



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:00 PM UTC

PDB ID : 8X28 / pdb_00008x28
Title : Crystal structure of H5 hemagglutinin from human-infecting H5N8 influenza virus
Authors : Jin, X.Y.; Han, P.; Song, H.; Qi, J.X.
Deposited on : 2023-11-09
Resolution : 3.19 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

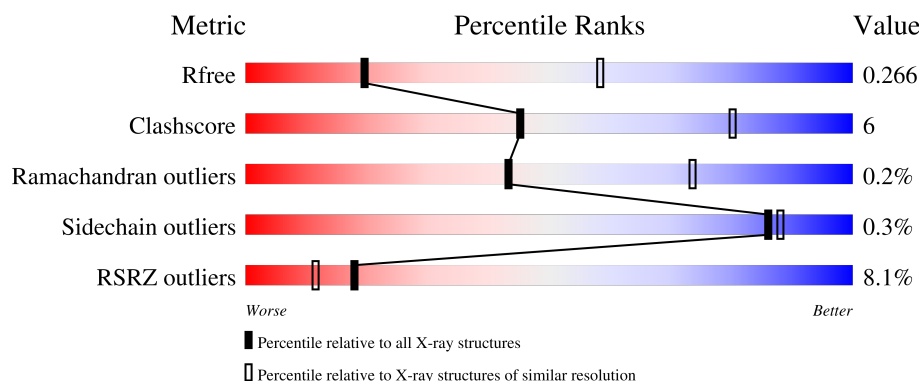
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	506	
1	B	506	
1	C	506	
1	D	506	
1	E	506	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	506	11% 82% 14%

2 Entry composition [i](#)

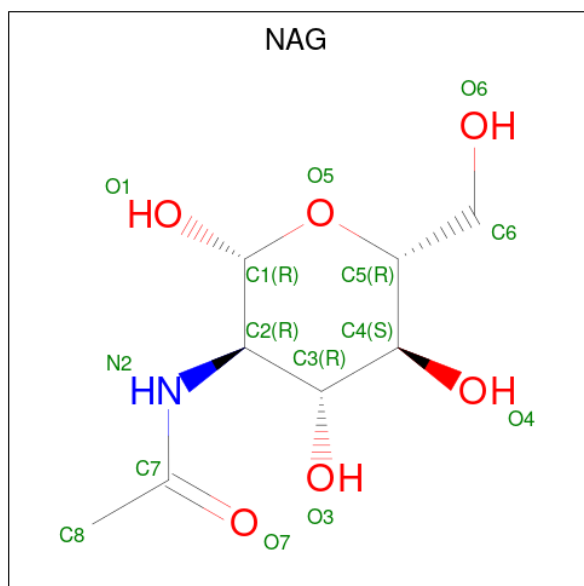
There are 2 unique types of molecules in this entry. The entry contains 23525 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	0	0
			3883	2441	676	744	22			
1	C	484	Total	C	N	O	S	0	0	0
			3878	2438	675	743	22			
1	D	484	Total	C	N	O	S	0	0	0
			3878	2438	675	743	22			
1	B	491	Total	C	N	O	S	0	0	0
			3923	2469	682	750	22			
1	E	485	Total	C	N	O	S	0	0	0
			3883	2441	676	744	22			
1	F	485	Total	C	N	O	S	0	0	0
			3884	2442	676	744	22			

- 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).

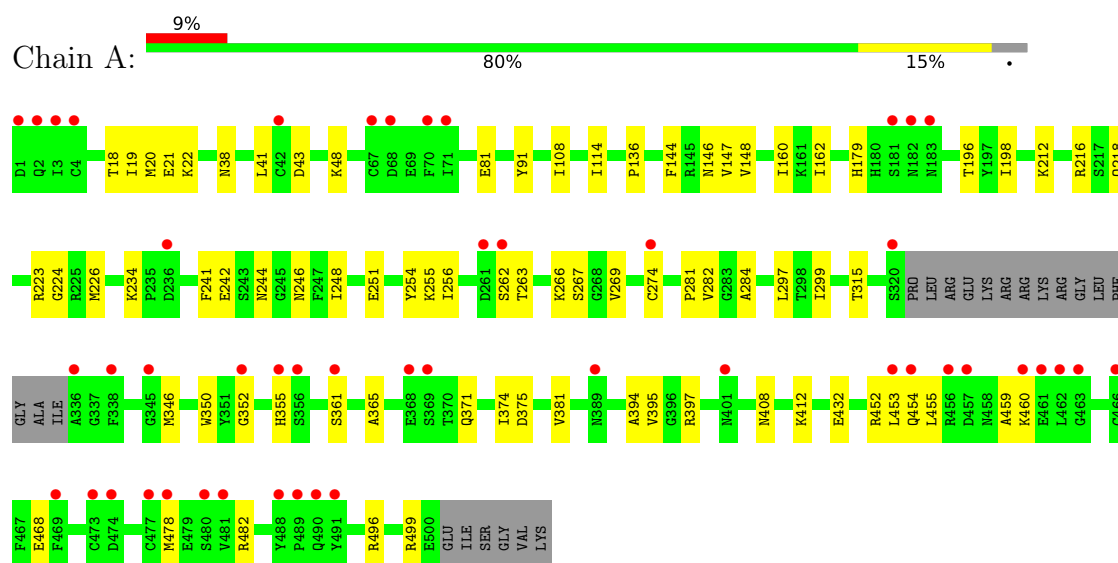


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1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

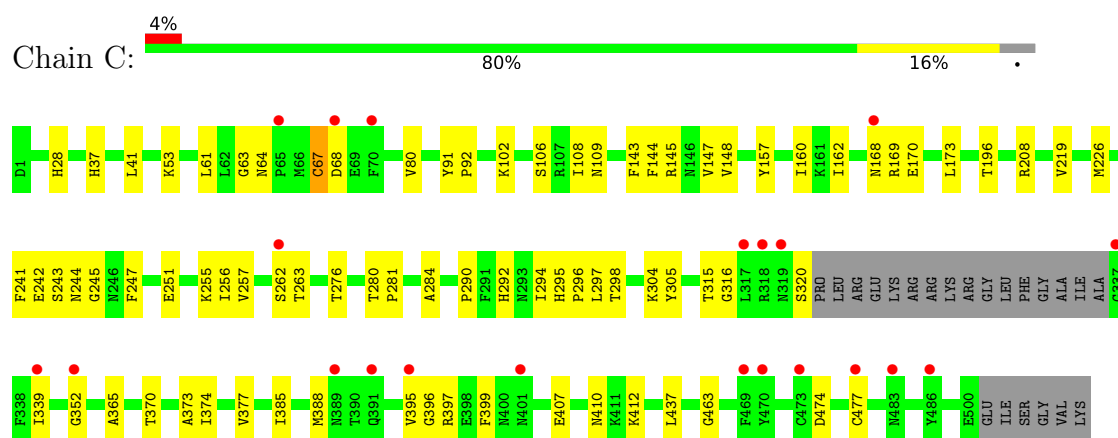
3 Residue-property plots [i](#)

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.

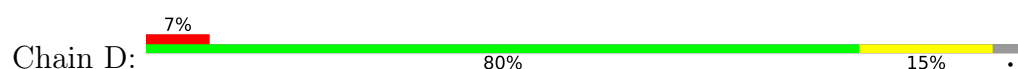
• Molecule 1: Hemagglutinin

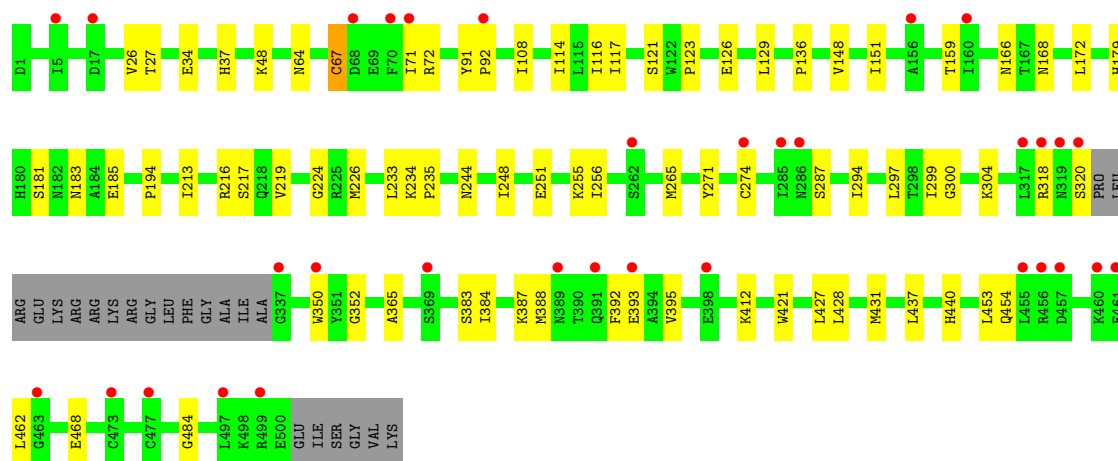


• Molecule 1: Hemagglutinin

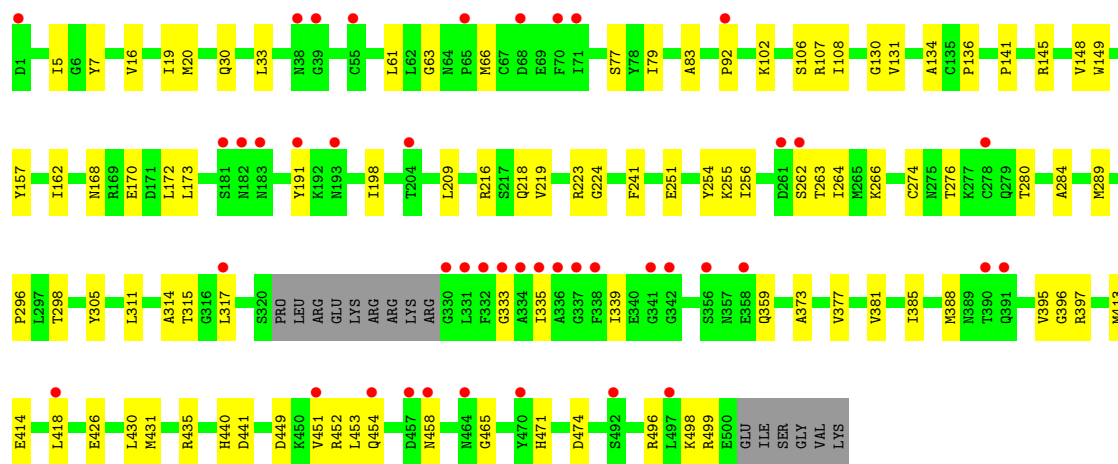
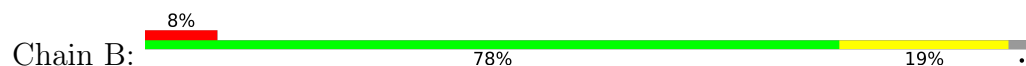


• Molecule 1: Hemagglutinin

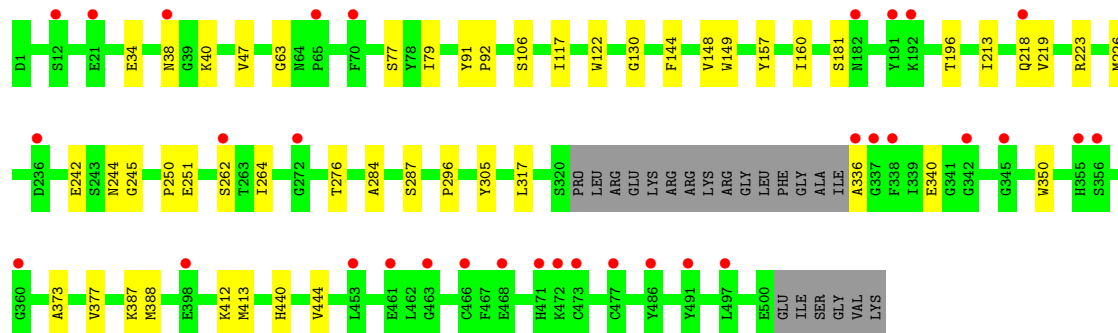
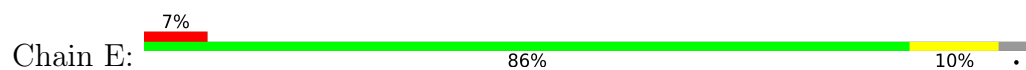




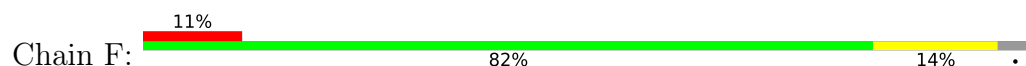
• Molecule 1: Hemagglutinin

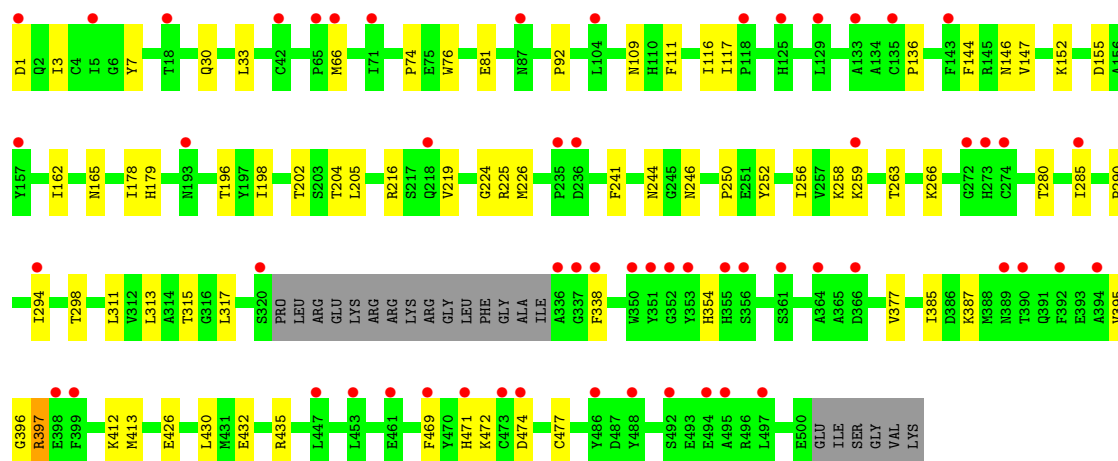


• Molecule 1: Hemagglutinin



• Molecule 1: Hemagglutinin





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.93Å 267.38Å 131.19Å 90.00° 99.46° 90.00°	Depositor
Resolution (Å)	32.04 – 3.19 32.04 – 3.19	Depositor EDS
% Data completeness (in resolution range)	99.6 (32.04-3.19) 88.0 (32.04-3.19)	Depositor EDS
R_{merge}	0.35	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.79 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.242 , 0.259 0.251 , 0.266	Depositor DCC
R_{free} test set	1999 reflections (2.43%)	wwPDB-VP
Wilson B-factor (Å ²)	48.2	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 59.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	23525	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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: NAG

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	0.17	0/3972	0.41	0/5379
1	B	0.12	0/4013	0.34	0/5434
1	C	0.16	0/3967	0.40	0/5372
1	D	0.14	0/3967	0.35	0/5372
1	E	0.12	0/3972	0.32	0/5379
1	F	0.17	0/3973	0.39	0/5381
All	All	0.15	0/23864	0.37	0/32317

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 [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	3883	0	3738	50	0
1	B	3923	0	3779	61	0
1	C	3878	0	3732	51	0
1	D	3878	0	3733	50	0
1	E	3883	0	3738	31	0
1	F	3884	0	3742	50	0
2	A	28	0	26	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	42	0	39	0	0
2	C	42	0	39	0	0
2	D	28	0	26	0	0
2	E	28	0	26	0	0
2	F	28	0	26	0	0
All	All	23525	0	22644	273	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 6.

All (273) 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:E:47:VAL:HG23	1:E:77:SER:HB3	1.62	0.81
1:B:397:ARG:HH22	1:F:412:LYS:HB2	1.47	0.78
1:A:41:LEU:HG	1:A:269:VAL:HG23	1.68	0.75
1:A:412:LYS:HG3	1:C:397:ARG:HH21	1.52	0.74
1:B:263:THR:HG21	1:B:396:GLY:H	1.54	0.73
1:B:7:TYR:HB2	1:B:317:LEU:HD13	1.71	0.72
1:C:64:ASN:HB3	1:C:67:CYS:HB2	1.71	0.72
1:E:276:THR:HG21	1:E:284:ALA:HB1	1.74	0.70
1:F:263:THR:HG21	1:F:396:GLY:H	1.56	0.69
1:B:276:THR:HG21	1:B:284:ALA:HB1	1.75	0.69
1:B:333:GLY:HA3	1:B:441:ASP:HB3	1.75	0.68
1:B:216:ARG:HH21	1:B:224:GLY:HA2	1.58	0.68
1:C:61:LEU:HD21	1:C:173:LEU:HD21	1.76	0.67
1:D:320:SER:HB3	1:D:437:LEU:HD13	1.77	0.67
1:F:469:PHE:HB3	1:F:471:HIS:O	1.94	0.67
1:A:452:ARG:HG2	1:A:453:LEU:H	1.60	0.66
1:B:395:VAL:HG22	1:F:412:LYS:HE2	1.77	0.66
1:A:216:ARG:HH21	1:A:224:GLY:HA2	1.60	0.65
1:E:79:ILE:HB	1:E:264:ILE:HD13	1.79	0.64
1:C:280:THR:HG22	1:C:298:THR:HG22	1.79	0.64
1:F:109:ASN:HB2	1:F:258:LYS:HB2	1.81	0.62
1:A:148:VAL:HG13	1:A:251:GLU:HB2	1.81	0.62
1:C:263:THR:HG21	1:C:396:GLY:H	1.63	0.62
1:D:71:ILE:HG22	1:D:72:ARG:HG2	1.80	0.62
1:F:432:GLU:HA	1:F:435:ARG:HD2	1.82	0.61
1:F:216:ARG:HH21	1:F:224:GLY:HA2	1.65	0.61
1:E:218:GLN:HE21	1:E:223:ARG:HH11	1.49	0.61
1:E:148:VAL:HG23	1:E:251:GLU:HB2	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:LYS:HB3	1:A:468:GLU:HB3	1.82	0.60
1:A:397:ARG:NH2	1:D:412:LYS:HG3	2.17	0.60
1:C:315:THR:HA	1:C:377:VAL:HG11	1.83	0.59
1:D:64:ASN:HB3	1:D:67:CYS:HB2	1.84	0.59
1:B:92:PRO:HB3	1:B:219:VAL:HG13	1.83	0.59
1:D:26:VAL:HA	1:D:318:ARG:HB3	1.83	0.59
1:C:276:THR:HG21	1:C:284:ALA:HB1	1.84	0.58
1:D:159:THR:HG22	1:D:244:ASN:HB3	1.86	0.58
1:B:5:ILE:HD11	1:B:451:VAL:HG21	1.86	0.58
1:C:162:ILE:HG22	1:C:241:PHE:HB2	1.86	0.57
1:A:397:ARG:HH22	1:D:412:LYS:HG3	1.69	0.57
1:B:280:THR:HG22	1:B:298:THR:HG22	1.86	0.57
1:F:33:LEU:HB2	1:F:311:LEU:HB2	1.86	0.57
1:C:196:THR:HG22	1:C:244:ASN:HB3	1.86	0.56
1:F:315:THR:HA	1:F:377:VAL:HG11	1.87	0.56
1:D:114:ILE:HG21	1:D:255:LYS:HE3	1.88	0.56
1:A:408:ASN:OD1	1:C:395:VAL:HG21	2.06	0.56
1:C:320:SER:HA	1:C:437:LEU:HD13	1.87	0.56
1:B:452:ARG:C	1:B:454:GLN:H	2.14	0.56
1:B:16:VAL:HG21	1:B:314:ALA:HB2	1.87	0.55
1:F:7:TYR:HB2	1:F:317:LEU:HD13	1.88	0.55
1:D:108:ILE:HD12	1:D:256:ILE:HG23	1.88	0.55
1:C:68:ASP:OD2	1:C:145:ARG:HG3	2.06	0.55
1:A:218:GLN:HB3	1:A:223:ARG:HG2	1.88	0.55
1:A:394:ALA:HA	1:D:412:LYS:HE3	1.88	0.55
1:D:166:ASN:HB2	1:D:233:LEU:HD23	1.89	0.54
1:D:216:ARG:HH21	1:D:224:GLY:HA2	1.71	0.54
1:A:108:ILE:HD12	1:A:256:ILE:HG23	1.89	0.54
1:A:299:ILE:HG23	1:A:395:VAL:HG12	1.90	0.54
1:D:234:LYS:HD3	1:D:235:PRO:HD3	1.90	0.54
1:F:162:ILE:HG22	1:F:241:PHE:HB2	1.89	0.54
1:A:263:THR:HB	1:A:395:VAL:HB	1.90	0.54
1:C:109:ASN:HB3	1:C:257:VAL:HG23	1.90	0.54
1:A:19:ILE:HG23	1:A:20:MET:HG3	1.90	0.54
1:E:336:ALA:HB3	1:E:340:GLU:HG3	1.90	0.54
1:D:462:LEU:HD21	1:D:468:GLU:HB2	1.90	0.53
1:A:371:GLN:HA	1:A:374:ILE:HG12	1.90	0.53
1:B:162:ILE:HG23	1:B:241:PHE:HB2	1.91	0.53
1:E:63:GLY:O	1:E:144:PHE:HD1	1.92	0.53
1:A:160:ILE:O	1:A:242:GLU:HA	2.08	0.53
1:F:1:ASP:HB2	1:F:472:LYS:HG2	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:VAL:HG23	1:C:251:GLU:HB2	1.91	0.53
1:D:37:HIS:HB3	1:D:294:ILE:HD13	1.89	0.53
1:F:280:THR:HG22	1:F:298:THR:HG22	1.91	0.53
1:A:81:GLU:O	1:A:266:LYS:HA	2.09	0.52
1:B:61:LEU:HD21	1:B:173:LEU:HD21	1.92	0.52
1:A:455:LEU:HD13	1:A:459:ALA:HB3	1.91	0.52
1:C:168:ASN:HB3	1:C:255:LYS:HE2	1.90	0.52
1:D:27:THR:HG23	1:D:318:ARG:HB2	1.92	0.52
1:C:91:TYR:CD1	1:C:226:MET:HG3	2.45	0.52
1:D:454:GLN:HE22	1:D:484:GLY:HA2	1.74	0.52
1:B:452:ARG:HG2	1:B:453:LEU:H	1.74	0.52
1:C:399:PHE:HB2	1:C:407:GLU:HG3	1.92	0.51
1:B:106:SER:HB2	1:B:262:SER:O	2.10	0.51
1:D:92:PRO:HB3	1:D:219:VAL:HG13	1.91	0.51
1:C:28:HIS:H	1:C:316:GLY:HA3	1.76	0.51
1:C:463:GLY:HA2	1:D:453:LEU:HD13	1.93	0.51
1:F:81:GLU:O	1:F:266:LYS:HA	2.10	0.51
1:F:290:PRO:HG3	1:F:385:ILE:HA	1.92	0.50
1:C:160:ILE:O	1:C:242:GLU:HA	2.10	0.50
1:B:414:GLU:O	1:B:418:LEU:HG	2.10	0.50
1:B:102:LYS:HE2	1:B:264:ILE:HG13	1.94	0.50
1:B:77:SER:HA	1:B:107:ARG:HD3	1.92	0.50
1:D:48:LYS:HE2	1:D:271:TYR:CE2	2.46	0.50
1:B:296:PRO:HG3	1:B:305:TYR:CE2	2.47	0.50
1:A:355:HIS:O	1:A:361:SER:HA	2.12	0.50
1:F:202:THR:HG23	1:F:204:THR:H	1.76	0.50
1:F:3:ILE:HB	1:F:469:PHE:CZ	2.47	0.49
1:C:397:ARG:HH11	1:C:410:ASN:HD21	1.58	0.49
1:D:181:SER:HB2	1:D:213:ILE:HG12	1.93	0.49
1:D:383:SER:O	1:D:387:LYS:HB2	2.12	0.49
1:B:311:LEU:HD21	1:B:426:GLU:HG2	1.93	0.49
1:A:38:ASN:ND2	1:A:284:ALA:HB3	2.28	0.49
1:D:183:ASN:ND2	1:D:185:GLU:HB3	2.28	0.49
1:A:38:ASN:HD21	1:A:284:ALA:HB3	1.76	0.49
1:A:91:TYR:CD1	1:A:226:MET:HG3	2.48	0.49
1:D:91:TYR:CD1	1:D:226:MET:HG3	2.48	0.49
1:A:452:ARG:C	1:A:454:GLN:H	2.21	0.48
1:D:265:MET:HE3	1:D:299:ILE:HD12	1.94	0.48
1:C:169:ARG:O	1:C:169:ARG:HG2	2.13	0.48
1:B:458:ASN:HB3	1:B:471:HIS:CD2	2.48	0.48
1:F:258:LYS:HG3	1:F:259:LYS:H	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ILE:HG21	1:A:255:LYS:HE3	1.94	0.48
1:A:212:LYS:HD3	1:C:208:ARG:HB2	1.96	0.48
1:D:148:VAL:HG23	1:D:251:GLU:HB2	1.95	0.48
1:E:440:HIS:O	1:E:444:VAL:HG23	2.14	0.48
1:D:121:SER:C	1:D:123:PRO:HD3	2.38	0.48
1:C:144:PHE:HB2	1:C:147:VAL:HG12	1.95	0.47
1:D:388:MET:HE1	1:D:421:TRP:CH2	2.49	0.47
1:B:198:ILE:HB	1:B:209:LEU:HB2	1.96	0.47
1:A:315:THR:HG22	1:A:381:VAL:HG21	1.96	0.47
1:D:34:GLU:HG2	1:D:287:SER:HB2	1.95	0.47
1:B:435:ARG:HE	1:F:435:ARG:NH2	2.13	0.47
1:E:157:TYR:CZ	1:E:245:GLY:HA2	2.50	0.47
1:B:30:GLN:HE21	1:B:289:MET:HE1	1.80	0.47
1:F:395:VAL:HG23	1:F:396:GLY:O	2.14	0.47
1:E:317:LEU:HD11	1:E:350:TRP:CG	2.50	0.47
1:F:111:PHE:HE1	1:F:256:ILE:HG12	1.79	0.47
1:C:281:PRO:HD3	1:C:297:LEU:O	2.15	0.47
1:C:373:ALA:O	1:C:377:VAL:HG23	2.14	0.47
1:C:292:HIS:ND1	1:C:294:ILE:HG22	2.30	0.46
1:D:352:GLY:HA3	1:D:365:ALA:HA	1.97	0.46
1:B:317:LEU:HD23	1:B:440:HIS:CG	2.51	0.46
1:F:3:ILE:HB	1:F:469:PHE:CE2	2.50	0.46
1:C:37:HIS:HB3	1:C:294:ILE:CD1	2.45	0.46
1:C:63:GLY:O	1:C:144:PHE:HA	2.16	0.46
1:A:352:GLY:HA3	1:A:365:ALA:HA	1.97	0.46
1:D:126:GLU:HB3	1:D:151:ILE:HG13	1.98	0.46
1:A:281:PRO:HD3	1:A:297:LEU:O	2.15	0.46
1:E:38:ASN:CG	1:E:284:ALA:HB3	2.41	0.46
1:B:131:VAL:CG1	1:B:141:PRO:HB2	2.45	0.46
1:F:196:THR:HA	1:F:244:ASN:OD1	2.16	0.46
1:E:106:SER:HB2	1:E:262:SER:O	2.16	0.46
1:B:108:ILE:HD12	1:B:256:ILE:HG23	1.98	0.46
1:B:381:VAL:O	1:B:385:ILE:HG13	2.16	0.46
1:F:144:PHE:HB2	1:F:147:VAL:HG12	1.98	0.46
1:A:412:LYS:CG	1:C:397:ARG:HH21	2.27	0.45
1:B:449:ASP:HB3	1:F:338:PHE:CZ	2.50	0.45
1:F:387:LYS:HD3	1:F:387:LYS:HA	1.77	0.45
1:D:72:ARG:HA	1:D:72:ARG:HD3	1.59	0.45
1:D:395:VAL:HG12	1:D:395:VAL:O	2.17	0.45
1:E:34:GLU:HG2	1:E:287:SER:HB2	1.98	0.45
1:F:397:ARG:HA	1:F:397:ARG:HD3	1.67	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:285:ILE:HG12	1:F:294:ILE:HD12	1.99	0.45
1:A:452:ARG:HG2	1:A:453:LEU:N	2.28	0.45
1:F:92:PRO:HB3	1:F:219:VAL:HB	1.98	0.45
1:A:198:ILE:HD11	1:A:246:ASN:O	2.17	0.45
1:C:68:ASP:CG	1:C:145:ARG:HG3	2.42	0.45
1:C:102:LYS:O	1:C:106:SER:HB3	2.16	0.45
1:D:304:LYS:HG2	1:D:421:TRP:CE2	2.52	0.45
1:A:43:ASP:OD1	1:A:48:LYS:HA	2.17	0.45
1:B:458:ASN:HB3	1:B:471:HIS:HD2	1.81	0.45
1:A:196:THR:HA	1:A:244:ASN:ND2	2.32	0.45
1:C:294:ILE:HG23	1:C:295:HIS:H	1.82	0.44
1:E:160:ILE:O	1:E:242:GLU:HA	2.16	0.44
1:B:339:ILE:HG12	1:B:465:GLY:HA3	1.99	0.44
1:E:181:SER:HB2	1:E:213:ILE:HG12	1.99	0.44
1:F:196:THR:HG21	1:F:246:ASN:HB2	2.00	0.44
1:A:374:ILE:HG13	1:A:375:ASP:N	2.33	0.44
2:A:601:NAG:O7	1:D:217:SER:HB2	2.17	0.44
1:B:148:VAL:HG23	1:B:251:GLU:HB2	1.98	0.44
1:B:496:ARG:HA	1:B:499:ARG:HD3	1.99	0.44
1:C:474:ASP:N	1:C:477:CYS:HB3	2.32	0.44
1:B:218:GLN:HB3	1:B:223:ARG:HG2	1.98	0.44
1:F:116:ILE:HD11	1:F:250:PRO:HB2	1.98	0.44
1:F:426:GLU:O	1:F:430:LEU:HG	2.18	0.44
1:C:92:PRO:HB3	1:C:219:VAL:HB	2.00	0.44
1:B:131:VAL:HG12	1:B:141:PRO:HB2	1.99	0.44
1:B:19:ILE:HG23	1:B:20:MET:HG3	2.00	0.44
1:A:179:HIS:HB2	1:A:248:ILE:HD11	2.00	0.44
1:C:412:LYS:HD3	1:D:393:GLU:HB3	2.00	0.44
1:F:117:ILE:HD12	1:F:250:PRO:HG2	2.00	0.44
1:A:262:SER:HA	1:A:395:VAL:HG11	1.99	0.43
1:C:106:SER:HB2	1:C:262:SER:O	2.18	0.43
1:B:430:LEU:HD11	1:E:387:LYS:HE3	2.00	0.43
1:E:412:LYS:HE3	1:F:413:MET:HE1	2.00	0.43
1:B:413:MET:HB2	1:E:413:MET:HE2	1.99	0.43
1:E:388:MET:HE3	1:E:388:MET:HB3	1.84	0.43
1:A:350:TRP:CH2	1:A:374:ILE:HG22	2.54	0.43
1:C:168:ASN:C	1:C:170:GLU:H	2.24	0.43
1:D:427:LEU:O	1:D:431:MET:HG3	2.19	0.43
1:E:296:PRO:HG3	1:E:305:TYR:CE2	2.54	0.43
1:F:202:THR:H	1:F:205:LEU:HB3	1.83	0.43
1:B:296:PRO:HG3	1:B:305:TYR:CZ	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:LEU:O	1:B:254:TYR:OH	2.32	0.43
1:B:359:GLN:HE21	1:B:474:ASP:HB2	1.84	0.43
1:B:388:MET:HE2	1:B:388:MET:HB2	1.89	0.43
1:C:53:LYS:HE3	1:C:53:LYS:HB2	1.94	0.43
1:E:196:THR:HA	1:E:244:ASN:ND2	2.34	0.43
1:A:267:SER:OG	1:A:269:VAL:HG22	2.19	0.43
1:C:370:THR:O	1:C:374:ILE:HG23	2.19	0.43
1:B:168:ASN:C	1:B:170:GLU:H	2.26	0.43
1:E:412:LYS:HD3	1:F:395:VAL:HG22	2.01	0.43
1:F:474:ASP:O	1:F:477:CYS:HB2	2.19	0.43
1:D:114:ILE:HD11	1:D:172:LEU:HD21	2.01	0.42
1:B:172:LEU:HD23	1:B:255:LYS:HA	2.01	0.42
1:C:304:LYS:HE3	1:C:388:MET:HE2	2.01	0.42
1:D:183:ASN:HD22	1:D:185:GLU:HB3	1.83	0.42
1:E:122:TRP:HZ3	1:E:160:ILE:HG21	1.84	0.42
1:A:18:THR:OG1	1:A:21:GLU:HB2	2.19	0.42
1:B:157:TYR:CE2	1:B:191:TYR:HD2	2.37	0.42
1:E:40:LYS:HE3	1:E:40:LYS:HB2	1.85	0.42
1:F:179:HIS:CD2	1:F:226:MET:HE2	2.54	0.42
1:D:126:GLU:HG2	1:D:129:LEU:HD13	2.02	0.42
1:D:300:GLY:HA2	1:D:392:PHE:CD1	2.54	0.42
1:B:315:THR:HA	1:B:377:VAL:HG11	2.02	0.42
1:D:168:ASN:HB3	1:D:255:LYS:HE2	2.01	0.42
1:D:384:ILE:HG12	1:D:428:LEU:HD21	2.00	0.42
1:F:92:PRO:HB2	1:F:225:ARG:HE	1.83	0.42
1:F:202:THR:HG22	1:F:205:LEU:HB2	2.02	0.42
1:A:21:GLU:O	1:A:22:LYS:HD3	2.20	0.42
1:A:144:PHE:HB2	1:A:147:VAL:HG12	2.02	0.42
1:C:243:SER:OG	1:C:247:PHE:HB2	2.20	0.42
1:B:63:GLY:HA3	1:B:145:ARG:H	1.84	0.42
1:B:498:LYS:HD2	1:B:498:LYS:HA	1.64	0.42
1:F:146:ASN:HB3	1:F:252:TYR:HB2	2.00	0.42
1:F:152:LYS:HD2	1:F:155:ASP:HA	2.02	0.42
1:B:335:ILE:HG23	1:B:441:ASP:HA	2.02	0.42
1:B:431:MET:O	1:B:435:ARG:HD2	2.20	0.42
1:E:91:TYR:CD1	1:E:226:MET:HG3	2.54	0.42
1:F:66:MET:HE2	1:F:66:MET:HB3	1.97	0.42
1:C:296:PRO:HG3	1:C:305:TYR:CE2	2.55	0.42
1:C:339:ILE:O	1:C:339:ILE:HG22	2.20	0.42
1:F:178:ILE:HB	1:F:198:ILE:HD12	2.00	0.42
1:A:346:MET:SD	1:A:352:GLY:HA3	2.60	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:GLU:OE2	1:D:431:MET:HG2	2.20	0.41
1:D:304:LYS:HE3	1:D:388:MET:HE2	2.02	0.41
1:B:33:LEU:HB2	1:B:311:LEU:HB2	2.01	0.41
1:E:92:PRO:HB3	1:E:219:VAL:HB	2.02	0.41
1:E:373:ALA:O	1:E:377:VAL:HG23	2.19	0.41
1:A:496:ARG:HA	1:A:499:ARG:HB2	2.01	0.41
1:F:30:GLN:O	1:F:313:LEU:N	2.53	0.41
1:A:162:ILE:HG22	1:A:241:PHE:HB2	2.03	0.41
1:C:290:PRO:HG3	1:C:385:ILE:HA	2.02	0.41
1:B:83:ALA:HA	1:B:266:LYS:HD2	2.02	0.41
1:B:134:ALA:O	1:B:136:PRO:HD3	2.19	0.41
1:A:478:MET:O	1:A:482:ARG:HG3	2.20	0.41
1:C:157:TYR:CZ	1:C:245:GLY:HA2	2.56	0.41
1:D:116:ILE:HG13	1:D:117:ILE:N	2.35	0.41
1:B:66:MET:HE2	1:B:66:MET:HB3	1.89	0.41
1:E:412:LYS:HE2	1:F:397:ARG:NH2	2.36	0.41
1:D:350:TRP:CZ3	1:D:440:HIS:HE1	2.39	0.41
1:B:130:GLY:HA3	1:B:149:TRP:O	2.20	0.41
1:B:311:LEU:HD23	1:B:311:LEU:HA	1.89	0.41
1:E:196:THR:HA	1:E:244:ASN:HD21	1.85	0.41
1:F:3:ILE:HD12	1:F:354:HIS:O	2.20	0.41
1:F:315:THR:HG22	1:F:315:THR:O	2.21	0.41
1:B:373:ALA:O	1:B:377:VAL:HG23	2.21	0.41
1:A:234:LYS:HE3	1:A:234:LYS:HB3	1.83	0.40
1:C:41:LEU:HD13	1:C:80:VAL:HG11	2.03	0.40
1:C:108:ILE:HD12	1:C:256:ILE:HG23	2.03	0.40
1:C:352:GLY:HA3	1:C:365:ALA:HA	2.03	0.40
1:D:297:LEU:HD22	1:D:395:VAL:O	2.20	0.40
1:B:397:ARG:HH22	1:F:412:LYS:CB	2.27	0.40
1:E:130:GLY:HA3	1:E:149:TRP:HB3	2.03	0.40
1:A:146:ASN:ND2	1:A:254:TYR:OH	2.55	0.40
1:C:108:ILE:HD13	1:C:108:ILE:HA	1.92	0.40
1:C:143:PHE:CG	1:C:144:PHE:N	2.88	0.40
1:D:148:VAL:CG2	1:D:251:GLU:HB2	2.50	0.40
1:D:179:HIS:HB2	1:D:248:ILE:HD11	2.03	0.40
1:B:79:ILE:HB	1:B:264:ILE:HD13	2.03	0.40
1:B:452:ARG:O	1:B:453:LEU:HB2	2.20	0.40
1:F:76:TRP:HH2	1:F:111:PHE:CD2	2.40	0.40
1:E:117:ILE:HD12	1:E:250:PRO:HG2	2.03	0.40
1:A:267:SER:OG	1:A:281:PRO:O	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	481/506 (95%)	459 (95%)	21 (4%)	1 (0%)	43	73
1	B	487/506 (96%)	462 (95%)	25 (5%)	0	100	100
1	C	480/506 (95%)	455 (95%)	25 (5%)	0	100	100
1	D	480/506 (95%)	463 (96%)	15 (3%)	2 (0%)	30	62
1	E	481/506 (95%)	459 (95%)	22 (5%)	0	100	100
1	F	481/506 (95%)	452 (94%)	27 (6%)	2 (0%)	30	62
All	All	2890/3036 (95%)	2750 (95%)	135 (5%)	5 (0%)	43	73

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	136	PRO
1	A	136	PRO
1	F	136	PRO
1	F	74	PRO
1	D	194	PRO

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	428/445 (96%)	426 (100%)	2 (0%)	81	85
1	B	431/445 (97%)	430 (100%)	1 (0%)	87	89
1	C	428/445 (96%)	427 (100%)	1 (0%)	87	89

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	428/445 (96%)	426 (100%)	2 (0%)	81	85
1	E	427/445 (96%)	427 (100%)	0	100	100
1	F	428/445 (96%)	426 (100%)	2 (0%)	81	85
All	All	2570/2670 (96%)	2562 (100%)	8 (0%)	86	88

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	274	CYS
1	A	282	VAL
1	C	67	CYS
1	D	67	CYS
1	D	274	CYS
1	B	274	CYS
1	F	165	ASN
1	F	397	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	HIS
1	A	64	ASN
1	A	125	HIS
1	A	146	ASN
1	A	168	ASN
1	A	193	ASN
1	A	240	HIS
1	A	273	HIS
1	C	125	HIS
1	C	146	ASN
1	C	193	ASN
1	C	240	HIS
1	C	389	ASN
1	C	408	ASN
1	C	458	ASN
1	D	110	HIS
1	D	183	ASN
1	D	454	GLN
1	B	182	ASN
1	B	275	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	355	HIS
1	B	410	ASN
1	E	28	HIS
1	E	125	HIS
1	E	193	ASN
1	E	240	HIS
1	E	424	ASN
1	F	15	GLN
1	F	37	HIS
1	F	125	HIS
1	F	424	ASN
1	F	446	ASN

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](#)

14 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	F	602	1	14,14,15	2.03	5 (35%)	17,19,21	1.98	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	601	1	14,14,15	2.04	4 (28%)	17,19,21	2.58	5 (29%)
2	NAG	A	602	1	14,14,15	2.02	4 (28%)	17,19,21	1.11	1 (5%)
2	NAG	B	601	1	14,14,15	2.04	4 (28%)	17,19,21	1.13	2 (11%)
2	NAG	B	603	1	14,14,15	2.02	4 (28%)	17,19,21	1.11	1 (5%)
2	NAG	B	602	1	14,14,15	2.07	4 (28%)	17,19,21	1.09	2 (11%)
2	NAG	F	601	1	14,14,15	1.92	3 (21%)	17,19,21	2.49	3 (17%)
2	NAG	C	602	1	14,14,15	2.06	4 (28%)	17,19,21	1.09	1 (5%)
2	NAG	E	601	1	14,14,15	2.06	4 (28%)	17,19,21	1.10	2 (11%)
2	NAG	E	602	1	14,14,15	2.05	4 (28%)	17,19,21	1.07	2 (11%)
2	NAG	D	602	1	14,14,15	2.09	4 (28%)	17,19,21	1.21	3 (17%)
2	NAG	C	603	1	14,14,15	2.02	4 (28%)	17,19,21	1.14	1 (5%)
2	NAG	C	601	1	14,14,15	2.01	3 (21%)	17,19,21	0.98	1 (5%)
2	NAG	D	601	1	14,14,15	2.05	4 (28%)	17,19,21	1.21	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	F	602	1	-	0/6/23/26	0/1/1/1
2	NAG	A	601	1	-	3/6/23/26	0/1/1/1
2	NAG	A	602	1	-	0/6/23/26	0/1/1/1
2	NAG	B	601	1	-	0/6/23/26	0/1/1/1
2	NAG	B	603	1	-	0/6/23/26	0/1/1/1
2	NAG	B	602	1	-	3/6/23/26	0/1/1/1
2	NAG	F	601	1	-	1/6/23/26	0/1/1/1
2	NAG	C	602	1	-	0/6/23/26	0/1/1/1
2	NAG	E	601	1	-	0/6/23/26	0/1/1/1
2	NAG	E	602	1	-	0/6/23/26	0/1/1/1
2	NAG	D	602	1	-	0/6/23/26	0/1/1/1
2	NAG	C	603	1	-	0/6/23/26	0/1/1/1
2	NAG	C	601	1	-	0/6/23/26	0/1/1/1
2	NAG	D	601	1	-	1/6/23/26	0/1/1/1

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	602	NAG	O5-C1	4.74	1.51	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	602	NAG	O5-C1	4.69	1.51	1.43
2	B	602	NAG	O5-C1	4.69	1.51	1.43
2	A	601	NAG	O5-C1	4.67	1.51	1.43
2	D	601	NAG	O5-C1	4.61	1.51	1.43
2	E	601	NAG	O5-C1	4.59	1.51	1.43
2	E	602	NAG	O5-C1	4.57	1.51	1.43
2	F	602	NAG	O5-C1	4.53	1.51	1.43
2	A	602	NAG	O5-C1	4.49	1.51	1.43
2	B	601	NAG	O5-C1	4.43	1.51	1.43
2	C	603	NAG	O5-C1	4.42	1.51	1.43
2	C	601	NAG	O5-C1	4.41	1.51	1.43
2	B	603	NAG	O5-C1	4.34	1.51	1.43
2	F	601	NAG	C7-N2	3.91	1.47	1.34
2	D	601	NAG	C7-N2	3.90	1.46	1.34
2	B	603	NAG	C7-N2	3.89	1.46	1.34
2	B	601	NAG	C7-N2	3.88	1.46	1.34
2	E	602	NAG	C7-N2	3.85	1.46	1.34
2	C	601	NAG	C7-N2	3.85	1.46	1.34
2	A	602	NAG	C7-N2	3.84	1.46	1.34
2	C	603	NAG	C7-N2	3.84	1.46	1.34
2	E	601	NAG	C7-N2	3.82	1.46	1.34
2	F	601	NAG	O5-C1	3.81	1.50	1.43
2	B	602	NAG	C7-N2	3.81	1.46	1.34
2	D	602	NAG	C7-N2	3.80	1.46	1.34
2	C	602	NAG	C7-N2	3.78	1.46	1.34
2	A	601	NAG	C7-N2	3.70	1.46	1.34
2	F	602	NAG	C7-N2	3.59	1.45	1.34
2	F	601	NAG	C2-N2	2.79	1.50	1.46
2	E	601	NAG	C2-N2	2.58	1.50	1.46
2	B	603	NAG	C2-N2	2.55	1.50	1.46
2	B	601	NAG	C2-N2	2.53	1.50	1.46
2	A	602	NAG	C2-N2	2.52	1.50	1.46
2	C	603	NAG	C2-N2	2.52	1.50	1.46
2	C	601	NAG	C2-N2	2.50	1.50	1.46
2	F	602	NAG	C2-N2	2.48	1.50	1.46
2	E	602	NAG	C2-N2	2.48	1.50	1.46
2	D	602	NAG	C2-N2	2.47	1.50	1.46
2	D	601	NAG	C2-N2	2.44	1.50	1.46
2	B	602	NAG	C2-N2	2.44	1.50	1.46
2	C	602	NAG	C2-N2	2.44	1.50	1.46
2	B	601	NAG	O5-C5	2.40	1.48	1.43
2	F	602	NAG	O5-C5	2.38	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	602	NAG	O5-C5	2.35	1.48	1.43
2	C	602	NAG	O5-C5	2.34	1.48	1.43
2	D	602	NAG	O5-C5	2.33	1.48	1.43
2	B	602	NAG	O5-C5	2.32	1.47	1.43
2	A	602	NAG	O5-C5	2.30	1.47	1.43
2	B	603	NAG	O5-C5	2.28	1.47	1.43
2	C	603	NAG	O5-C5	2.22	1.47	1.43
2	D	601	NAG	O5-C5	2.19	1.47	1.43
2	E	601	NAG	O5-C5	2.17	1.47	1.43
2	A	601	NAG	O7-C7	-2.14	1.18	1.23
2	F	602	NAG	O7-C7	-2.03	1.18	1.23
2	A	601	NAG	C8-C7	2.02	1.54	1.50

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	601	NAG	C1-O5-C5	-7.35	102.33	112.19
2	F	602	NAG	C1-C2-N2	-5.87	101.18	110.43
2	A	601	NAG	C8-C7-N2	5.65	125.48	116.12
2	F	601	NAG	C1-C2-N2	-5.30	102.09	110.43
2	A	601	NAG	C4-C3-C2	5.25	118.71	111.02
2	A	601	NAG	O7-C7-N2	-5.18	112.83	121.98
2	F	602	NAG	C2-N2-C7	4.40	128.79	122.90
2	F	601	NAG	C2-N2-C7	3.72	127.89	122.90
2	A	601	NAG	C2-N2-C7	3.32	127.35	122.90
2	C	602	NAG	C1-O5-C5	2.76	115.89	112.19
2	B	602	NAG	C1-O5-C5	2.71	115.82	112.19
2	D	601	NAG	C1-O5-C5	2.40	115.40	112.19
2	D	602	NAG	C8-C7-N2	2.39	120.08	116.12
2	E	602	NAG	C8-C7-N2	2.39	120.07	116.12
2	F	602	NAG	C3-C4-C5	2.38	114.54	110.23
2	B	601	NAG	C8-C7-N2	2.37	120.04	116.12
2	E	602	NAG	C2-N2-C7	-2.35	119.75	122.90
2	C	601	NAG	C8-C7-N2	2.34	120.00	116.12
2	B	603	NAG	C8-C7-N2	2.34	120.00	116.12
2	D	602	NAG	C2-N2-C7	-2.33	119.78	122.90
2	B	601	NAG	C2-N2-C7	-2.31	119.80	122.90
2	A	602	NAG	C8-C7-N2	2.31	119.95	116.12
2	C	603	NAG	C8-C7-N2	2.28	119.91	116.12
2	E	601	NAG	C8-C7-N2	2.23	119.81	116.12
2	D	601	NAG	C8-C7-N2	2.19	119.76	116.12
2	B	602	NAG	C8-C7-N2	2.10	119.60	116.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	601	NAG	C1-O5-C5	2.06	114.95	112.19
2	D	602	NAG	C1-O5-C5	2.05	114.94	112.19
2	A	601	NAG	O3-C3-C2	2.01	113.58	109.40

There are no chirality outliers.

All (8) torsion outliers are listed below:

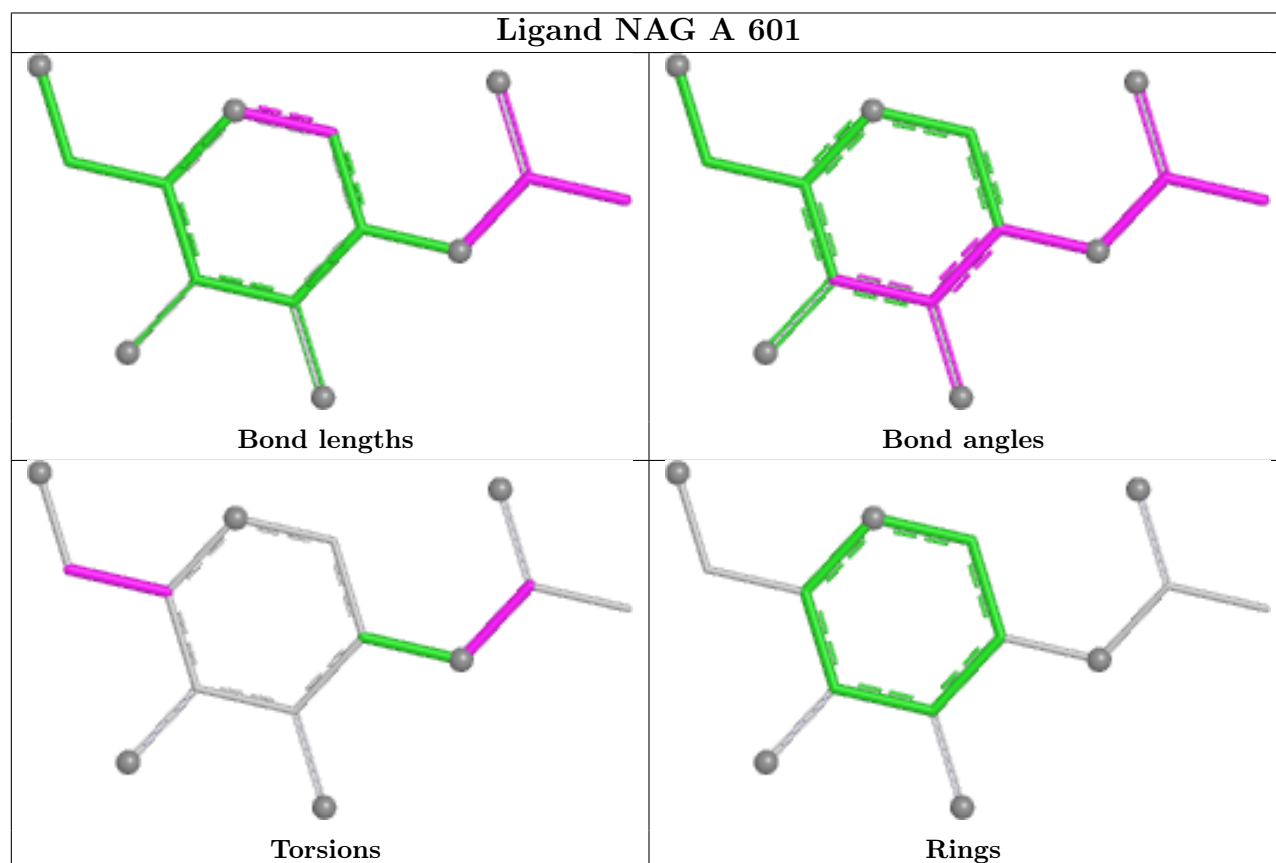
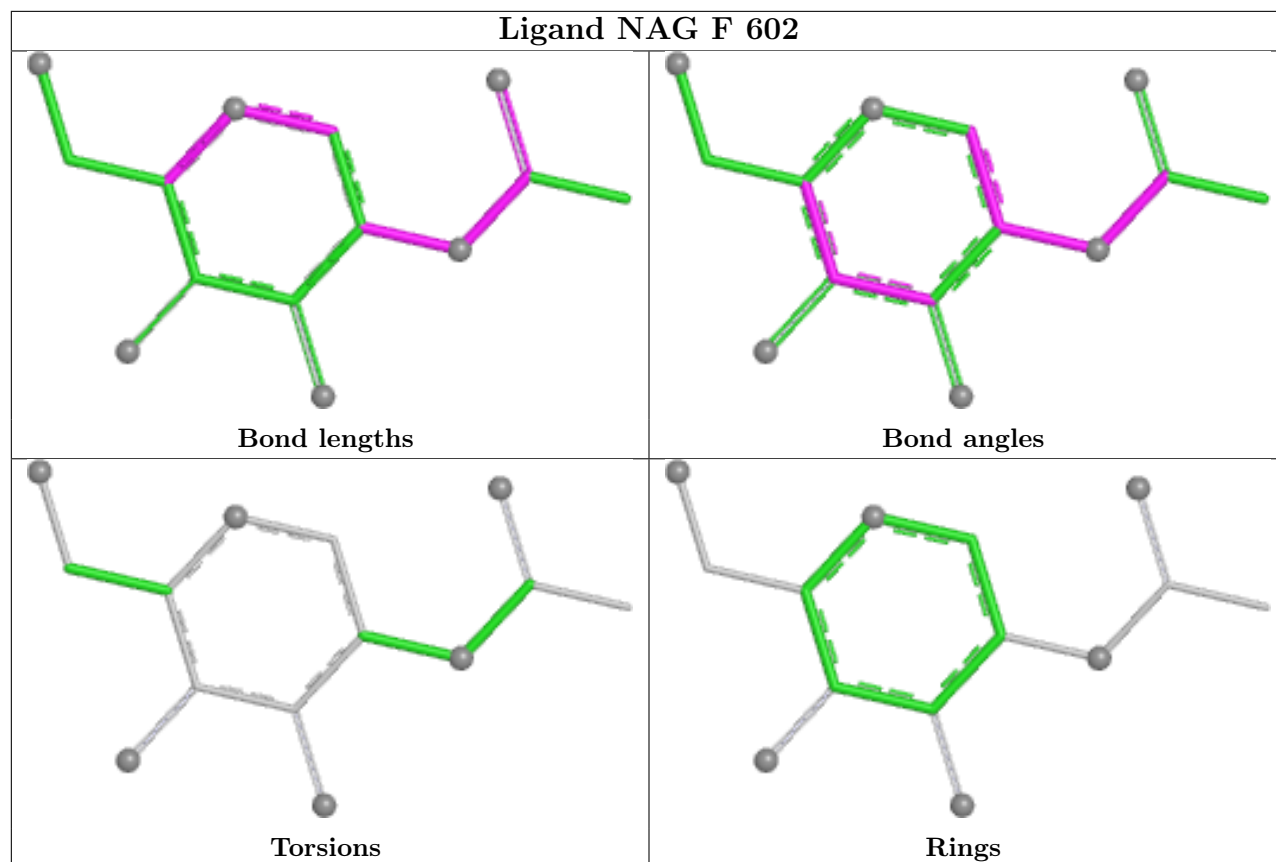
Mol	Chain	Res	Type	Atoms
2	F	601	NAG	C3-C2-N2-C7
2	A	601	NAG	C8-C7-N2-C2
2	A	601	NAG	O7-C7-N2-C2
2	B	602	NAG	C4-C5-C6-O6
2	D	601	NAG	O5-C5-C6-O6
2	A	601	NAG	O5-C5-C6-O6
2	B	602	NAG	O5-C5-C6-O6
2	B	602	NAG	C1-C2-N2-C7

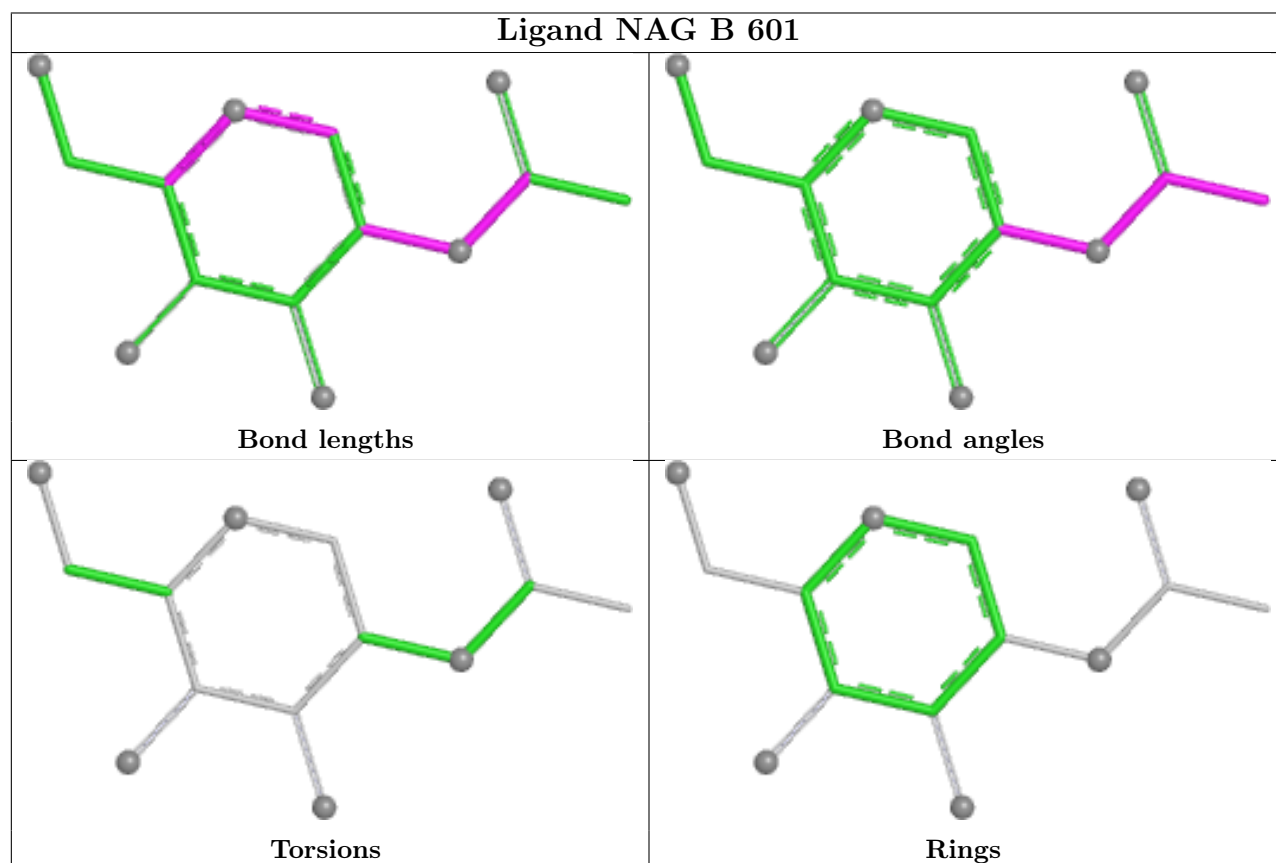
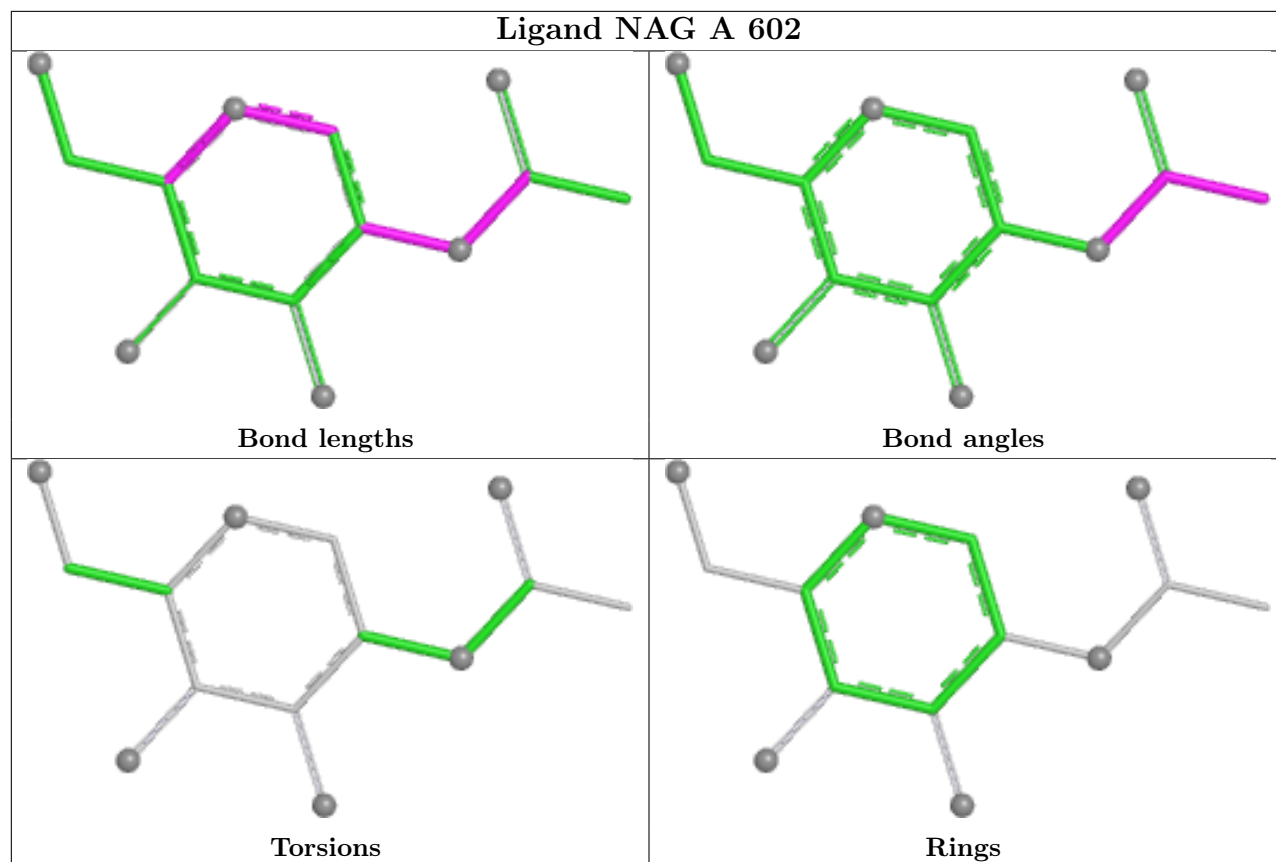
There are no ring outliers.

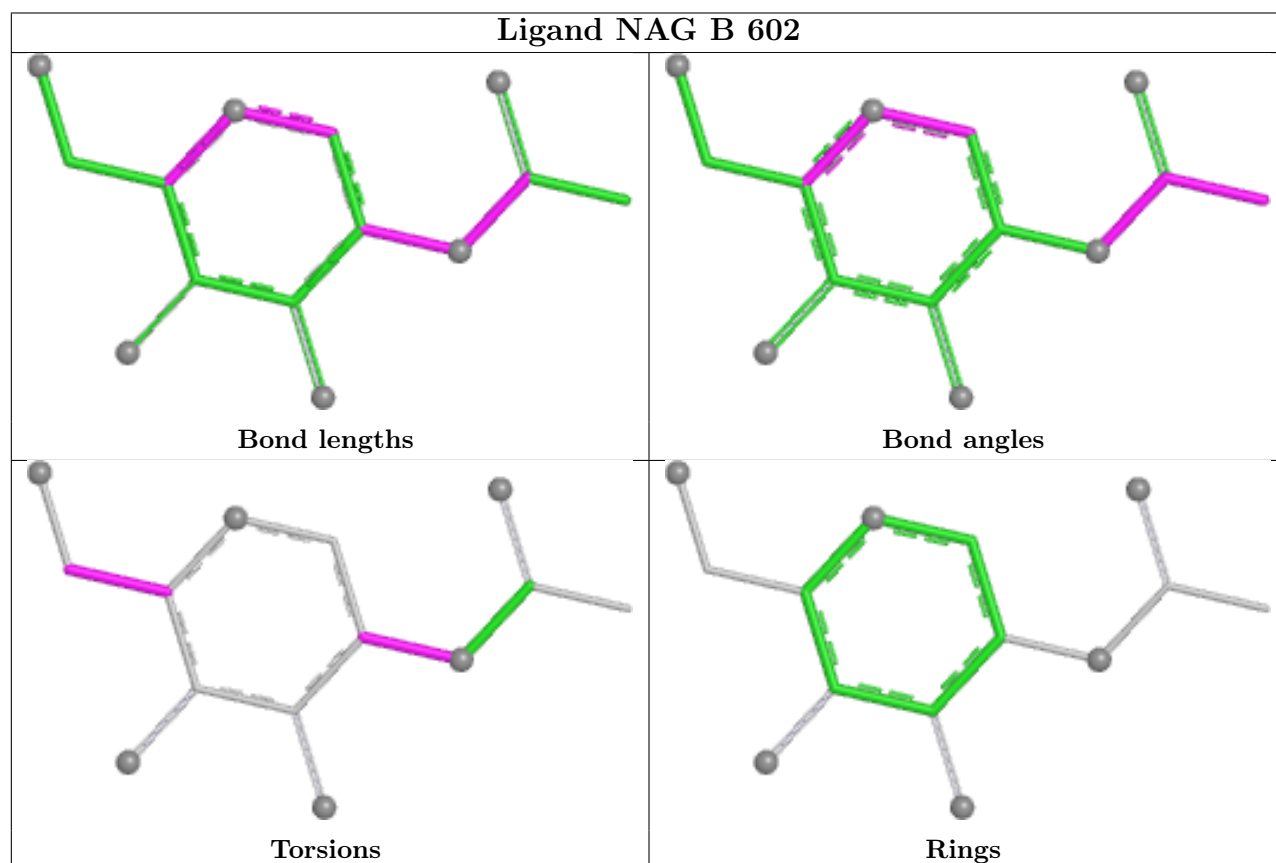
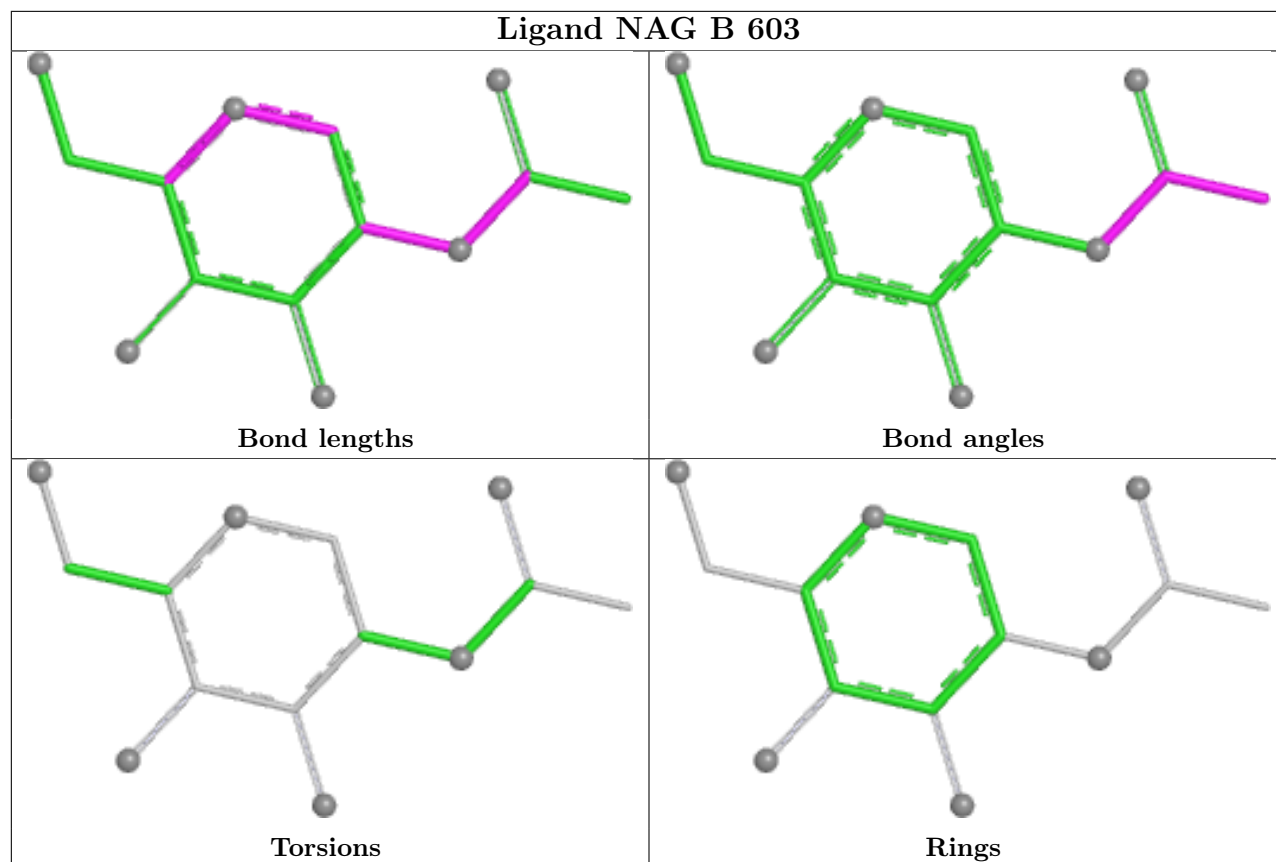
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	NAG	1	0

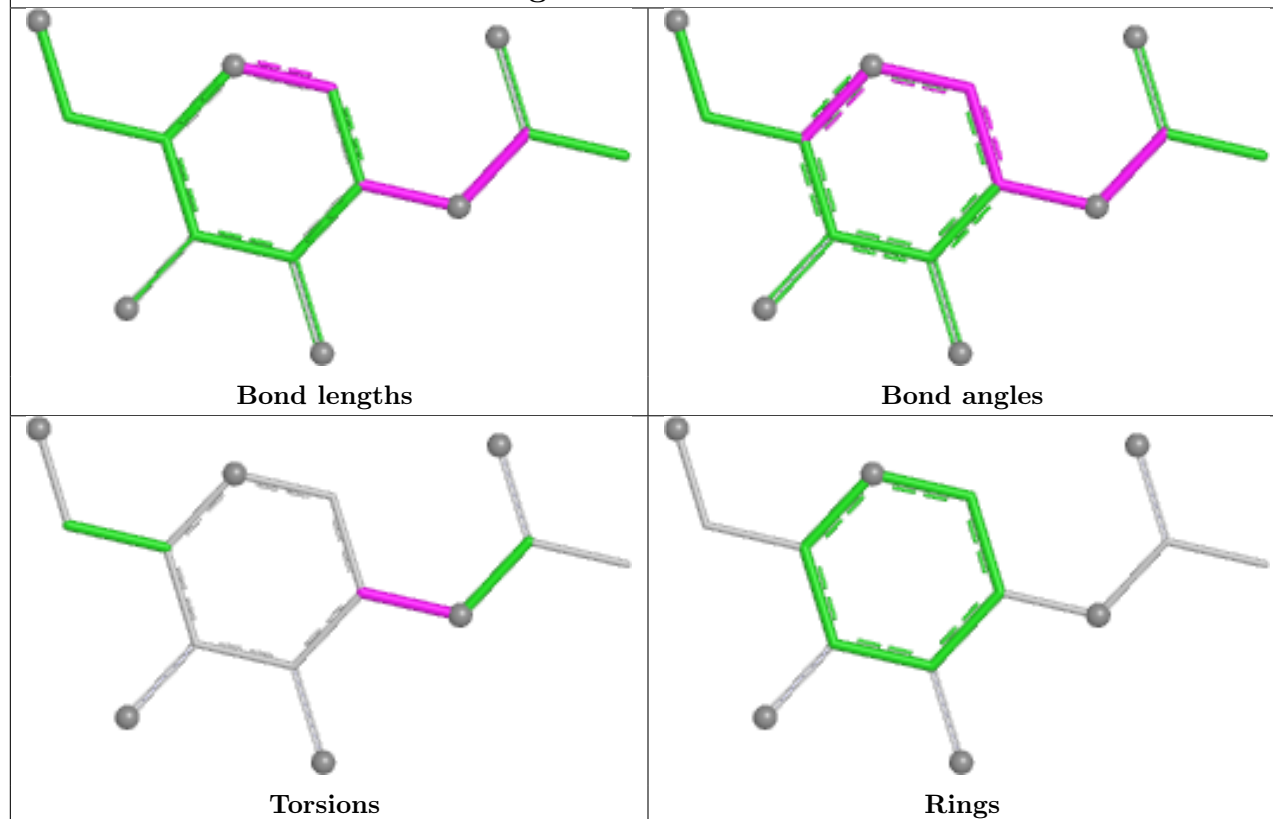
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



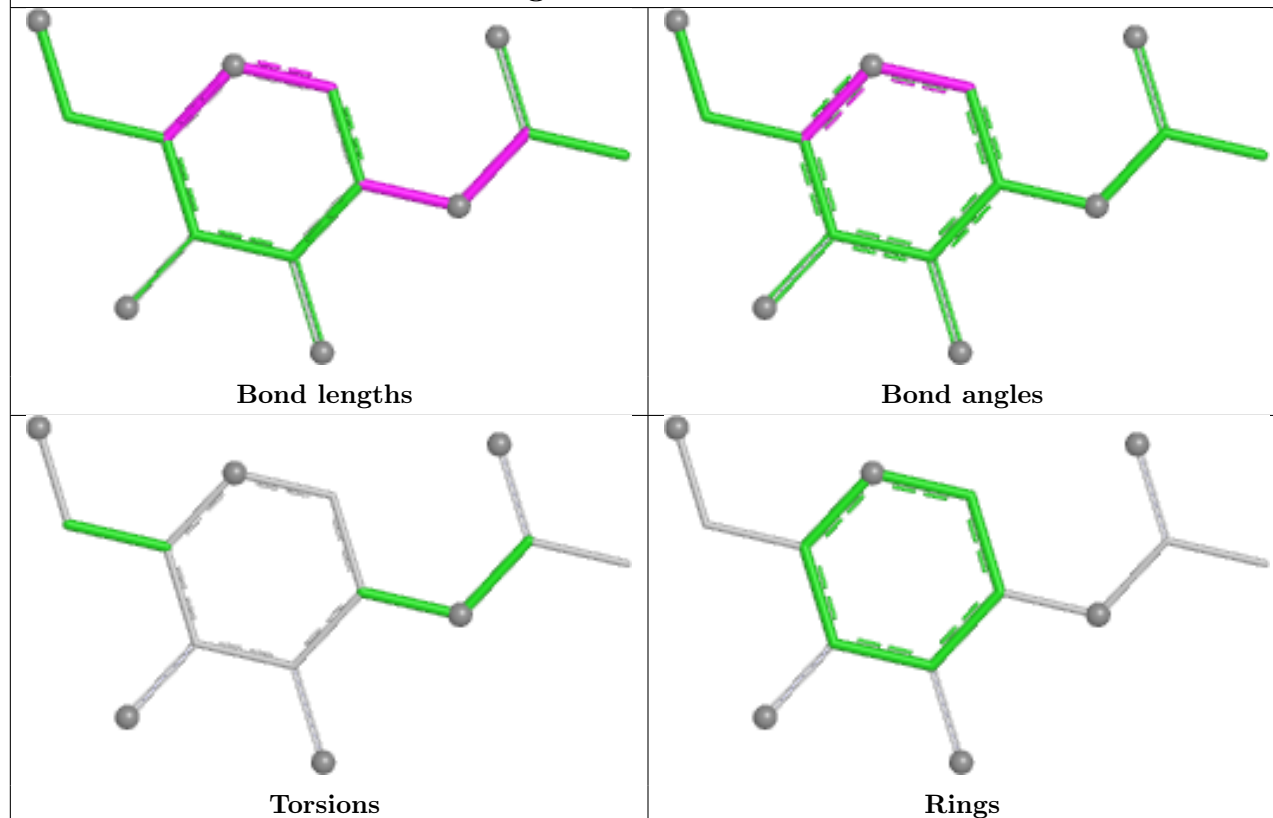


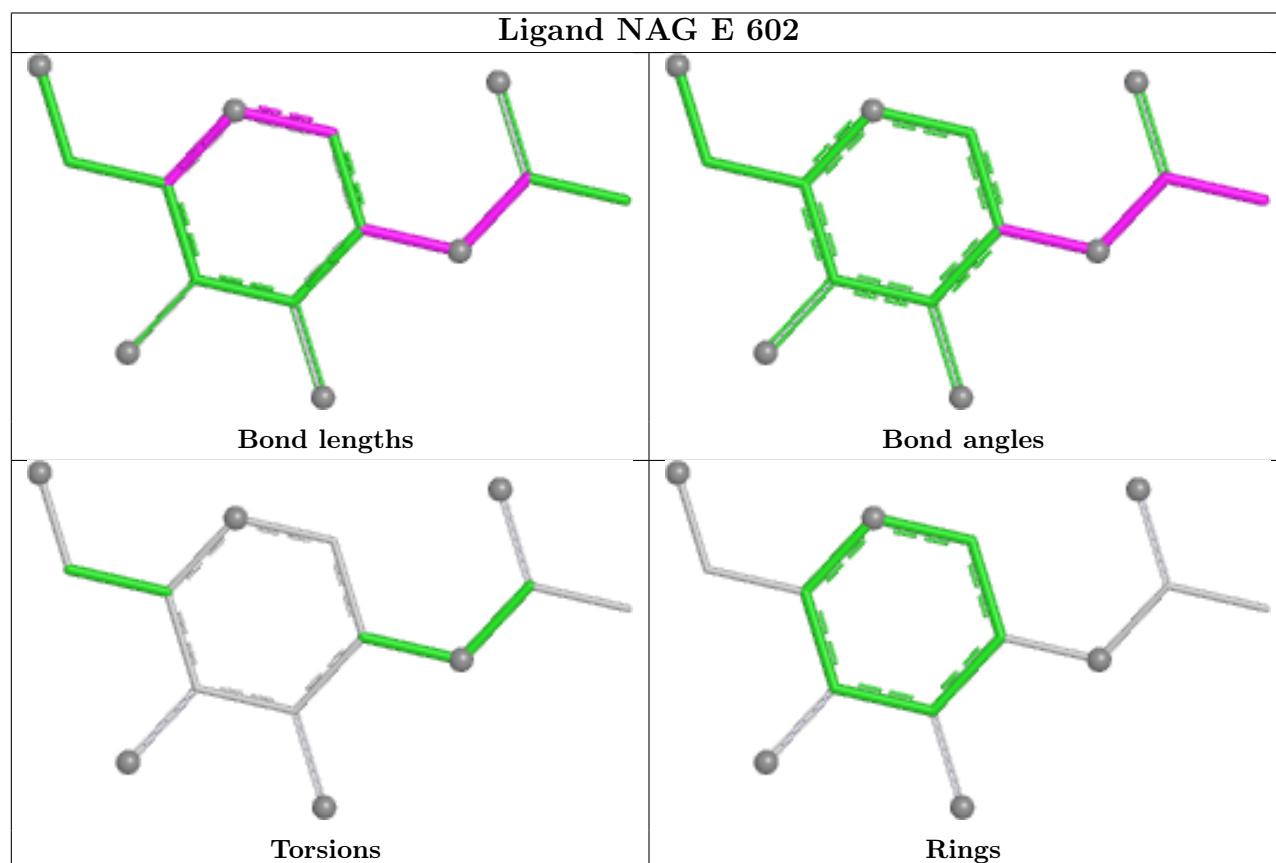
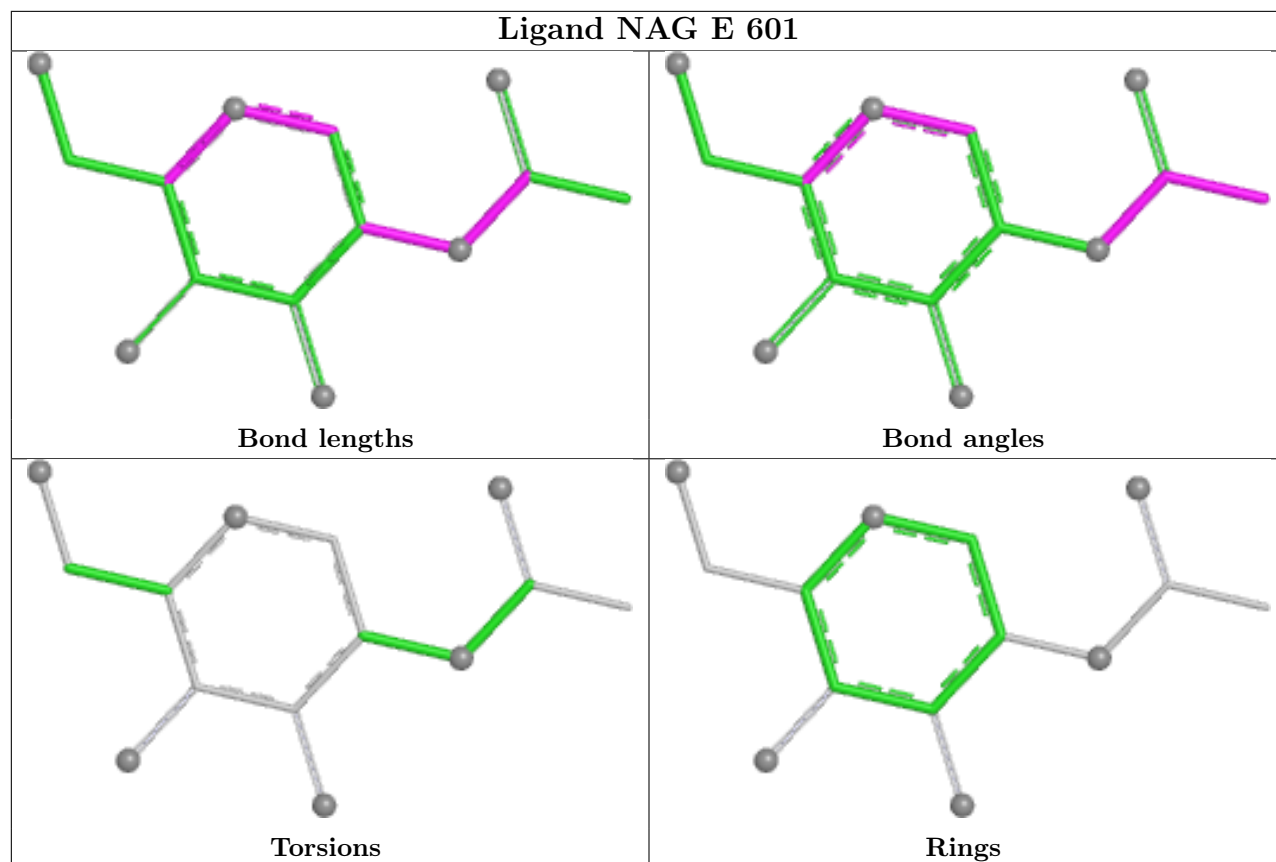


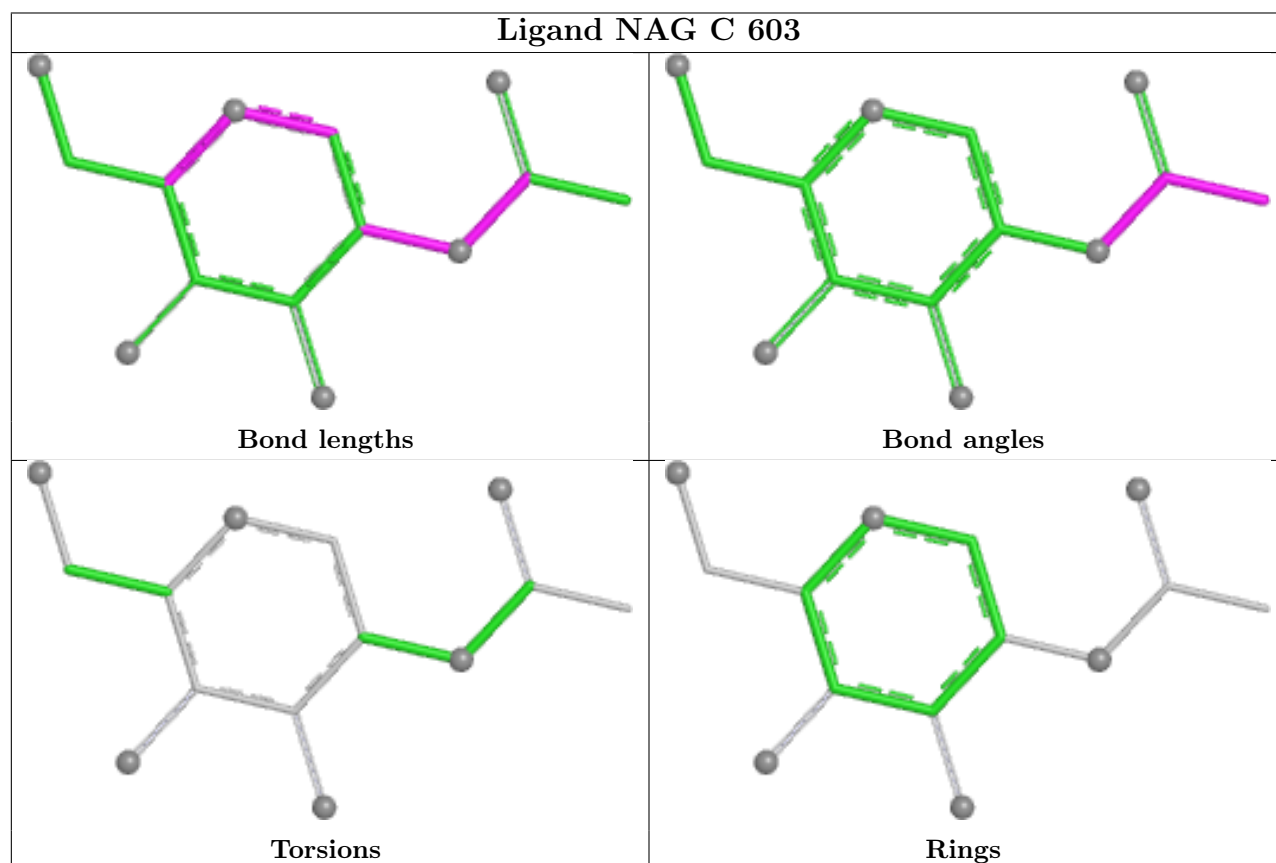
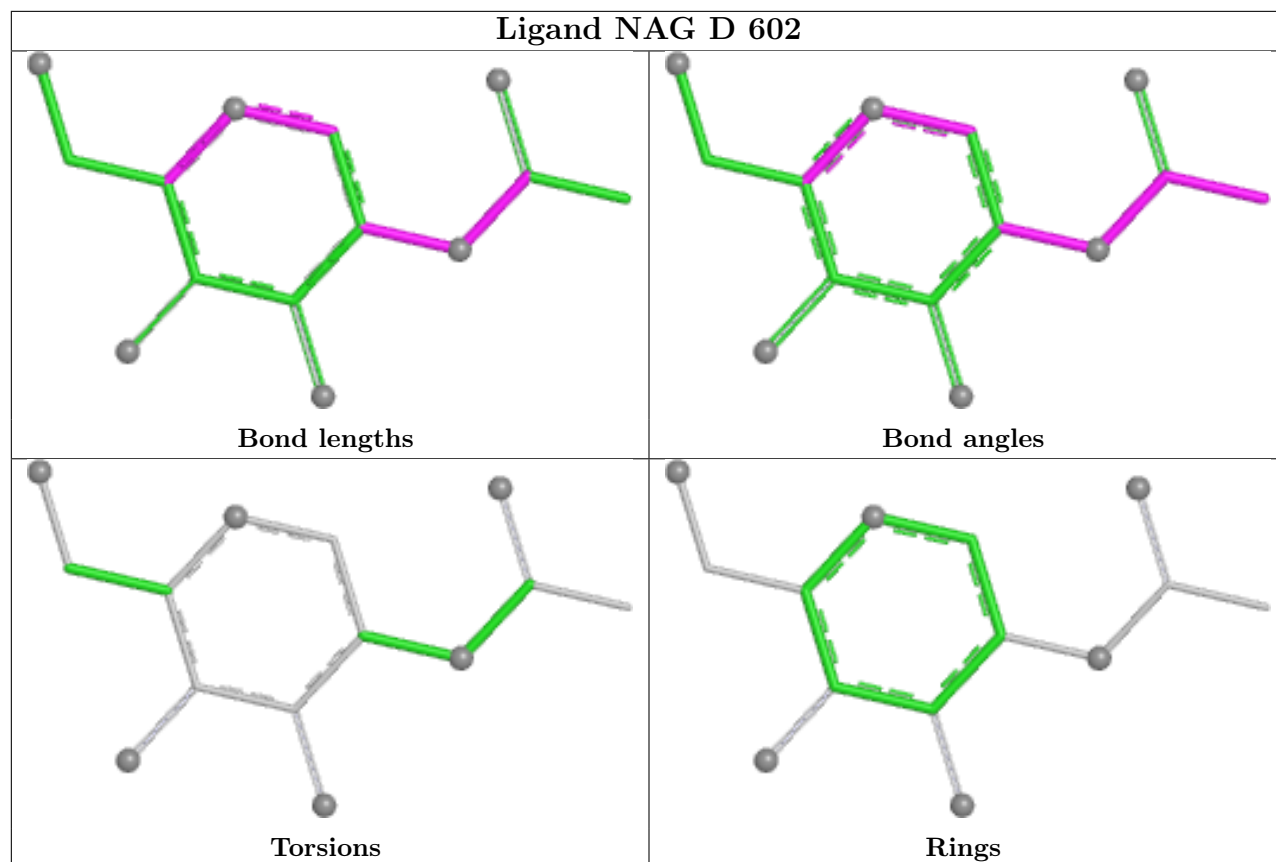
Ligand NAG F 601

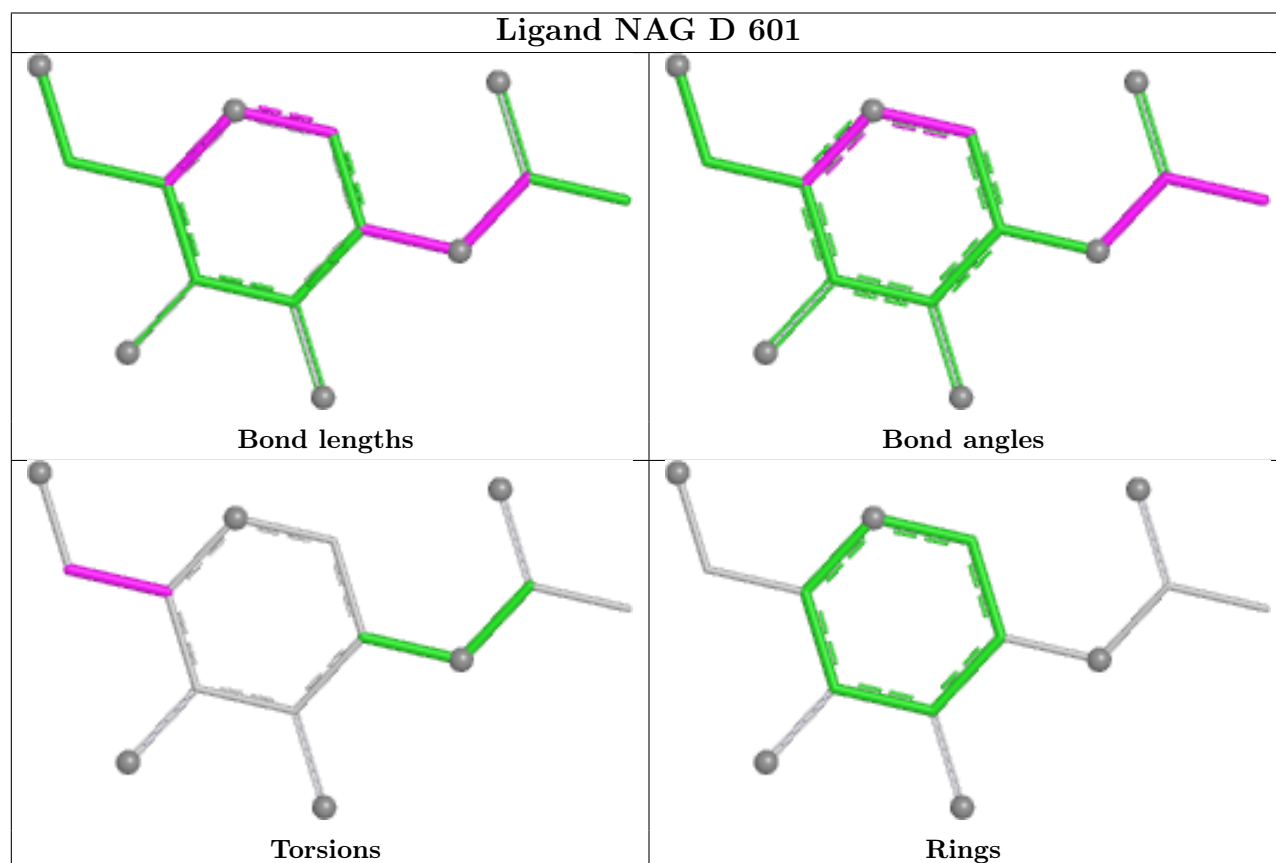
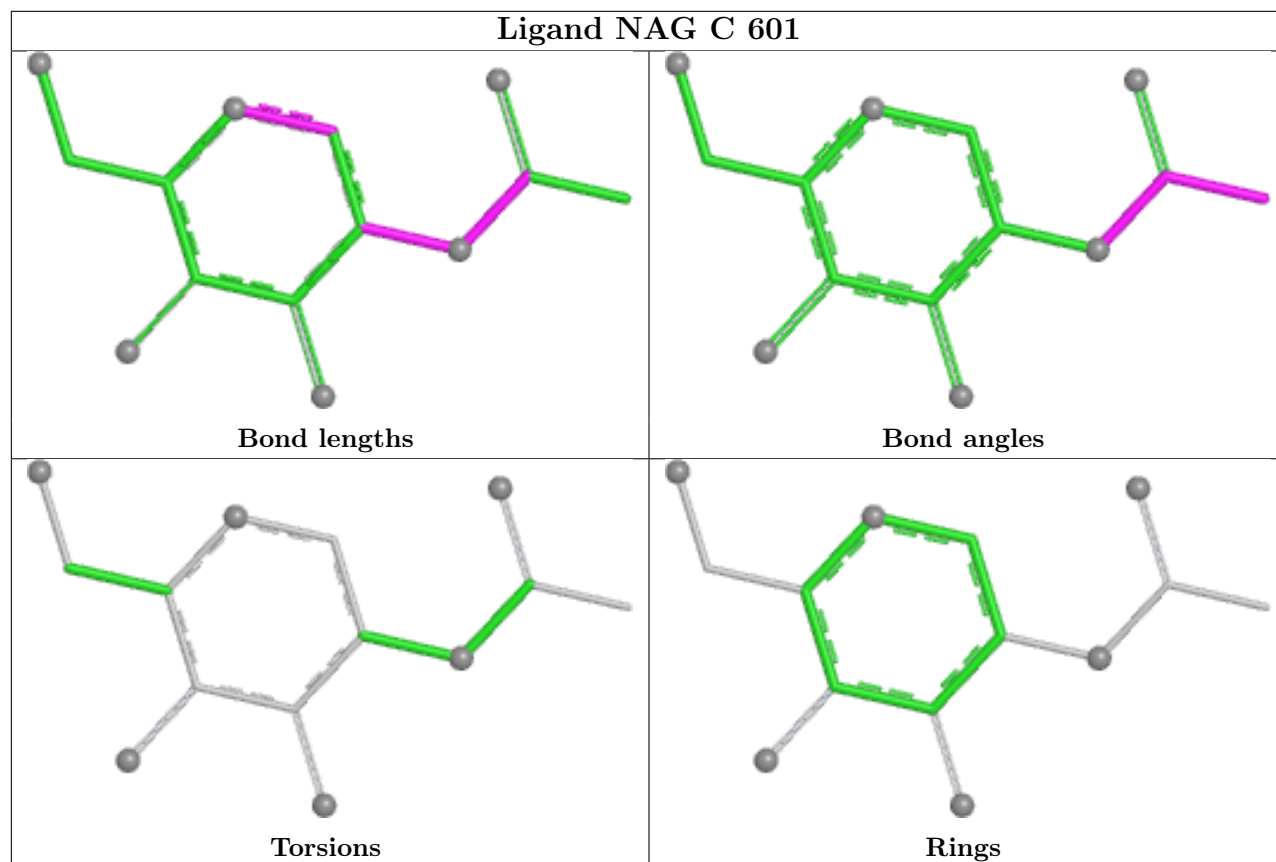


Ligand NAG C 602









5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	485/506 (95%)	0.78	48 (9%)	13 8	33, 63, 161, 195	0
1	B	491/506 (97%)	0.83	43 (8%)	15 10	39, 77, 131, 168	0
1	C	484/506 (95%)	0.49	21 (4%)	40 24	24, 50, 132, 148	0
1	D	484/506 (95%)	0.66	33 (6%)	23 15	32, 58, 142, 166	0
1	E	485/506 (95%)	0.70	33 (6%)	23 15	31, 62, 147, 164	0
1	F	485/506 (95%)	1.01	58 (11%)	9 6	43, 86, 164, 185	0
All	All	2914/3036 (95%)	0.74	236 (8%)	18 11	24, 68, 147, 195	0

All (236) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	352	GLY	5.1
1	B	335	ILE	4.9
1	A	477	CYS	4.9
1	B	331	LEU	4.7
1	E	338	PHE	4.7
1	B	332	PHE	4.7
1	F	497	LEU	4.7
1	F	473	CYS	4.6
1	B	336	ALA	4.6
1	F	66	MET	4.4
1	B	333	GLY	4.2
1	A	473	CYS	4.1
1	D	477	CYS	3.9
1	D	350	TRP	3.9
1	F	337	GLY	3.8
1	A	469	PHE	3.8
1	B	334	ALA	3.7
1	E	182	ASN	3.7
1	E	486	TYR	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	70	PHE	3.7
1	E	38	ASN	3.6
1	A	460	LYS	3.6
1	F	338	PHE	3.6
1	E	473	CYS	3.6
1	F	392	PHE	3.5
1	F	492	SER	3.5
1	B	38	ASN	3.4
1	A	71	ILE	3.4
1	D	320	SER	3.4
1	D	71	ILE	3.4
1	A	182	ASN	3.3
1	B	262	SER	3.3
1	B	356	SER	3.3
1	C	486	TYR	3.3
1	A	338	PHE	3.2
1	B	182	ASN	3.2
1	A	461	GLU	3.2
1	A	4	CYS	3.2
1	C	469	PHE	3.2
1	B	1	ASP	3.2
1	A	462	LEU	3.2
1	F	353	TYR	3.2
1	F	135	CYS	3.1
1	F	218	GLN	3.1
1	E	463	GLY	3.1
1	E	491	TYR	3.1
1	F	1	ASP	3.1
1	B	55	CYS	3.1
1	A	181	SER	3.1
1	E	477	CYS	3.1
1	D	68	ASP	3.0
1	C	317	LEU	3.0
1	F	471	HIS	3.0
1	E	337	GLY	3.0
1	D	92	PRO	3.0
1	B	330	GLY	3.0
1	E	218	GLN	3.0
1	A	355	HIS	2.9
1	B	68	ASP	2.9
1	E	70	PHE	2.9
1	C	70	PHE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	399	PHE	2.9
1	F	236	ASP	2.9
1	A	336	ALA	2.9
1	D	70	PHE	2.9
1	A	480	SER	2.9
1	F	5	ILE	2.9
1	F	356	SER	2.9
1	E	336	ALA	2.9
1	F	350	TRP	2.9
1	D	473	CYS	2.9
1	F	351	TYR	2.9
1	B	261	ASP	2.8
1	E	272	GLY	2.8
1	A	456	ARG	2.8
1	D	318	ARG	2.8
1	B	204	THR	2.8
1	D	389	ASN	2.7
1	B	470	TYR	2.7
1	D	317	LEU	2.7
1	B	418	LEU	2.7
1	A	2	GLN	2.7
1	E	356	SER	2.7
1	F	157	TYR	2.7
1	E	398	GLU	2.7
1	A	356	SER	2.7
1	F	104	LEU	2.7
1	B	338	PHE	2.7
1	A	320	SER	2.7
1	C	262	SER	2.7
1	F	320	SER	2.7
1	A	1	ASP	2.7
1	D	286	ASN	2.7
1	D	456	ARG	2.6
1	B	497	LEU	2.6
1	A	345	GLY	2.6
1	D	156	ALA	2.6
1	F	336	ALA	2.6
1	B	191	TYR	2.6
1	E	191	TYR	2.6
1	D	285	ILE	2.6
1	B	183	ASN	2.6
1	C	352	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	358	GLU	2.6
1	D	455	LEU	2.6
1	B	390	THR	2.6
1	A	68	ASP	2.6
1	A	183	ASN	2.6
1	C	319	ASN	2.6
1	A	478	MET	2.6
1	D	274	CYS	2.6
1	F	274	CYS	2.6
1	C	68	ASP	2.6
1	E	345	GLY	2.6
1	D	319	ASN	2.6
1	B	193	ASN	2.6
1	F	453	LEU	2.6
1	F	398	GLU	2.6
1	B	391	GLN	2.5
1	C	389	ASN	2.5
1	A	70	PHE	2.5
1	E	471	HIS	2.5
1	B	341	GLY	2.5
1	A	481	VAL	2.5
1	A	488	TYR	2.5
1	E	65	PRO	2.5
1	C	318	ARG	2.5
1	E	342	GLY	2.5
1	A	42	CYS	2.5
1	A	368	GLU	2.5
1	B	454	GLN	2.5
1	F	364	ALA	2.4
1	E	262	SER	2.4
1	F	71	ILE	2.4
1	E	497	LEU	2.4
1	E	236	ASP	2.4
1	D	463	GLY	2.4
1	D	499	ARG	2.4
1	B	492	SER	2.4
1	C	473	CYS	2.4
1	D	398	GLU	2.4
1	A	369	SER	2.4
1	F	235	PRO	2.4
1	A	389	ASN	2.4
1	D	17	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	366	ASP	2.4
1	F	474	ASP	2.4
1	F	494	GLU	2.4
1	C	65	PRO	2.4
1	C	339	ILE	2.3
1	E	355	HIS	2.3
1	F	488	TYR	2.3
1	F	143	PHE	2.3
1	B	451	VAL	2.3
1	A	489	PRO	2.3
1	A	401	ASN	2.3
1	A	454	GLN	2.3
1	F	469	PHE	2.3
1	E	21	GLU	2.3
1	F	495	ALA	2.3
1	A	453	LEU	2.3
1	A	261	ASP	2.3
1	C	391	GLN	2.3
1	C	395	VAL	2.3
1	D	5	ILE	2.3
1	F	65	PRO	2.3
1	E	12	SER	2.3
1	F	273	HIS	2.3
1	A	67	CYS	2.3
1	A	274	CYS	2.3
1	F	259	LYS	2.3
1	D	461	GLU	2.3
1	F	394	ALA	2.3
1	A	262	SER	2.3
1	A	491	TYR	2.3
1	D	460	LYS	2.3
1	F	389	ASN	2.3
1	A	474	ASP	2.3
1	A	463	GLY	2.2
1	C	337	GLY	2.2
1	C	401	ASN	2.2
1	B	458	ASN	2.2
1	C	477	CYS	2.2
1	A	236	ASP	2.2
1	A	457	ASP	2.2
1	F	355	HIS	2.2
1	F	87	ASN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	337	GLY	2.2
1	B	65	PRO	2.2
1	F	129	LEU	2.2
1	E	192	LYS	2.2
1	F	390	THR	2.2
1	D	391	GLN	2.2
1	D	160	ILE	2.2
1	E	360	GLY	2.2
1	E	466	CYS	2.2
1	F	118	PRO	2.2
1	F	272	GLY	2.2
1	F	125	HIS	2.2
1	C	470	TYR	2.2
1	D	393	GLU	2.2
1	B	92	PRO	2.2
1	B	464	ASN	2.1
1	B	39	GLY	2.1
1	B	342	GLY	2.1
1	F	361	SER	2.1
1	A	466	CYS	2.1
1	D	457	ASP	2.1
1	F	18	THR	2.1
1	D	262	SER	2.1
1	B	181	SER	2.1
1	C	483	ASN	2.1
1	D	497	LEU	2.1
1	B	71	ILE	2.1
1	B	317	LEU	2.1
1	E	453	LEU	2.1
1	F	486	TYR	2.1
1	F	133	ALA	2.1
1	D	369	SER	2.1
1	B	457	ASP	2.1
1	A	490	GLN	2.1
1	E	461	GLU	2.1
1	F	461	GLU	2.1
1	A	361	SER	2.0
1	A	3	ILE	2.0
1	F	193	ASN	2.0
1	F	447	LEU	2.0
1	B	278	CYS	2.0
1	F	42	CYS	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	352	GLY	2.0
1	B	337	GLY	2.0
1	F	285	ILE	2.0
1	F	294	ILE	2.0
1	C	168	ASN	2.0
1	E	472	LYS	2.0
1	E	468	GLU	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.

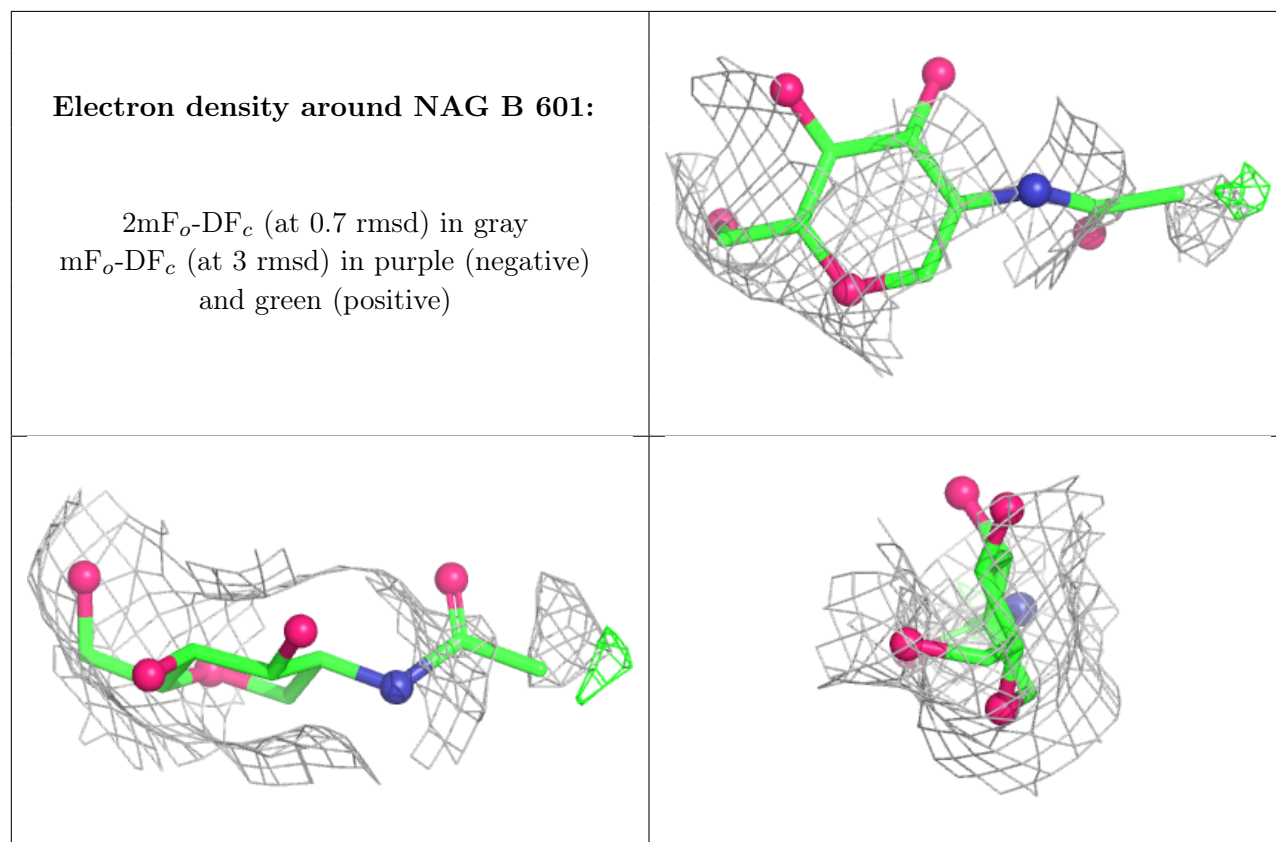
6.4 Ligands [i](#)

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	NAG	B	601	14/15	0.63	0.15	73,117,133,136	0
2	NAG	C	601	14/15	0.67	0.19	64,115,135,142	0
2	NAG	A	602	14/15	0.69	0.12	71,116,131,133	0
2	NAG	C	603	14/15	0.70	0.14	88,123,145,146	0
2	NAG	B	603	14/15	0.72	0.14	83,111,121,126	0
2	NAG	F	602	14/15	0.73	0.11	81,121,138,145	0
2	NAG	E	602	14/15	0.74	0.15	95,124,139,140	0
2	NAG	E	601	14/15	0.75	0.15	62,84,111,112	0
2	NAG	B	602	14/15	0.76	0.17	85,105,123,124	0
2	NAG	D	602	14/15	0.79	0.13	105,123,126,127	0
2	NAG	A	601	14/15	0.80	0.22	66,92,105,108	0
2	NAG	D	601	14/15	0.85	0.11	47,60,83,88	0
2	NAG	F	601	14/15	0.86	0.13	66,93,104,104	0
2	NAG	C	602	14/15	0.86	0.13	52,64,85,87	0

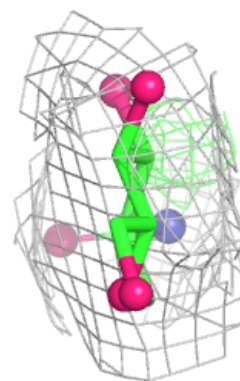
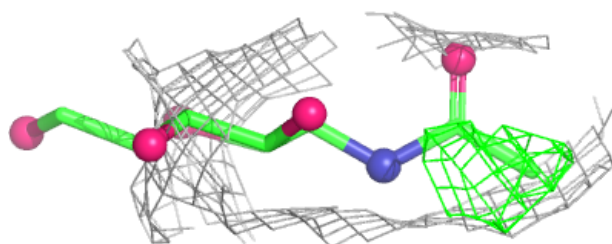
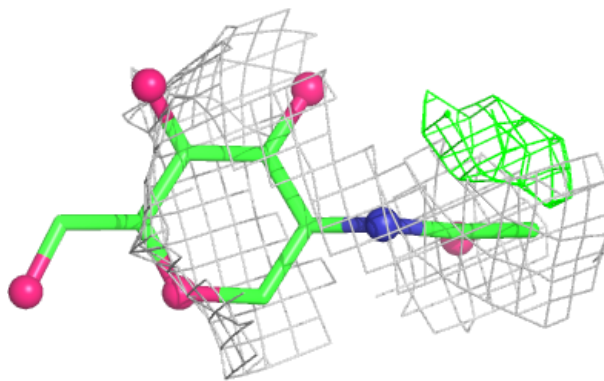
The following is a graphical depiction of the model fit to experimental electron density of all

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.

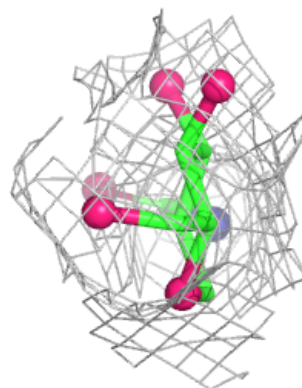
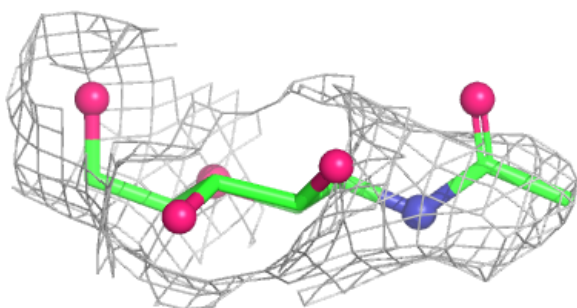
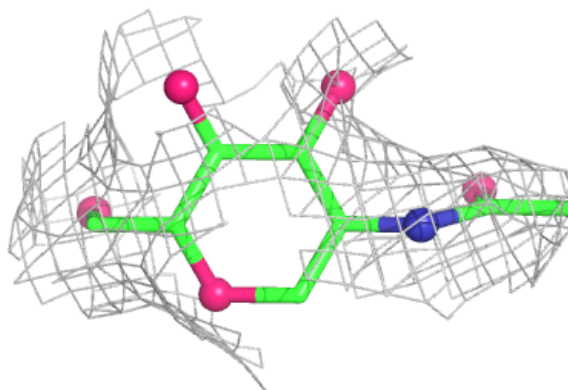


Electron density around NAG C 601:

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

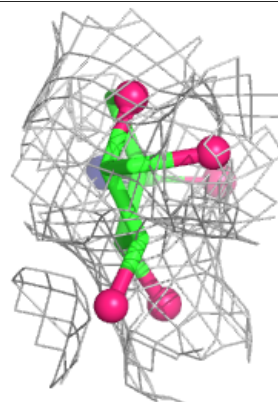
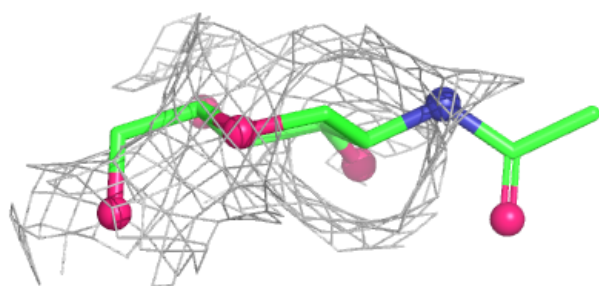
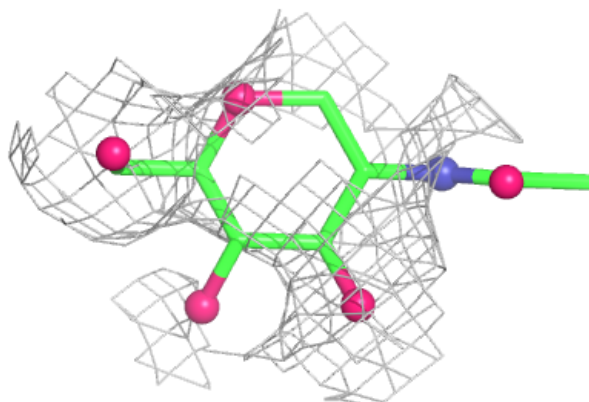
**Electron density around NAG A 602:**

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



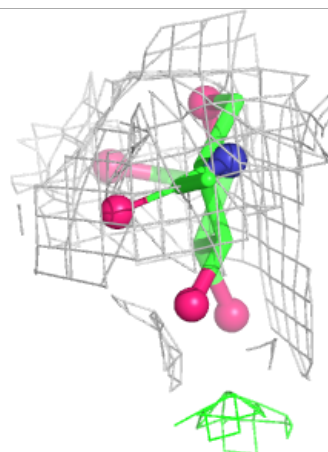
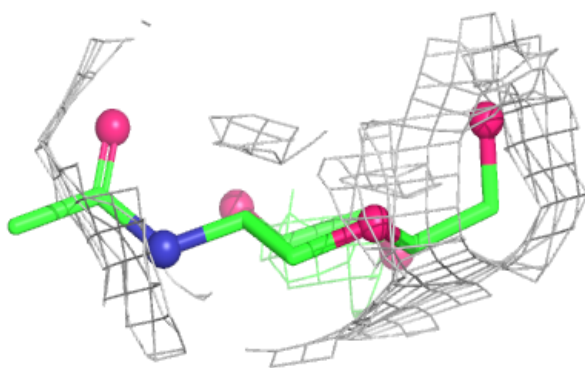
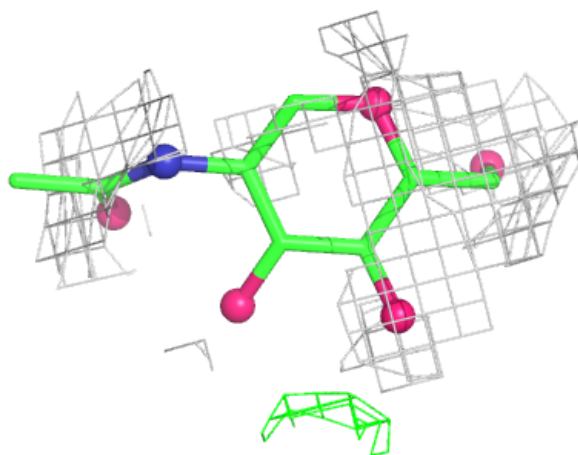
Electron density around NAG C 603:

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



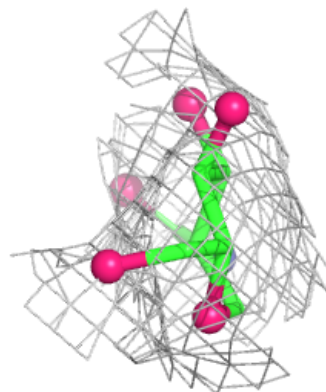
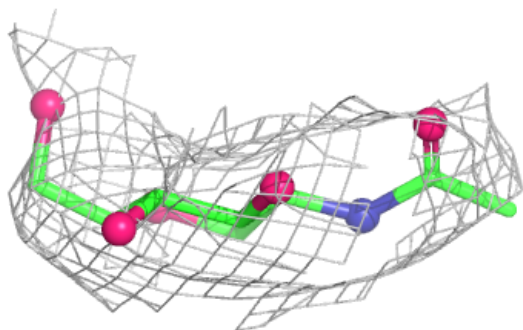
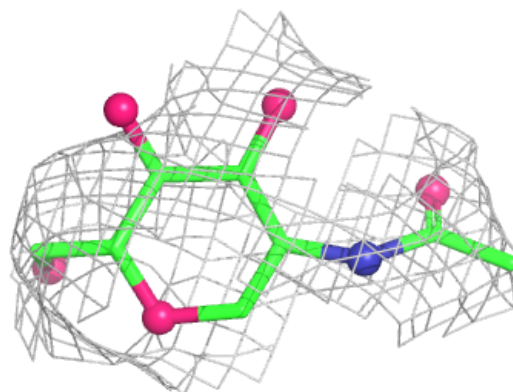
Electron density around NAG B 603:

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

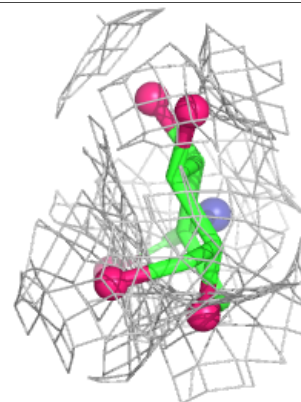
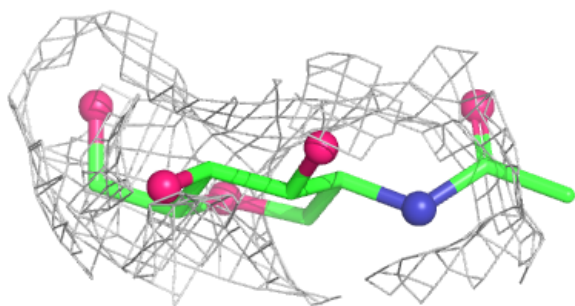
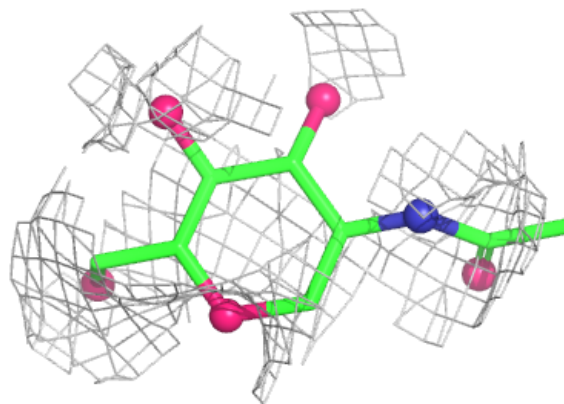


Electron density around NAG F 602:

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

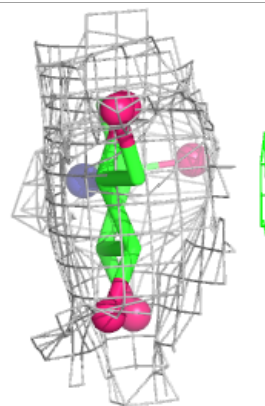
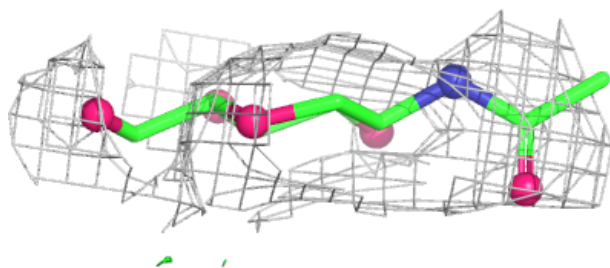
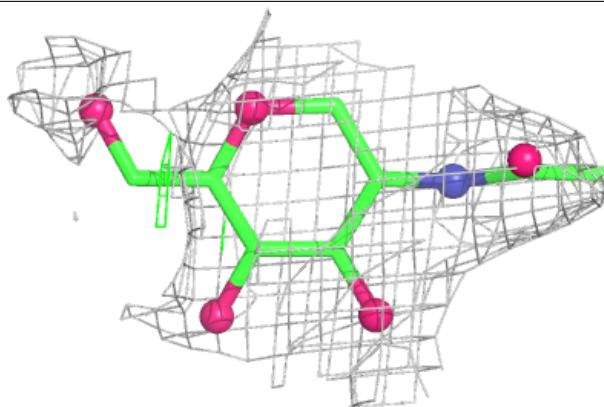
**Electron density around NAG E 602:**

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

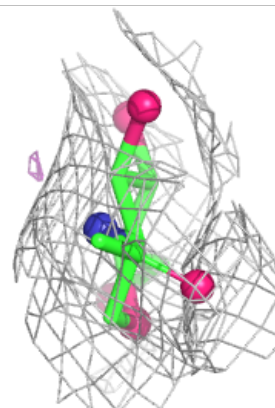
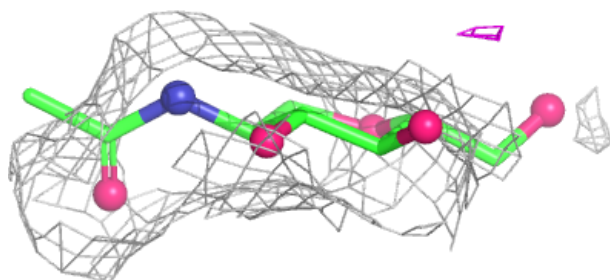
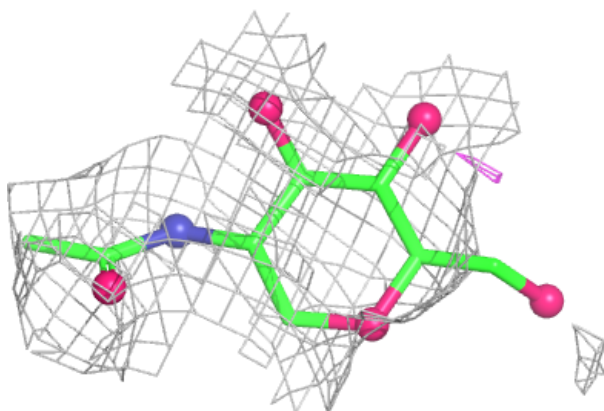


Electron density around NAG E 601:

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

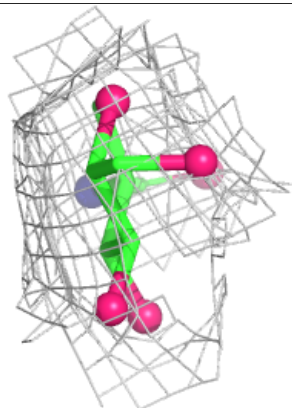
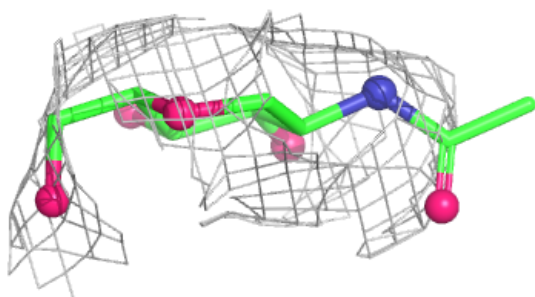
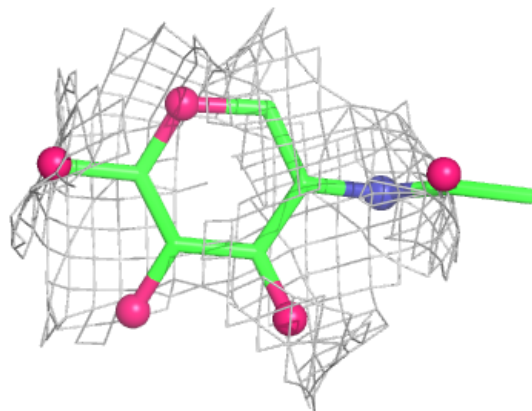
**Electron density around NAG B 602:**

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



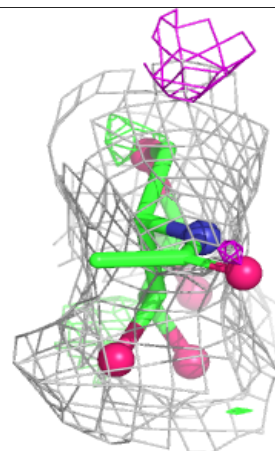
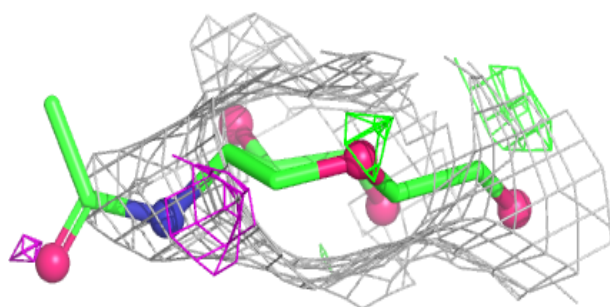
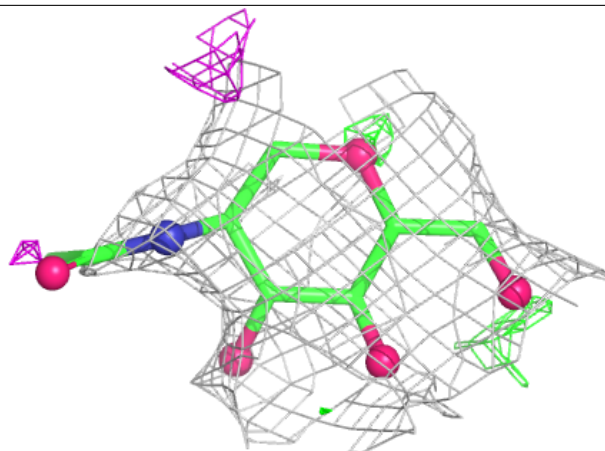
Electron density around NAG D 602:

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

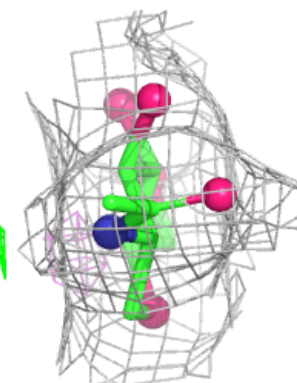
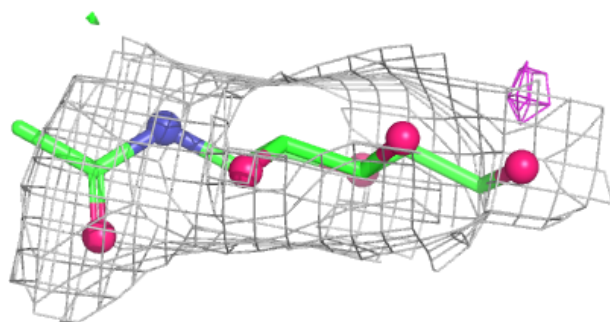
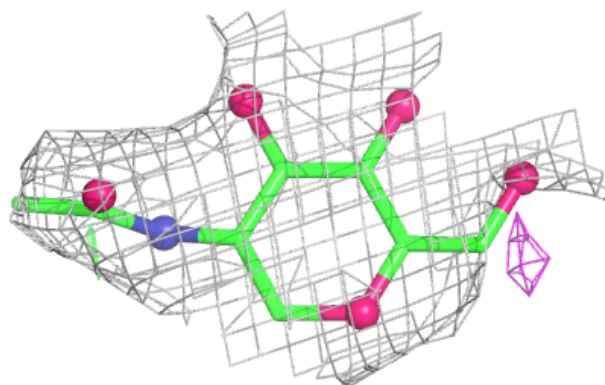


Electron density around NAG A 601:

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

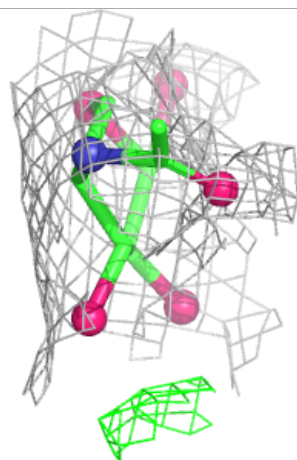
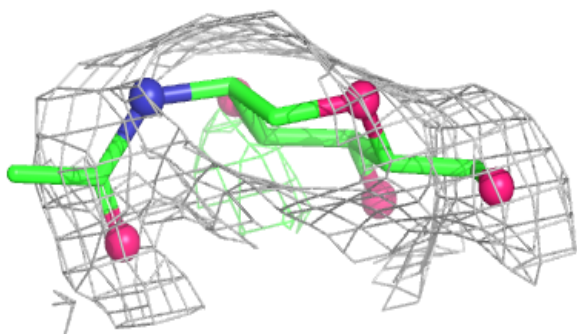
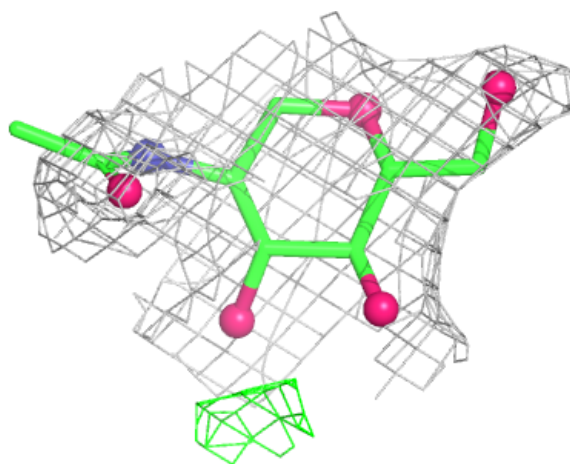
**Electron density around NAG D 601:**

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



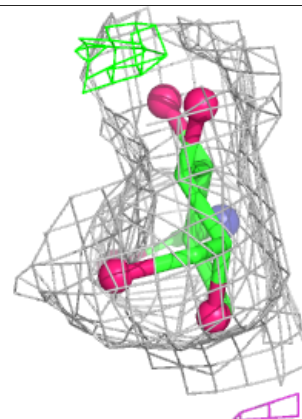
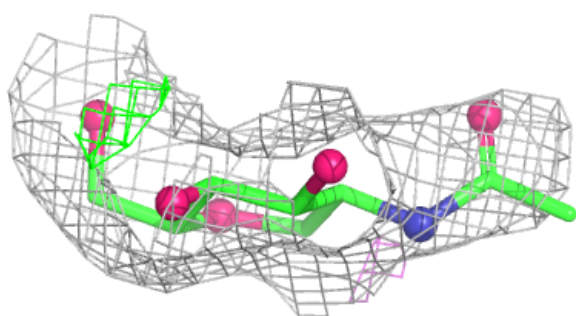
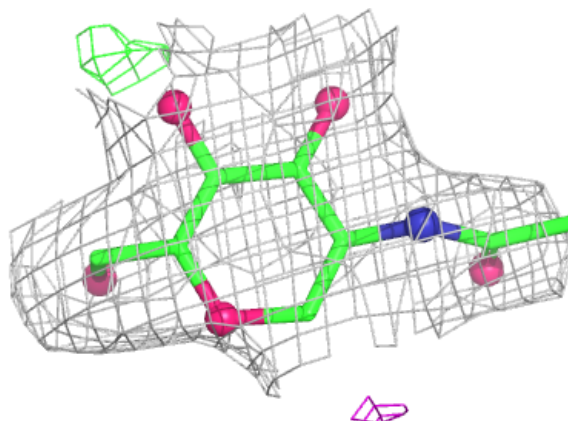
Electron density around NAG F 601:

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



Electron density around NAG C 602:

$2mF_o-DF_c$ (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.