Full wwPDB X-ray Structure Validation Report ⓘ

Nov 4, 2021 – 12:05 am GMT

PDB ID	:	7ANA
Title	:	A single sulfatase is required for metabolism of colonic mucin O-glycans and intestinal colonization by a symbiotic human gut bacterium (BT1622-S1_20)
Authors	:	Sofia de Jesus Vaz Luis, A.; Basle, A.; Martens, E.C.; Cartmell, A.
Deposited on	:	2020-10-11
Resolution	:	2.30 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:

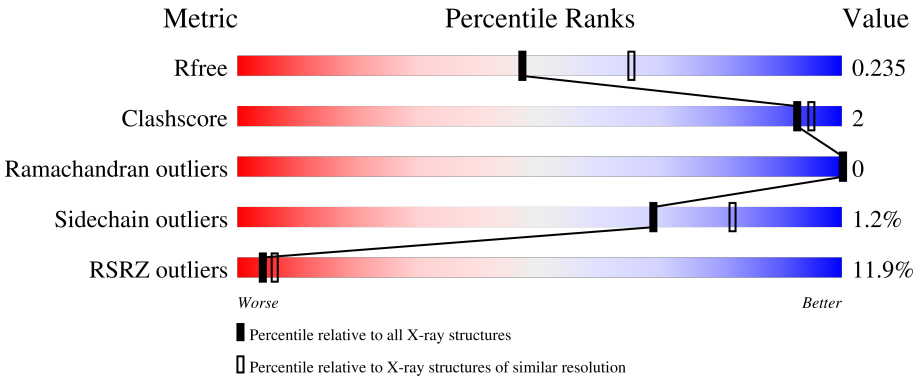
MolProbity	:	4.02b-467
Mogul	:	1.8.4 (270009), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	AAA	503	20% 89% 6% 6%
1	BBB	503	2% 90% 5% 6%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7799 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 N-acetylgalactosamine-6-sulfatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	475	Total	C	N	O	S	0	0	0
			3785	2412	646	705	22			
1	BBB	475	Total	C	N	O	S	0	1	0
			3796	2418	650	706	22			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-2	MET	-	initiating methionine	UNP Q8A7A3
AAA	-1	GLY	-	expression tag	UNP Q8A7A3
AAA	0	SER	-	expression tag	UNP Q8A7A3
AAA	1	SER	-	expression tag	UNP Q8A7A3
AAA	2	HIS	-	expression tag	UNP Q8A7A3
AAA	3	HIS	-	expression tag	UNP Q8A7A3
AAA	4	HIS	-	expression tag	UNP Q8A7A3
AAA	5	HIS	-	expression tag	UNP Q8A7A3
AAA	6	HIS	-	expression tag	UNP Q8A7A3
AAA	7	HIS	-	expression tag	UNP Q8A7A3
AAA	8	SER	-	expression tag	UNP Q8A7A3
AAA	9	SER	-	expression tag	UNP Q8A7A3
AAA	10	GLY	-	expression tag	UNP Q8A7A3
AAA	11	LEU	-	expression tag	UNP Q8A7A3
AAA	12	VAL	-	expression tag	UNP Q8A7A3
AAA	13	PRO	-	expression tag	UNP Q8A7A3
AAA	14	ARG	-	expression tag	UNP Q8A7A3
AAA	15	GLY	-	expression tag	UNP Q8A7A3
AAA	16	SER	-	expression tag	UNP Q8A7A3
AAA	17	HIS	-	expression tag	UNP Q8A7A3
AAA	18	MET	-	expression tag	UNP Q8A7A3
AAA	19	ALA	-	expression tag	UNP Q8A7A3
AAA	20	SER	-	expression tag	UNP Q8A7A3
BBB	-2	MET	-	initiating methionine	UNP Q8A7A3
BBB	-1	GLY	-	expression tag	UNP Q8A7A3

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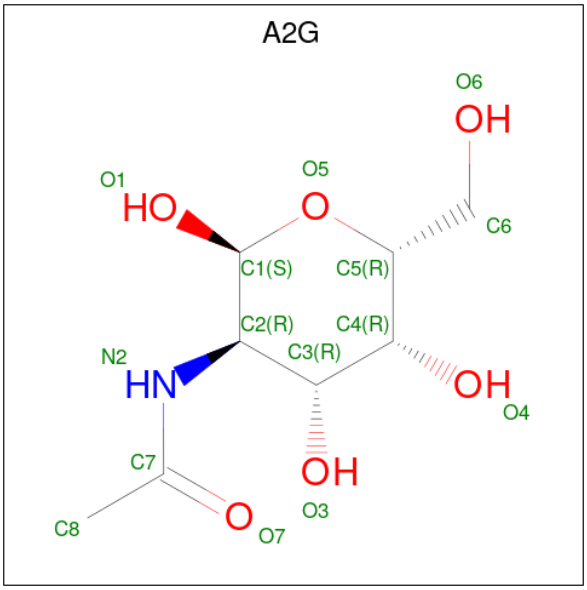
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	0	SER	-	expression tag	UNP Q8A7A3
BBB	1	SER	-	expression tag	UNP Q8A7A3
BBB	2	HIS	-	expression tag	UNP Q8A7A3
BBB	3	HIS	-	expression tag	UNP Q8A7A3
BBB	4	HIS	-	expression tag	UNP Q8A7A3
BBB	5	HIS	-	expression tag	UNP Q8A7A3
BBB	6	HIS	-	expression tag	UNP Q8A7A3
BBB	7	HIS	-	expression tag	UNP Q8A7A3
BBB	8	SER	-	expression tag	UNP Q8A7A3
BBB	9	SER	-	expression tag	UNP Q8A7A3
BBB	10	GLY	-	expression tag	UNP Q8A7A3
BBB	11	LEU	-	expression tag	UNP Q8A7A3
BBB	12	VAL	-	expression tag	UNP Q8A7A3
BBB	13	PRO	-	expression tag	UNP Q8A7A3
BBB	14	ARG	-	expression tag	UNP Q8A7A3
BBB	15	GLY	-	expression tag	UNP Q8A7A3
BBB	16	SER	-	expression tag	UNP Q8A7A3
BBB	17	HIS	-	expression tag	UNP Q8A7A3
BBB	18	MET	-	expression tag	UNP Q8A7A3
BBB	19	ALA	-	expression tag	UNP Q8A7A3
BBB	20	SER	-	expression tag	UNP Q8A7A3

- Molecule 2 is 2-acetamido-2-deoxy-alpha-D-galactopyranose (three-letter code: A2G) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).

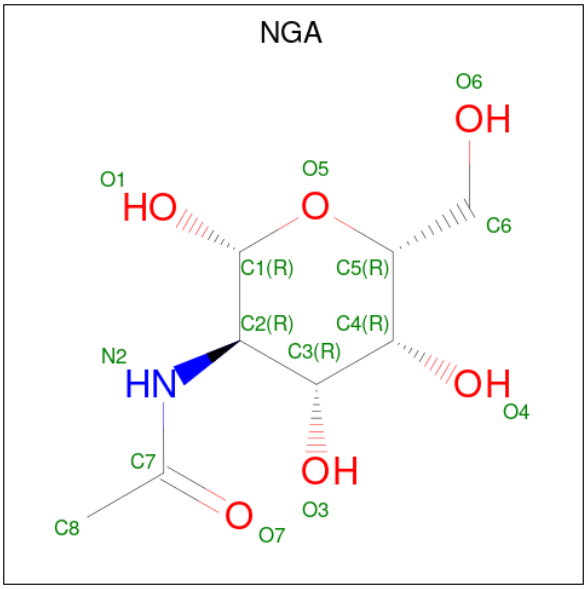


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total C N O 15 8 1 6	0	0
2	BBB	1	Total C N O 15 8 1 6	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

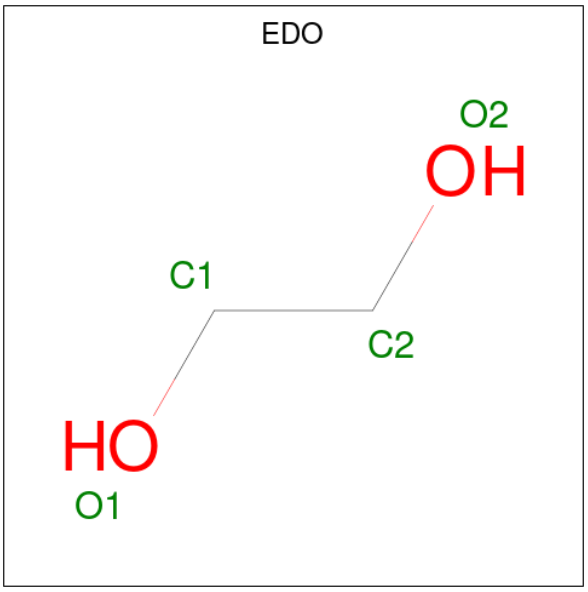
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total Ca 1 1	0	0
3	BBB	1	Total Ca 1 1	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-galactopyranose (three-letter code: NGA) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	BBB	1	Total C N O 15 8 1 6	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	BBB	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

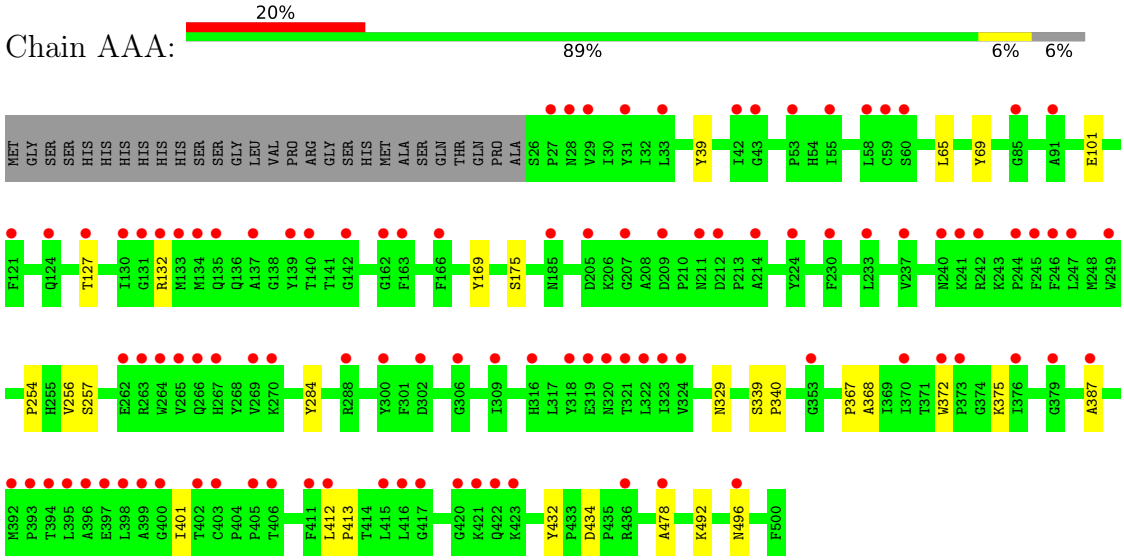
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	52	Total O 52 52	0	0
6	BBB	115	Total O 115 115	0	0

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.

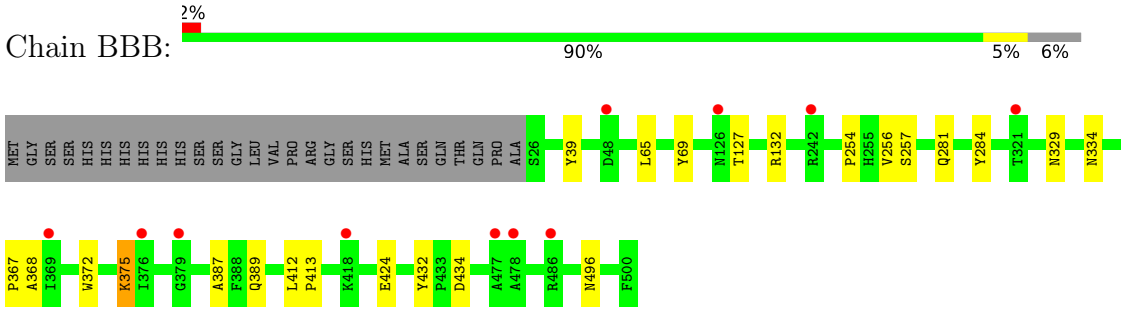
• Molecule 1: N-acetylgalactosamine-6-sulfatase

Chain AAA:



• Molecule 1: N-acetylgalactosamine-6-sulfatase

Chain BBB:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	83.25Å 83.25Å 390.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.22 – 2.30 70.12 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (70.22-2.30) 99.8 (70.12-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.211 , 0.235 0.216 , 0.235	Depositor DCC
R_{free} test set	3073 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	47.6	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7799	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, A2G, EDO, NGA

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	AAA	0.64	0/3899	0.74	1/5289 (0.0%)
1	BBB	0.63	0/3910	0.76	2/5303 (0.0%)
All	All	0.63	0/7809	0.75	3/10592 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BBB	389	GLN	CB-CA-C	-6.84	96.72	110.40
1	AAA	496	ASN	CB-CA-C	-5.49	99.42	110.40
1	BBB	496	ASN	CB-CA-C	-5.41	99.59	110.40

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	AAA	3785	0	3612	12	0
1	BBB	3796	0	3624	10	0
2	AAA	15	0	12	0	0
2	BBB	15	0	12	1	0
3	AAA	1	0	0	0	0
3	BBB	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	BBB	15	0	15	1	0
5	BBB	4	0	6	1	0
6	AAA	52	0	0	0	0
6	BBB	115	0	0	1	0
All	All	7799	0	7281	23	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 2.

All (23) 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)
5:BBB:602:EDO:H21	6:BBB:718:HOH:O	1.97	0.65
1:AAA:127:THR:O	1:AAA:132:ARG:NH1	2.41	0.54
1:BBB:127:THR:O	1:BBB:132:ARG:NH1	2.41	0.53
1:AAA:478:ALA:HB2	4:BBB:601:NGA:H82	1.90	0.52
1:BBB:39:TYR:HA	1:BBB:367:PRO:HD3	1.95	0.48
1:BBB:65:LEU:HB2	1:BBB:368:ALA:HB3	1.98	0.46
1:BBB:372:TRP:CE2	1:BBB:375:LYS:HG3	2.51	0.46
1:AAA:39:TYR:HA	1:AAA:367:PRO:HD3	1.97	0.45
1:AAA:256:VAL:HG23	1:AAA:284:TYR:CE2	2.51	0.45
1:BBB:256:VAL:HG23	1:BBB:284:TYR:CE2	2.51	0.45
1:AAA:65:LEU:HB2	1:AAA:368:ALA:HB3	1.98	0.45
1:BBB:334:ASN:ND2	2:BBB:603:A2G:H8	2.32	0.44
1:BBB:69:TYR:O	1:BBB:387:ALA:HA	2.18	0.43
1:AAA:432:TYR:CZ	1:AAA:434:ASP:HB3	2.53	0.43
1:AAA:69:TYR:O	1:AAA:387:ALA:HA	2.19	0.43
1:AAA:372:TRP:CE2	1:AAA:375:LYS:HG3	2.54	0.43
1:AAA:256:VAL:HB	1:AAA:257:SER:HA	2.01	0.42
1:BBB:432:TYR:CZ	1:BBB:434:ASP:HB3	2.54	0.42
1:AAA:412:LEU:N	1:AAA:413:PRO:CD	2.83	0.42
1:BBB:412:LEU:N	1:BBB:413:PRO:CD	2.83	0.42
1:AAA:339:SER:N	1:AAA:340:PRO:CD	2.83	0.41
1:BBB:256:VAL:HB	1:BBB:257:SER:HA	2.03	0.41
1:AAA:169:TYR:CE1	1:AAA:175:SER:HA	2.56	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	AAA	473/503 (94%)	457 (97%)	16 (3%)	0	100	100
1	BBB	474/503 (94%)	459 (97%)	15 (3%)	0	100	100
All	All	947/1006 (94%)	916 (97%)	31 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	400/425 (94%)	395 (99%)	5 (1%)	69	82
1	BBB	401/425 (94%)	396 (99%)	5 (1%)	71	84
All	All	801/850 (94%)	791 (99%)	10 (1%)	69	84

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	101	GLU
1	AAA	254	PRO
1	AAA	329	ASN
1	AAA	401	ILE
1	AAA	492	LYS
1	BBB	254	PRO
1	BBB	281	GLN
1	BBB	329	ASN

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Mol	Chain	Res	Type
1	BBB	375	LYS
1	BBB	424	GLU

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)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

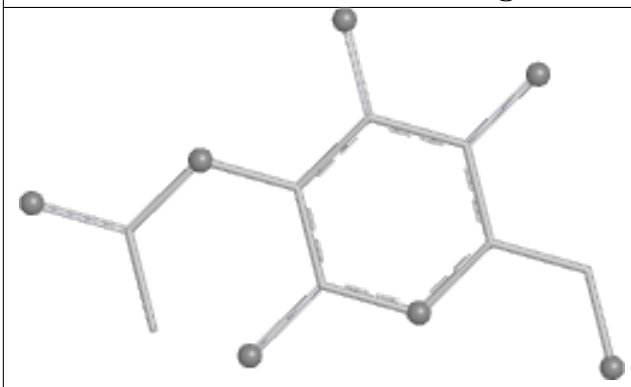
There are no ring outliers.

No monomer is involved in short contacts.

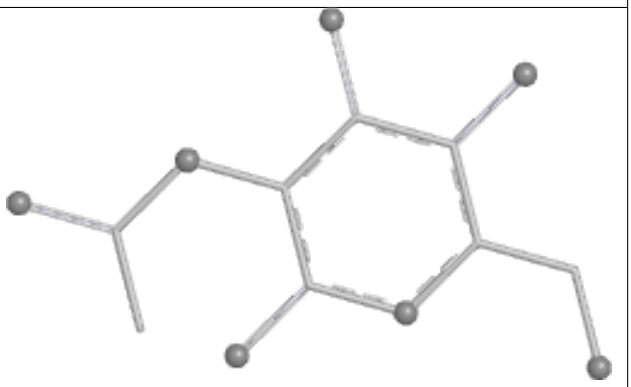
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

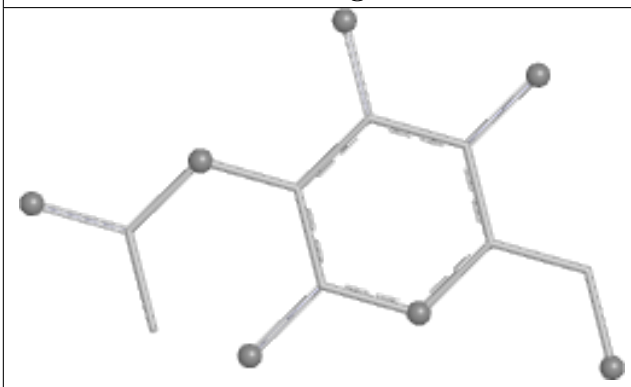
Ligand A2G AAA 701



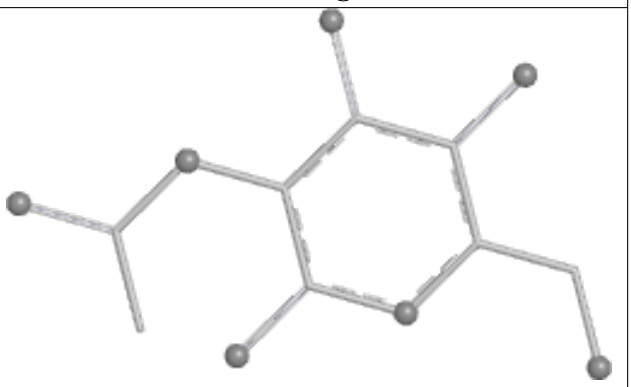
Bond lengths



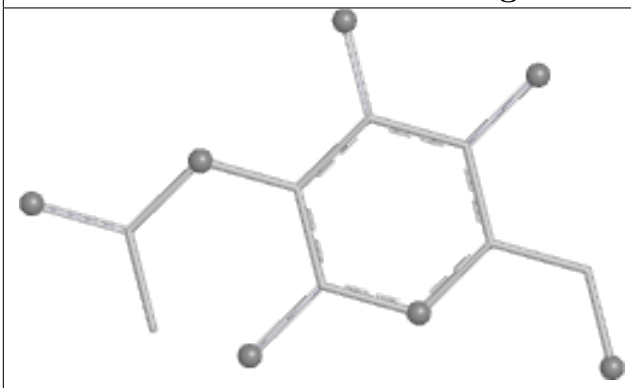
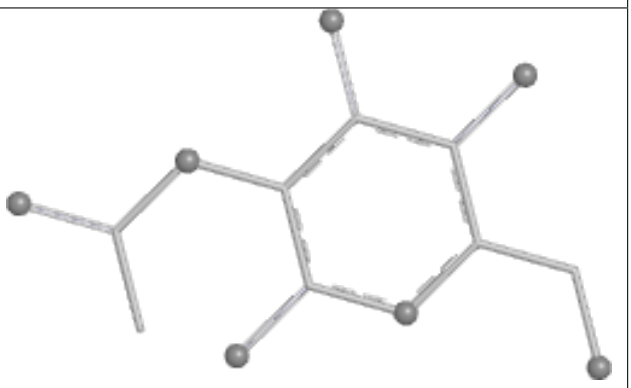
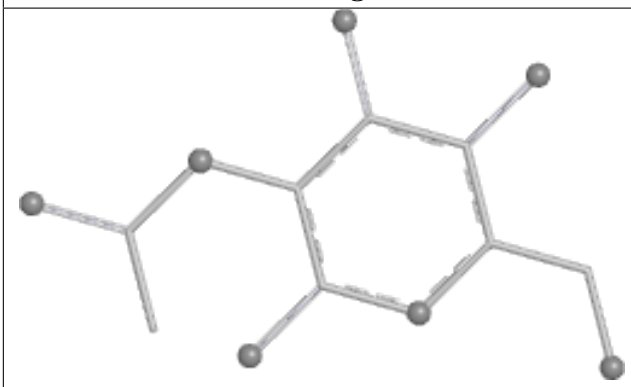
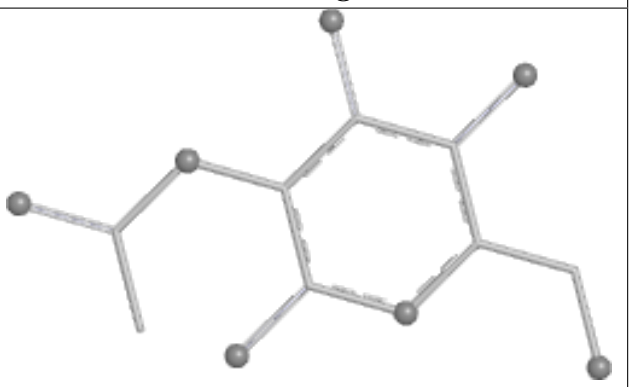
Bond angles



Torsions



Rings

Ligand A2G BBB 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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>2	OWAB(Å^2)	Q<0.9
1	AAA	475/503 (94%)	1.25	102 (21%) 0 1	45, 68, 120, 143	0
1	BBB	475/503 (94%)	0.62	11 (2%) 60 67	35, 48, 69, 92	0
All	All	950/1006 (94%)	0.93	113 (11%) 4 6	35, 55, 109, 143	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	237	VAL	9.9
1	AAA	247	LEU	6.8
1	AAA	402	THR	5.9
1	AAA	263	ARG	5.6
1	AAA	58	LEU	5.5
1	AAA	387	ALA	5.4
1	AAA	245	PHE	5.4
1	AAA	322	LEU	4.9
1	AAA	416	LEU	4.8
1	AAA	397	GLU	4.6
1	AAA	233	LEU	4.5
1	AAA	417	GLY	4.4
1	AAA	55	ILE	4.3
1	AAA	399	ALA	4.3
1	AAA	207	GLY	4.2
1	AAA	133	MET	4.1
1	AAA	131	GLY	4.1
1	AAA	411	PHE	4.0
1	AAA	395	LEU	4.0
1	AAA	373	PRO	3.9
1	AAA	139	TYR	3.9
1	AAA	244	PRO	3.8
1	AAA	214	ALA	3.8
1	AAA	209	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	AAA	376	ILE	3.8
1	AAA	266	GLN	3.8
1	AAA	400	GLY	3.7
1	AAA	415	LEU	3.6
1	AAA	270	LYS	3.5
1	AAA	31	TYR	3.4
1	AAA	163	PHE	3.4
1	AAA	288	ARG	3.4
1	AAA	264	TRP	3.4
1	AAA	309	ILE	3.4
1	AAA	132	ARG	3.4
1	BBB	477	ALA	3.3
1	AAA	423	LYS	3.3
1	AAA	211	ASN	3.3
1	AAA	403	CYS	3.3
1	AAA	53	PRO	3.2
1	AAA	398	LEU	3.1
1	AAA	212	ASP	3.1
1	AAA	127	THR	3.0
1	AAA	319	GLU	3.0
1	AAA	230	PHE	3.0
1	AAA	59	CYS	3.0
1	AAA	130	ILE	2.9
1	AAA	140	THR	2.9
1	AAA	166	PHE	2.9
1	AAA	124	GLN	2.8
1	AAA	27	PRO	2.7
1	AAA	394	THR	2.7
1	AAA	412	LEU	2.7
1	AAA	135	GLN	2.7
1	AAA	320	ASN	2.7
1	BBB	478	ALA	2.7
1	AAA	300	TYR	2.7
1	AAA	321	THR	2.7
1	AAA	241	LYS	2.7
1	AAA	405	PRO	2.7
1	BBB	48	ASP	2.6
1	AAA	185	ASN	2.6
1	AAA	240	ASN	2.6
1	AAA	324	VAL	2.6
1	AAA	379	GLY	2.6
1	AAA	134	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	BBB	379	GLY	2.5
1	BBB	418	LYS	2.5
1	AAA	162	GLY	2.5
1	AAA	224	TYR	2.5
1	AAA	43	GLY	2.5
1	AAA	478	ALA	2.5
1	AAA	323	ILE	2.5
1	AAA	496	ASN	2.5
1	AAA	396	ALA	2.5
1	AAA	267	HIS	2.4
1	AAA	318	TYR	2.4
1	AAA	420	GLY	2.4
1	AAA	60	SER	2.4
1	AAA	142	GLY	2.4
1	AAA	269	VAL	2.4
1	AAA	85	GLY	2.4
1	AAA	436	ARG	2.4
1	AAA	242	ARG	2.3
1	BBB	486	ARG	2.3
1	AAA	406	THR	2.3
1	AAA	353	GLY	2.3
1	AAA	91	ALA	2.3
1	AAA	137	ALA	2.3
1	AAA	316	HIS	2.3
1	BBB	242	ARG	2.3
1	AAA	372	TRP	2.3
1	AAA	28	ASN	2.3
1	AAA	205	ASP	2.2
1	AAA	29	VAL	2.2
1	AAA	262	GLU	2.2
1	AAA	422	GLN	2.2
1	BBB	321	THR	2.2
1	AAA	246	PHE	2.2
1	BBB	126	ASN	2.2
1	AAA	33	LEU	2.2
1	AAA	306	GLY	2.2
1	AAA	249	TRP	2.1
1	AAA	421	LYS	2.1
1	AAA	393	PRO	2.1
1	BBB	376	ILE	2.1
1	AAA	121	PHE	2.1
1	AAA	392	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	AAA	302	ASP	2.1
1	AAA	42	ILE	2.1
1	AAA	265	VAL	2.0
1	AAA	370	ILE	2.0
1	BBB	369	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

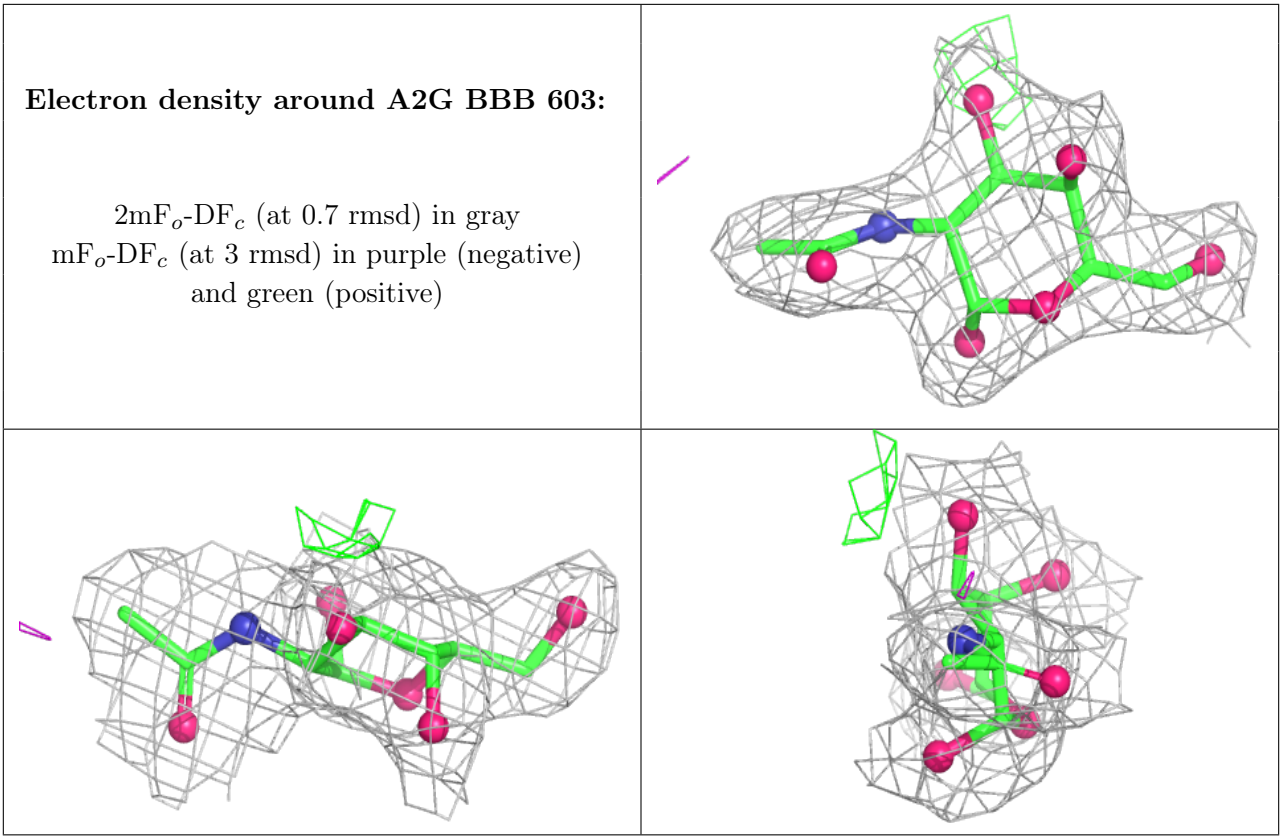
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	BBB	602	4/4	0.70	0.21	56,60,60,62	0
4	NGA	BBB	601	15/15	0.86	0.18	62,63,66,66	0
2	A2G	BBB	603	15/15	0.89	0.14	44,45,47,48	0
2	A2G	AAA	701	15/15	0.93	0.13	46,47,48,48	0
3	CA	AAA	702	1/1	0.95	0.11	69,69,69,69	0
3	CA	BBB	604	1/1	0.96	0.10	64,64,64,64	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.

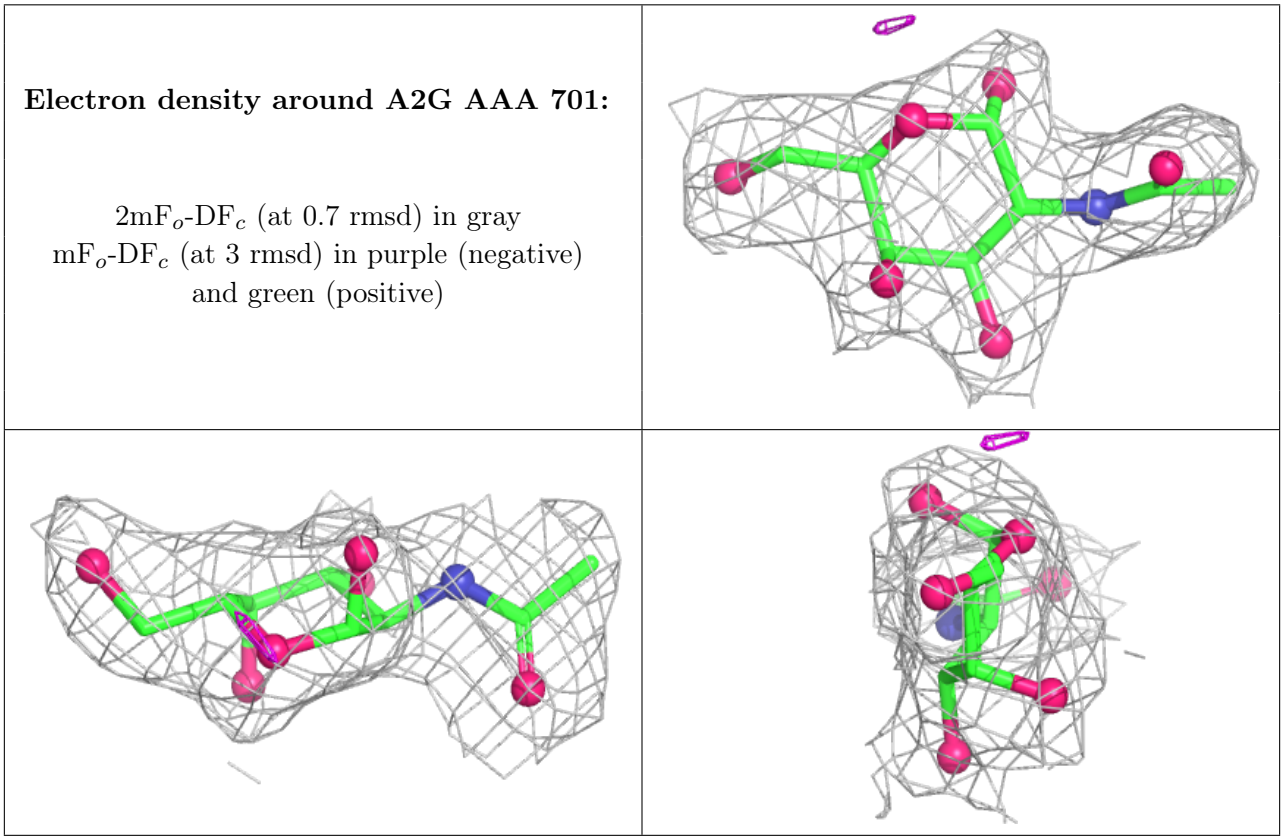
Electron density around A2G BBB 603:

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



Electron density around A2G AAA 701:

$2mF_o$-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.