Full wwPDB X-ray Structure Validation Report ⓘ

Dec 5, 2024 – 04:23 PM EST

PDB ID	:	9DIP
Title	:	Crystal structure of H5 hemagglutinin from the influenza virus A/Texas/37/2024 (H5N1) with LSTa
Authors	:	Lin, T.H.; Zhu, Y.; Wilson, I.A.
Deposited on	:	2024-09-05
Resolution	:	2.32 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:

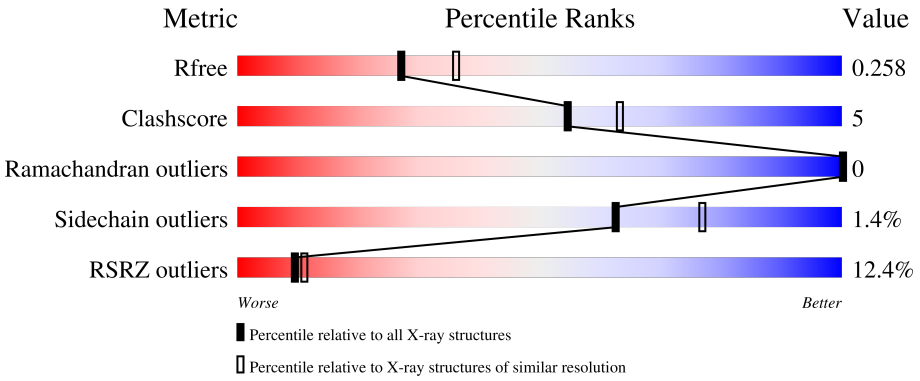
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.32 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.



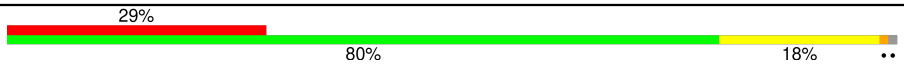
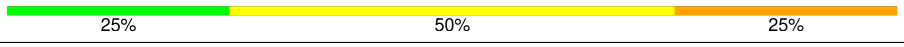
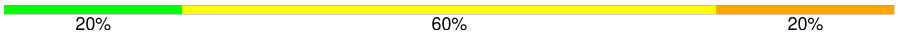
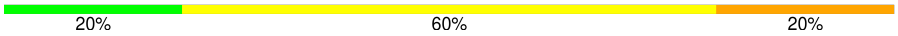
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	7250 (2.34-2.30)
Clashscore	180529	8063 (2.34-2.30)
Ramachandran outliers	177936	7993 (2.34-2.30)
Sidechain outliers	177891	7993 (2.34-2.30)
RSRZ outliers	164620	7250 (2.34-2.30)

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	A	325	2% 87% 11%
1	C	325	6% 89% 10%
1	I	325	6% 89% 10%
2	B	176	11% 87% 11%
2	D	176	39% 87% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	J	176	
3	E	4	
4	F	5	
4	H	5	
5	G	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GLC	F	1	X	-	-	-
4	GLC	H	1	X	-	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12264 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 Hemagglutinin HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2546	1611	444	476	15			
1	C	322	Total	C	N	O	S	0	0	0
			2546	1611	444	476	15			
1	I	322	Total	C	N	O	S	0	0	0
			2546	1611	444	476	15			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	expression tag	UNP A0A6B7HPT9
A	8	ASP	-	expression tag	UNP A0A6B7HPT9
A	9	PRO	-	expression tag	UNP A0A6B7HPT9
A	10	GLY	-	expression tag	UNP A0A6B7HPT9
A	111	MET	LEU	conflict	UNP A0A6B7HPT9
A	122	GLN	LEU	conflict	UNP A0A6B7HPT9
A	199	ILE	THR	conflict	UNP A0A6B7HPT9
A	214	ALA	VAL	conflict	UNP A0A6B7HPT9
C	7	ALA	-	expression tag	UNP A0A6B7HPT9
C	8	ASP	-	expression tag	UNP A0A6B7HPT9
C	9	PRO	-	expression tag	UNP A0A6B7HPT9
C	10	GLY	-	expression tag	UNP A0A6B7HPT9
C	111	MET	LEU	conflict	UNP A0A6B7HPT9
C	122	GLN	LEU	conflict	UNP A0A6B7HPT9
C	199	ILE	THR	conflict	UNP A0A6B7HPT9
C	214	ALA	VAL	conflict	UNP A0A6B7HPT9
I	7	ALA	-	expression tag	UNP A0A6B7HPT9
I	8	ASP	-	expression tag	UNP A0A6B7HPT9
I	9	PRO	-	expression tag	UNP A0A6B7HPT9
I	10	GLY	-	expression tag	UNP A0A6B7HPT9
I	111	MET	LEU	conflict	UNP A0A6B7HPT9
I	122	GLN	LEU	conflict	UNP A0A6B7HPT9
I	199	ILE	THR	conflict	UNP A0A6B7HPT9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	214	ALA	VAL	conflict	UNP A0A6B7HPT9

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	174	Total	C	N	O	S	0	0	0
			1412	878	245	281	8			
2	D	174	Total	C	N	O	S	0	0	0
			1412	878	245	281	8			
2	J	174	Total	C	N	O	S	0	0	0
			1412	878	245	281	8			

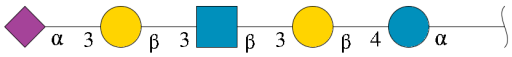
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	-	expression tag	UNP A0A6B7HQ27
B	176	GLY	-	expression tag	UNP A0A6B7HQ27
D	175	SER	-	expression tag	UNP A0A6B7HQ27
D	176	GLY	-	expression tag	UNP A0A6B7HQ27
J	175	SER	-	expression tag	UNP A0A6B7HQ27
J	176	GLY	-	expression tag	UNP A0A6B7HQ27

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galacto pyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	4	Total	C	N	O	0	0	0
			57	31	2	24			

- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galacto pyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-alpha-D-glucopyranose.

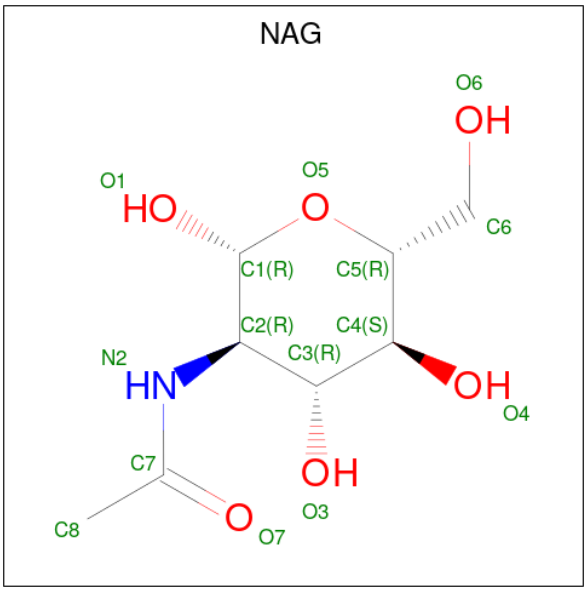


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	F	5	Total C N O 68 37 2 29	0	0	0
4	H	5	Total C N O 68 37 2 29	0	0	0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	G	2	Total C N O 28 16 2 10	0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 7 is water.

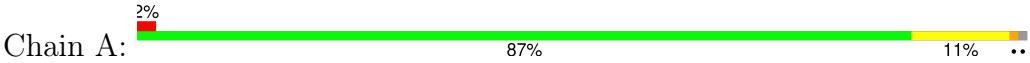
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	36	Total O 36 36	0	0
7	B	9	Total O 9 9	0	0
7	C	45	Total O 45 45	0	0
7	D	4	Total O 4 4	0	0
7	I	39	Total O 39 39	0	0
7	J	8	Total O 8 8	0	0

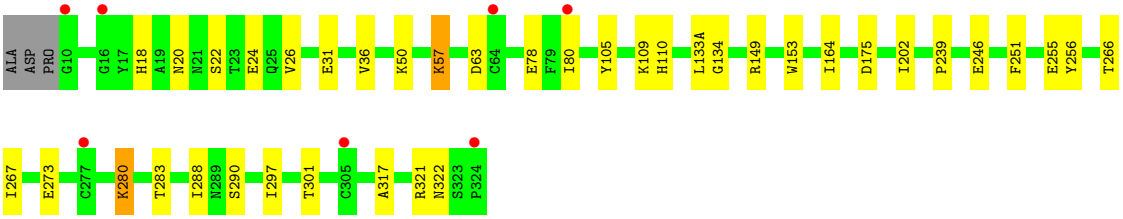
3 Residue-property plots (i)

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: Hemagglutinin HA1

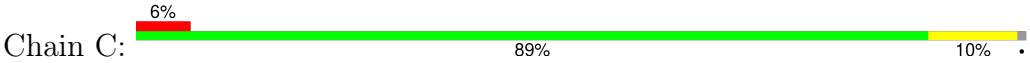
Chain A:

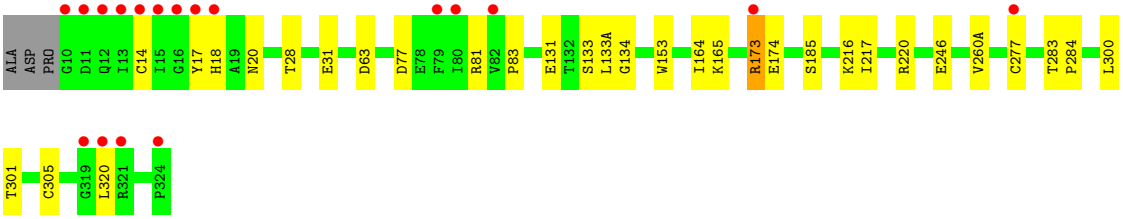




• Molecule 1: Hemagglutinin HA1

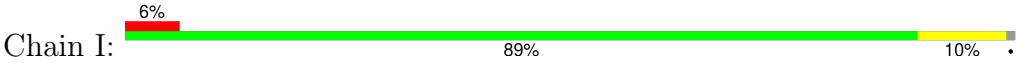
Chain C:

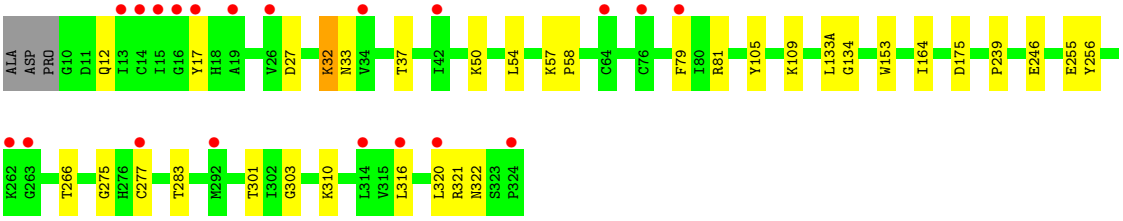




• Molecule 1: Hemagglutinin HA1

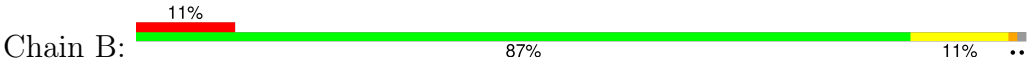
Chain I:

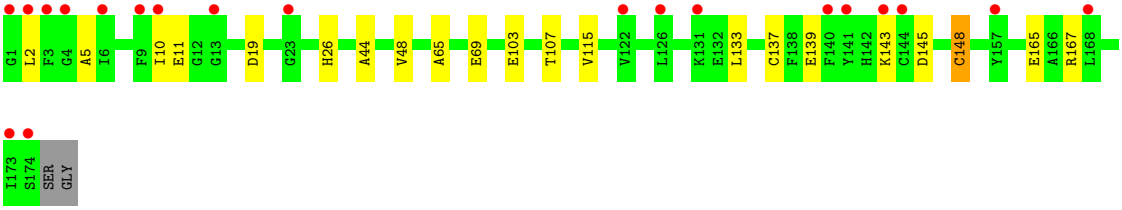




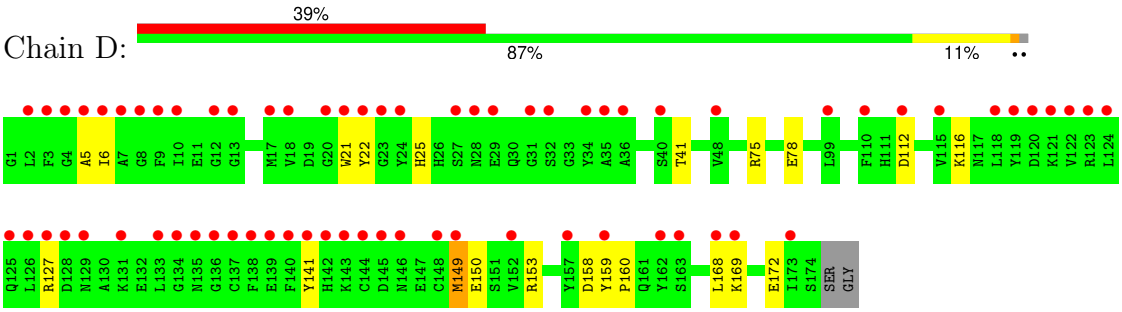
• Molecule 2: Hemagglutinin HA2

Chain B:

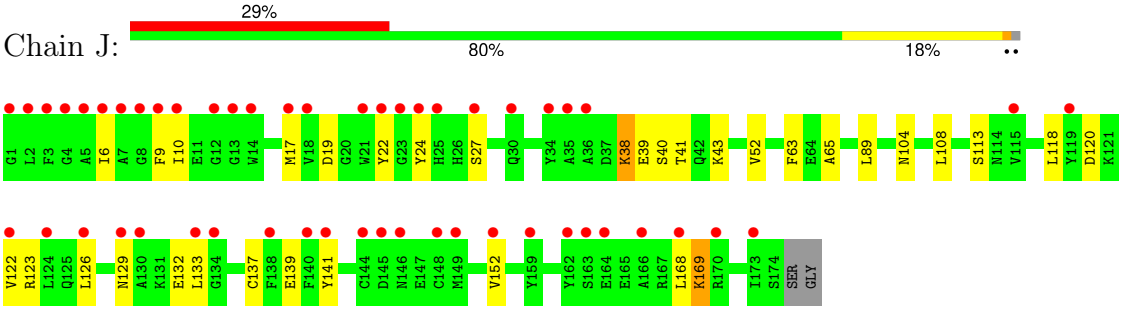




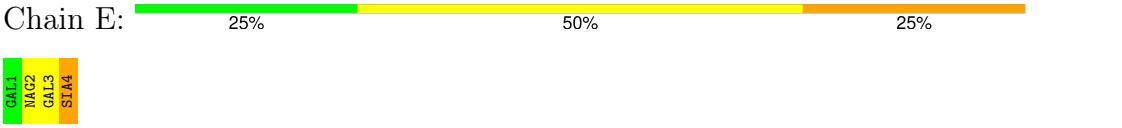
• Molecule 2: Hemagglutinin HA2



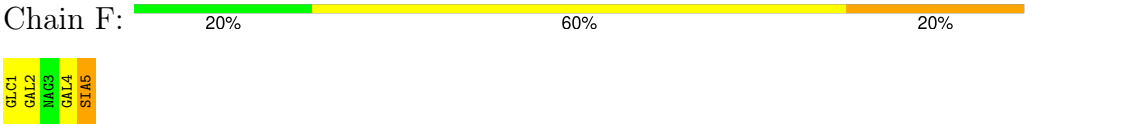
• Molecule 2: Hemagglutinin HA2



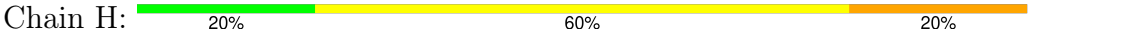
• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



• Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-alpha-D-glucopyranose



• Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose-(1-4)-alpha-D-glucopyranose



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	103.54Å 74.76Å 131.10Å 90.00° 96.21° 90.00°	Depositor
Resolution (Å)	31.18 – 2.32 31.18 – 2.32	Depositor EDS
% Data completeness (in resolution range)	98.3 (31.18-2.32) 98.6 (31.18-2.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 2.32Å)	Xtriage
Refinement program	PHENIX (1.21rc1_5127: ???)	Depositor
R, R_{free}	0.216 , 0.258 0.217 , 0.258	Depositor DCC
R_{free} test set	4347 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	57.9	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 39.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12264	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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: GLC, NAG, GAL, SIA

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	0.25	0/2610	0.49	0/3548
1	C	0.25	0/2610	0.49	0/3548
1	I	0.25	0/2610	0.49	0/3548
2	B	0.30	0/1439	0.48	0/1934
2	D	0.25	0/1439	0.46	0/1934
2	J	0.25	0/1439	0.46	0/1934
All	All	0.25	0/12147	0.48	0/16446

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	2546	0	2495	29	0
1	C	2546	0	2495	20	0
1	I	2546	0	2496	24	0
2	B	1412	0	1319	14	0
2	D	1412	0	1321	14	0
2	J	1412	0	1322	26	0
3	E	57	0	49	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	68	0	58	1	0
4	H	68	0	58	1	0
5	G	28	0	25	0	0
6	A	14	0	13	0	0
6	I	14	0	13	0	0
7	A	36	0	0	3	0
7	B	9	0	0	0	0
7	C	45	0	0	1	0
7	D	4	0	0	0	0
7	I	39	0	0	0	0
7	J	8	0	0	0	0
All	All	12264	0	11664	111	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 (111) 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:26:VAL:HG21	1:A:317:ALA:HB2	1.73	0.71
1:A:273:GLU:N	1:A:273:GLU:OE2	2.22	0.70
2:D:75:ARG:NH1	2:D:78:GLU:OE2	2.25	0.69
1:A:290:SER:N	7:A:501:HOH:O	2.21	0.69
2:D:127:ARG:NH1	2:D:159:TYR:OH	2.26	0.68
1:C:216:LYS:O	1:C:220:ARG:NH2	2.26	0.68
1:I:283:THR:HG22	1:I:301:THR:HG22	1.78	0.65
2:J:17:MET:HE2	2:J:19:ASP:H	1.61	0.64
1:A:18:HIS:HE1	1:A:20:ASN:HB3	1.62	0.64
1:A:31:GLU:OE1	1:A:321:ARG:NH2	2.32	0.63
2:D:22:TYR:H	2:D:41:THR:HG22	1.63	0.63
2:D:127:ARG:NH1	2:J:132:GLU:O	2.32	0.63
1:C:81:ARG:HH12	1:C:83:PRO:HB3	1.63	0.63
1:A:57:LYS:HD3	1:A:57:LYS:H	1.64	0.63
1:A:280:LYS:NZ	7:A:501:HOH:O	2.06	0.63
1:I:57:LYS:HG2	1:I:58:PRO:HD2	1.82	0.62
2:D:149:MET:SD	2:D:153:ARG:NH2	2.74	0.61
2:B:103:GLU:O	2:B:107:THR:OG1	2.17	0.61
1:A:283:THR:HG22	1:A:301:THR:HG22	1.83	0.61
2:J:38:LYS:HD3	2:J:38:LYS:H	1.65	0.61
1:I:50:LYS:HD2	1:I:275:GLY:HA3	1.82	0.61
2:B:19:ASP:N	2:B:19:ASP:OD1	2.35	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:22:TYR:H	2:J:41:THR:HG22	1.68	0.59
1:A:78:GLU:HG3	1:A:149:ARG:HD3	1.85	0.58
1:A:22:SER:OG	1:A:24:GLU:OE1	2.11	0.57
2:J:133:LEU:HD12	2:J:137:CYS:HB2	1.87	0.56
2:B:145:ASP:OD1	2:B:148:CYS:N	2.34	0.56
1:C:165:LYS:NZ	7:C:401:HOH:O	2.33	0.55
2:D:150:GLU:OE1	2:D:153:ARG:NH1	2.39	0.55
2:J:39:GLU:O	2:J:43:LYS:HG3	2.07	0.54
1:A:50:LYS:HE3	1:A:273:GLU:HG2	1.90	0.53
1:I:79:PHE:HE2	1:I:81:ARG:HE	1.57	0.52
1:I:134:GLY:HA3	1:I:153:TRP:HB3	1.91	0.52
1:I:316:LEU:HD23	2:J:52:VAL:HG22	1.92	0.52
2:D:6:ILE:HG12	2:D:112:ASP:HA	1.90	0.52
2:J:40:SER:HA	2:J:43:LYS:NZ	2.24	0.52
1:I:255:GLU:HG2	1:I:256:TYR:CD2	2.45	0.52
1:I:310:LYS:HB2	2:J:89:LEU:HD21	1.92	0.52
1:A:255:GLU:HG2	1:A:256:TYR:CD2	2.45	0.51
2:D:168:LEU:O	2:D:172:GLU:HG2	2.11	0.51
1:C:14:CYS:HB2	2:D:25:HIS:HB3	1.92	0.50
1:A:22:SER:OG	1:A:36:VAL:O	2.29	0.50
1:A:288:ILE:HD11	1:A:297:ILE:HD12	1.94	0.49
1:A:22:SER:HB3	1:A:322:ASN:ND2	2.27	0.49
1:A:105:TYR:CZ	1:A:109:LYS:HD2	2.47	0.49
2:B:2:LEU:O	2:J:113:SER:OG	2.19	0.49
1:C:18:HIS:HB2	2:D:21:TRP:HA	1.95	0.49
2:J:9:PHE:CD1	2:J:10:ILE:HG13	2.47	0.49
2:B:11:GLU:N	2:B:11:GLU:OE1	2.46	0.49
2:J:9:PHE:HD1	2:J:10:ILE:HG13	1.78	0.48
1:A:133(A):LEU:O	3:E:4:SIA:H113	2.13	0.48
1:A:202:ILE:HD11	1:A:251:PHE:HA	1.94	0.48
1:I:17:TYR:HB2	1:I:320:LEU:HD22	1.95	0.48
1:C:131:GLU:OE2	1:C:133:SER:OG	2.22	0.48
2:J:133:LEU:HD21	2:J:139:GLU:HB2	1.95	0.48
1:I:105:TYR:CE2	1:I:109:LYS:HD2	2.49	0.48
1:A:80:ILE:O	1:A:80:ILE:HG13	2.14	0.47
1:C:133(A):LEU:O	4:F:5:SIA:H113	2.15	0.47
1:C:164:ILE:O	1:C:246:GLU:HA	2.15	0.47
1:C:17:TYR:HB2	1:C:320:LEU:HD22	1.96	0.46
1:C:320:LEU:HD21	2:D:22:TYR:HE1	1.80	0.46
2:J:40:SER:HA	2:J:43:LYS:HZ3	1.80	0.46
1:I:266:THR:HG22	2:J:65:ALA:HB1	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:141:TYR:O	2:D:169:LYS:HB3	2.16	0.45
2:D:5:ALA:HB2	2:D:116:LYS:HB2	1.98	0.45
1:I:321:ARG:HD3	2:J:6:ILE:HG21	1.98	0.45
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.99	0.45
1:A:175:ASP:OD1	1:A:239:PRO:HD3	2.16	0.45
1:I:32:LYS:HG2	1:I:33:ASN:HB2	1.99	0.45
1:C:131:GLU:HG2	1:C:133(A):LEU:HD12	1.98	0.44
2:B:133:LEU:HD21	2:B:139:GLU:HB2	1.99	0.44
1:I:133(A):LEU:O	4:H:5:SIA:H113	2.18	0.44
1:C:18:HIS:HE1	1:C:20:ASN:HB3	1.83	0.44
1:A:18:HIS:CE1	1:A:20:ASN:HB3	2.48	0.44
1:C:284:PRO:HD3	1:C:300:LEU:O	2.18	0.44
1:I:321:ARG:HG2	2:J:108:LEU:HD22	2.00	0.44
1:A:110:HIS:ND1	2:B:69:GLU:OE1	2.49	0.44
1:C:134:GLY:HA3	1:C:153:TRP:HB3	2.00	0.44
1:I:37:THR:OG1	1:I:320:LEU:N	2.51	0.44
2:J:168:LEU:HB2	2:J:169:LYS:NZ	2.32	0.43
2:J:122:VAL:HG22	2:J:152:VAL:HG12	2.00	0.43
1:C:174:GLU:HG2	1:C:260(A):VAL:HG22	2.00	0.43
2:B:133:LEU:HD12	2:B:137:CYS:HB2	1.99	0.43
2:J:24:TYR:OH	2:J:118:LEU:HD11	2.19	0.43
2:B:44:ALA:O	2:B:48:VAL:HG22	2.19	0.43
1:A:266:THR:HG22	2:B:65:ALA:HB1	2.01	0.43
1:A:288:ILE:HG22	7:A:501:HOH:O	2.18	0.43
2:B:5:ALA:HB1	2:B:115:VAL:HG12	2.00	0.43
1:I:303:GLY:HA2	2:J:63:PHE:CD2	2.53	0.43
1:A:164:ILE:O	1:A:246:GLU:HA	2.18	0.42
1:I:164:ILE:O	1:I:246:GLU:HA	2.19	0.42
1:C:185:SER:HB2	1:C:217:ILE:HG12	2.01	0.42
1:I:37:THR:HG23	1:I:322:ASN:HB2	2.00	0.42
2:B:5:ALA:O	2:B:10:ILE:HB	2.18	0.42
1:I:54:LEU:HD21	2:J:63:PHE:HE2	1.84	0.42
1:A:109:LYS:HB3	1:A:267:ILE:HD11	2.01	0.42
1:C:173:ARG:NE	1:C:173:ARG:HA	2.35	0.42
1:I:316:LEU:HD12	2:J:104:ASN:OD1	2.20	0.42
1:C:301:THR:HB	1:C:305:CYS:SG	2.60	0.42
2:D:158:ASP:CG	2:D:160:PRO:HD2	2.40	0.42
2:J:126:LEU:O	2:J:129:ASN:HB3	2.19	0.41
2:B:143:LYS:HD3	2:B:143:LYS:HA	1.90	0.41
1:C:28:THR:HG23	1:C:31:GLU:H	1.85	0.41
1:A:24:GLU:CD	1:A:24:GLU:N	2.74	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:LYS:HD2	1:A:50:LYS:HA	1.88	0.41
1:C:283:THR:HG22	1:C:301:THR:HG22	2.02	0.41
1:I:12:GLN:HB3	2:J:27:SER:HB3	2.01	0.41
1:I:175:ASP:OD1	1:I:239:PRO:HD3	2.20	0.41
2:B:165:GLU:OE1	2:B:165:GLU:N	2.51	0.41
1:I:37:THR:HG1	1:I:320:LEU:H	1.68	0.41
2:J:141:TYR:O	2:J:169:LYS:HD3	2.21	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	320/325 (98%)	314 (98%)	6 (2%)	0	100	100
1	C	320/325 (98%)	312 (98%)	8 (2%)	0	100	100
1	I	320/325 (98%)	310 (97%)	10 (3%)	0	100	100
2	B	172/176 (98%)	170 (99%)	2 (1%)	0	100	100
2	D	172/176 (98%)	165 (96%)	7 (4%)	0	100	100
2	J	172/176 (98%)	170 (99%)	2 (1%)	0	100	100
All	All	1476/1503 (98%)	1441 (98%)	35 (2%)	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	A	285/287 (99%)	282 (99%)	3 (1%)	70 83
1	C	285/287 (99%)	281 (99%)	4 (1%)	62 77
1	I	285/287 (99%)	282 (99%)	3 (1%)	70 83
2	B	149/150 (99%)	146 (98%)	3 (2%)	50 67
2	D	149/150 (99%)	148 (99%)	1 (1%)	81 90
2	J	149/150 (99%)	145 (97%)	4 (3%)	40 56
All	All	1302/1311 (99%)	1284 (99%)	18 (1%)	62 77

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LYS
1	A	63	ASP
1	A	280	LYS
2	B	26	HIS
2	B	148	CYS
2	B	167	ARG
1	C	63	ASP
1	C	77	ASP
1	C	173	ARG
1	C	277	CYS
2	D	149	MET
1	I	27	ASP
1	I	32	LYS
1	I	277	CYS
2	J	38	LYS
2	J	120	ASP
2	J	123	ARG
2	J	169	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	322	ASN
2	B	26	HIS
1	I	40	GLN
1	I	142	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

16 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	$\#\|Z\| > 2$
3	GAL	E	1	3	12,12,12	0.65	0	17,17,17	0.85	0
3	NAG	E	2	3	14,14,15	0.76	0	17,19,21	1.36	1 (5%)
3	GAL	E	3	3	11,11,12	0.67	0	15,15,17	1.16	1 (6%)
3	SIA	E	4	3	20,20,21	1.63	2 (10%)	21,28,31	1.87	5 (23%)
4	GLC	F	1	4	12,12,12	0.55	0	17,17,17	1.26	2 (11%)
4	GAL	F	2	4	11,11,12	0.74	0	15,15,17	1.26	3 (20%)
4	NAG	F	3	4	14,14,15	0.76	0	17,19,21	0.85	0
4	GAL	F	4	4	11,11,12	0.76	0	15,15,17	1.10	1 (6%)
4	SIA	F	5	4	20,20,21	1.61	2 (10%)	21,28,31	1.87	5 (23%)
5	NAG	G	1	1,5	14,14,15	0.67	0	17,19,21	1.19	1 (5%)
5	NAG	G	2	5	14,14,15	0.70	0	17,19,21	0.78	0
4	GLC	H	1	4	12,12,12	0.52	0	17,17,17	0.77	0
4	GAL	H	2	4	11,11,12	0.75	0	15,15,17	1.00	1 (6%)
4	NAG	H	3	4	14,14,15	0.71	0	17,19,21	0.83	1 (5%)
4	GAL	H	4	4	11,11,12	0.73	0	15,15,17	1.11	1 (6%)
4	SIA	H	5	4	20,20,21	1.61	2 (10%)	21,28,31	1.78	4 (19%)

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
3	GAL	E	1	3	-	0/2/22/22	0/1/1/1
3	NAG	E	2	3	-	1/6/23/26	0/1/1/1
3	GAL	E	3	3	-	1/2/19/22	0/1/1/1
3	SIA	E	4	3	-	3/18/34/38	0/1/1/1
4	GLC	F	1	4	1/1/5/5	1/2/22/22	0/1/1/1
4	GAL	F	2	4	-	2/2/19/22	0/1/1/1
4	NAG	F	3	4	-	0/6/23/26	0/1/1/1
4	GAL	F	4	4	-	0/2/19/22	0/1/1/1
4	SIA	F	5	4	-	0/18/34/38	0/1/1/1
5	NAG	G	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
4	GLC	H	1	4	1/1/5/5	0/2/22/22	0/1/1/1
4	GAL	H	2	4	-	1/2/19/22	0/1/1/1
4	NAG	H	3	4	-	0/6/23/26	0/1/1/1
4	GAL	H	4	4	-	2/2/19/22	0/1/1/1
4	SIA	H	5	4	-	6/18/34/38	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	5	SIA	C2-C1	5.83	1.59	1.52
3	E	4	SIA	C2-C1	5.79	1.59	1.52
4	H	5	SIA	C2-C1	5.64	1.59	1.52
3	E	4	SIA	O6-C2	2.15	1.47	1.43
4	F	5	SIA	O6-C2	2.09	1.47	1.43
4	H	5	SIA	O6-C2	2.03	1.47	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	4	SIA	O1A-C1-C2	-5.19	111.64	122.85
4	H	5	SIA	O1A-C1-C2	-5.17	111.67	122.85
4	F	5	SIA	O1A-C1-C2	-5.09	111.85	122.85
3	E	2	NAG	O5-C1-C2	-4.41	104.47	111.29
3	E	4	SIA	O6-C2-C3	-3.88	105.34	110.56
4	F	5	SIA	O6-C2-C3	-3.63	105.67	110.56
4	H	5	SIA	O6-C2-C3	-3.54	105.80	110.56
4	H	4	GAL	O3-C3-C2	-3.02	103.89	110.05
4	F	4	GAL	O3-C3-C2	-2.99	103.96	110.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	1	GLC	C4-C3-C2	2.83	115.80	110.83
3	E	3	GAL	O3-C3-C2	-2.80	104.33	110.05
4	F	5	SIA	C6-C5-N5	-2.80	106.43	110.91
5	G	1	NAG	C1-O5-C5	2.75	115.88	112.19
4	F	2	GAL	C1-O5-C5	2.57	115.64	112.19
4	F	5	SIA	O1B-C1-C2	2.46	119.12	112.71
4	H	5	SIA	O1B-C1-C2	2.46	119.11	112.71
3	E	4	SIA	O1B-C1-O1A	2.40	129.53	124.08
3	E	4	SIA	O1B-C1-C2	2.35	118.82	112.71
4	F	2	GAL	C1-C2-C3	2.29	112.98	109.64
3	E	4	SIA	C6-C5-N5	-2.27	107.29	110.91
4	H	5	SIA	O1B-C1-O1A	2.27	129.22	124.08
4	F	2	GAL	O3-C3-C2	-2.25	105.47	110.05
4	F	1	GLC	C3-C4-C5	2.20	114.21	110.23
4	F	5	SIA	O1B-C1-O1A	2.18	129.03	124.08
4	H	2	GAL	O3-C3-C2	-2.05	105.88	110.05
4	H	3	NAG	C1-O5-C5	2.01	114.88	112.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	F	1	GLC	C1
4	H	1	GLC	C1

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	4	GAL	O5-C5-C6-O6
4	H	4	GAL	C4-C5-C6-O6
4	H	5	SIA	C6-C7-C8-O8
5	G	1	NAG	O5-C5-C6-O6
3	E	4	SIA	C6-C7-C8-O8
3	E	2	NAG	O5-C5-C6-O6
4	F	1	GLC	O5-C5-C6-O6
4	F	2	GAL	C4-C5-C6-O6
4	H	5	SIA	O7-C7-C8-O8
4	H	5	SIA	C6-C7-C8-C9
4	F	2	GAL	O5-C5-C6-O6
4	H	2	GAL	C4-C5-C6-O6
4	H	5	SIA	C7-C8-C9-O9
4	H	5	SIA	O7-C7-C8-C9
3	E	3	GAL	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	E	4	SIA	C6-C7-C8-C9
3	E	4	SIA	O7-C7-C8-O8
4	H	5	SIA	O8-C8-C9-O9

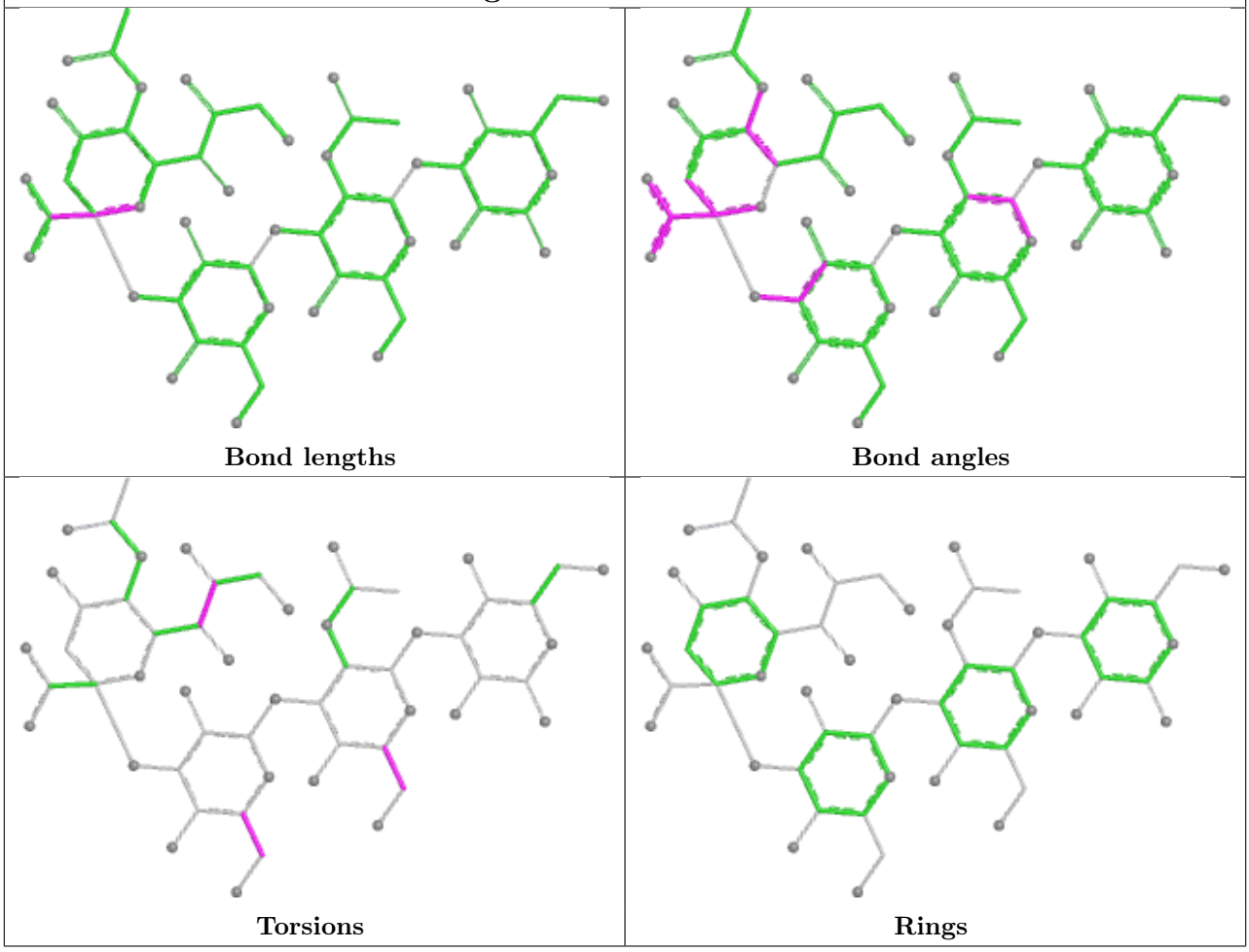
There are no ring outliers.

3 monomers are involved in 3 short contacts:

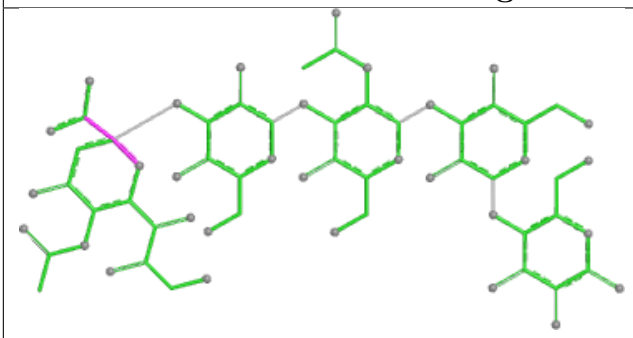
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	5	SIA	1	0
3	E	4	SIA	1	0
4	H	5	SIA	1	0

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

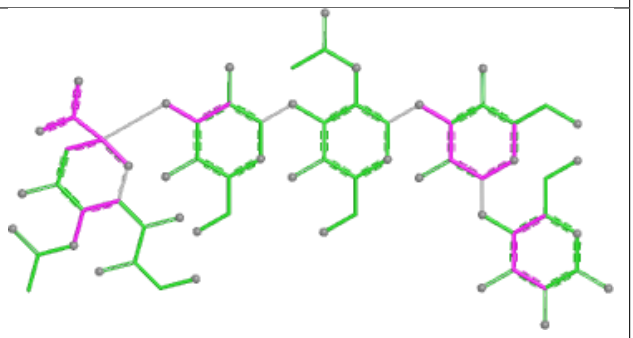
Oligosaccharide Chain E



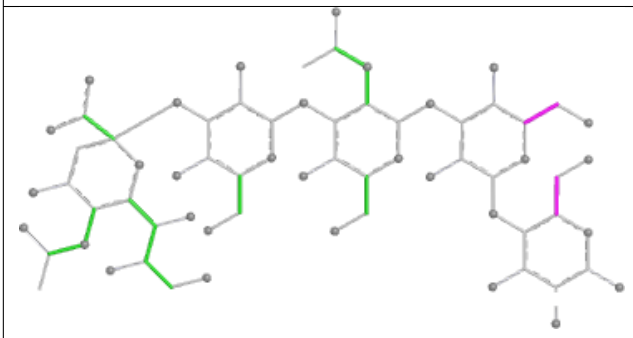
Oligosaccharide Chain F



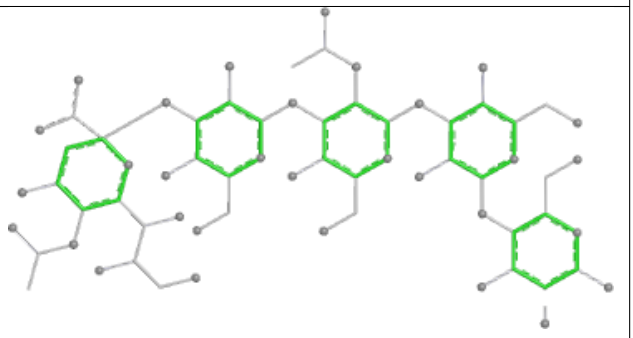
Bond lengths



Bond angles

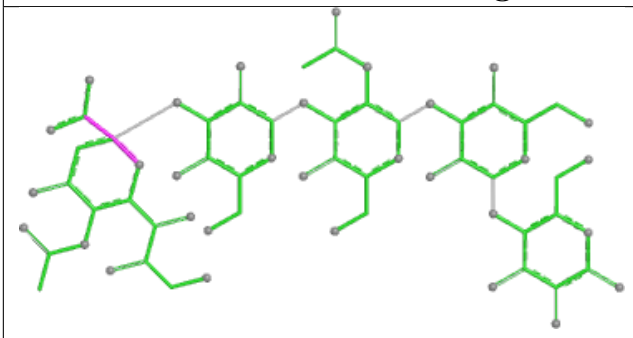


Torsions

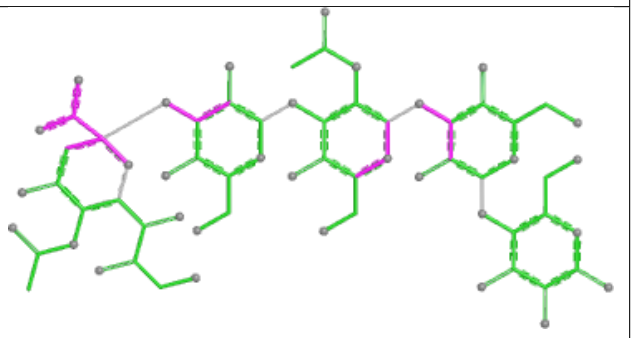


Rings

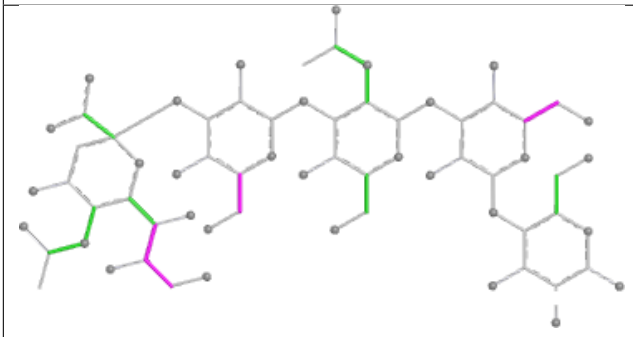
Oligosaccharide Chain H



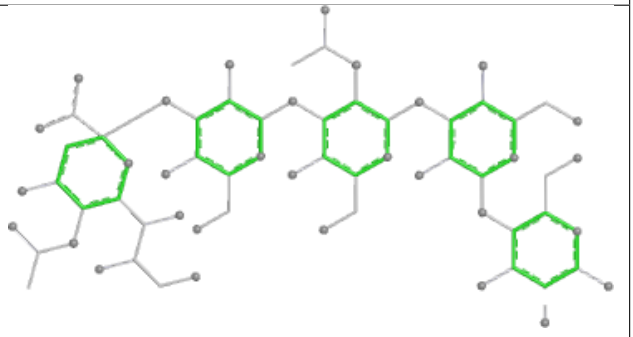
Bond lengths



Bond angles

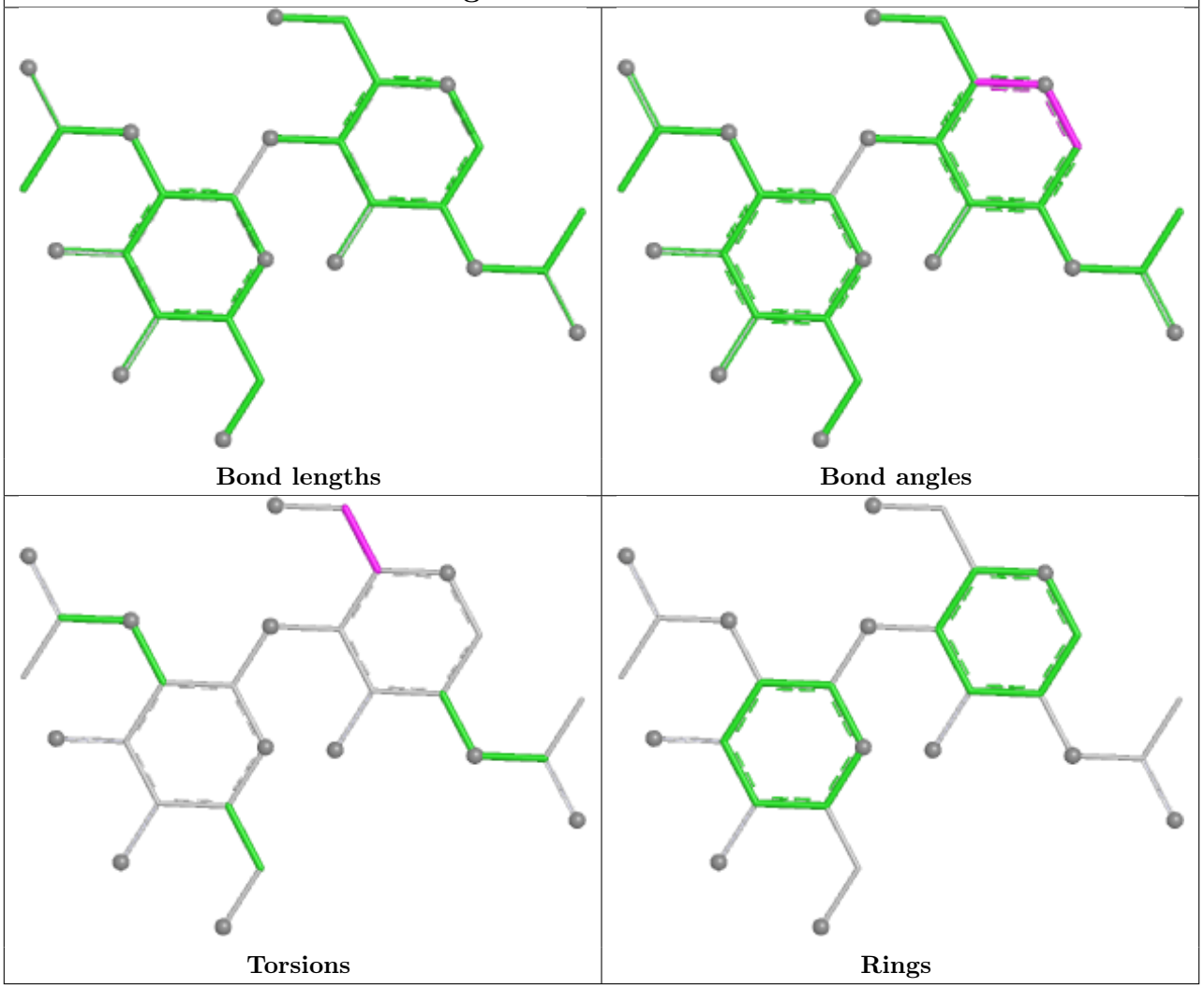


Torsions



Rings

Oligosaccharide Chain G



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	$\#\|Z\| > 2$
6	NAG	A	401	1	14,14,15	0.72	0	17,19,21	1.04	1 (5%)
6	NAG	I	401	1	14,14,15	0.73	0	17,19,21	1.13	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
6	NAG	A	401	1	-	3/6/23/26	0/1/1/1
6	NAG	I	401	1	-	2/6/23/26	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(^{o})	Ideal(^{o})
6	I	401	NAG	C1-O5-C5	3.15	116.41	112.19
6	A	401	NAG	C1-O5-C5	2.24	115.19	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

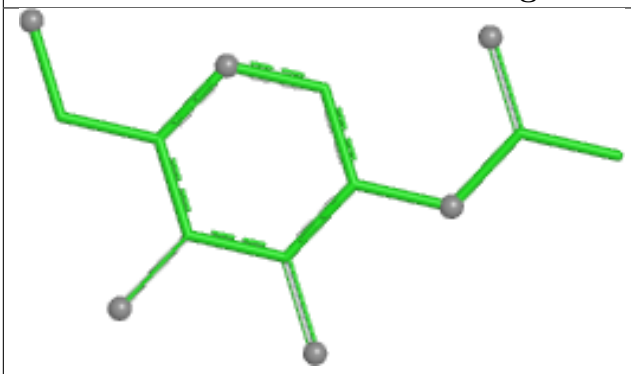
Mol	Chain	Res	Type	Atoms
6	A	401	NAG	C8-C7-N2-C2
6	A	401	NAG	O7-C7-N2-C2
6	I	401	NAG	O5-C5-C6-O6
6	I	401	NAG	C4-C5-C6-O6
6	A	401	NAG	O5-C5-C6-O6

There are no ring outliers.

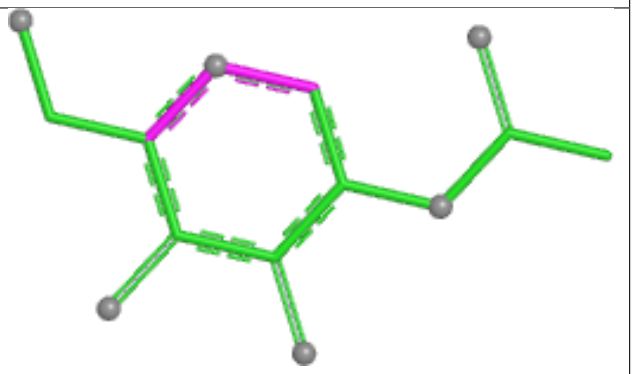
No monomer is involved in short contacts.

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.

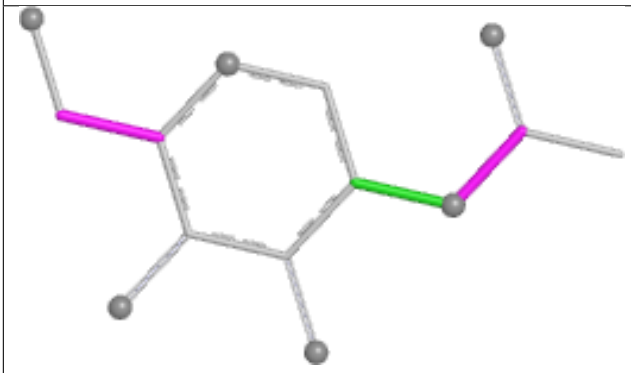
Ligand NAG A 401



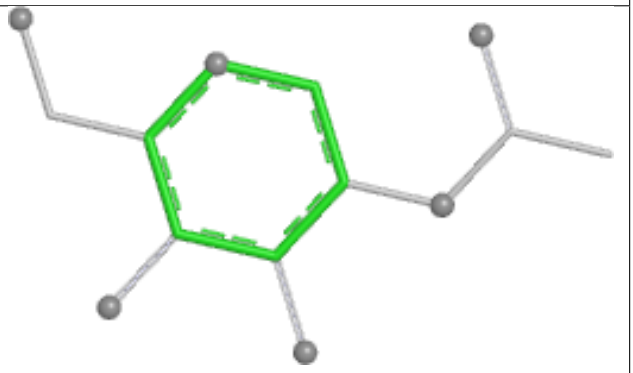
Bond lengths



Bond angles

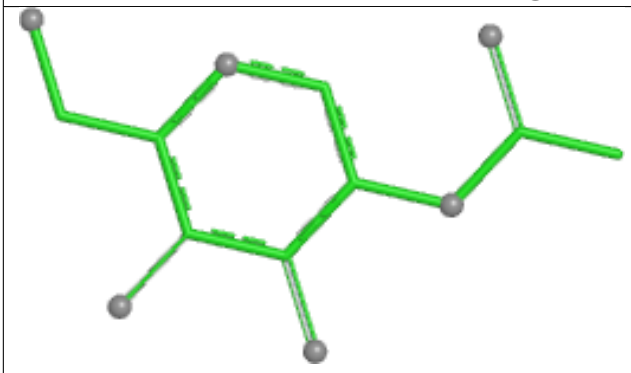


Torsions

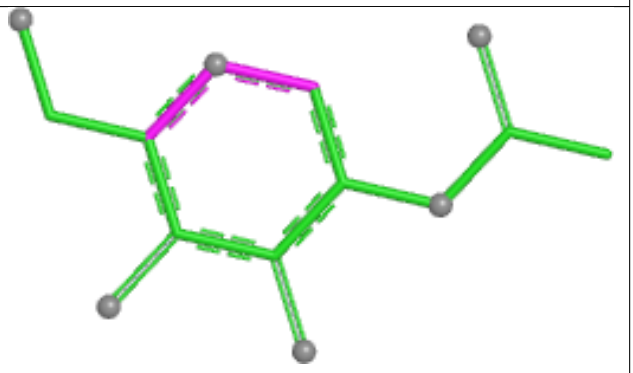


Rings

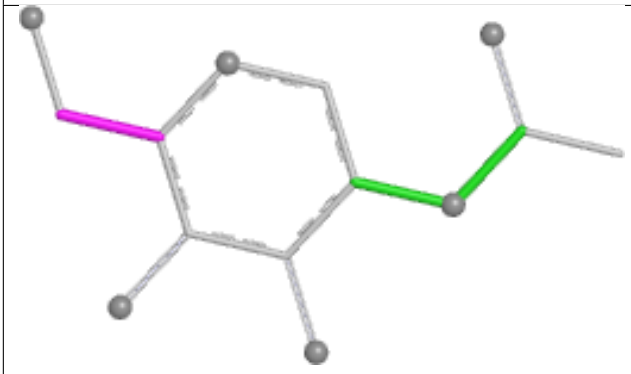
Ligand NAG I 401



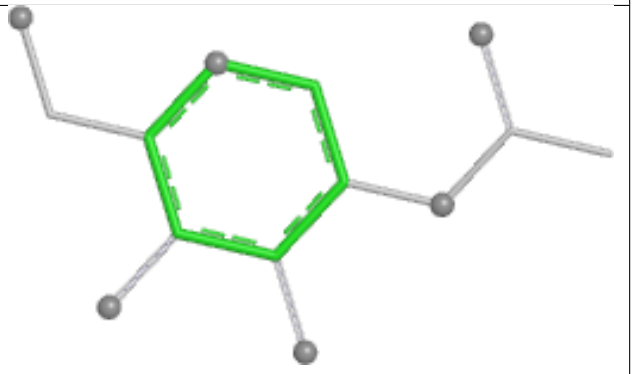
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	A	322/325 (99%)	0.27	7 (2%) 62 64	45, 64, 96, 125	0
1	C	322/325 (99%)	0.23	18 (5%) 31 34	38, 59, 117, 201	0
1	I	322/325 (99%)	0.38	20 (6%) 28 31	42, 65, 111, 158	0
2	B	174/176 (98%)	0.80	20 (11%) 11 13	44, 97, 136, 165	0
2	D	174/176 (98%)	1.52	69 (39%) 1 1	43, 135, 188, 200	0
2	J	174/176 (98%)	1.39	51 (29%) 1 2	43, 122, 162, 179	0
All	All	1488/1503 (99%)	0.62	185 (12%) 9 11	38, 70, 160, 201	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	5	ALA	6.5
1	C	13	ILE	6.5
2	J	6	ILE	6.3
2	D	152	VAL	5.5
2	D	140	PHE	5.5
2	J	140	PHE	5.1
2	J	149	MET	5.1
2	D	6	ILE	4.8
2	D	2	LEU	4.8
2	J	36	ALA	4.8
2	J	9	PHE	4.6
2	J	2	LEU	4.5
2	D	122	VAL	4.5
2	D	4	GLY	4.4
2	J	10	ILE	4.4
1	I	13	ILE	4.3
2	D	138	PHE	4.2
2	D	141	TYR	4.2
2	J	7	ALA	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	10	GLY	4.2
2	J	173	ILE	4.2
2	J	27	SER	4.1
1	I	316	LEU	4.1
2	J	4	GLY	3.9
1	I	320	LEU	3.9
2	D	10	ILE	3.9
2	D	3	PHE	3.8
2	J	3	PHE	3.8
1	I	17	TYR	3.7
2	B	3	PHE	3.7
2	D	9	PHE	3.7
2	D	126	LEU	3.7
2	J	115	VAL	3.6
1	I	16	GLY	3.6
2	D	119	TYR	3.6
2	J	24	TYR	3.6
1	I	15	ILE	3.6
2	D	7	ALA	3.5
2	D	5	ALA	3.5
2	B	126	LEU	3.4
2	B	173	ILE	3.4
1	C	277	CYS	3.4
2	D	35	ALA	3.4
2	D	27	SER	3.4
2	B	2	LEU	3.4
2	J	145	ASP	3.4
2	J	21	TRP	3.4
2	B	122	VAL	3.4
2	D	136	GLY	3.3
2	J	124	LEU	3.3
2	D	143	LYS	3.2
2	D	36	ALA	3.2
1	C	14	CYS	3.2
2	J	168	LEU	3.2
1	C	16	GLY	3.2
1	C	79	PHE	3.1
2	D	28	ASN	3.1
2	D	22	TYR	3.1
1	A	80	ILE	3.1
1	C	12	GLN	3.1
2	D	133	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	319	GLY	3.1
2	D	159	TYR	3.1
2	B	6	ILE	3.1
2	D	144	CYS	3.0
2	D	173	ILE	3.0
2	J	159	TYR	3.0
2	J	12	GLY	3.0
2	J	14	TRP	2.9
2	J	126	LEU	2.9
2	D	169	LYS	2.9
2	D	142	HIS	2.9
2	D	23	GLY	2.9
2	D	118	LEU	2.9
2	D	21	TRP	2.9
1	C	11	ASP	2.9
2	D	162	TYR	2.9
2	B	1	GLY	2.8
2	D	125	GLN	2.8
1	C	15	ILE	2.8
2	D	157	TYR	2.8
2	D	145	ASP	2.8
1	I	263	GLY	2.8
2	J	141	TYR	2.8
2	D	123	ARG	2.8
2	J	144	CYS	2.8
2	J	148	CYS	2.7
2	D	134	GLY	2.7
2	J	134	GLY	2.7
1	C	321	ARG	2.7
2	D	120	ASP	2.7
2	B	140	PHE	2.7
2	D	34	TYR	2.7
2	J	119	TYR	2.7
1	I	76	CYS	2.7
2	D	124	LEU	2.7
2	D	168	LEU	2.7
2	D	129	ASN	2.7
2	J	35	ALA	2.7
2	B	9	PHE	2.6
2	B	4	GLY	2.6
2	D	8	GLY	2.6
2	J	17	MET	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	J	22	TYR	2.6
2	J	30	GLN	2.6
2	D	12	GLY	2.6
2	J	138	PHE	2.6
1	C	80	ILE	2.6
2	B	143	LYS	2.5
1	I	42	ILE	2.5
2	B	174	SER	2.5
2	D	29	GLU	2.5
1	A	10	GLY	2.5
2	D	131	LYS	2.5
2	B	141	TYR	2.5
1	C	324	PRO	2.5
2	J	1	GLY	2.5
1	I	26	VAL	2.5
2	D	48	VAL	2.5
1	A	324	PRO	2.5
2	D	128	ASP	2.4
2	B	23	GLY	2.4
1	I	79	PHE	2.4
2	B	168	LEU	2.4
2	B	131	LYS	2.4
1	I	19	ALA	2.4
1	C	82	VAL	2.4
1	I	324	PRO	2.4
2	B	144	CYS	2.4
2	B	157	TYR	2.4
2	J	130	ALA	2.4
2	J	34	TYR	2.3
2	J	162	TYR	2.3
1	A	64	CYS	2.3
1	A	277	CYS	2.3
2	D	139	GLU	2.3
2	D	20	GLY	2.3
1	A	305	CYS	2.3
2	D	110	PHE	2.3
2	D	163	SER	2.3
2	J	133	LEU	2.3
2	D	18	VAL	2.3
2	D	112	ASP	2.3
2	D	146	ASN	2.2
2	D	115	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	127	ARG	2.2
2	J	18	VAL	2.2
2	J	122	VAL	2.2
2	J	152	VAL	2.2
2	J	170	ARG	2.2
1	I	64	CYS	2.2
2	D	148	CYS	2.2
2	D	32	SER	2.2
2	D	40	SER	2.2
2	D	31	GLY	2.2
2	J	8	GLY	2.2
2	J	13	GLY	2.2
2	D	149	MET	2.2
2	B	10	ILE	2.2
1	C	320	LEU	2.2
2	D	99	LEU	2.2
1	C	17	TYR	2.2
1	C	18	HIS	2.2
2	J	164	GLU	2.1
2	D	135	ASN	2.1
2	J	146	ASN	2.1
2	D	24	TYR	2.1
2	D	17	MET	2.1
1	C	173	ARG	2.1
1	I	277	CYS	2.1
2	J	166	ALA	2.1
1	I	14	CYS	2.1
1	I	262	LYS	2.1
2	D	137	CYS	2.1
1	I	314	LEU	2.1
1	I	34	VAL	2.0
1	A	16	GLY	2.0
2	B	13	GLY	2.0
2	D	13	GLY	2.0
2	J	23	GLY	2.0
2	D	121	LYS	2.0
2	J	25	HIS	2.0
2	J	163	SER	2.0
2	J	129	ASN	2.0
1	I	292	MET	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)

SUGAR-RSR INFOmissingINFO

6.4 Ligands (i)

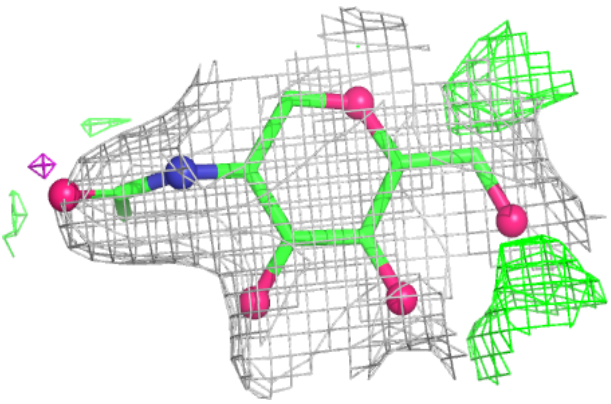
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

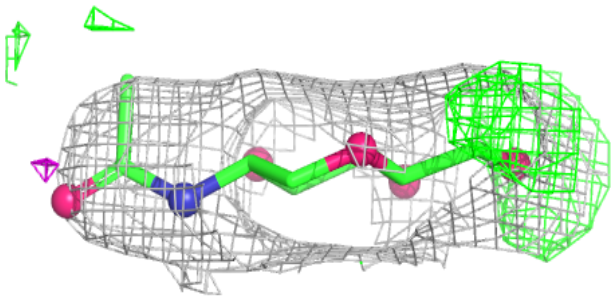
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	A	401	14/15	0.78	0.13	71,75,91,91	0
6	NAG	I	401	14/15	0.86	0.09	61,71,85,90	0

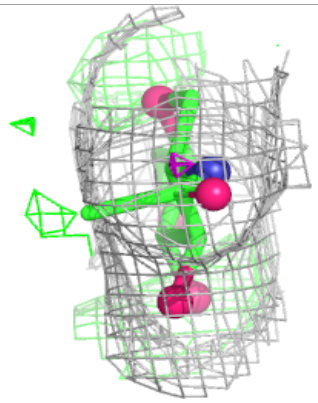
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAG A 401:

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

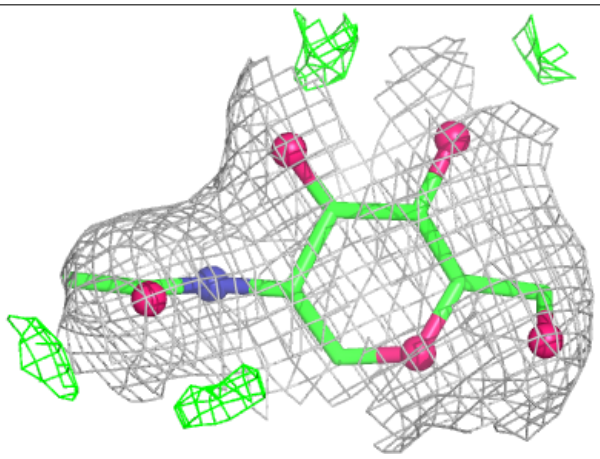


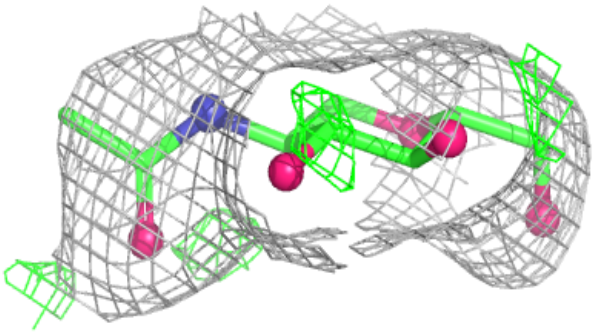


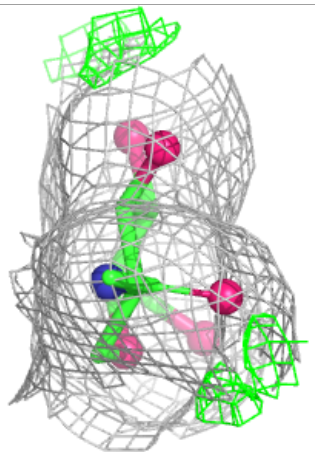


Electron density around NAG I 401:

$2mF_o$-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.