



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:32 AM UTC

PDB ID : 8HJ8 / pdb_00008hj8
Title : Crystal structure of barley exohydrolase isoform ExoI E220A mutant in complex with 2-deoxy-2-fluoro-D-glucopyranosides
Authors : Luang, S.; Streltsov, V.A.; Hrmova, M.
Deposited on : 2022-11-22
Resolution : 1.95 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

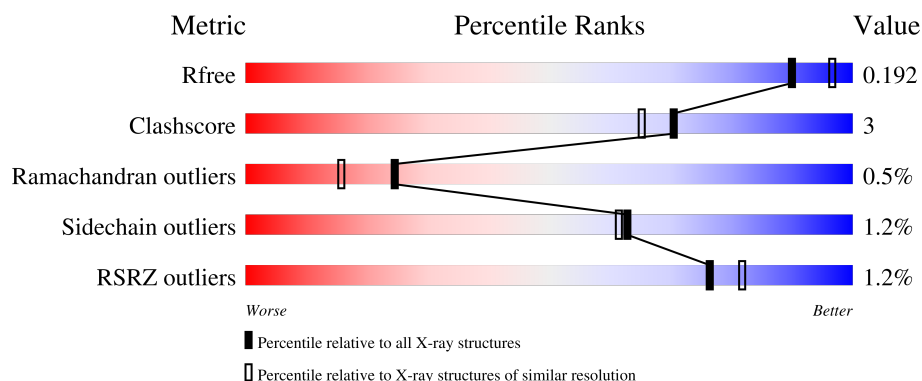
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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

Mol	Chain	Length	Quality of chain
1	A	609	% 85% 12% .

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5400 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.

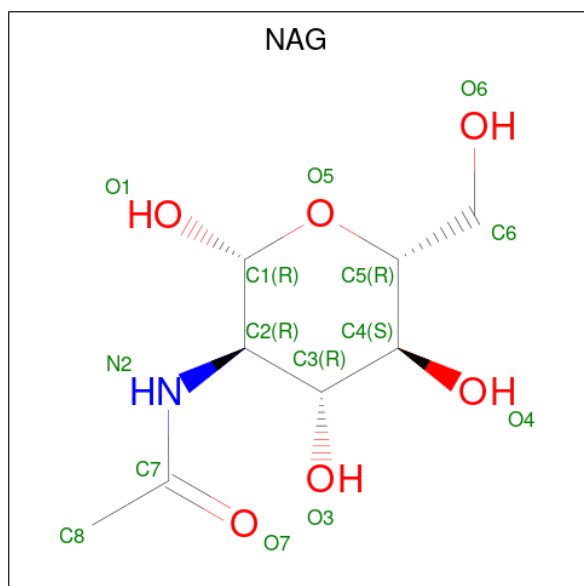
- Molecule 1 is a protein called Glyco_hydro_3 domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	606	4617	2918	802	868	29	0	14	0

There are 5 discrepancies between the modelled and reference sequences:

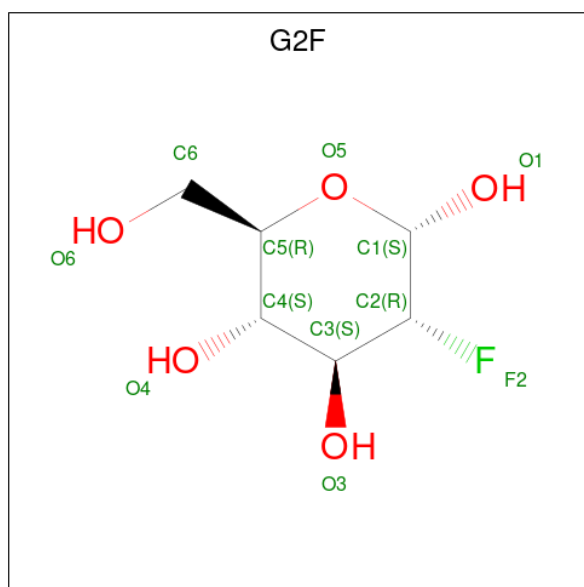
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	HIS	-	expression tag	UNP A0A8I6XKI1
A	-2	HIS	-	expression tag	UNP A0A8I6XKI1
A	-1	ALA	-	expression tag	UNP A0A8I6XKI1
A	220	ALA	GLU	engineered mutation	UNP A0A8I6XKI1
A	320	LYS	ASN	conflict	UNP A0A8I6XKI1

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



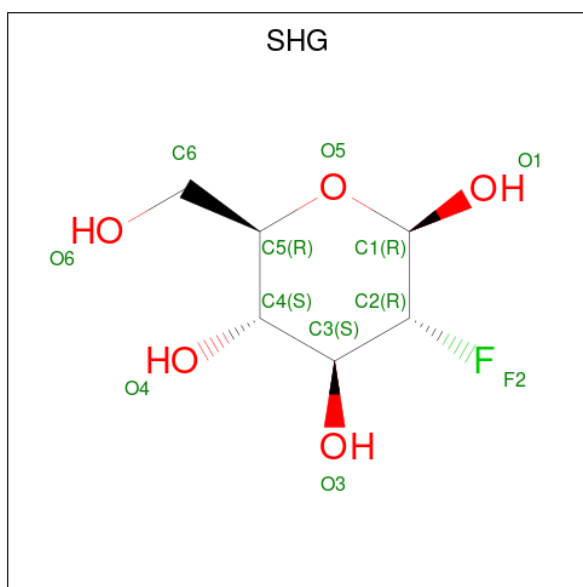
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is 2-deoxy-2-fluoro-alpha-D-glucopyranose (CCD ID: G2F) (formula: $C_6H_{11}FO_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	F	O	0	0
			11	6	1	4		

- Molecule 4 is 2-deoxy-2-fluoro-beta-D-glucopyranose (CCD ID: SHG) (formula: $C_6H_{11}FO_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	O	0	0
			12	6	1	5		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



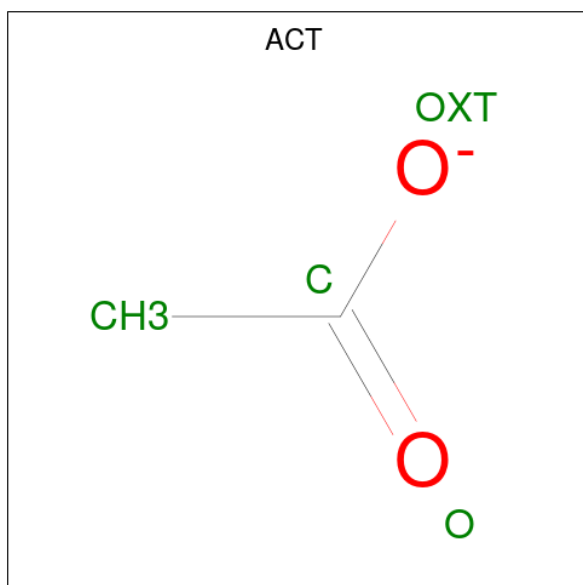
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



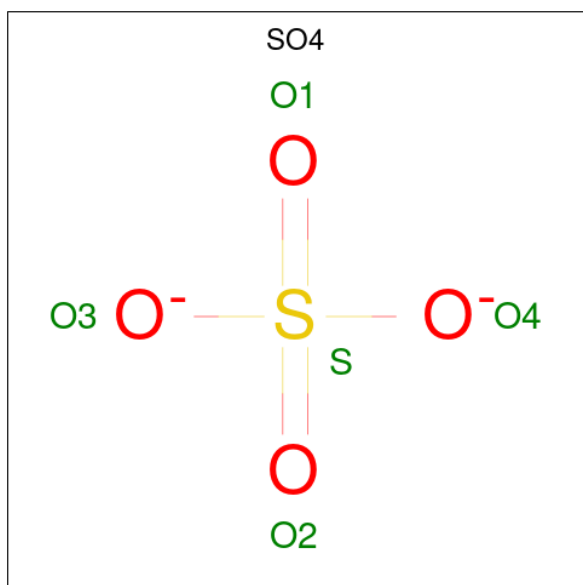
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		

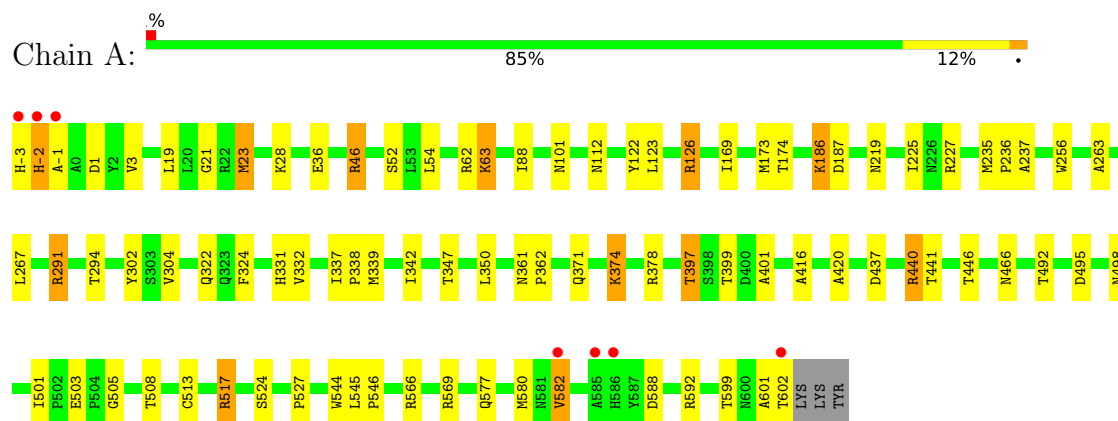
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	629	Total	O	0	0
			629	629		

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: Glyco_hydro_3 domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	100.50Å 100.50Å 182.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	88.06 – 1.95 88.06 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.3 (88.06-1.95) 99.3 (88.06-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 1.95Å)	Xtriage
Refinement program	REFMAC 7.0.005	Depositor
R, R_{free}	0.144 , 0.184 0.158 , 0.192	Depositor DCC
R_{free} test set	3452 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5400	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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: ACT, NAG, SO4, SHG, GOL, G2F

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	1.81	58/4769 (1.2%)	1.40	19/6474 (0.3%)

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

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	517[B]	ARG	CZ-NH1	8.65	1.44	1.32
1	A	1	ASP	CA-C	8.32	1.64	1.52
1	A	503	GLU	CD-OE2	7.74	1.40	1.25
1	A	440[A]	ARG	CZ-NH2	7.36	1.43	1.33
1	A	126	ARG	CD-NE	-7.31	1.36	1.46
1	A	546	PRO	N-CA	7.24	1.56	1.47
1	A	-2	HIS	N-CA	7.09	1.55	1.46
1	A	440[A]	ARG	CZ-NH1	7.03	1.42	1.32
1	A	23	MET	C-O	-7.01	1.15	1.23
1	A	592	ARG	NE-CZ	6.97	1.40	1.33
1	A	-1	ALA	N-CA	6.84	1.55	1.46
1	A	601	ALA	CA-C	6.82	1.61	1.52
1	A	513	CYS	CA-C	6.56	1.61	1.52
1	A	545	LEU	N-CA	6.49	1.53	1.46
1	A	401	ALA	CA-C	6.48	1.60	1.53
1	A	446	THR	CB-OG1	6.26	1.53	1.43
1	A	362	PRO	C-O	6.24	1.31	1.24
1	A	304	VAL	N-CA	6.10	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	LYS	C-O	-6.09	1.16	1.23
1	A	592	ARG	CD-NE	6.09	1.54	1.46
1	A	599	THR	CA-C	-6.07	1.45	1.52
1	A	361	ASN	CG-ND2	-5.98	1.20	1.33
1	A	338	PRO	CA-C	5.97	1.59	1.52
1	A	495	ASP	CA-C	5.90	1.60	1.52
1	A	440[A]	ARG	NE-CZ	5.90	1.39	1.33
1	A	371	GLN	CD-NE2	-5.87	1.21	1.33
1	A	52	SER	CA-C	-5.86	1.45	1.52
1	A	36	GLU	C-O	5.81	1.30	1.23
1	A	-1	ALA	CA-C	5.80	1.60	1.52
1	A	256	TRP	CA-C	5.78	1.59	1.52
1	A	237	ALA	CA-C	5.64	1.60	1.52
1	A	582	VAL	CA-CB	5.62	1.62	1.54
1	A	350	LEU	N-CA	-5.58	1.39	1.46
1	A	378	ARG	C-O	-5.58	1.17	1.24
1	A	592	ARG	CZ-NH2	5.58	1.40	1.33
1	A	347	THR	CA-C	5.58	1.59	1.52
1	A	322	GLN	CA-C	5.57	1.59	1.52
1	A	21	GLY	C-O	-5.55	1.16	1.24
1	A	263	ALA	N-CA	5.52	1.52	1.46
1	A	416	ALA	C-O	-5.51	1.17	1.23
1	A	492	THR	N-CA	5.46	1.53	1.46
1	A	46	ARG	N-CA	5.40	1.52	1.46
1	A	337	ILE	CA-C	-5.37	1.48	1.52
1	A	342	ILE	C-O	5.34	1.30	1.24
1	A	588	ASP	CA-C	5.34	1.59	1.52
1	A	331	HIS	N-CA	5.32	1.52	1.46
1	A	225	ILE	C-O	5.32	1.30	1.24
1	A	501	ILE	C-O	-5.32	1.17	1.24
1	A	517[B]	ARG	CD-NE	5.32	1.53	1.46
1	A	324	PHE	CA-CB	5.27	1.61	1.53
1	A	582	VAL	N-CA	5.25	1.52	1.46
1	A	62	ARG	CA-CB	-5.16	1.44	1.53
1	A	302	TYR	CA-CB	5.12	1.61	1.53
1	A	174	THR	C-O	-5.06	1.17	1.24
1	A	397	THR	C-N	-5.05	1.26	1.33
1	A	332	VAL	CA-C	5.04	1.59	1.52
1	A	88	ILE	CA-C	5.04	1.57	1.53
1	A	219	ASN	C-O	-5.00	1.18	1.23

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	ARG	NE-CZ-NH1	9.86	131.36	121.50
1	A	126	ARG	NE-CZ-NH2	-8.96	111.13	119.20
1	A	112	ASN	N-CA-C	8.69	121.85	111.33
1	A	267	LEU	N-CA-C	8.38	120.50	111.36
1	A	46	ARG	NE-CZ-NH2	7.77	126.19	119.20
1	A	592	ARG	NE-CZ-NH2	7.39	125.85	119.20
1	A	397	THR	N-CA-C	-6.42	99.56	109.52
1	A	440[A]	ARG	CG-CD-NE	-6.02	98.76	112.00
1	A	3	VAL	N-CA-CB	-5.97	103.70	111.82
1	A	126	ARG	CD-NE-CZ	5.80	132.51	124.40
1	A	291	ARG	NE-CZ-NH2	5.66	124.29	119.20
1	A	123	LEU	N-CA-C	-5.64	105.14	111.28
1	A	291	ARG	NE-CZ-NH1	-5.49	116.01	121.50
1	A	374	LYS	CG-CD-CE	5.48	123.90	111.30
1	A	498	ASN	OD1-CG-ND2	-5.35	117.25	122.60
1	A	420	ALA	N-CA-C	5.30	117.97	111.82
1	A	440[A]	ARG	CD-NE-CZ	5.28	131.79	124.40
1	A	62	ARG	NE-CZ-NH2	-5.28	114.45	119.20
1	A	28	LYS	N-CA-C	5.17	116.60	111.07

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	-3	HIS	Peptide
1	A	187	ASP	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4617	0	4570	26	0
2	A	42	0	39	0	0
3	A	11	0	9	0	0
4	A	12	0	11	2	0
5	A	30	0	40	1	0
6	A	44	0	33	4	0
7	A	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	629	0	0	15	0
All	All	5400	0	4702	32	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 3.

All (32) 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:A:709:GOL:H32	8:A:806:HOH:O	1.64	0.96
1:A:122:TYR:CE2	1:A:126:ARG:HD2	2.16	0.80
1:A:399:THR:HG23	8:A:923:HOH:O	1.87	0.74
1:A:466[A]:ASN:OD1	1:A:508:THR:OG1	2.08	0.71
1:A:566[B]:ARG:CZ	8:A:806:HOH:O	2.47	0.61
4:A:705:SHG:H6A	8:A:1260:HOH:O	2.04	0.58
1:A:517[B]:ARG:HG2	8:A:1226:HOH:O	2.04	0.56
4:A:705:SHG:H6	8:A:1293:HOH:O	2.07	0.55
1:A:291:ARG:HD3	8:A:1075:HOH:O	2.09	0.53
1:A:227[B]:ARG:NH1	8:A:805:HOH:O	2.24	0.51
1:A:577:GLN:HB3	1:A:580[B]:MET:SD	2.52	0.50
1:A:294:THR:HG23	6:A:715:ACT:OXT	2.13	0.49
1:A:374:LYS:NZ	8:A:812:HOH:O	2.46	0.49
6:A:713:ACT:CH3	8:A:1389:HOH:O	2.60	0.48
1:A:46:ARG:HD2	8:A:1038:HOH:O	2.13	0.47
1:A:397:THR:OG1	1:A:399:THR:HG22	2.14	0.47
1:A:235:MET:N	1:A:236:PRO:CD	2.77	0.47
1:A:566[B]:ARG:NE	8:A:806:HOH:O	2.47	0.47
1:A:577:GLN:OE1	1:A:580[B]:MET:HE1	2.15	0.47
1:A:122:TYR:CZ	1:A:126:ARG:HD2	2.50	0.46
1:A:339[B]:MET:HG2	8:A:1312:HOH:O	2.16	0.45
6:A:718:ACT:H3	8:A:1376:HOH:O	2.16	0.44
1:A:19:LEU:O	1:A:23:MET:HG3	2.17	0.44
1:A:527:PRO:HD3	1:A:569:ARG:HD3	2.00	0.44
1:A:524:SER:O	1:A:544:TRP:HA	2.19	0.43
1:A:122:TYR:CD2	1:A:126:ARG:HD2	2.55	0.42
1:A:169:ILE:O	1:A:173[A]:MET:HG2	2.19	0.41
1:A:122:TYR:O	1:A:126:ARG:HD3	2.21	0.41
1:A:437:ASP:HB3	1:A:441:THR:HG21	2.03	0.41
6:A:719:ACT:H2	8:A:807:HOH:O	2.21	0.41

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	613/609 (101%)	588 (96%)	22 (4%)	3 (0%)	24 16

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-2	HIS
1	A	505	GLY
1	A	582	VAL

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	495/489 (101%)	489 (99%)	6 (1%)	63 61

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LEU
1	A	63	LYS
1	A	101	ASN
1	A	186[A]	LYS
1	A	440[A]	ARG
1	A	602	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	487	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](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 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	$\# Z > 2$
2	NAG	A	703	1	14,14,15	0.82	1 (7%)	17,19,21	1.37	3 (17%)
5	GOL	A	706	-	5,5,5	0.35	0	5,5,5	1.23	1 (20%)
6	ACT	A	719	-	3,3,3	0.81	0	3,3,3	0.88	0
6	ACT	A	718	-	3,3,3	1.06	0	3,3,3	2.21	2 (66%)
5	GOL	A	708	-	5,5,5	0.70	0	5,5,5	1.18	1 (20%)
4	SHG	A	705	-	12,12,12	2.92	5 (41%)	16,17,17	3.57	8 (50%)
6	ACT	A	712	-	3,3,3	1.10	0	3,3,3	1.10	0
2	NAG	A	702	1	14,14,15	1.99	3 (21%)	17,19,21	2.92	4 (23%)
5	GOL	A	707	-	5,5,5	0.57	0	5,5,5	0.97	0
6	ACT	A	716	-	3,3,3	0.66	0	3,3,3	1.49	0
6	ACT	A	717	-	3,3,3	0.89	0	3,3,3	0.37	0
6	ACT	A	714	-	3,3,3	0.77	0	3,3,3	1.44	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ACT	A	720	-	3,3,3	0.89	0	3,3,3	0.62	0
6	ACT	A	713	-	3,3,3	0.76	0	3,3,3	1.31	0
7	SO4	A	724	-	4,4,4	0.61	0	6,6,6	0.38	0
3	G2F	A	704	-	11,11,12	2.14	4 (36%)	12,15,17	2.02	2 (16%)
6	ACT	A	721	-	3,3,3	1.11	0	3,3,3	0.18	0
6	ACT	A	715	-	3,3,3	0.89	0	3,3,3	0.98	0
5	GOL	A	710	-	5,5,5	0.51	0	5,5,5	1.07	0
6	ACT	A	711	-	3,3,3	1.06	0	3,3,3	0.65	0
2	NAG	A	701	1	14,14,15	0.93	0	17,19,21	2.42	9 (52%)
7	SO4	A	723	-	4,4,4	0.61	0	6,6,6	0.50	0
5	GOL	A	709	-	5,5,5	0.60	0	5,5,5	0.72	0
7	SO4	A	722	-	4,4,4	0.92	0	6,6,6	1.11	1 (16%)

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
5	GOL	A	707	-	-	4/4/4/4	-
2	NAG	A	703	1	-	0/6/23/26	0/1/1/1
5	GOL	A	706	-	-	3/4/4/4	-
5	GOL	A	708	-	-	2/4/4/4	-
4	SHG	A	705	-	-	2/2/22/22	0/1/1/1
2	NAG	A	701	1	-	0/6/23/26	0/1/1/1
2	NAG	A	702	1	-	2/6/23/26	0/1/1/1
5	GOL	A	709	-	-	1/4/4/4	-
3	G2F	A	704	-	-	0/2/19/22	0/1/1/1
5	GOL	A	710	-	-	0/4/4/4	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	705	SHG	C2-C1	5.96	1.58	1.52
2	A	702	NAG	C1-C2	5.15	1.59	1.52
3	A	704	G2F	C1-C2	5.09	1.59	1.52
4	A	705	SHG	C2-C3	5.05	1.57	1.52
4	A	705	SHG	O1-C1	4.54	1.53	1.39
2	A	702	NAG	O5-C1	4.19	1.50	1.43
4	A	705	SHG	O5-C1	3.09	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	704	G2F	C2-C3	2.78	1.55	1.51
3	A	704	G2F	O5-C5	2.66	1.48	1.43
3	A	704	G2F	O3-C3	2.49	1.49	1.43
4	A	705	SHG	O3-C3	2.27	1.48	1.43
2	A	703	NAG	C1-C2	2.15	1.55	1.52
2	A	702	NAG	O5-C5	2.07	1.47	1.43

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	702	NAG	C1-O5-C5	8.19	123.16	112.19
4	A	705	SHG	C1-O5-C5	7.84	128.82	113.65
4	A	705	SHG	O3-C3-C2	7.77	124.00	109.63
4	A	705	SHG	F2-C2-C1	6.23	114.79	107.81
2	A	702	NAG	O5-C5-C6	5.56	118.48	107.66
3	A	704	G2F	F2-C2-C1	5.55	112.63	108.26
2	A	701	NAG	C1-C2-N2	5.18	118.60	110.43
2	A	702	NAG	O5-C1-C2	-4.43	104.44	111.29
2	A	701	NAG	C4-C3-C2	-4.39	104.58	111.02
2	A	701	NAG	O5-C5-C4	-3.47	102.40	110.83
4	A	705	SHG	O1-C1-C2	3.33	123.12	109.33
3	A	704	G2F	O3-C3-C2	3.28	115.42	109.55
6	A	718	ACT	O-C-CH3	-2.94	110.47	122.53
2	A	702	NAG	C3-C4-C5	-2.84	105.08	110.23
2	A	703	NAG	O5-C1-C2	-2.71	107.09	111.29
4	A	705	SHG	O5-C5-C6	2.67	113.06	106.44
2	A	701	NAG	C6-C5-C4	2.59	119.37	113.02
2	A	701	NAG	O5-C5-C6	2.55	112.63	107.66
5	A	706	GOL	C3-C2-C1	-2.54	102.47	111.80
4	A	705	SHG	F2-C2-C3	2.41	110.90	108.81
6	A	718	ACT	OXT-C-CH3	2.34	124.87	115.05
4	A	705	SHG	C3-C4-C5	-2.34	105.99	110.23
2	A	701	NAG	C3-C4-C5	-2.31	106.04	110.23
2	A	701	NAG	O4-C4-C5	2.27	114.92	109.32
2	A	701	NAG	O7-C7-C8	-2.23	118.08	122.05
7	A	722	SO4	O4-S-O2	2.19	121.03	109.56
5	A	708	GOL	O1-C1-C2	2.13	119.96	110.38
2	A	703	NAG	O5-C5-C4	-2.05	105.84	110.83
2	A	703	NAG	O4-C4-C5	2.03	114.33	109.32
4	A	705	SHG	C6-C5-C4	2.03	118.00	113.02
2	A	701	NAG	O3-C3-C2	2.01	113.58	109.40
6	A	714	ACT	OXT-C-CH3	2.01	123.47	115.05

There are no chirality outliers.

All (14) torsion outliers are listed below:

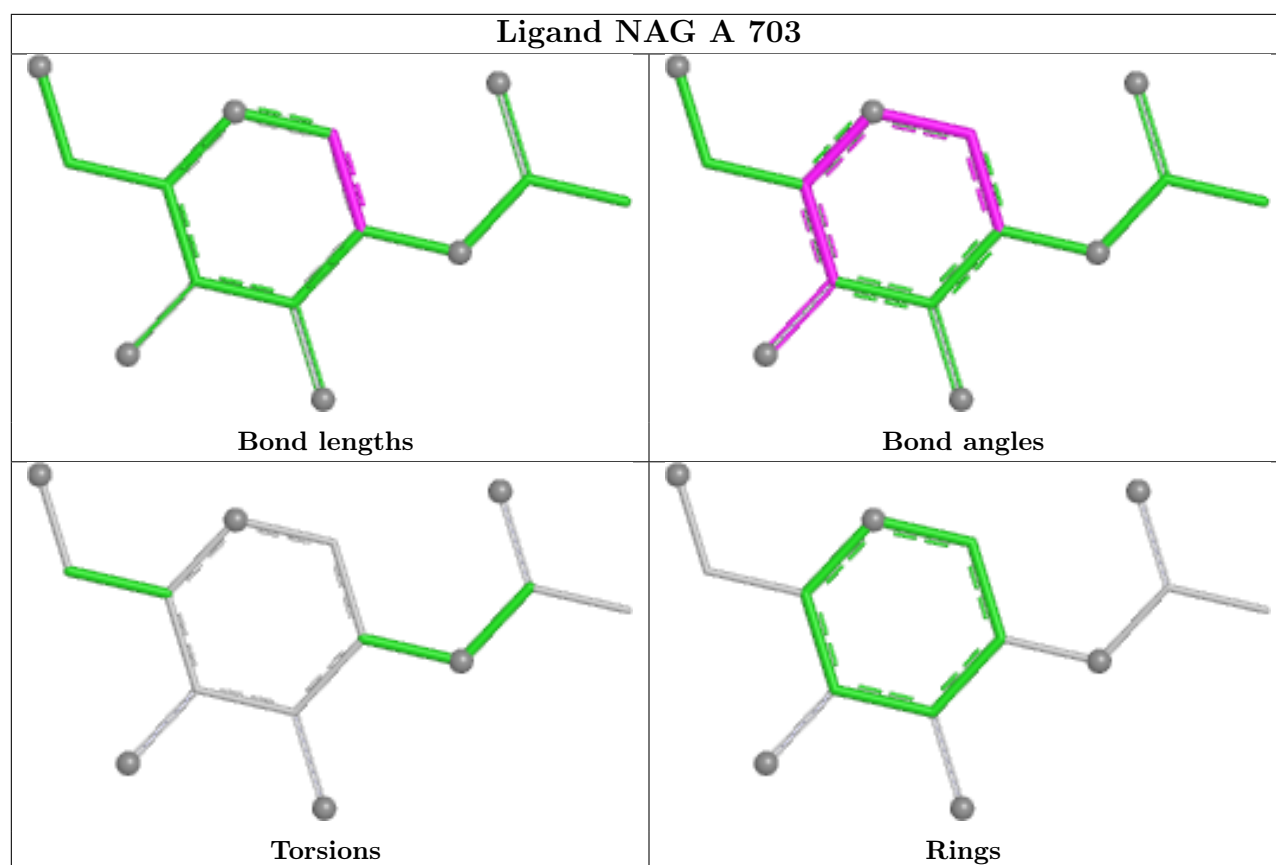
Mol	Chain	Res	Type	Atoms
5	A	706	GOL	O1-C1-C2-O2
5	A	707	GOL	C1-C2-C3-O3
5	A	707	GOL	O2-C2-C3-O3
5	A	708	GOL	C1-C2-C3-O3
4	A	705	SHG	O5-C5-C6-O6
4	A	705	SHG	C4-C5-C6-O6
2	A	702	NAG	C4-C5-C6-O6
5	A	706	GOL	O1-C1-C2-C3
5	A	707	GOL	O1-C1-C2-C3
5	A	709	GOL	O1-C1-C2-C3
5	A	708	GOL	O2-C2-C3-O3
2	A	702	NAG	O5-C5-C6-O6
5	A	707	GOL	O1-C1-C2-O2
5	A	706	GOL	C1-C2-C3-O3

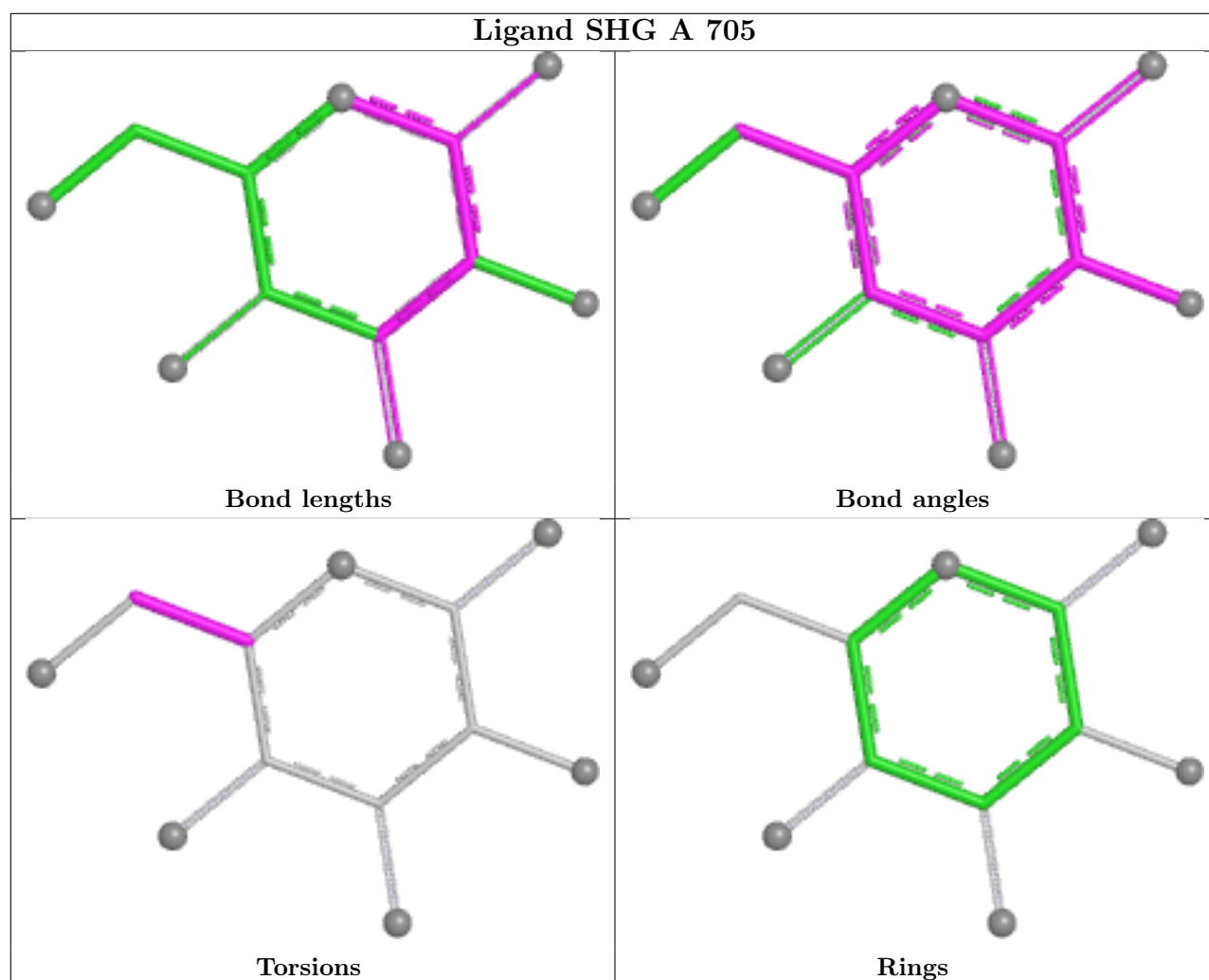
There are no ring outliers.

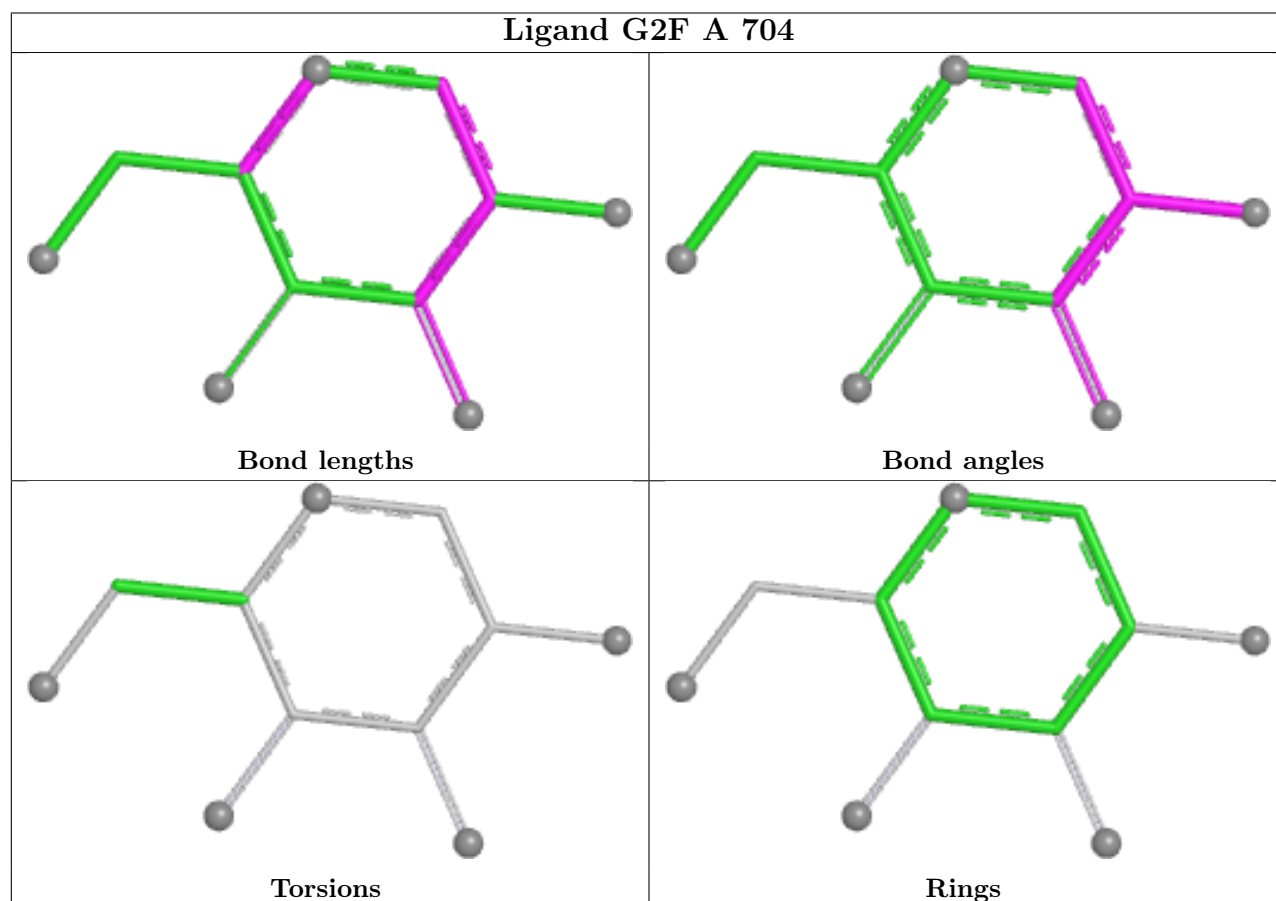
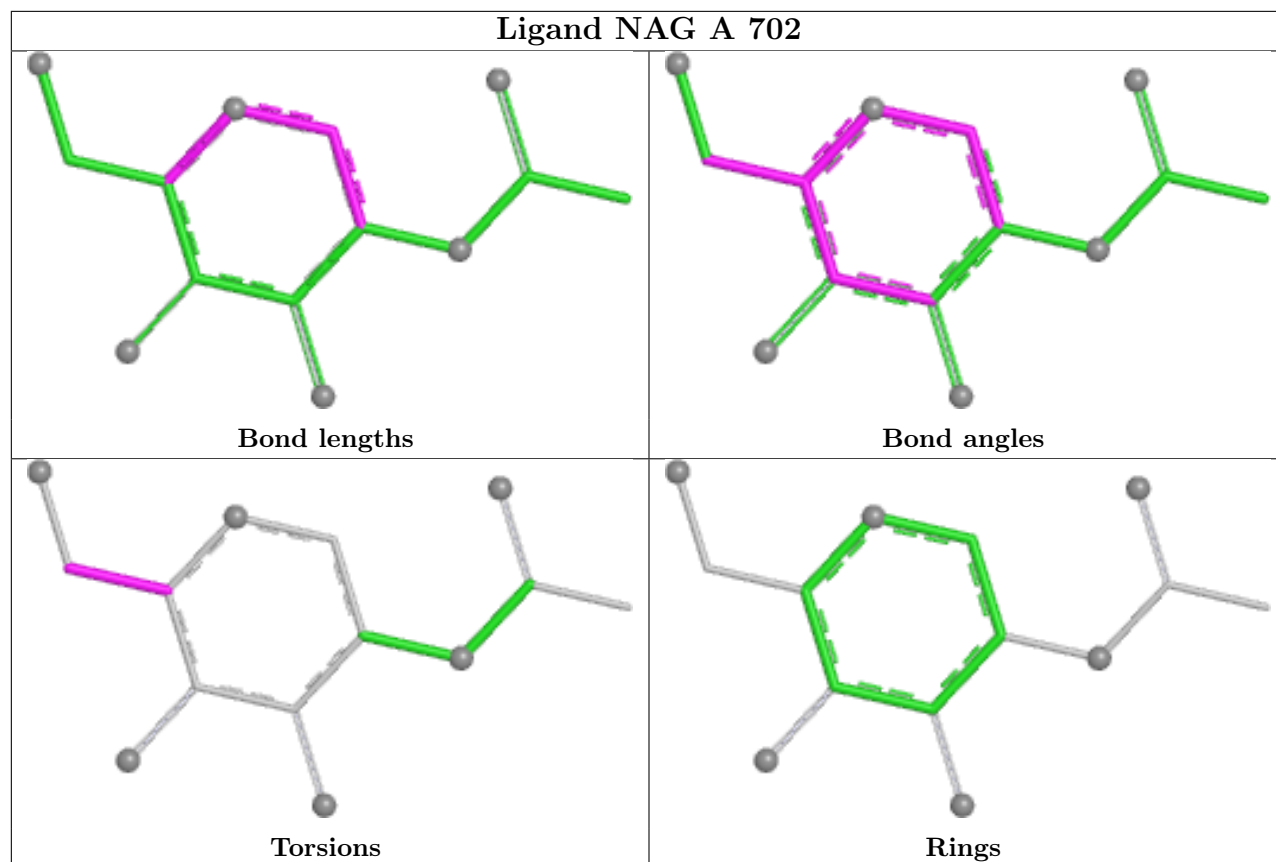
6 monomers are involved in 7 short contacts:

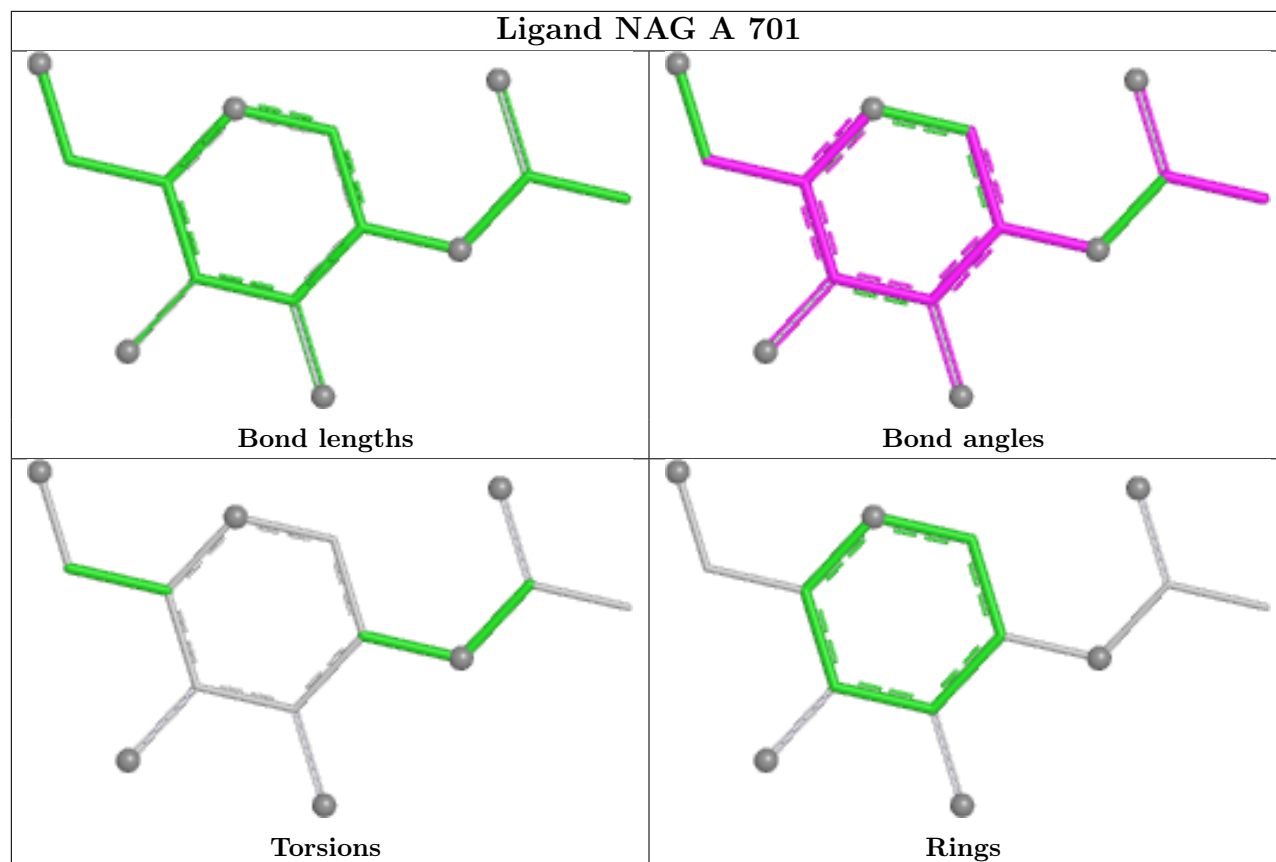
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	719	ACT	1	0
6	A	718	ACT	1	0
4	A	705	SHG	2	0
6	A	713	ACT	1	0
6	A	715	ACT	1	0
5	A	709	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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 [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	606/609 (99%)	-0.26	7 (1%) 76 82	24, 34, 51, 106	8 (1%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	586	HIS	3.9
1	A	582	VAL	3.7
1	A	-2	HIS	3.7
1	A	602	THR	3.6
1	A	-3	HIS	3.3
1	A	-1	ALA	3.2
1	A	585	ALA	2.5

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 oligosaccharides 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, 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	ACT	A	712	4/4	0.56	0.28	61,76,86,89	0

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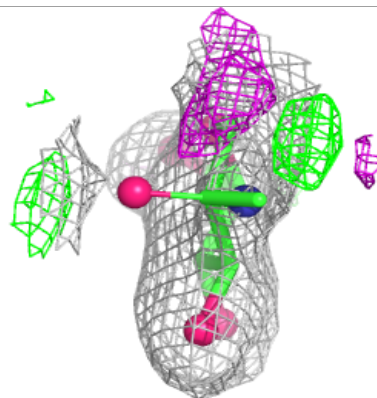
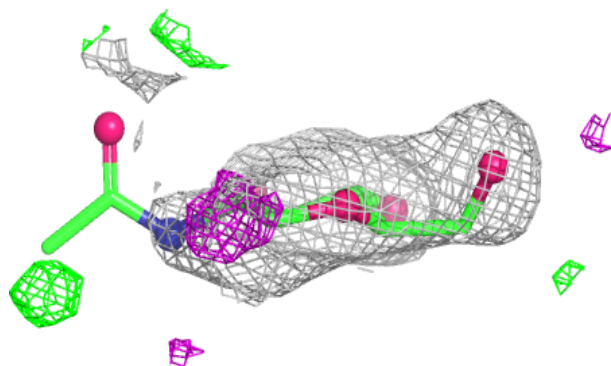
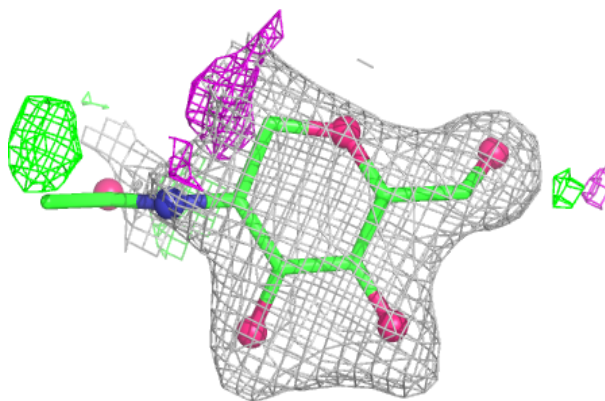
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	SO4	A	723	5/5	0.63	0.11	99,106,112,120	0
6	ACT	A	720	4/4	0.71	0.21	72,83,87,88	0
6	ACT	A	717	4/4	0.74	0.20	66,76,76,81	0
6	ACT	A	719	4/4	0.74	0.16	63,74,75,79	0
2	NAG	A	702	14/15	0.75	0.14	58,87,102,106	0
2	NAG	A	701	14/15	0.76	0.14	78,90,94,97	0
7	SO4	A	724	5/5	0.76	0.13	85,107,127,127	0
5	GOL	A	709	6/6	0.80	0.15	65,71,80,81	0
6	ACT	A	711	4/4	0.81	0.15	64,74,75,79	0
6	ACT	A	713	4/4	0.82	0.14	48,60,63,66	0
6	ACT	A	714	4/4	0.83	0.15	64,70,71,74	0
6	ACT	A	718	4/4	0.85	0.19	35,51,57,58	0
6	ACT	A	721	4/4	0.85	0.21	73,73,81,84	0
6	ACT	A	715	4/4	0.87	0.15	66,69,70,72	0
4	SHG	A	705	12/12	0.88	0.11	38,47,53,55	0
6	ACT	A	716	4/4	0.88	0.17	60,63,67,75	0
2	NAG	A	703	14/15	0.88	0.11	52,57,83,90	0
5	GOL	A	708	6/6	0.89	0.13	43,57,67,89	0
5	GOL	A	706	6/6	0.89	0.22	37,41,44,51	6
5	GOL	A	707	6/6	0.89	0.18	51,74,81,96	0
5	GOL	A	710	6/6	0.90	0.12	64,69,72,75	0
7	SO4	A	722	5/5	0.93	0.07	49,50,66,68	0
3	G2F	A	704	11/12	0.95	0.08	30,34,39,40	0

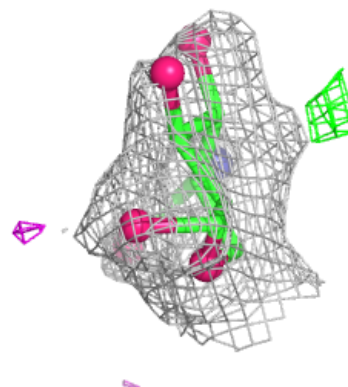
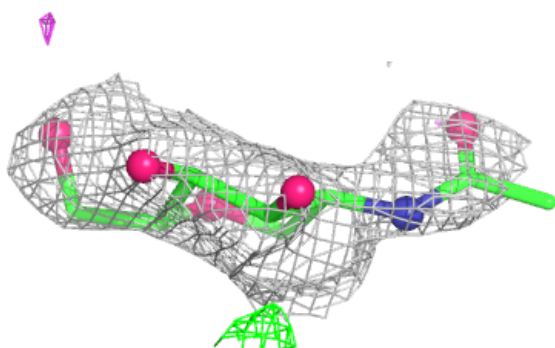
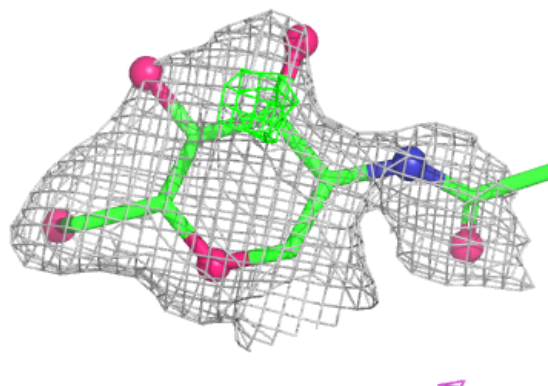
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAG A 702:

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

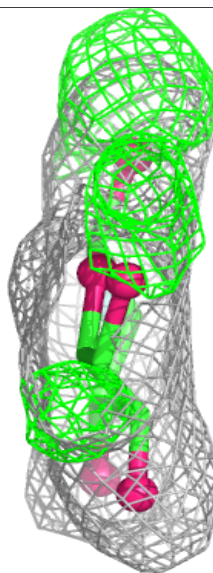
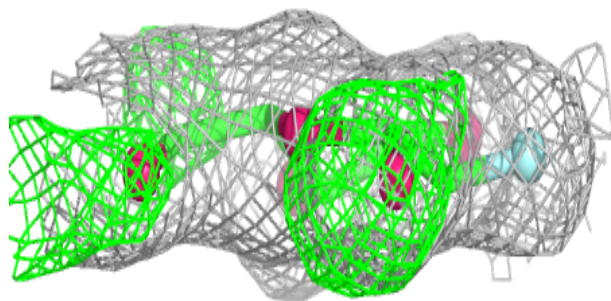
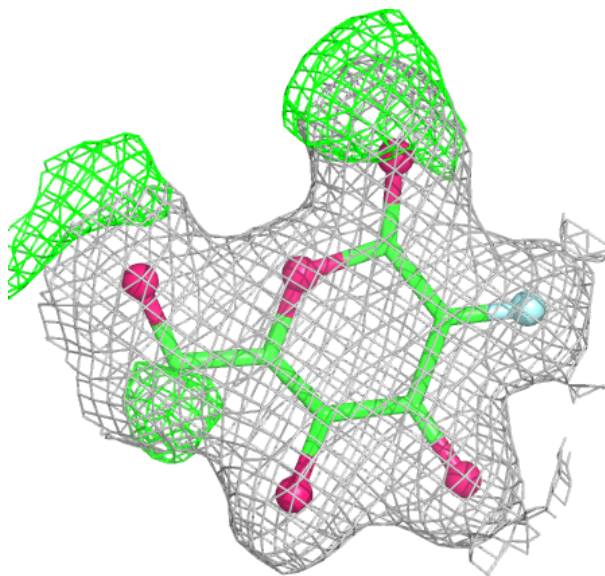
**Electron density around NAG A 701:**

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



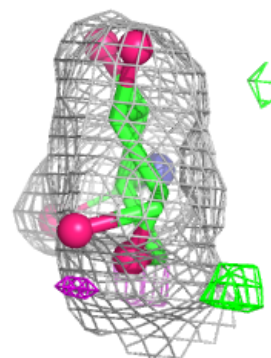
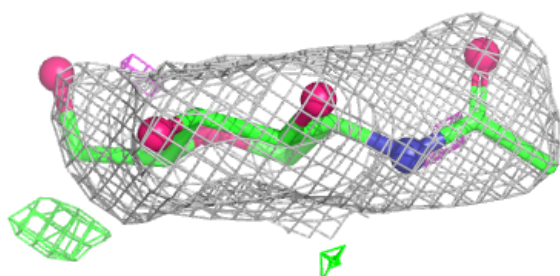
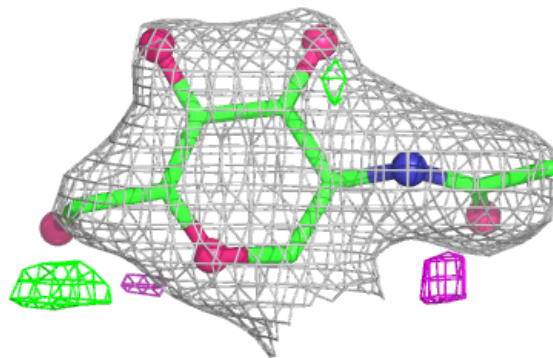
Electron density around SHG A 705:

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



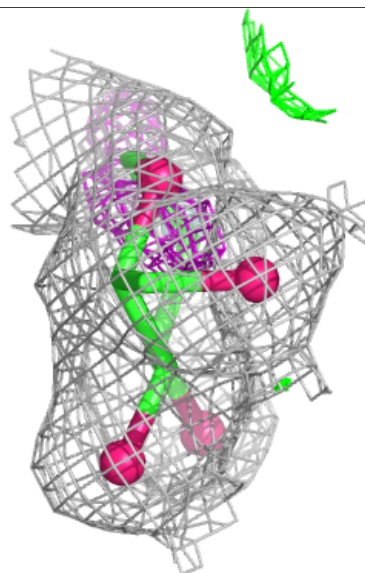
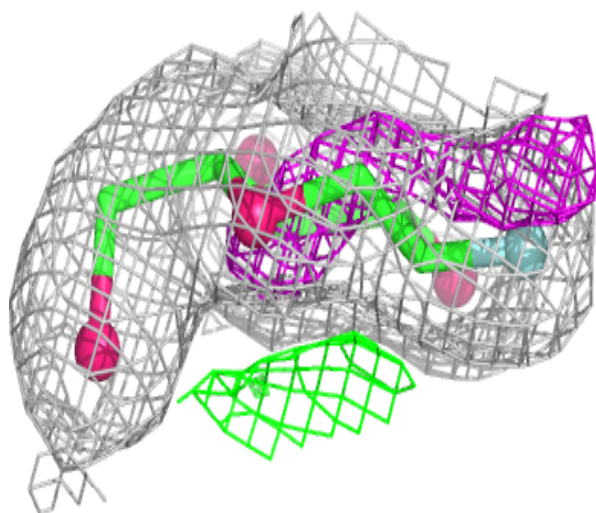
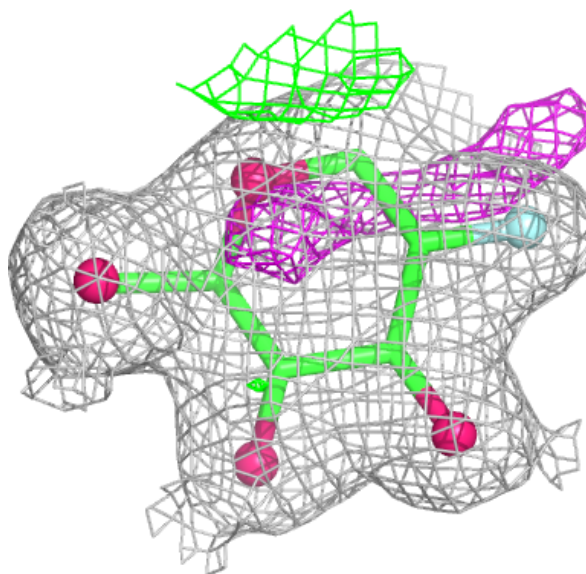
Electron density around NAG A 703:

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



Electron density around G2F A 704:

$2mF_o-DF_c$ (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.