:190:PHE:HB3	2.00	0.43
1:B:210:GLY:HA2	1:B:213:ILE:HD12	2.00	0.43
1:B:528:THR:O	1:B:531:PHE:HB3	2.17	0.43
1:B:32:PHE:HB3	1:B:35:ILE:HD11	2.01	0.43
1:A:458:PRO:HA	1:A:465:TYR:CD1	2.53	0.43
1:A:286:TRP:CZ3	5:A:1504:5O2:H18	2.54	0.43
1:B:352:SER:O	1:B:395:ARG:HG3	2.19	0.43
1:B:74:ASP:HB2	7:B:712:HOH:O	2.19	0.43
1:B:497:SER:HB2	1:B:498:PRO:CA	2.48	0.42
1:B:24:ALA:HB3	1:B:140:GLN:HG3	2.02	0.42
1:A:32:PHE:HB3	1:A:35:ILE:HD11	2.01	0.42
1:A:210:GLY:HA2	1:A:213:ILE:HD12	2.01	0.42
1:B:458:PRO:HA	1:B:465:TYR:CD1	2.54	0.41
1:A:160:ALA:HB2	1:A:169:GLY:CA	2.50	0.41
1:B:160:ALA:HB2	1:B:169:GLY:CA	2.50	0.41
1:A:352:SER:O	1:A:395:ARG:HG3	2.20	0.41
1:A:24:ALA:HB3	1:A:140:GLN:HG3	2.02	0.41
1:A:512:SER:OG	1:A:519:GLU:HB3	2.21	0.41
1:A:257:CYS:HA	1:A:258:PRO:HD3	1.92	0.41
1:A:36:PRO:HB2	1:A:53:LYS:HD3	2.04	0.40
1:B:525:ARG:HG2	1:B:528:THR:HB	2.02	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	536/543 (99%)	519 (97%)	16 (3%)	1 (0%)	47 68
1	B	536/543 (99%)	521 (97%)	13 (2%)	2 (0%)	34 54
All	All	1072/1086 (99%)	1040 (97%)	29 (3%)	3 (0%)	41 61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	497	SER
1	A	342	GLY
1	B	342	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	443/443 (100%)	429 (97%)	14 (3%)	39 65
1	B	443/443 (100%)	430 (97%)	13 (3%)	42 69
All	All	886/886 (100%)	859 (97%)	27 (3%)	40 68

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	TYR
1	A	84	GLU
1	A	146	LEU
1	A	161	LEU
1	A	200	PHE
1	A	251	LEU
1	A	295	PHE
1	A	337	TYR
1	A	356	ARG
1	A	372	ASP
1	A	424	ARG
1	A	494	ASP
1	A	525	ARG

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Mol	Chain	Res	Type
1	A	541	SER
1	B	61	ASP
1	B	84	GLU
1	B	146	LEU
1	B	149	MET
1	B	200	PHE
1	B	251	LEU
1	B	269	LEU
1	B	295	PHE
1	B	337	TYR
1	B	413	GLN
1	B	496	LYS
1	B	497	SER
1	B	524	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	HIS
1	A	287	HIS
1	B	223	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](#)

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

5.5 Carbohydrates [i](#)

5 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	C	1	1,2	14,14,15	0.36	0	17,19,21	0.62	1 (5%)
2	FUC	C	2	2	10,10,11	0.47	0	14,14,16	0.70	0
3	NAG	D	1	1,3	14,14,15	0.33	0	17,19,21	0.95	1 (5%)
3	NAG	D	2	3	14,14,15	0.33	0	17,19,21	0.58	0
3	FUC	D	3	3	10,10,11	0.45	0	14,14,16	0.62	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	C	1	1,2	-	0/6/23/26	0/1/1/1
2	FUC	C	2	2	-	-	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	FUC	D	3	3	-	-	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	NAG	C1-O5-C5	3.13	116.44	112.19
2	C	1	NAG	C1-O5-C5	2.17	115.14	112.19

There are no chirality outliers.

There are no torsion outliers.

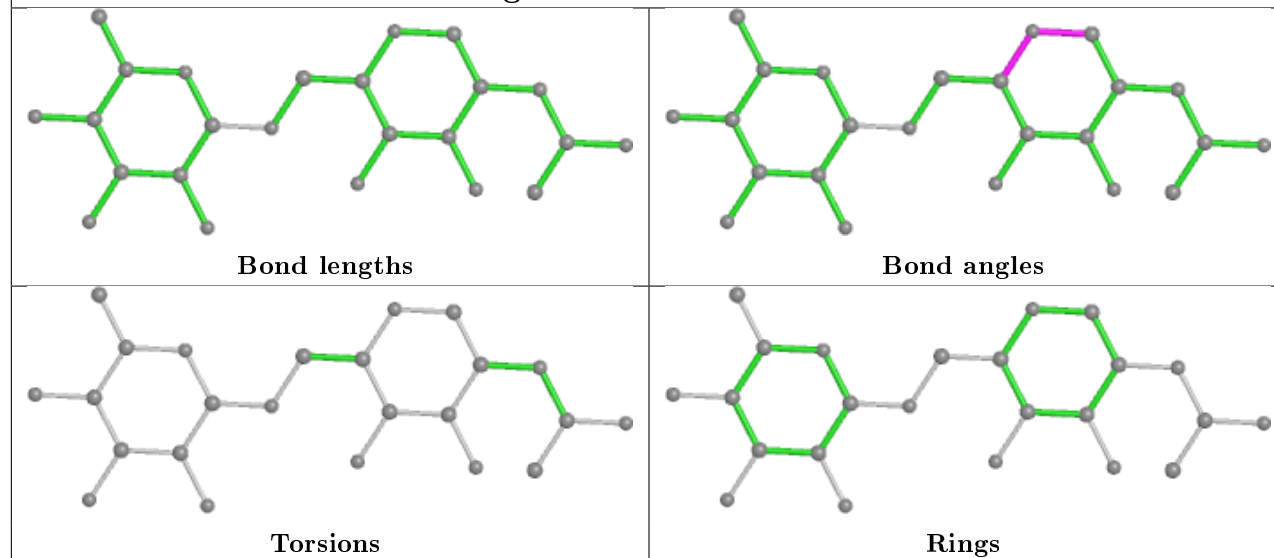
There are no ring outliers.

1 monomer is involved in 1 short contact:

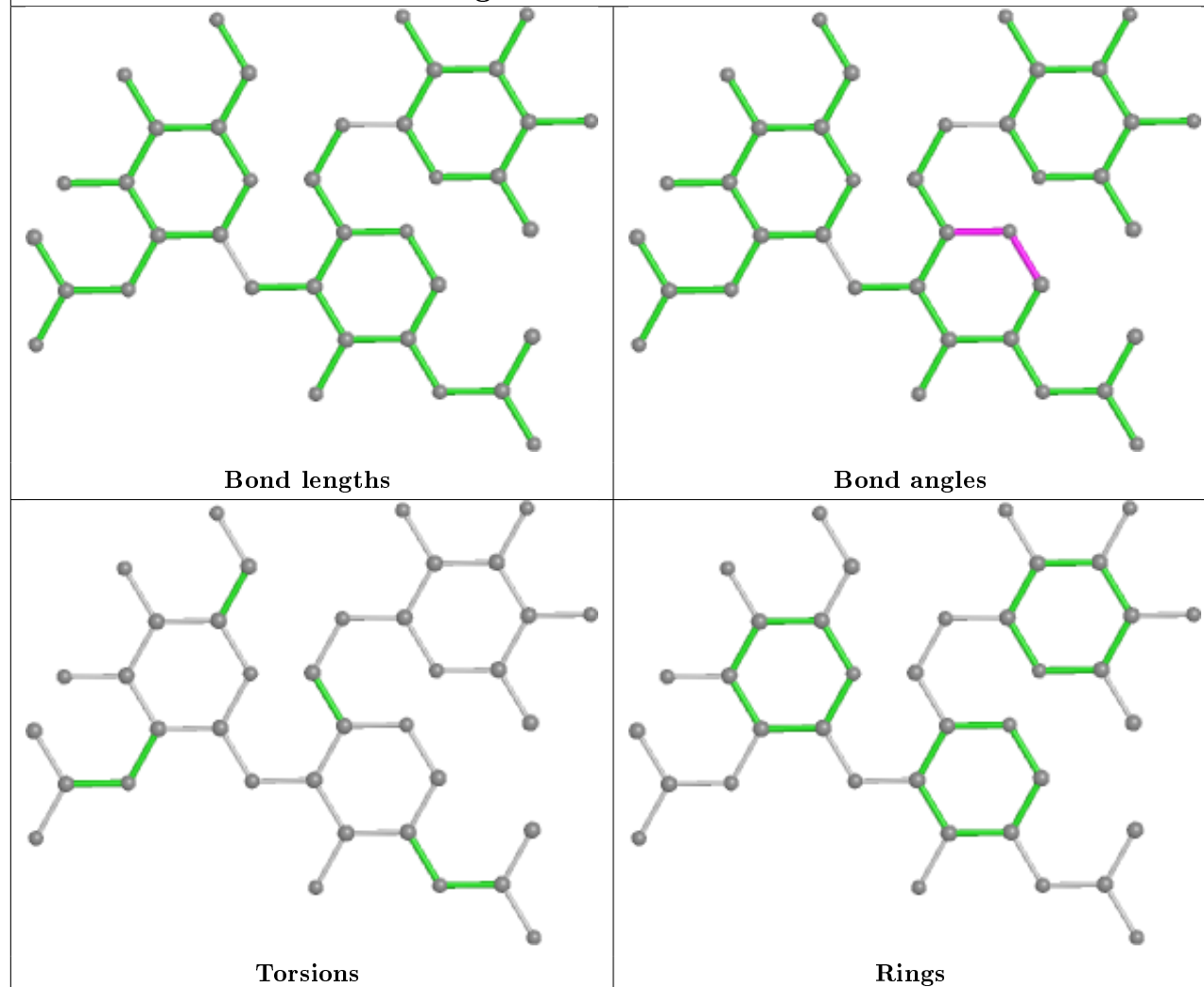
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2	NAG	1	0

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



Oligosaccharide Chain D



5.6 Ligand geometry

5 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	601	1	14,14,15	0.38	0	17,19,21	0.58	0
5	5O2	A	1504	-	54,56,56	2.44	15 (27%)	64,79,79	1.33	5 (7%)
6	P6G	B	606	-	18,18,18	2.33	6 (33%)	17,17,17	1.60	4 (23%)
5	5O2	B	605	-	54,56,56	2.61	16 (29%)	64,79,79	1.35	8 (12%)
4	NAG	A	1503	1	14,14,15	0.41	0	17,19,21	0.79	1 (5%)

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	NAG	B	601	1	-	0/6/23/26	0/1/1/1
5	5O2	A	1504	-	-	10/18/25/25	0/8/8/8
6	P6G	B	606	-	-	7/16/16/16	-
5	5O2	B	605	-	-	6/18/25/25	0/8/8/8
4	NAG	A	1503	1	-	0/6/23/26	0/1/1/1

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	605	5O2	C39-C37	7.70	1.52	1.40
5	A	1504	5O2	C6-N2	7.61	1.50	1.40
5	B	605	5O2	C6-N2	7.10	1.49	1.40
5	B	605	5O2	C30-C39	7.07	1.51	1.38
5	A	1504	5O2	C39-C37	6.51	1.50	1.40
5	A	1504	5O2	C30-C39	6.42	1.49	1.38
5	B	605	5O2	C31-C33	5.54	1.51	1.42
5	B	605	5O2	C14-C16	5.22	1.50	1.42
5	A	1504	5O2	C14-C16	5.18	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	605	5O2	C7-C14	4.90	1.51	1.43
6	B	606	P6G	O10-C9	4.78	1.62	1.42
5	A	1504	5O2	C7-C14	4.65	1.51	1.43
5	A	1504	5O2	C30-C31	4.02	1.50	1.43
6	B	606	P6G	O16-C15	4.01	1.59	1.42
5	B	605	5O2	N4-N5	3.88	1.41	1.34
5	A	1504	5O2	C5-C6	3.85	1.48	1.40
5	A	1504	5O2	C31-C33	3.83	1.48	1.42
6	B	606	P6G	O13-C12	3.82	1.58	1.42
5	B	605	5O2	C5-C6	3.74	1.48	1.40
6	B	606	P6G	O4-C3	3.68	1.58	1.42
6	B	606	P6G	O19-C18	3.57	1.60	1.42
5	B	605	5O2	C30-C31	3.55	1.49	1.43
5	B	605	5O2	C4-C6	3.54	1.48	1.41
5	A	1504	5O2	C4-C6	3.53	1.48	1.41
5	B	605	5O2	N5-N6	3.44	1.41	1.34
5	B	605	5O2	C37-N8	3.33	1.36	1.32
5	A	1504	5O2	N5-N6	3.31	1.40	1.34
5	A	1504	5O2	N4-N5	3.23	1.40	1.34
6	B	606	P6G	O7-C6	2.79	1.54	1.42
5	B	605	5O2	C27-C26	2.65	1.40	1.36
5	B	605	5O2	C26-N4	2.42	1.37	1.34
5	A	1504	5O2	C37-N8	2.37	1.35	1.32
5	A	1504	5O2	C3-C2	2.24	1.41	1.36
5	A	1504	5O2	C27-C26	2.17	1.39	1.36
5	B	605	5O2	C3-C2	2.17	1.41	1.36
5	A	1504	5O2	C27-N6	-2.16	1.33	1.35
5	B	605	5O2	C17-C18	2.01	1.40	1.36

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1504	5O2	C37-N8-C33	5.53	124.49	117.67
5	B	605	5O2	C37-N8-C33	4.65	123.41	117.67
5	A	1504	5O2	N4-N5-N6	-4.17	104.17	107.31
5	B	605	5O2	N4-N5-N6	-3.59	104.61	107.31
5	A	1504	5O2	C39-C37-N8	-3.51	120.69	123.68
6	B	606	P6G	O1-C2-C3	3.36	131.29	111.81
5	B	605	5O2	C39-C37-N8	-3.29	120.87	123.68
5	A	1504	5O2	C5-C6-C4	-3.10	116.68	120.61
5	B	605	5O2	C5-C6-C4	-3.07	116.72	120.61
6	B	606	P6G	O13-C12-C11	2.80	123.03	110.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1503	NAG	C1-O5-C5	2.73	115.89	112.19
5	B	605	5O2	C8-C7-C14	-2.48	116.23	121.31
6	B	606	P6G	O4-C3-C2	2.47	120.92	110.07
5	B	605	5O2	C39-C30-N7	2.42	123.97	119.54
5	B	605	5O2	C20-N2-C6	-2.41	116.75	118.90
5	A	1504	5O2	C8-C7-C14	-2.39	116.41	121.31
5	B	605	5O2	C41-C40-C39	-2.25	108.21	112.84
6	B	606	P6G	O7-C6-C5	2.03	119.57	110.39

There are no chirality outliers.

All (23) torsion outliers are listed below:

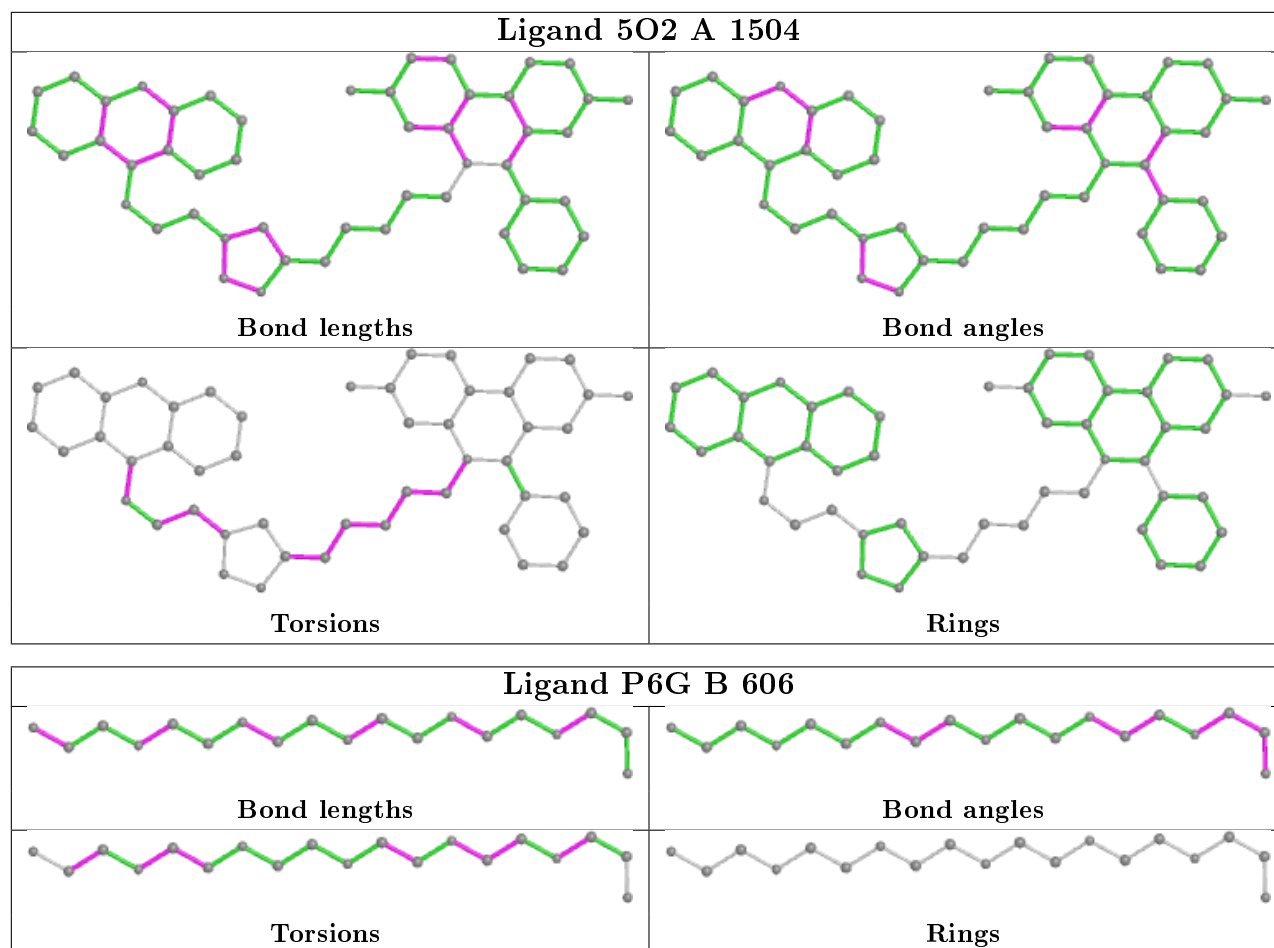
Mol	Chain	Res	Type	Atoms
5	A	1504	5O2	N2-C20-C21-C22
5	A	1504	5O2	C24-C25-C26-N4
5	A	1504	5O2	C29-C28-N6-N5
5	A	1504	5O2	C29-C28-N6-C27
5	A	1504	5O2	N6-C28-C29-N7
5	B	605	5O2	C29-C28-N6-C27
5	B	605	5O2	N6-C28-C29-N7
6	B	606	P6G	C14-C15-O16-C17
5	A	1504	5O2	C20-C21-C22-C24
5	A	1504	5O2	C22-C24-C25-C26
6	B	606	P6G	O4-C5-C6-O7
6	B	606	P6G	O13-C14-C15-O16
6	B	606	P6G	O16-C17-C18-O19
5	B	605	5O2	C31-C30-N7-C29
5	A	1504	5O2	C21-C22-C24-C25
5	B	605	5O2	C20-C21-C22-C24
5	A	1504	5O2	C21-C20-N2-C7
5	B	605	5O2	C21-C22-C24-C25
6	B	606	P6G	C5-C6-O7-C8
6	B	606	P6G	O7-C8-C9-O10
5	B	605	5O2	C29-C28-N6-N5
5	A	1504	5O2	C31-C30-N7-C29
6	B	606	P6G	C2-C3-O4-C5

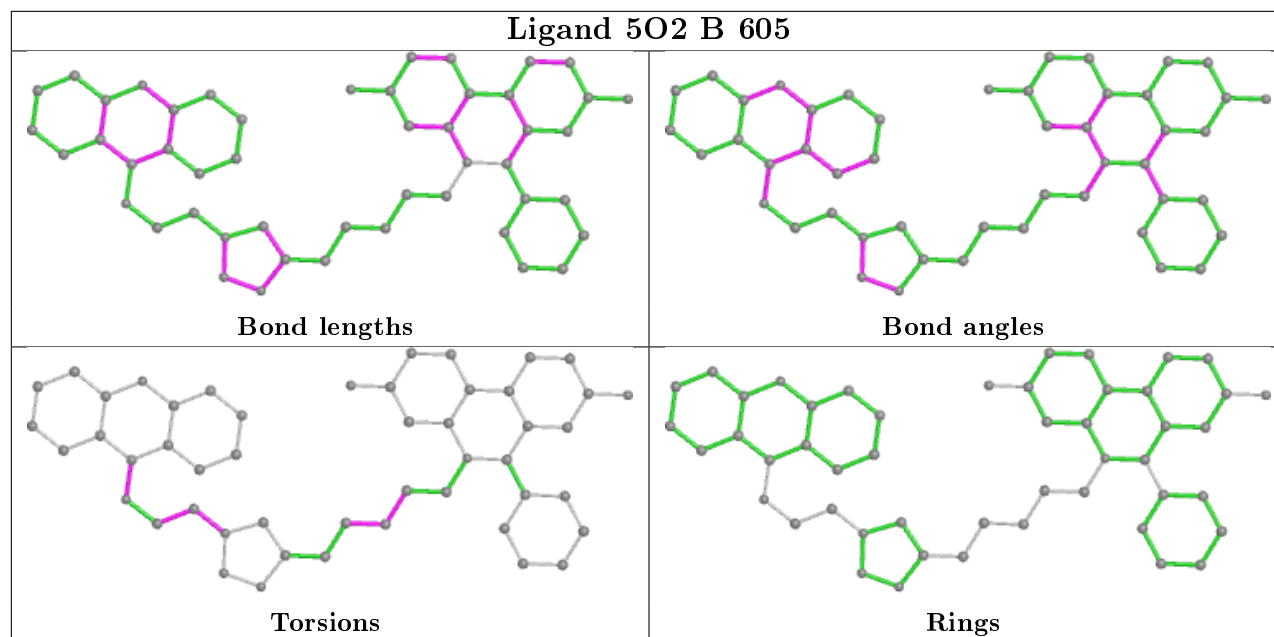
There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1504	5O2	2	0
6	B	606	P6G	2	0
5	B	605	5O2	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	538/543 (99%)	-0.27	11 (2%) 65 68	42, 61, 91, 141	0
1	B	537/543 (98%)	0.03	16 (2%) 50 53	48, 66, 97, 152	0
All	All	1075/1086 (98%)	-0.12	27 (2%) 57 61	42, 64, 95, 152	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	259	PRO	5.7
1	B	542	ALA	5.2
1	B	541	SER	4.5
1	B	259	PRO	4.4
1	B	543	THR	4.1
1	A	543	THR	3.6
1	A	542	ALA	3.3
1	A	373	LEU	3.3
1	A	496	LYS	2.8
1	A	380	LEU	2.8
1	B	203	SER	2.8
1	B	204	ALA	2.6
1	B	121	GLY	2.6
1	B	105	TYR	2.5
1	B	109	ALA	2.4
1	B	3	ARG	2.4
1	B	7	GLN	2.3
1	B	122	GLY	2.3
1	A	165	ARG	2.2
1	B	353	LEU	2.2
1	A	470	ARG	2.1
1	A	540	LEU	2.1
1	A	493	ARG	2.1
1	A	539	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	9	LEU	2.1
1	B	360	LEU	2.1
1	B	18	ARG	2.1

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

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

6.3 Carbohydrates [i](#)

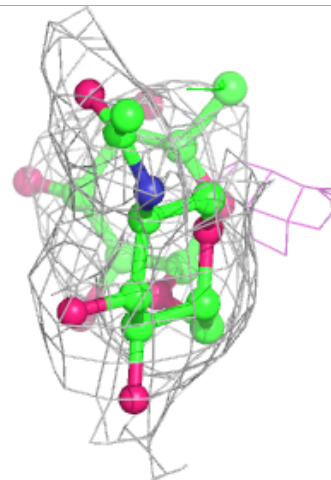
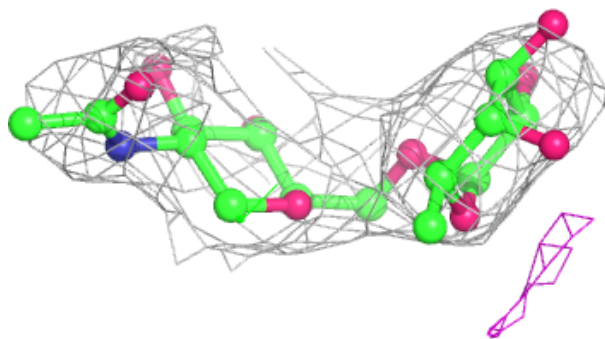
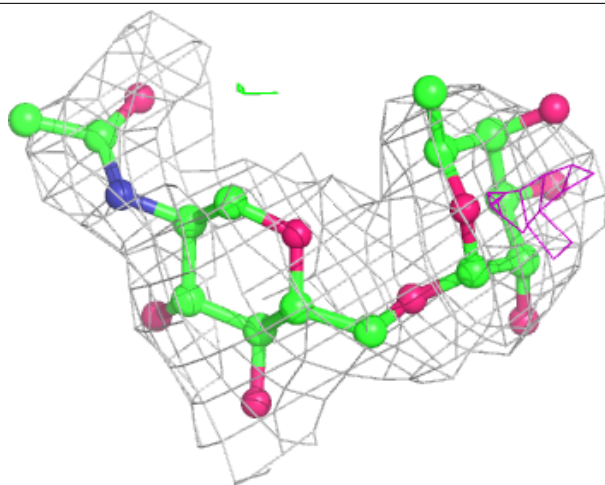
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

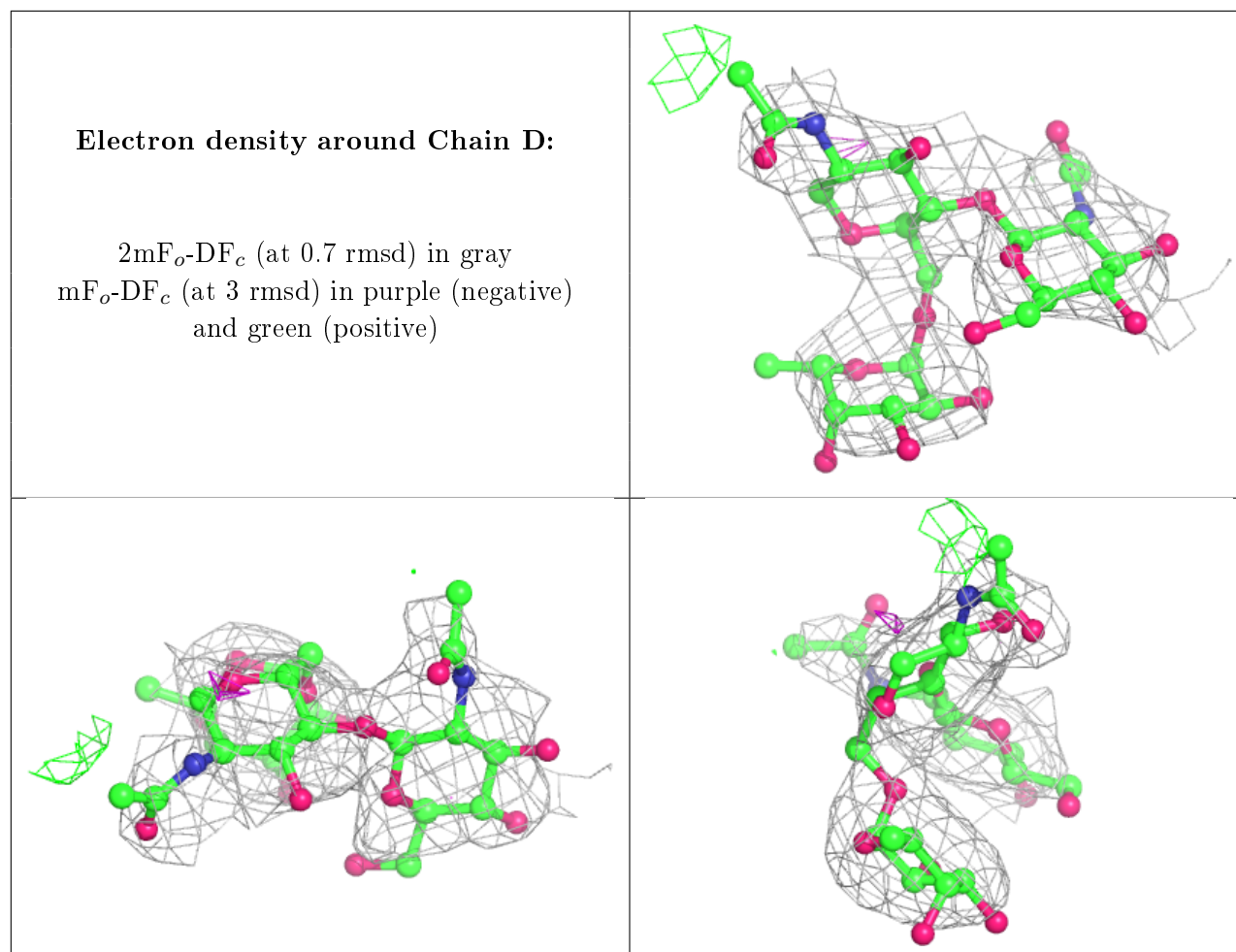
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	D	2	14/15	0.83	0.46	135,136,137,137	0
3	NAG	D	1	14/15	0.85	0.43	127,131,134,136	0
2	NAG	C	1	14/15	0.86	0.24	107,110,119,123	0
3	FUC	D	3	10/11	0.91	0.46	132,134,135,136	0
2	FUC	C	2	10/11	0.92	0.45	127,130,132,134	0

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)





6.4 Ligands [i](#)

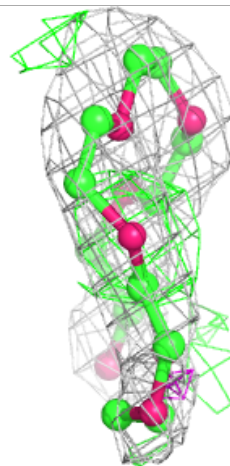
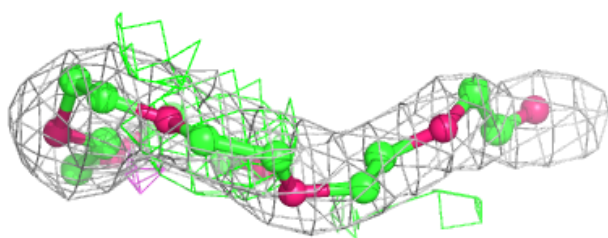
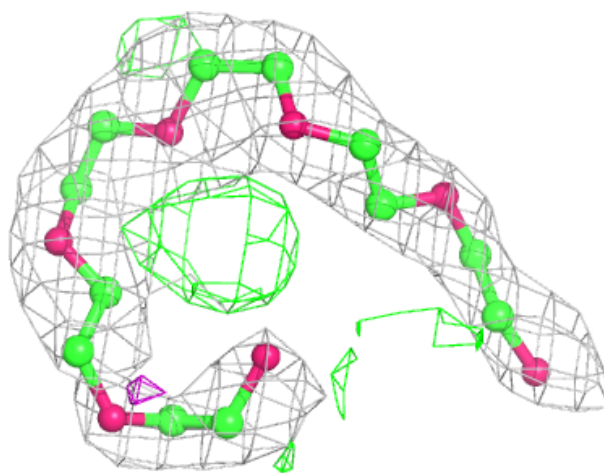
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	B	601	14/15	0.83	0.22	125,128,131,131	0
6	P6G	B	606	19/19	0.85	0.25	65,80,85,85	0
4	NAG	A	1503	14/15	0.87	0.19	108,111,114,114	0
5	5O2	B	605	49/49	0.90	0.20	44,97,112,114	0
5	5O2	A	1504	49/49	0.93	0.20	47,88,97,99	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.

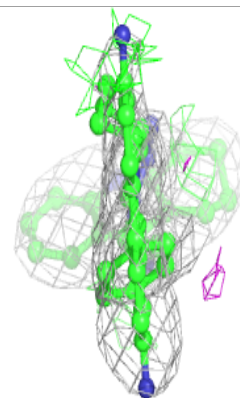
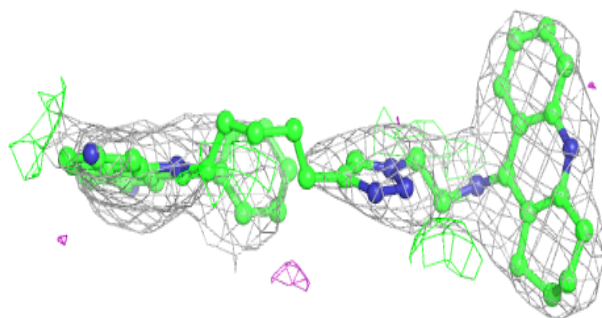
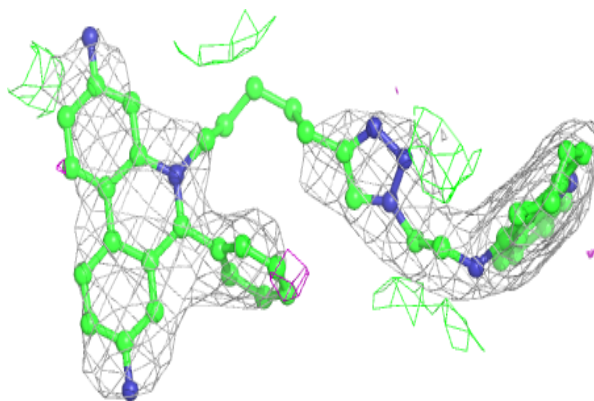
Electron density around P6G B 606:

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

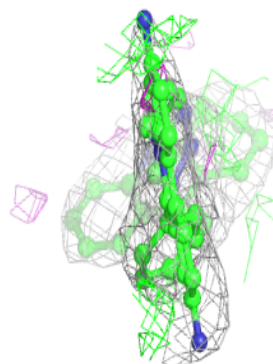
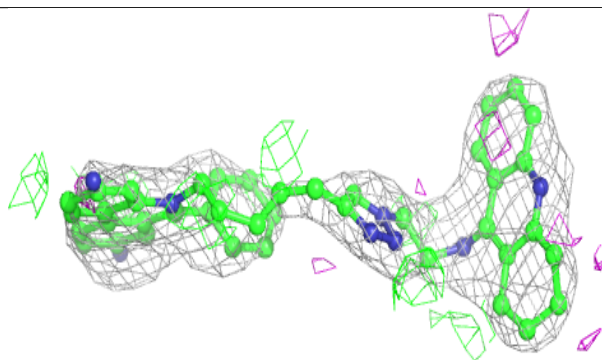
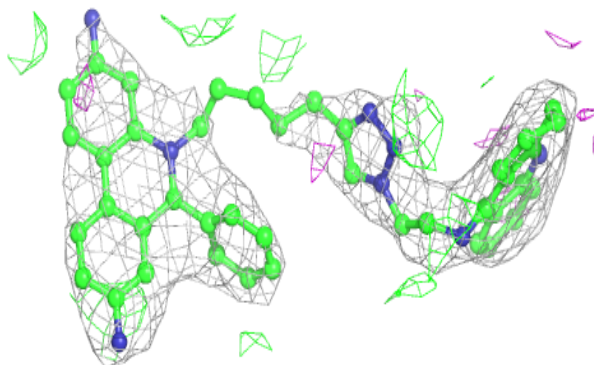


Electron density around 5O2 B 605:

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

**Electron density around 5O2 A 1504:**

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



6.5 Other polymers

There are no such residues in this entry.