



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:44 AM UTC

PDB ID : 7QXO / pdb_00007qxo
Title : The structure of T. forsythia NanH
Authors : Rafferty, J.; Stafford, G.; Satur, M.
Deposited on : 2022-01-26
Resolution : 1.90 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

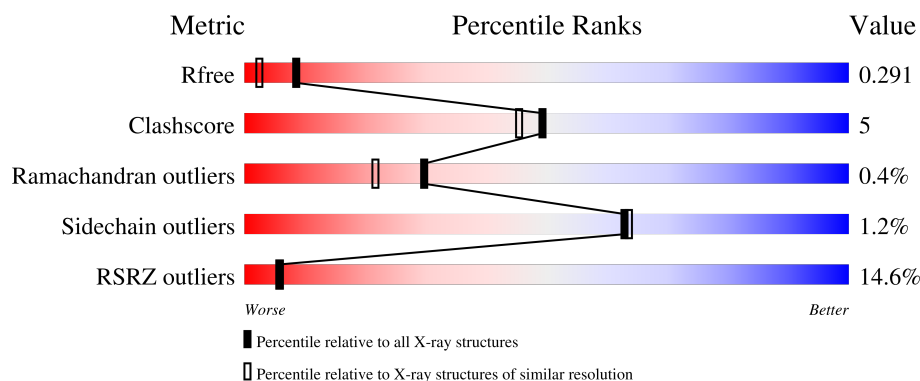
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	519	11% 87% 12%
1	B	519	18% 90% 9%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 16620 atoms, of which 8091 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.

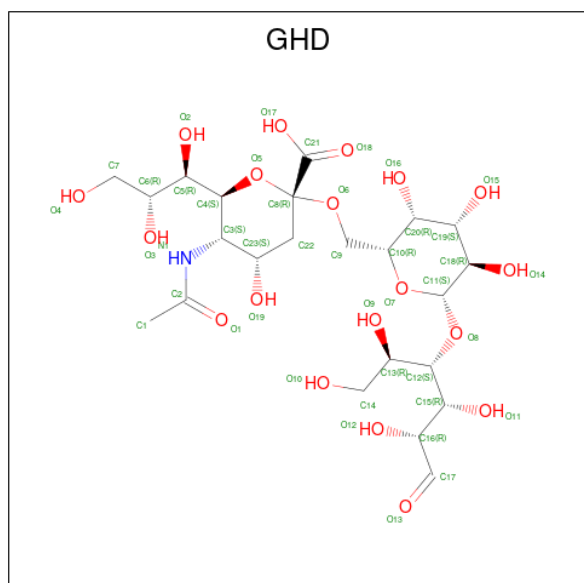
- Molecule 1 is a protein called BNR/Asp-box repeat protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	519	Total	C	H	N	O	S	126	0	0
			8027	2504	4005	724	774	20			
1	B	519	Total	C	H	N	O	S	127	1	0
			8038	2507	4010	725	776	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	237	ALA	ASP	engineered mutation	UNP G8UIQ1
B	237	ALA	ASP	engineered mutation	UNP G8UIQ1

- Molecule 2 is (2 {R},4 {S},5 {S},6 {S})-5-acetamido-4-oxidanyl-6-[(1 {R},2 {R})-1,2,3-tris(oxidanyl)propyl]-2-[[[(2 {R},3 {R},4 {S},5 {R},6 {S})-3,4,5-tris(oxidanyl)-6-[(2 {R},3 {S},4 {R},5 {R})-1,2,4,5-tetrakis(oxidanyl)-6-oxidanylidene-hexan-3-yl]oxy-oxan-2-yl]methoxy]oxane-2-carboxylic acid (CCD ID: GHD) (formula: C₂₃H₃₉NO₁₉) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	11	0
			81	23	38	1	19		
2	B	1	Total	C	H	N	O	11	0
			81	23	38	1	19		

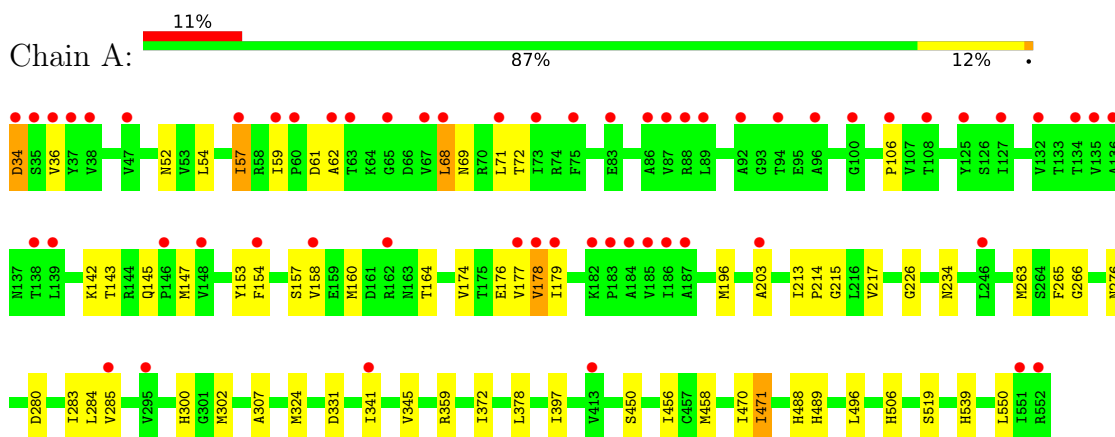
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	211	Total	O	0	0
			211	211		
3	B	182	Total	O	0	0
			182	182		

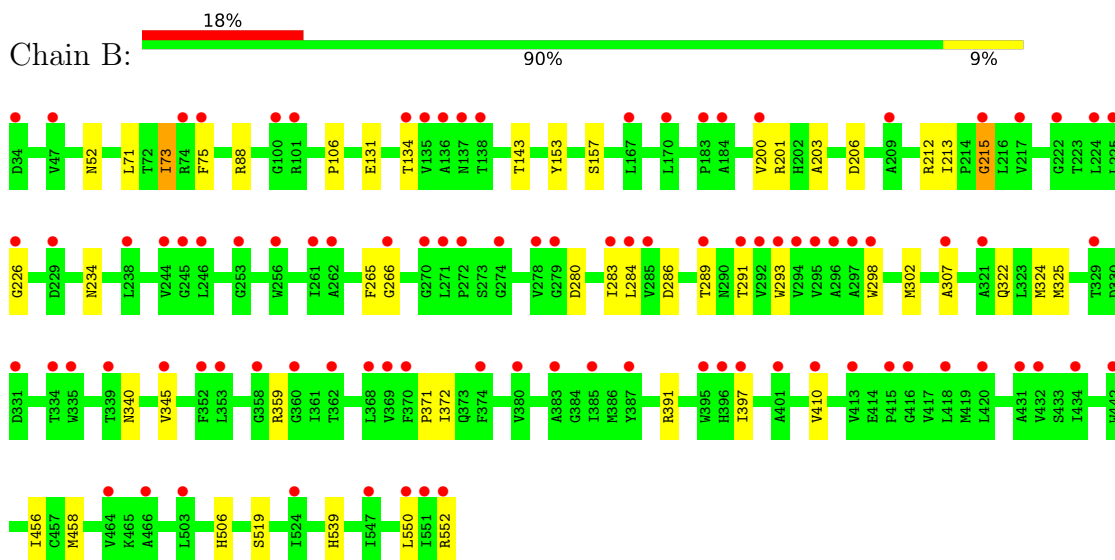
3 Residue-property plots [i](#)

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: BNR/Asp-box repeat protein



- Molecule 1: BNR/Asp-box repeat protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	79.87Å 79.87Å 349.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.64 – 1.90 72.64 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (72.64-1.90) 99.9 (72.64-1.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.252 , 0.290 0.253 , 0.291	Depositor DCC
R_{free} test set	4483 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	33.0	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 25.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16620	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GHD

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	1.01	0/4100	1.26	3/5568 (0.1%)
1	B	1.04	0/4106	1.25	3/5576 (0.1%)
All	All	1.03	0/8206	1.26	6/11144 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331	ASP	CA-CB-CG	5.31	117.91	112.60
1	B	215	GLY	CA-C-O	-5.18	116.90	120.94
1	B	75	PHE	CA-C-N	5.13	124.97	120.10
1	B	75	PHE	C-N-CA	5.13	124.97	120.10
1	A	214	PRO	CA-C-N	5.09	125.11	121.65
1	A	214	PRO	C-N-CA	5.09	125.11	121.65

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4022	4005	3990	46	0
1	B	4028	4010	3994	41	0
2	A	43	38	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	43	38	0	0	0
3	A	211	0	0	2	0
3	B	182	0	0	1	0
All	All	8529	8091	7984	87	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (87) 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:263:MET:HE1	1:A:324:MET:HB2	1.35	1.08
1:A:160:MET:HG3	1:A:196:MET:HE1	1.36	1.06
1:B:322:GLN:HB3	1:B:324:MET:CE	1.98	0.92
1:A:263:MET:HE1	1:A:324:MET:CB	2.04	0.87
1:A:302:MET:HE1	1:A:307:ALA:HA	1.57	0.87
1:B:322:GLN:HB3	1:B:324:MET:HE2	1.56	0.85
1:A:263:MET:CE	1:A:324:MET:HB2	2.07	0.83
1:B:324:MET:HE1	1:B:340:ASN:ND2	1.95	0.81
1:B:200:VAL:O	1:B:201:ARG:HD2	1.83	0.79
1:B:322:GLN:CB	1:B:324:MET:CE	2.63	0.76
1:A:62:ALA:HB2	1:A:147:MET:HE3	1.68	0.73
1:A:263:MET:CE	1:A:324:MET:CB	2.67	0.71
1:B:212:ARG:NH2	3:B:701:HOH:O	2.23	0.71
1:A:302:MET:HE1	1:A:307:ALA:CA	2.22	0.69
1:B:298:TRP:HE3	1:B:324:MET:HE3	1.57	0.68
1:B:322:GLN:CB	1:B:324:MET:HE2	2.24	0.67
1:B:302:MET:HE1	1:B:307:ALA:HA	1.79	0.64
1:A:34:ASP:OD2	1:A:61:ASP:HB2	1.99	0.63
1:A:62:ALA:CB	1:A:147:MET:HE3	2.28	0.62
1:A:276:ASN:OD1	1:A:300:HIS:HD2	1.85	0.60
1:A:300:HIS:HE1	3:A:858:HOH:O	1.84	0.59
1:B:324:MET:HE1	1:B:340:ASN:CG	2.27	0.59
1:B:289:THR:OG1	1:B:291:THR:HG22	2.02	0.59
1:A:59:ILE:HG21	1:A:147:MET:HE1	1.87	0.57
1:A:164:THR:HG21	1:A:196:MET:HE2	1.86	0.57
1:B:71:LEU:C	1:B:71:LEU:HD12	2.31	0.55
1:B:322:GLN:CB	1:B:324:MET:HE3	2.37	0.55
1:A:68:LEU:HD21	1:A:177:VAL:CG2	2.37	0.55
1:A:488:HIS:HD2	1:A:489:HIS:ND1	2.05	0.55
1:B:88:ARG:NH1	1:B:131:GLU:OE2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:GLN:HB2	1:B:324:MET:HE3	1.90	0.54
1:B:302:MET:HE1	1:B:307:ALA:CA	2.38	0.53
1:A:71:LEU:HD11	1:A:174:VAL:HG11	1.90	0.53
1:A:57:ILE:HD11	1:A:154:PHE:CD1	2.45	0.52
1:A:213:ILE:HG21	1:A:280:ASP:HA	1.91	0.52
1:A:263:MET:CE	1:A:324:MET:HB3	2.40	0.52
3:A:702:HOH:O	1:B:302:MET:HA	2.09	0.52
1:B:293:TRP:HE3	1:B:325:MET:HE2	1.75	0.51
1:B:213:ILE:HG21	1:B:280:ASP:HA	1.91	0.50
1:B:286:ASP:HB3	1:B:291:THR:HG22	1.94	0.50
1:B:345:VAL:HB	1:B:397:ILE:HD12	1.93	0.50
1:A:217:VAL:HB	1:A:285:VAL:HG23	1.93	0.50
1:B:284:LEU:HD12	1:B:284:LEU:C	2.36	0.50
1:B:283:ILE:O	1:B:359:ARG:HA	2.12	0.49
1:A:283:ILE:O	1:A:359:ARG:HA	2.13	0.49
1:A:345:VAL:HB	1:A:397:ILE:HD12	1.94	0.49
1:A:284:LEU:HD12	1:A:284:LEU:C	2.38	0.48
1:A:54:LEU:HD22	1:A:158:VAL:CG1	2.44	0.48
1:A:143:THR:CG2	1:A:145:GLN:H	2.27	0.48
1:A:341:ILE:CG2	1:A:341:ILE:O	2.61	0.47
1:A:160:MET:HG3	1:A:196:MET:CE	2.25	0.47
1:B:286:ASP:OD1	1:B:391:ARG:NH1	2.48	0.47
1:B:322:GLN:HB2	1:B:324:MET:CE	2.43	0.47
1:A:52:ASN:O	1:A:157:SER:HA	2.15	0.47
1:B:302:MET:HE1	1:B:307:ALA:CB	2.45	0.47
1:B:371:PRO:HG3	1:B:410:VAL:HG12	1.98	0.46
1:B:52:ASN:O	1:B:157:SER:HA	2.15	0.46
1:B:106:PRO:HD3	1:B:153:TYR:CD2	2.51	0.46
1:A:36:VAL:HG22	1:A:59:ILE:HD13	1.98	0.46
1:A:302:MET:CE	1:A:307:ALA:HA	2.40	0.45
1:A:106:PRO:HD3	1:A:153:TYR:CD2	2.51	0.45
1:A:506:HIS:HA	1:A:550:LEU:O	2.16	0.45
1:A:69:ASN:HB2	1:A:178:VAL:CG2	2.47	0.44
1:B:506:HIS:HA	1:B:550:LEU:O	2.17	0.44
1:B:71:LEU:CD1	1:B:73:ILE:HD12	2.48	0.44
1:A:36:VAL:HG13	1:A:59:ILE:HD13	2.00	0.44
1:B:458:MET:HE1	1:B:519:SER:O	2.17	0.44
1:B:293:TRP:CE3	1:B:325:MET:HE2	2.51	0.43
1:A:203:ALA:HB2	1:A:539:HIS:CE1	2.53	0.43
1:B:302:MET:HE1	1:B:307:ALA:HB2	2.00	0.43
1:A:470:ILE:HG23	1:A:471:ILE:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:LEU:N	1:A:496:LEU:HD22	2.33	0.43
1:B:200:VAL:C	1:B:201:ARG:HD2	2.42	0.43
1:A:378:LEU:HD12	1:A:378:LEU:N	2.34	0.42
1:A:458:MET:HE1	1:A:519:SER:O	2.19	0.42
1:B:203:ALA:HB2	1:B:539:HIS:CE1	2.54	0.42
1:B:215:GLY:O	1:B:226:GLY:HA2	2.19	0.42
1:B:302:MET:CE	1:B:307:ALA:HA	2.49	0.42
1:B:201:ARG:NH2	1:B:206:ASP:OD2	2.53	0.42
1:A:215:GLY:O	1:A:226:GLY:HA2	2.20	0.42
1:A:72:THR:OG1	1:A:176:GLU:HB3	2.20	0.41
1:A:62:ALA:HB2	1:A:147:MET:CE	2.44	0.41
1:A:372:ILE:C	1:A:372:ILE:HD12	2.46	0.41
1:A:59:ILE:HD12	1:A:179:ILE:HD11	2.02	0.41
1:B:372:ILE:HD12	1:B:372:ILE:C	2.46	0.41
1:A:265:PHE:O	1:A:266:GLY:C	2.64	0.40
1:B:265:PHE:O	1:B:266:GLY:C	2.65	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	517/519 (100%)	494 (96%)	21 (4%)	2 (0%)	30	22
1	B	518/519 (100%)	495 (96%)	21 (4%)	2 (0%)	30	22
All	All	1035/1038 (100%)	989 (96%)	42 (4%)	4 (0%)	30	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	234	ASN
1	B	234	ASN

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Mol	Chain	Res	Type
1	A	456	ILE
1	B	456	ILE

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	445/445 (100%)	438 (98%)	7 (2%)	55	54
1	B	446/445 (100%)	442 (99%)	4 (1%)	70	73
All	All	891/890 (100%)	880 (99%)	11 (1%)	63	63

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ASP
1	A	57	ILE
1	A	68	LEU
1	A	142	LYS
1	A	178	VAL
1	A	450	SER
1	A	471	ILE
1	B	73	ILE
1	B	134	THR
1	B	143	THR
1	B	552	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	ASN
1	A	300	HIS
1	A	488	HIS
1	B	42	GLN
1	B	163	ASN

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Mol	Chain	Res	Type
1	B	396	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](#)

2 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	GHD	B	601	-	43,44,44	0.71	2 (4%)	58,64,64	1.43	9 (15%)
2	GHD	A	601	-	43,44,44	1.03	2 (4%)	58,64,64	1.66	10 (17%)

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	GHD	B	601	-	-	22/45/84/84	0/2/2/2
2	GHD	A	601	-	-	25/45/84/84	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	GHD	O6-C8	4.18	1.47	1.40
2	B	601	GHD	O6-C8	2.83	1.45	1.40
2	A	601	GHD	O17-C21	-2.82	1.20	1.30
2	B	601	GHD	O17-C21	-2.25	1.22	1.30

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	GHD	C6-C5-C4	5.26	122.94	113.05
2	A	601	GHD	C22-C23-C3	4.93	117.34	109.72
2	B	601	GHD	C6-C5-C4	4.88	122.22	113.05
2	A	601	GHD	O2-C5-C4	-4.55	99.61	109.44
2	B	601	GHD	C4-C3-N1	3.99	117.27	110.91
2	A	601	GHD	C4-C3-N1	3.48	116.45	110.91
2	A	601	GHD	C8-C22-C23	3.45	117.71	110.73
2	A	601	GHD	C3-N1-C2	3.02	130.17	123.11
2	B	601	GHD	O5-C4-C3	-2.93	107.16	109.84
2	B	601	GHD	O2-C5-C4	-2.85	103.29	109.44
2	A	601	GHD	C8-O5-C4	-2.83	107.73	114.36
2	B	601	GHD	C8-O5-C4	-2.71	108.00	114.36
2	B	601	GHD	C22-C23-C3	2.50	113.59	109.72
2	B	601	GHD	C22-C8-C21	2.43	116.88	111.39
2	B	601	GHD	C8-C22-C23	2.38	115.54	110.73
2	B	601	GHD	C3-N1-C2	2.34	128.58	123.11
2	A	601	GHD	O8-C12-C13	2.21	111.03	107.98
2	A	601	GHD	C19-C20-C10	2.15	114.14	110.23
2	A	601	GHD	O6-C8-O5	2.09	115.74	109.97

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GHD	O1-C2-N1-C3
2	A	601	GHD	C4-C3-N1-C2
2	A	601	GHD	C3-C4-C5-C6
2	A	601	GHD	C3-C4-C5-O2
2	A	601	GHD	O5-C4-C5-C6
2	A	601	GHD	O5-C4-C5-O2
2	A	601	GHD	O17-C21-C8-O6
2	A	601	GHD	C21-C8-O6-C9
2	A	601	GHD	C22-C8-O6-C9

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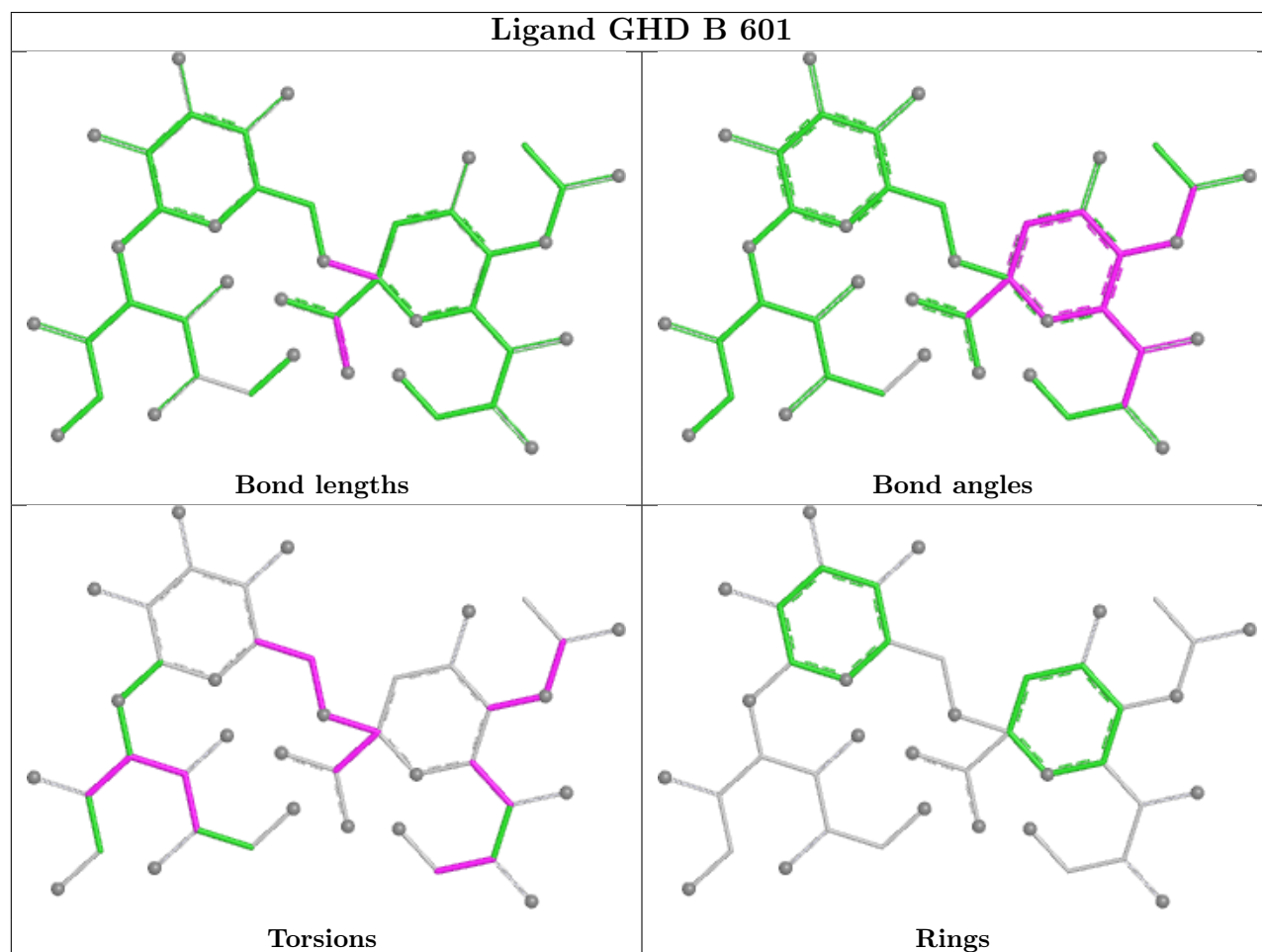
Mol	Chain	Res	Type	Atoms
2	A	601	GHD	O5-C8-O6-C9
2	A	601	GHD	O8-C12-C13-O9
2	A	601	GHD	O8-C12-C13-C14
2	A	601	GHD	O9-C13-C14-O10
2	A	601	GHD	C13-C12-C15-O11
2	A	601	GHD	O8-C12-C15-O11
2	A	601	GHD	C13-C12-C15-C16
2	A	601	GHD	O8-C12-C15-C16
2	A	601	GHD	C13-C12-O8-C11
2	B	601	GHD	C4-C3-N1-C2
2	B	601	GHD	C3-C4-C5-C6
2	B	601	GHD	C3-C4-C5-O2
2	B	601	GHD	O5-C4-C5-C6
2	B	601	GHD	O5-C4-C5-O2
2	B	601	GHD	C5-C6-C7-O4
2	B	601	GHD	O3-C6-C7-O4
2	B	601	GHD	O17-C21-C8-O6
2	B	601	GHD	C21-C8-O6-C9
2	B	601	GHD	C22-C8-O6-C9
2	B	601	GHD	O5-C8-O6-C9
2	B	601	GHD	O8-C12-C15-C16
2	B	601	GHD	C10-C9-O6-C8
2	B	601	GHD	O7-C10-C9-O6
2	A	601	GHD	C12-C13-C14-O10
2	A	601	GHD	C1-C2-N1-C3
2	B	601	GHD	O1-C2-N1-C3
2	B	601	GHD	C1-C2-N1-C3
2	B	601	GHD	C20-C10-C9-O6
2	A	601	GHD	C10-C9-O6-C8
2	B	601	GHD	O8-C12-C15-O11
2	B	601	GHD	O18-C21-C8-O6
2	A	601	GHD	C5-C6-C7-O4
2	A	601	GHD	O3-C6-C7-O4
2	B	601	GHD	C15-C12-C13-O9
2	A	601	GHD	O7-C11-O8-C12
2	A	601	GHD	C18-C11-O8-C12
2	B	601	GHD	O18-C21-C8-C22
2	B	601	GHD	O11-C15-C16-C17

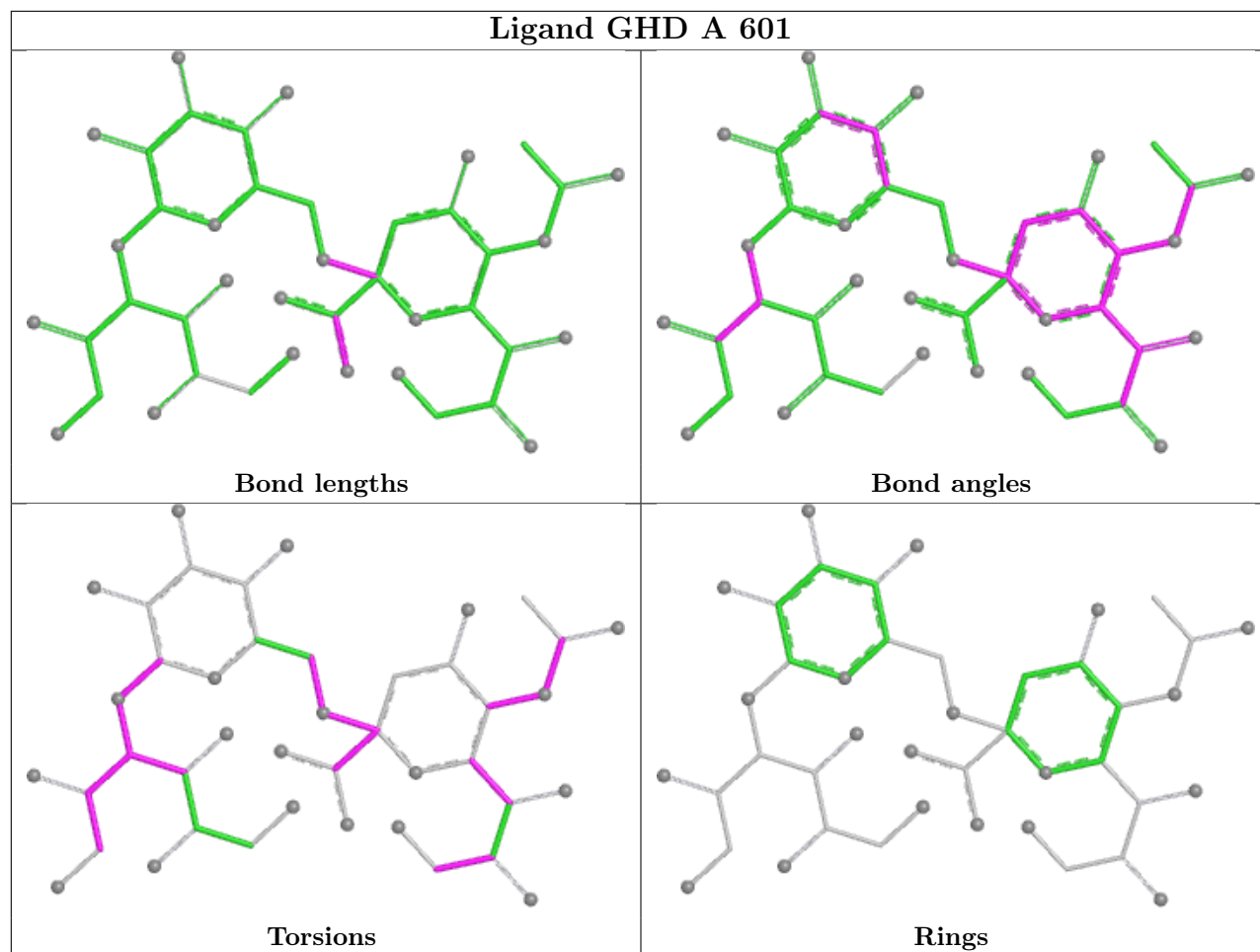
There are no ring outliers.

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 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	519/519 (100%)	0.79	58 (11%)	10 10	24, 42, 69, 92	0
1	B	519/519 (100%)	1.27	94 (18%)	3 3	21, 46, 61, 80	1 (0%)
All	All	1038/1038 (100%)	1.03	152 (14%)	6 6	21, 44, 63, 92	1 (0%)

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	34	ASP	4.4
1	B	358	GLY	4.3
1	B	547	ILE	4.2
1	A	132	VAL	4.2
1	A	135	VAL	3.8
1	B	294	VAL	3.8
1	A	35	SER	3.8
1	B	262	ALA	3.7
1	B	395	TRP	3.7
1	B	296	ALA	3.6
1	A	183	PRO	3.6
1	B	293	TRP	3.6
1	A	148	VAL	3.5
1	B	369	VAL	3.5
1	A	36	VAL	3.5
1	B	413	VAL	3.4
1	A	185	VAL	3.4
1	B	274	GLY	3.4
1	B	261	ILE	3.3
1	B	246	LEU	3.3
1	B	345	VAL	3.3
1	B	420	LEU	3.3
1	B	552	ARG	3.3
1	A	341	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	34	ASP	3.2
1	A	413	VAL	3.2
1	B	167	LEU	3.2
1	A	92	ALA	3.2
1	A	184	ALA	3.2
1	B	292	VAL	3.2
1	B	401	ALA	3.1
1	A	65	GLY	3.1
1	A	178	VAL	3.0
1	B	335	TRP	3.0
1	A	67	VAL	3.0
1	A	177	VAL	3.0
1	B	138	THR	3.0
1	B	360	GLY	3.0
1	A	179	ILE	2.9
1	A	63	THR	2.9
1	A	134	THR	2.9
1	B	245	GLY	2.9
1	B	222	GLY	2.9
1	A	47	VAL	2.8
1	B	297	ALA	2.8
1	B	442	TRP	2.8
1	A	182	LYS	2.8
1	A	71	LEU	2.8
1	A	89	LEU	2.8
1	A	73	ILE	2.8
1	B	285	VAL	2.7
1	B	137	ASN	2.7
1	B	209	ALA	2.7
1	B	283	ILE	2.7
1	B	225	LEU	2.7
1	B	217	VAL	2.7
1	B	432	VAL	2.7
1	A	96	ALA	2.6
1	B	279	GLY	2.6
1	A	37	TYR	2.6
1	B	298	TRP	2.6
1	B	370	PHE	2.6
1	A	125	TYR	2.6
1	B	387	TYR	2.6
1	A	139	LEU	2.6
1	B	383	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	271	LEU	2.5
1	B	135	VAL	2.5
1	A	68	LEU	2.5
1	A	57	ILE	2.5
1	B	272	PRO	2.5
1	A	154	PHE	2.5
1	B	278	VAL	2.5
1	B	524	ILE	2.4
1	B	226	GLY	2.4
1	B	229	ASP	2.4
1	A	86	ALA	2.4
1	B	74	ARG	2.4
1	A	285	VAL	2.4
1	B	215	GLY	2.4
1	A	552	ARG	2.3
1	B	353	LEU	2.3
1	B	75	PHE	2.3
1	B	291	THR	2.3
1	B	136	ALA	2.3
1	B	434	ILE	2.3
1	B	100	GLY	2.3
1	B	295	VAL	2.3
1	B	410	VAL	2.3
1	B	368	LEU	2.3
1	A	187	ALA	2.3
1	A	127	ILE	2.3
1	B	238	LEU	2.3
1	A	186	ILE	2.3
1	B	244	VAL	2.3
1	B	224	LEU	2.3
1	A	88	ARG	2.2
1	B	352	PHE	2.2
1	A	38	VAL	2.2
1	A	138	THR	2.2
1	B	362	THR	2.2
1	B	284	LEU	2.2
1	B	418	LEU	2.2
1	B	550	LEU	2.2
1	A	106	PRO	2.2
1	A	146	PRO	2.2
1	B	416	GLY	2.2
1	B	307	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	374	PHE	2.2
1	B	397	ILE	2.2
1	B	134	THR	2.2
1	B	339	THR	2.2
1	A	60	PRO	2.2
1	B	551	ILE	2.2
1	A	158	VAL	2.2
1	B	266	GLY	2.2
1	A	162	ARG	2.2
1	B	385	ILE	2.1
1	B	334	THR	2.1
1	A	83	GLU	2.1
1	A	203	ALA	2.1
1	B	466	ALA	2.1
1	A	75	PHE	2.1
1	A	59	ILE	2.1
1	A	108	THR	2.1
1	B	256	TRP	2.1
1	B	329	THR	2.1
1	A	295	VAL	2.1
1	B	380	VAL	2.1
1	B	503	LEU	2.1
1	A	62	ALA	2.1
1	A	136	ALA	2.1
1	B	321	ALA	2.1
1	B	431	ALA	2.1
1	B	101	ARG	2.1
1	B	396	HIS	2.1
1	B	47	VAL	2.1
1	B	200	VAL	2.1
1	B	183	PRO	2.1
1	B	415	PRO	2.1
1	A	246	LEU	2.1
1	A	551	ILE	2.0
1	B	289	THR	2.0
1	A	100	GLY	2.0
1	B	464	VAL	2.0
1	B	170	LEU	2.0
1	B	184	ALA	2.0
1	B	331	ASP	2.0
1	A	94	THR	2.0
1	B	253	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	270	GLY	2.0
1	A	87	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

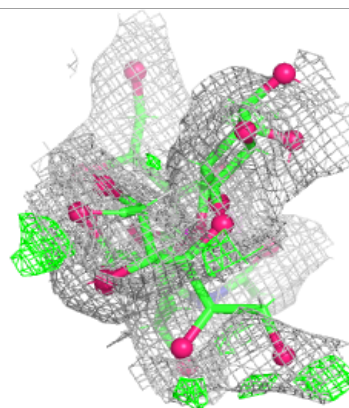
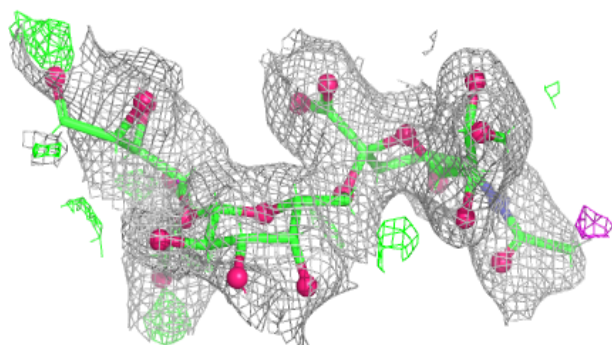
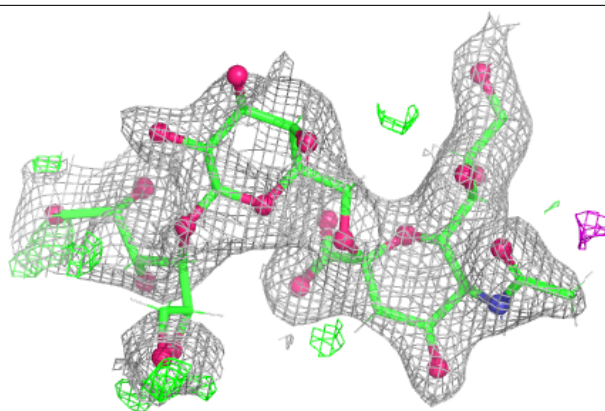
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GHD	B	601	43/43	0.77	0.15	30,51,92,97	11
2	GHD	A	601	43/43	0.88	0.11	27,33,68,72	11

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.

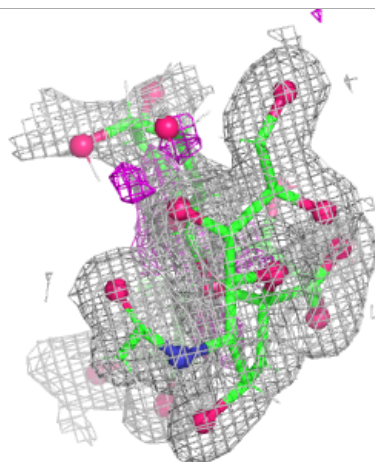
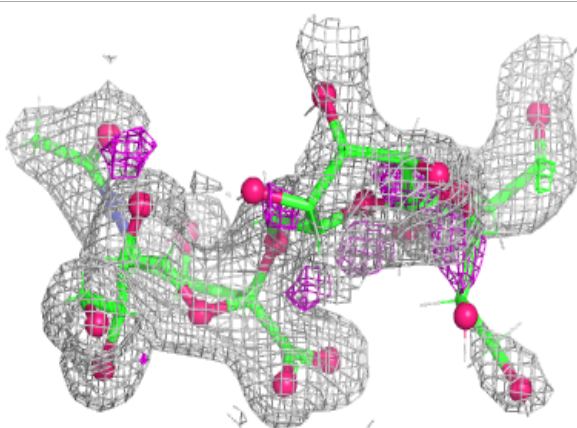
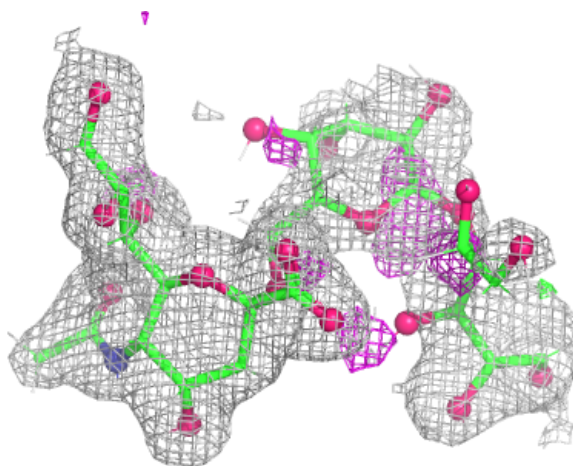
Electron density around GHD B 601:

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



Electron density around GHD A 601:

$2mF_o-DF_c$ (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.