



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:51 PM UTC

PDB ID : 8WDS / pdb_00008wds
Title : Crystal structure of BF.7 RBD complexed with human ACE2
Authors : Li, W.; Xie, Y.
Deposited on : 2023-09-16
Resolution : 3.40 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

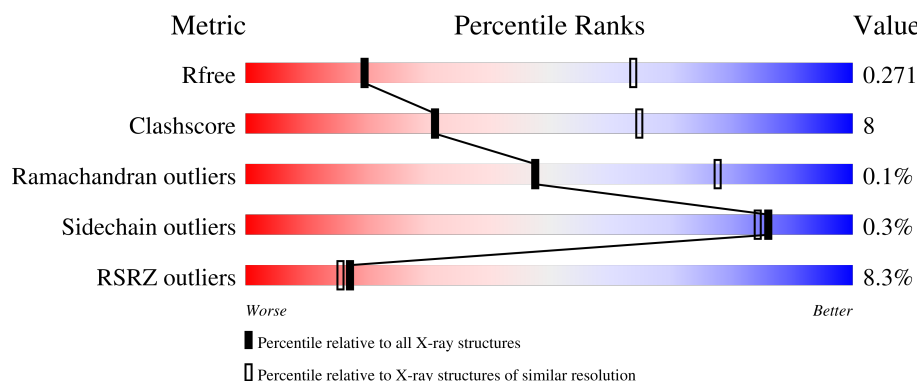
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	805	 59% 15% 26%
1	C	805	 9% 59% 15% 26%
2	B	247	 9% 57% 22% 21%
2	D	247	 10% 62% 16% 21%
3	E	2	 100%

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Mol	Chain	Length	Quality of chain
4	F	3	100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13009 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 Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	596	Total	C	N	O	S	0	1	0
			4870	3116	808	917	29			
1	C	596	Total	C	N	O	S	0	1	0
			4857	3110	801	917	29			

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	195	Total	C	N	O	S	0	1	0
			1559	1004	262	285	8			
2	D	195	Total	C	N	O	S	0	1	0
			1556	1003	261	284	8			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	301	MET	-	initiating methionine	UNP P0DTC2
B	302	HIS	-	expression tag	UNP P0DTC2
B	303	SER	-	expression tag	UNP P0DTC2
B	304	SER	-	expression tag	UNP P0DTC2
B	305	ALA	-	expression tag	UNP P0DTC2
B	306	LEU	-	expression tag	UNP P0DTC2
B	307	LEU	-	expression tag	UNP P0DTC2
B	308	CYS	-	expression tag	UNP P0DTC2
B	309	CYS	-	expression tag	UNP P0DTC2
B	310	LEU	-	expression tag	UNP P0DTC2
B	311	VAL	-	expression tag	UNP P0DTC2
B	312	LEU	-	expression tag	UNP P0DTC2
B	313	LEU	-	expression tag	UNP P0DTC2
B	314	THR	-	expression tag	UNP P0DTC2
B	315	GLY	-	expression tag	UNP P0DTC2
B	316	VAL	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	317	ARG	-	expression tag	UNP P0DTC2
B	318	ALA	-	expression tag	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	346	THR	ARG	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	452	ARG	LEU	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	486	VAL	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	542	HIS	-	expression tag	UNP P0DTC2
B	543	HIS	-	expression tag	UNP P0DTC2
B	544	HIS	-	expression tag	UNP P0DTC2
B	545	HIS	-	expression tag	UNP P0DTC2
B	546	HIS	-	expression tag	UNP P0DTC2
B	547	HIS	-	expression tag	UNP P0DTC2
D	301	MET	-	initiating methionine	UNP P0DTC2
D	302	HIS	-	expression tag	UNP P0DTC2
D	303	SER	-	expression tag	UNP P0DTC2
D	304	SER	-	expression tag	UNP P0DTC2
D	305	ALA	-	expression tag	UNP P0DTC2
D	306	LEU	-	expression tag	UNP P0DTC2
D	307	LEU	-	expression tag	UNP P0DTC2
D	308	CYS	-	expression tag	UNP P0DTC2
D	309	CYS	-	expression tag	UNP P0DTC2
D	310	LEU	-	expression tag	UNP P0DTC2
D	311	VAL	-	expression tag	UNP P0DTC2
D	312	LEU	-	expression tag	UNP P0DTC2
D	313	LEU	-	expression tag	UNP P0DTC2
D	314	THR	-	expression tag	UNP P0DTC2
D	315	GLY	-	expression tag	UNP P0DTC2
D	316	VAL	-	expression tag	UNP P0DTC2

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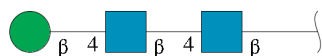
Chain	Residue	Modelled	Actual	Comment	Reference
D	317	ARG	-	expression tag	UNP P0DTC2
D	318	ALA	-	expression tag	UNP P0DTC2
D	339	ASP	GLY	variant	UNP P0DTC2
D	346	THR	ARG	variant	UNP P0DTC2
D	371	PHE	SER	variant	UNP P0DTC2
D	373	PRO	SER	variant	UNP P0DTC2
D	375	PHE	SER	variant	UNP P0DTC2
D	376	ALA	THR	variant	UNP P0DTC2
D	405	ASN	ASP	variant	UNP P0DTC2
D	408	SER	ARG	variant	UNP P0DTC2
D	417	ASN	LYS	variant	UNP P0DTC2
D	440	LYS	ASN	variant	UNP P0DTC2
D	452	ARG	LEU	variant	UNP P0DTC2
D	477	ASN	SER	variant	UNP P0DTC2
D	478	LYS	THR	variant	UNP P0DTC2
D	484	ALA	GLU	variant	UNP P0DTC2
D	486	VAL	PHE	variant	UNP P0DTC2
D	498	ARG	GLN	variant	UNP P0DTC2
D	501	TYR	ASN	variant	UNP P0DTC2
D	505	HIS	TYR	variant	UNP P0DTC2
D	542	HIS	-	expression tag	UNP P0DTC2
D	543	HIS	-	expression tag	UNP P0DTC2
D	544	HIS	-	expression tag	UNP P0DTC2
D	545	HIS	-	expression tag	UNP P0DTC2
D	546	HIS	-	expression tag	UNP P0DTC2
D	547	HIS	-	expression tag	UNP P0DTC2

- Molecule 3 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
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

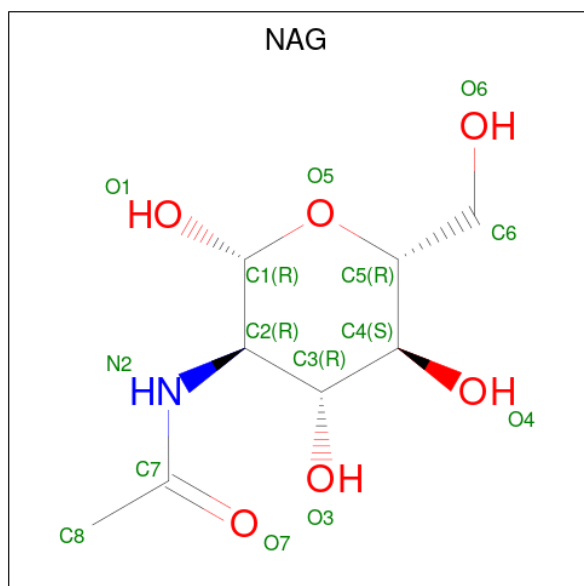


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		
5	C	1	Total	Zn	0	0
			1	1		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



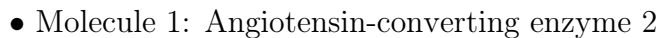
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		

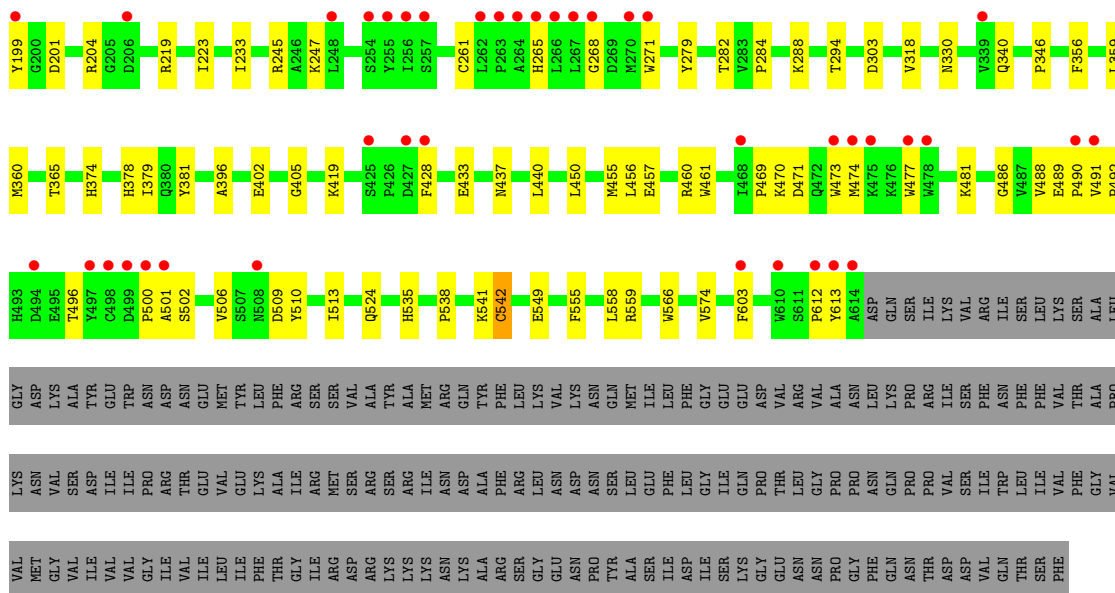
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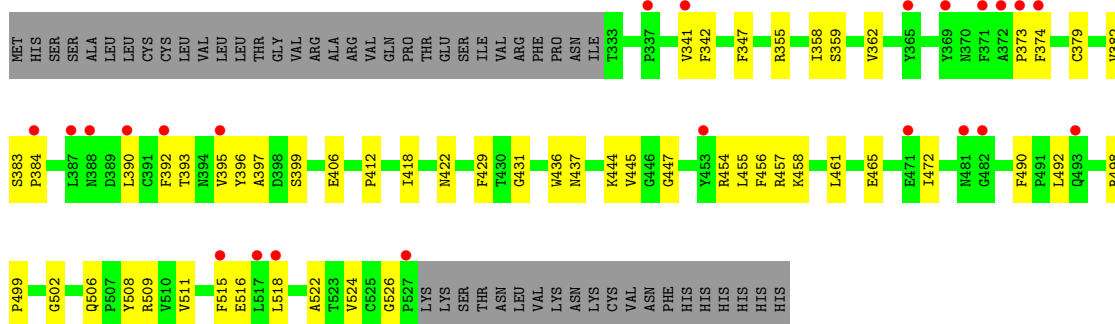
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 1: Angiotensin-converting enzyme 2

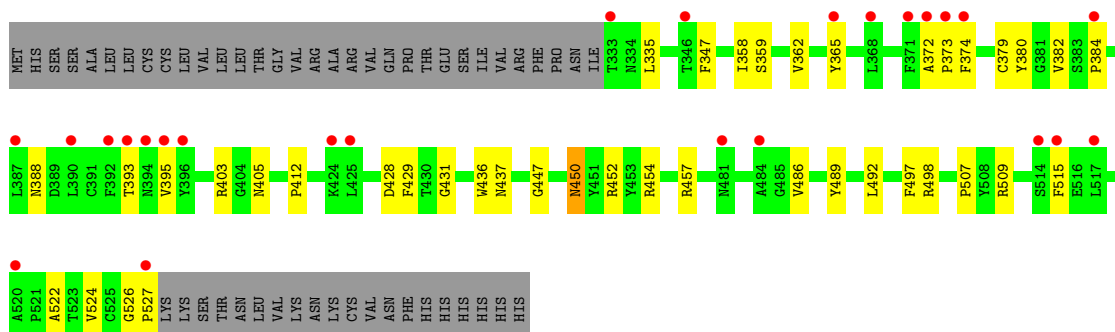




- Molecule 2: Spike protein S1



- Molecule 2: Spike protein S1



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%

MAG1
MAG2

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

Chain F:  100%

MAG1
MAG2
BNA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	122.69Å 137.35Å 154.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.42 – 3.40 29.42 – 3.40	Depositor EDS
% Data completeness (in resolution range)	87.1 (29.42-3.40) 86.9 (29.42-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 3.39Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.232 , 0.271 0.232 , 0.271	Depositor DCC
R_{free} test set	1543 reflections (4.22%)	wwPDB-VP
Wilson B-factor (Å ²)	60.2	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	13009	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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: ZN, NAG, BMA

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	0.20	0/5010	0.38	0/6806
1	C	0.20	0/4998	0.40	1/6793 (0.0%)
2	B	0.22	0/1606	0.43	0/2188
2	D	0.23	0/1606	0.40	0/2188
All	All	0.21	0/13220	0.40	1/17975 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	318	VAL	N-CA-C	-5.30	107.31	112.29

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	4870	0	4649	78	0
1	C	4857	0	4619	72	0
2	B	1559	0	1477	37	0
2	D	1556	0	1479	24	0
3	E	28	0	25	0	0
4	F	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	28	0	26	0	0
6	B	14	0	13	0	0
6	C	56	0	52	1	0
All	All	13009	0	12374	209	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 8.

All (209) 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:C:490:PRO:HA	1:C:612:PRO:HG2	1.65	0.79
1:C:116:LEU:HD21	1:C:187:LYS:HE2	1.66	0.78
1:C:455:MET:HE2	1:C:481:LYS:HG2	1.69	0.75
2:B:359:SER:HA	2:B:524:VAL:HG22	1.69	0.74
1:A:152:MET:HE3	1:A:164:ALA:HB3	1.70	0.71
2:B:373:PRO:HG2	2:B:437:ASN:HB3	1.72	0.71
2:D:373:PRO:HG2	2:D:437:ASN:HB3	1.73	0.70
2:B:393:THR:HA	2:B:522:ALA:HA	1.71	0.70
1:C:104:GLY:O	1:C:106:SER:N	2.24	0.70
1:C:489:GLU:HG3	1:C:613:TYR:HE1	1.56	0.70
1:A:157:ASP:OD1	1:A:158:TYR:N	2.29	0.66
1:A:88:ILE:HG22	1:A:94:LYS:HG3	1.75	0.66
1:C:500:PRO:HB2	1:C:506:VAL:HG11	1.78	0.66
1:C:457:GLU:HG2	1:C:513:ILE:HB	1.78	0.64
1:C:261:CYS:HB2	1:C:488:VAL:HB	1.80	0.64
1:A:474:MET:HE1	1:A:500:PRO:HD2	1.78	0.63
2:D:359:SER:HA	2:D:524:VAL:HG22	1.80	0.63
2:B:347:PHE:CE1	2:B:509:ARG:HD3	2.34	0.62
1:C:489:GLU:HG3	1:C:613:TYR:CE1	2.33	0.62
2:B:341:VAL:HG11	2:B:397:ALA:HB1	1.81	0.61
1:A:53:ASN:O	1:A:55:THR:HG23	2.02	0.60
2:B:358:ILE:HB	2:B:395:VAL:HB	1.82	0.60
2:D:393:THR:HA	2:D:522:ALA:HA	1.84	0.60
1:A:133:CYS:HA	1:A:141:CYS:HA	1.83	0.59
1:A:294:THR:HG23	1:A:365:THR:HA	1.84	0.59
1:A:457:GLU:HG2	1:A:513:ILE:HB	1.83	0.59
1:C:177:ARG:NH2	1:C:470:LYS:O	2.35	0.59
1:A:54:ILE:HD11	1:A:343:VAL:HG23	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:MET:HE1	1:A:161:ARG:HA	1.86	0.58
1:C:419:LYS:HE2	1:C:428:PHE:HB3	1.85	0.58
1:C:294:THR:HG23	1:C:365:THR:HA	1.85	0.58
1:A:524:GLN:HB3	1:A:574:VAL:HG11	1.85	0.58
1:C:157:ASP:OD1	1:C:158:TYR:N	2.37	0.57
1:A:499:ASP:O	1:A:502:SER:OG	2.22	0.57
2:B:347:PHE:CD2	2:B:399:SER:HB2	2.40	0.57
2:B:437:ASN:ND2	2:B:506:GLN:OE1	2.32	0.56
1:A:416:LYS:HD2	1:A:543:ASP:HB3	1.87	0.56
1:C:109:SER:O	1:C:112:LYS:N	2.37	0.55
1:A:527:GLU:HG3	1:A:539:LEU:HD22	1.89	0.55
1:C:271:TRP:NE1	1:C:502:SER:O	2.30	0.55
1:C:460:ARG:NH2	1:C:510:TYR:O	2.38	0.55
1:C:21:ILE:HD11	1:C:83:TYR:HA	1.88	0.55
2:D:362:VAL:HG23	2:D:526:GLY:HA3	1.88	0.54
2:D:388:ASN:HB3	2:D:527:PRO:HA	1.90	0.54
1:C:125:THR:O	1:C:129:THR:OG1	2.24	0.54
2:B:461:LEU:HG	2:B:465:GLU:HB3	1.89	0.54
1:A:104:GLY:O	1:A:107:VAL:HG12	2.07	0.54
1:C:233:ILE:HD13	1:C:450:LEU:HD13	1.91	0.53
2:D:452:ARG:HH21	2:D:492:LEU:HD12	1.72	0.53
1:C:492:PRO:HD3	1:C:613:TYR:CD2	2.44	0.52
1:A:144:LEU:HB2	1:A:168:TRP:CZ3	2.45	0.52
1:C:183:TYR:OH	1:C:509:ASP:OD1	2.27	0.52
1:A:293:VAL:HG11	1:A:418:LEU:HD22	1.92	0.52
1:C:161:ARG:NE	1:C:265:HIS:O	2.42	0.52
1:C:245:ARG:NH2	1:C:603:PHE:O	2.42	0.52
2:D:447:GLY:HA2	2:D:498:ARG:HG2	1.92	0.52
2:B:379:CYS:HB2	2:B:384:PRO:HD3	1.92	0.52
1:A:53:ASN:OD1	1:A:340:GLN:HG3	2.09	0.52
2:D:358:ILE:HB	2:D:395:VAL:HB	1.92	0.52
2:B:457:ARG:HD2	2:B:458:LYS:H	1.76	0.51
1:A:180:TYR:HA	1:A:183:TYR:HB3	1.92	0.51
1:A:20:THR:HG22	1:A:23:GLU:CD	2.36	0.51
1:C:378:HIS:HE1	1:C:402:GLU:HA	1.75	0.51
1:A:482:ARG:HD3	1:A:608:THR:O	2.11	0.51
2:B:355:ARG:HE	2:B:396:TYR:HB3	1.75	0.51
1:C:85:LEU:HD21	1:C:98:GLN:HB2	1.92	0.51
1:A:440:LEU:HD23	1:A:444:LEU:HG	1.92	0.51
1:A:119:ILE:HG23	1:A:179:LEU:HD22	1.92	0.51
2:B:490:PHE:CE2	2:B:492:LEU:HB2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:TRP:CD1	1:A:502:SER:HB2	2.46	0.51
1:A:269:ASP:OD1	1:A:272:GLY:N	2.36	0.50
1:A:351:LEU:HD22	1:A:355:ASP:OD2	2.11	0.50
1:A:284:PRO:HB2	1:A:285:PHE:CD2	2.47	0.50
1:C:180:TYR:HA	1:C:183:TYR:HB3	1.94	0.50
1:A:362:THR:HG23	1:A:368:ASP:HB3	1.92	0.49
1:C:396:ALA:HB1	1:C:566:TRP:HA	1.94	0.49
1:A:232:GLU:HB2	1:A:581:VAL:HG11	1.94	0.49
1:C:356:PHE:HB3	1:C:379:ILE:HD12	1.94	0.49
1:C:457:GLU:HG3	1:C:461:TRP:CE2	2.48	0.49
2:D:347:PHE:CE2	2:D:509:ARG:HB3	2.47	0.49
1:A:25:ALA:HB1	1:A:97:LEU:HD11	1.95	0.48
1:A:360:MET:HE1	1:A:371:THR:HB	1.95	0.48
1:C:524:GLN:HB3	1:C:574:VAL:HG11	1.94	0.48
1:A:168:TRP:CZ3	1:A:172:VAL:HG21	2.48	0.48
1:A:500:PRO:HB2	1:A:506:VAL:HG11	1.96	0.48
1:A:446:ILE:O	1:A:449:THR:HG22	2.14	0.48
1:A:53:ASN:O	1:A:54:ILE:C	2.56	0.48
1:C:31:LYS:HE3	2:D:489:TYR:HB3	1.96	0.48
2:B:437:ASN:HB2	2:B:508:TYR:CZ	2.48	0.47
1:C:20:THR:HG23	1:C:23:GLU:H	1.79	0.47
2:D:335:LEU:HD23	2:D:362:VAL:HG13	1.95	0.47
2:D:428:ASP:OD1	2:D:428:ASP:N	2.47	0.47
1:A:21:ILE:HD11	1:A:83:TYR:HA	1.96	0.47
1:A:169:ARG:HH22	1:A:271:TRP:HA	1.78	0.47
1:C:538:PRO:HD2	1:C:541:LYS:HD3	1.96	0.47
1:A:243:TYR:CE2	1:A:440:LEU:HD11	2.49	0.47
1:A:541:LYS:HE2	1:A:541:LYS:HB3	1.76	0.47
1:C:174:LYS:HA	1:C:496:THR:O	2.15	0.47
1:C:189:GLU:HG2	1:C:192:ARG:HH12	1.80	0.47
2:B:393:THR:HG21	2:B:518:LEU:HD12	1.96	0.47
2:D:454:ARG:HD3	2:D:457:ARG:HG3	1.97	0.47
1:A:450:LEU:HB2	1:A:451:PRO:HD3	1.98	0.46
2:B:444:LYS:HB3	2:B:444:LYS:HE2	1.83	0.46
1:A:594:TRP:CZ2	1:A:598:GLN:HG3	2.50	0.46
1:C:75:GLU:O	1:C:79:LEU:HG	2.16	0.46
1:A:284:PRO:HD3	1:A:440:LEU:HD13	1.98	0.46
1:A:233:ILE:HD13	1:A:450:LEU:HD13	1.97	0.46
1:C:107:VAL:HG21	1:C:193:ALA:HB1	1.97	0.46
1:C:288:LYS:HG3	1:C:433:GLU:HB2	1.98	0.46
1:A:75:GLU:O	1:A:79:LEU:HD12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:LEU:HB2	1:C:186:LEU:HD13	1.98	0.45
2:D:431:GLY:HA2	2:D:515:PHE:CD2	2.51	0.45
1:A:227:GLU:HG2	1:A:454:TYR:OH	2.16	0.45
2:B:445:VAL:HG22	2:B:499:PRO:HG3	1.99	0.45
2:B:502:GLY:O	2:B:506:GLN:HG3	2.17	0.45
1:A:476:LYS:HE2	1:A:476:LYS:HB2	1.76	0.45
1:A:381:TYR:CE1	1:A:558:LEU:HA	2.51	0.45
2:B:379:CYS:SG	2:B:384:PRO:HB3	2.56	0.45
1:C:25:ALA:HB1	1:C:97:LEU:HD11	1.97	0.45
1:C:181:GLU:HA	1:C:473:TRP:CH2	2.52	0.45
1:A:144:LEU:HB2	1:A:168:TRP:CH2	2.51	0.45
2:B:457:ARG:HD2	2:B:458:LYS:N	2.32	0.45
2:D:365:TYR:HB2	2:D:388:ASN:OD1	2.17	0.45
1:A:217:TYR:CE1	1:A:221:GLN:HG2	2.52	0.45
1:A:554:LEU:O	1:A:558:LEU:HG	2.17	0.45
2:B:342:PHE:CZ	2:B:511:VAL:HG11	2.52	0.45
1:C:346:PRO:HB3	1:C:360:MET:HG3	1.98	0.45
1:C:455:MET:CE	1:C:481:LYS:HG2	2.41	0.45
1:A:233:ILE:HG13	1:A:581:VAL:HG21	1.99	0.45
1:A:517:THR:HG22	1:A:579:MET:SD	2.56	0.45
1:C:374:HIS:HD1	1:C:405:GLY:C	2.25	0.45
1:A:245:ARG:NH2	1:A:603:PHE:O	2.50	0.45
2:B:447:GLY:HA2	2:B:498:ARG:HG2	1.99	0.45
1:A:248:LEU:HD12	1:A:262:LEU:HD22	1.98	0.44
1:C:247:LYS:HB2	1:C:282:THR:HG22	1.99	0.44
1:A:489:GLU:OE1	1:A:489:GLU:N	2.48	0.44
1:C:456:LEU:HD12	1:C:477:TRP:HH2	1.83	0.44
1:A:145:GLU:HA	1:A:146:PRO:HA	1.87	0.44
1:A:450:LEU:HD21	1:A:519:THR:HG21	2.00	0.44
1:A:499:ASP:OD1	1:A:499:ASP:N	2.49	0.44
2:B:395:VAL:HG22	2:B:515:PHE:HD1	1.82	0.44
2:D:497:PHE:CD2	2:D:507:PRO:HB3	2.53	0.44
1:C:340:GLN:HB2	6:C:902:NAG:H82	2.00	0.44
1:C:469:PRO:HB2	1:C:471:ASP:OD1	2.18	0.44
1:A:168:TRP:NE1	1:A:502:SER:HB2	2.33	0.44
1:C:555:PHE:O	1:C:559:ARG:HG2	2.18	0.43
1:A:85:LEU:HD21	1:A:98:GLN:HB2	1.99	0.43
2:B:412:PRO:HG3	2:B:429:PHE:HB3	1.99	0.43
2:B:374:PHE:O	2:B:436:TRP:HA	2.19	0.43
2:B:422:ASN:OD1	2:B:454:ARG:N	2.51	0.43
1:A:152:MET:O	1:A:161:ARG:NH1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:412:PRO:HG3	2:D:429:PHE:HB3	2.01	0.43
1:C:261:CYS:HB3	1:C:486:GLY:C	2.44	0.43
1:A:21:ILE:HD11	1:A:82:MET:O	2.18	0.43
1:C:131:LYS:HB3	1:C:143:LEU:HD23	2.00	0.43
1:C:162:LEU:HD11	1:C:491:VAL:HG23	2.01	0.43
2:D:372:ALA:CB	2:D:436:TRP:HB2	2.49	0.43
1:C:284:PRO:HD3	1:C:440:LEU:HG	2.01	0.43
1:C:549:GLU:H	1:C:549:GLU:CD	2.26	0.43
1:C:82:MET:SD	2:D:486:VAL:HG11	2.59	0.42
1:C:151:ILE:O	1:C:155:SER:HB3	2.19	0.42
1:A:30:ASP:O	1:A:34:HIS:ND1	2.39	0.42
1:A:580:ASN:OD1	1:A:581:VAL:N	2.53	0.42
2:B:362:VAL:HG23	2:B:526:GLY:HA3	2.02	0.42
1:C:500:PRO:O	1:C:506:VAL:HB	2.19	0.42
2:D:450:ASN:HD22	2:D:450:ASN:HA	1.55	0.42
1:A:453:THR:HG23	1:A:512:PHE:CD2	2.54	0.42
2:B:347:PHE:HD2	2:B:399:SER:HB2	1.83	0.42
1:C:178:PRO:HA	1:C:181:GLU:OE1	2.19	0.42
1:A:490:PRO:HA	1:A:612:PRO:HG2	2.01	0.42
1:A:492:PRO:HD3	1:A:613:TYR:CG	2.54	0.42
1:C:158:TYR:O	1:C:162:LEU:N	2.49	0.42
1:C:161:ARG:HH21	1:C:268:GLY:H	1.68	0.42
1:C:201:ASP:CG	1:C:219:ARG:HE	2.28	0.42
1:A:177:ARG:HH22	1:A:495:GLU:HB3	1.85	0.42
1:A:402:GLU:HB3	1:A:518:ARG:HG3	2.00	0.42
1:C:176:LEU:HD13	1:C:501:ALA:HB1	2.02	0.42
2:B:390:LEU:HD23	2:B:390:LEU:HA	1.85	0.42
1:C:381:TYR:CE1	1:C:558:LEU:HA	2.55	0.42
2:D:374:PHE:O	2:D:436:TRP:HA	2.20	0.42
2:B:490:PHE:HE2	2:B:492:LEU:HB2	1.84	0.41
1:C:279:TYR:OH	1:C:437:ASN:HB3	2.20	0.41
1:A:265:HIS:ND1	1:A:490:PRO:HG3	2.36	0.41
2:B:431:GLY:HA2	2:B:515:PHE:CD2	2.56	0.41
1:A:165:TRP:HA	1:A:270:MET:SD	2.60	0.41
1:A:165:TRP:CH2	1:A:490:PRO:HD2	2.55	0.41
1:A:459:TRP:CG	1:A:477:TRP:HE3	2.38	0.41
1:A:396:ALA:HB1	1:A:566:TRP:HA	2.02	0.41
2:B:382:VAL:HG22	2:B:383:SER:H	1.85	0.41
2:B:455:LEU:HG	2:B:456:PHE:CE1	2.56	0.41
1:C:105:SER:H	1:C:190:MET:CG	2.33	0.41
2:D:379:CYS:HB2	2:D:384:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:380:TYR:C	2:D:382:VAL:H	2.27	0.41
2:B:406:GLU:HB3	2:B:418:ILE:HG13	2.02	0.41
2:B:472:ILE:HD13	2:B:472:ILE:HA	1.89	0.41
1:C:187:LYS:HD2	1:C:199:TYR:CZ	2.55	0.40
1:C:474:MET:HE1	1:C:500:PRO:HD2	2.03	0.40
1:C:535:HIS:CD2	1:C:542:CYS:HB2	2.55	0.40
2:B:444:LYS:C	2:B:499:PRO:HD3	2.46	0.40
1:C:85:LEU:HD12	1:C:85:LEU:HA	1.95	0.40
1:C:204:ARG:CZ	1:C:223:ILE:HD11	2.51	0.40
1:C:303:ASP:OD1	1:C:303:ASP:N	2.53	0.40
1:A:455:MET:HE3	1:A:480:MET:HB2	2.02	0.40
1:C:48:TRP:CZ3	1:C:359:LEU:HB2	2.57	0.40
1:A:132:VAL:HG22	1:A:148:LEU:HD11	2.03	0.40
1:A:497:TYR:HB3	1:A:499:ASP:OD1	2.21	0.40
2:B:392:PHE:HB3	2:B:516:GLU:O	2.22	0.40
2:D:403:ARG:HH12	2:D:405:ASN:HD22	1.70	0.40
1:A:171:GLU:O	1:A:175:GLN:HG3	2.22	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	595/805 (74%)	576 (97%)	19 (3%)	0	100	100
1	C	595/805 (74%)	563 (95%)	31 (5%)	1 (0%)	43	71
2	B	194/247 (78%)	176 (91%)	18 (9%)	0	100	100
2	D	194/247 (78%)	185 (95%)	9 (5%)	0	100	100
All	All	1578/2104 (75%)	1500 (95%)	77 (5%)	1 (0%)	48	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	54	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	527/711 (74%)	526 (100%)	1 (0%)	87	85
1	C	525/711 (74%)	523 (100%)	2 (0%)	84	83
2	B	168/216 (78%)	168 (100%)	0	100	100
2	D	168/216 (78%)	167 (99%)	1 (1%)	78	80
All	All	1388/1854 (75%)	1384 (100%)	4 (0%)	86	84

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	C	330	ASN
1	C	542	CYS
2	D	450	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	210	ASN
1	A	472	GLN
1	A	508	ASN
1	A	552	GLN
1	A	556	ASN
2	B	519	HIS
1	C	58	ASN
1	C	61	ASN
1	C	63	ASN
1	C	194	ASN
1	C	210	ASN

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Mol	Chain	Res	Type
1	C	522	GLN
1	C	524	GLN
2	D	450	ASN
2	D	505	HIS

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 ⓘ

5 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	NAG	E	1	3,1	14,14,15	0.33	0	17,19,21	0.81	1 (5%)
3	NAG	E	2	3	14,14,15	0.56	0	17,19,21	0.91	1 (5%)
4	NAG	F	1	4,1	14,14,15	0.31	0	17,19,21	0.45	0
4	NAG	F	2	4	14,14,15	0.25	0	17,19,21	0.44	0
4	BMA	F	3	4	11,11,12	0.79	0	15,15,17	0.74	0

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	NAG	E	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	F	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	1/2/19/22	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(°)	Ideal(°)
3	E	2	NAG	C1-C2-N2	2.44	114.28	110.43
3	E	1	NAG	O4-C4-C5	2.24	114.83	109.32

There are no chirality outliers.

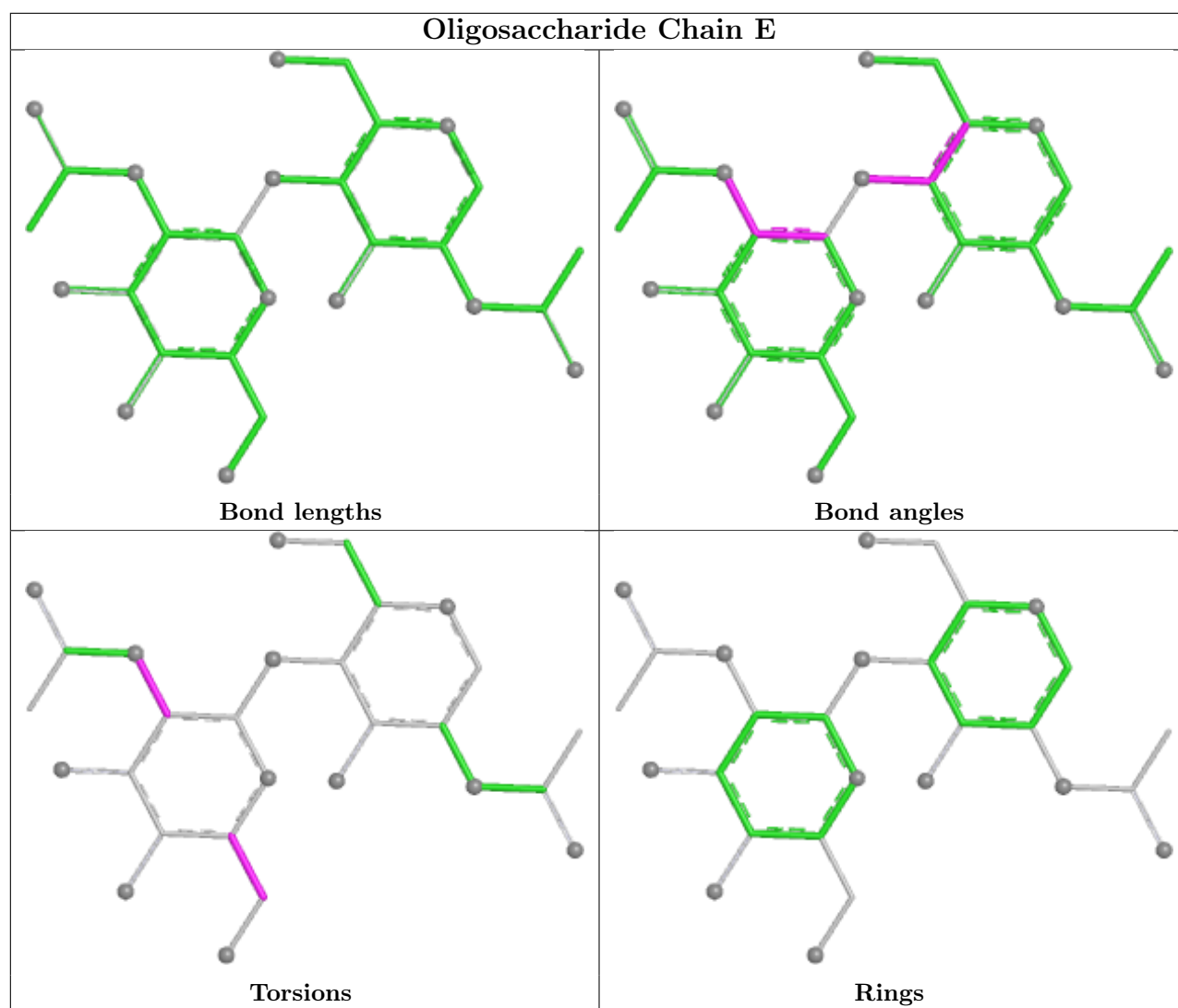
All (6) torsion outliers are listed below:

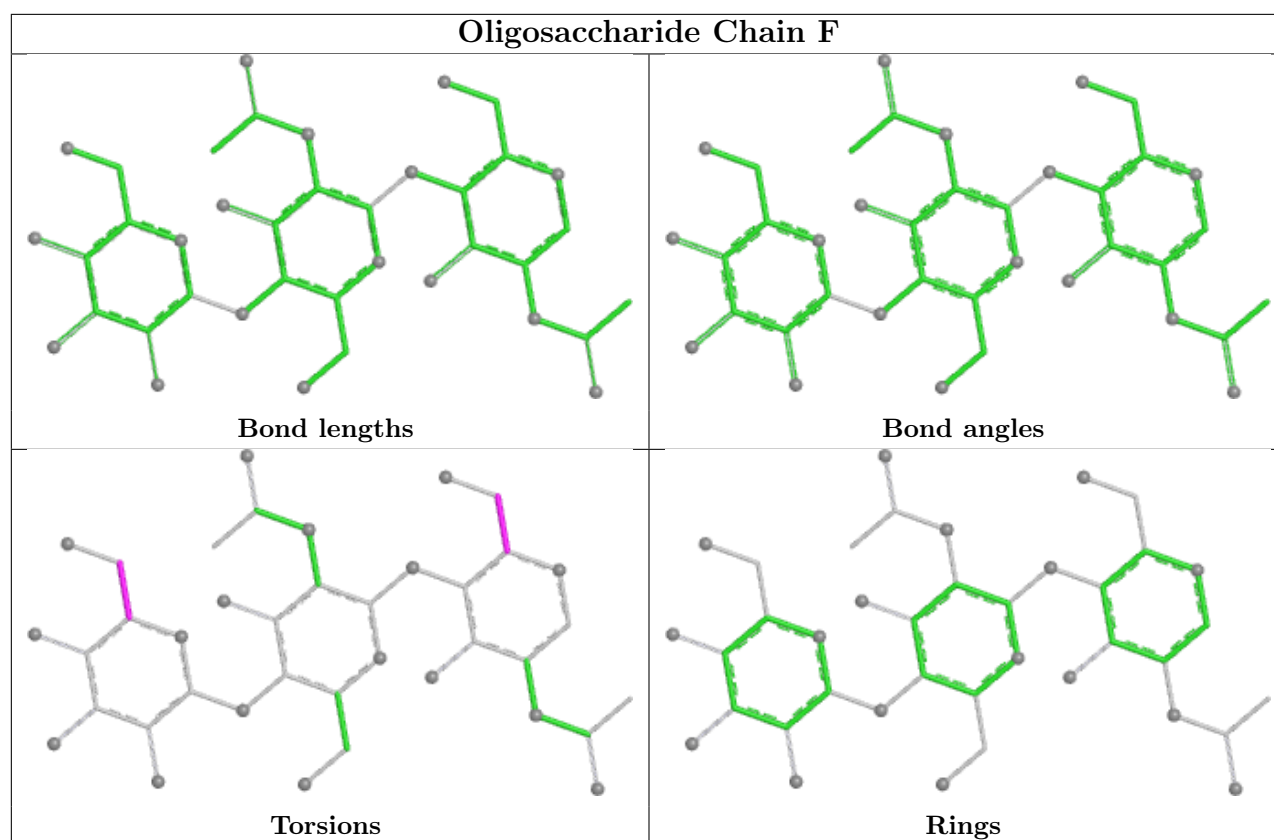
Mol	Chain	Res	Type	Atoms
4	F	3	BMA	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
3	E	2	NAG	C3-C2-N2-C7
4	F	1	NAG	O5-C5-C6-O6
3	E	2	NAG	C1-C2-N2-C7

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 oligosaccharide.





5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

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	C	902	1	14,14,15	0.60	0	17,19,21	0.65	0
6	NAG	A	902	1	14,14,15	0.41	0	17,19,21	0.44	0
6	NAG	C	905	1	14,14,15	0.45	0	17,19,21	0.78	0
6	NAG	A	903	1	14,14,15	0.48	0	17,19,21	0.45	0
6	NAG	C	903	1	14,14,15	0.42	0	17,19,21	0.42	0
6	NAG	B	601	2	14,14,15	0.26	0	17,19,21	0.40	0
6	NAG	C	904	1	14,14,15	0.34	0	17,19,21	0.70	0

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	C	902	1	-	1/6/23/26	0/1/1/1
6	NAG	A	902	1	-	1/6/23/26	0/1/1/1
6	NAG	C	905	1	-	2/6/23/26	0/1/1/1
6	NAG	A	903	1	-	3/6/23/26	0/1/1/1
6	NAG	C	903	1	-	0/6/23/26	0/1/1/1
6	NAG	B	601	2	-	2/6/23/26	0/1/1/1
6	NAG	C	904	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	903	NAG	O5-C5-C6-O6
6	A	903	NAG	C4-C5-C6-O6
6	C	904	NAG	O5-C5-C6-O6
6	C	904	NAG	C4-C5-C6-O6
6	C	904	NAG	C1-C2-N2-C7
6	B	601	NAG	C4-C5-C6-O6
6	B	601	NAG	O5-C5-C6-O6
6	C	905	NAG	C4-C5-C6-O6
6	A	902	NAG	C3-C2-N2-C7
6	A	903	NAG	C3-C2-N2-C7
6	C	902	NAG	C3-C2-N2-C7
6	C	904	NAG	C3-C2-N2-C7
6	C	905	NAG	O5-C5-C6-O6

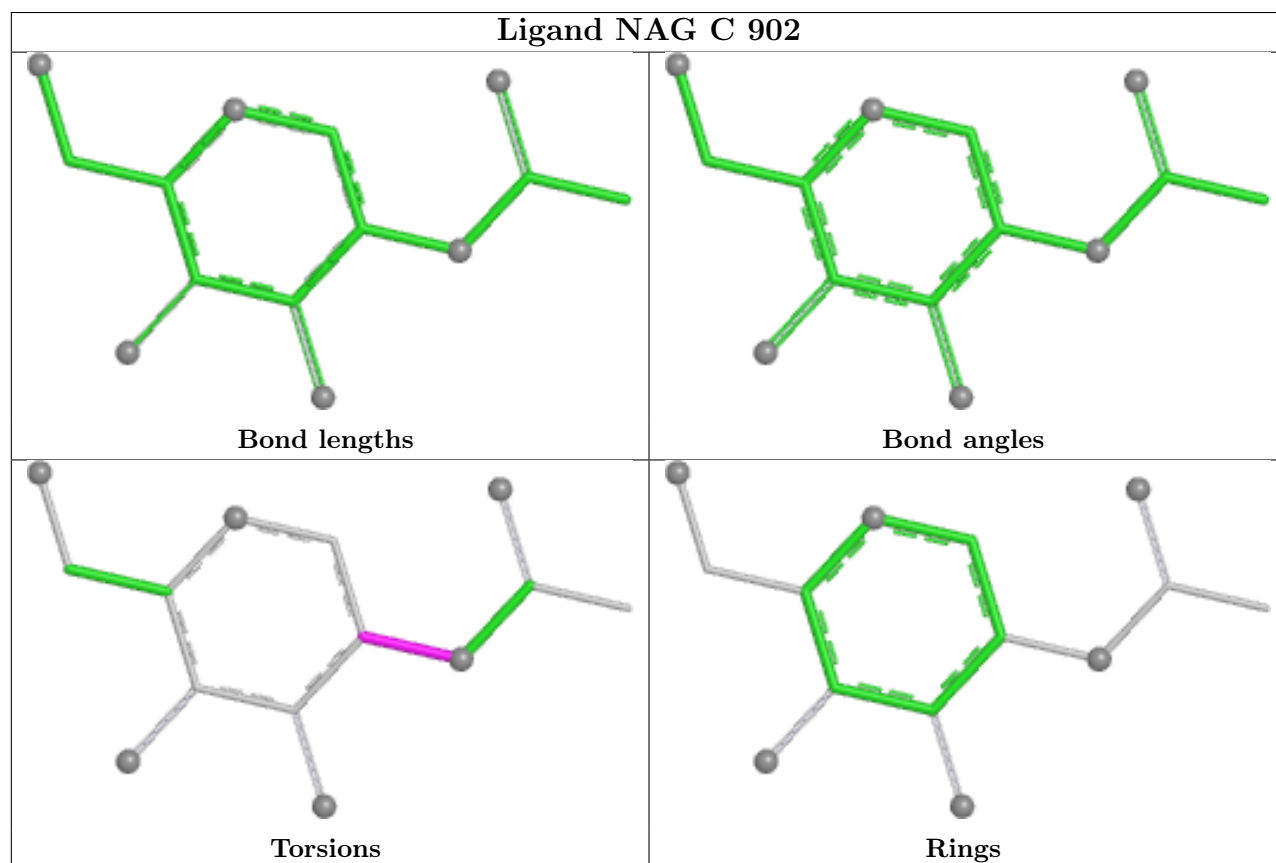
There are no ring outliers.

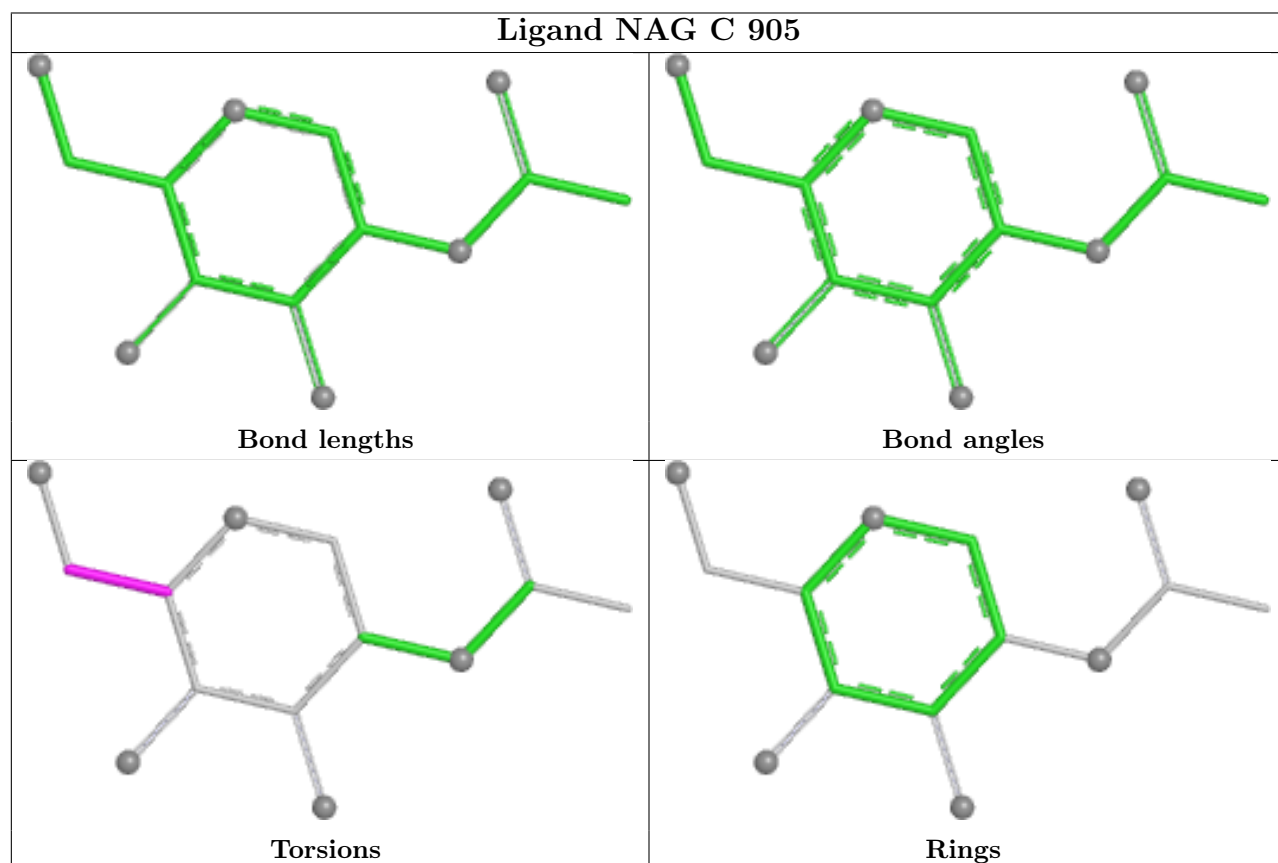
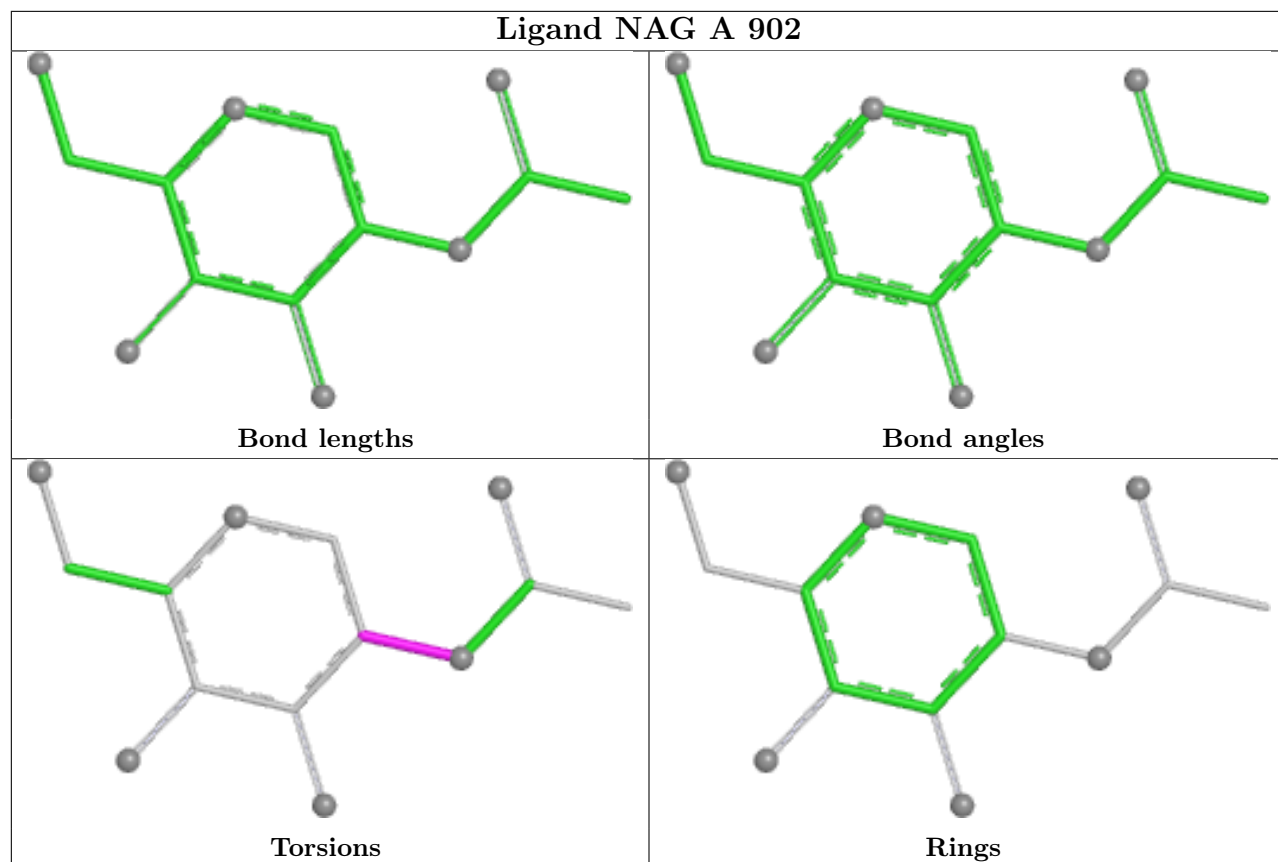
1 monomer is involved in 1 short contact:

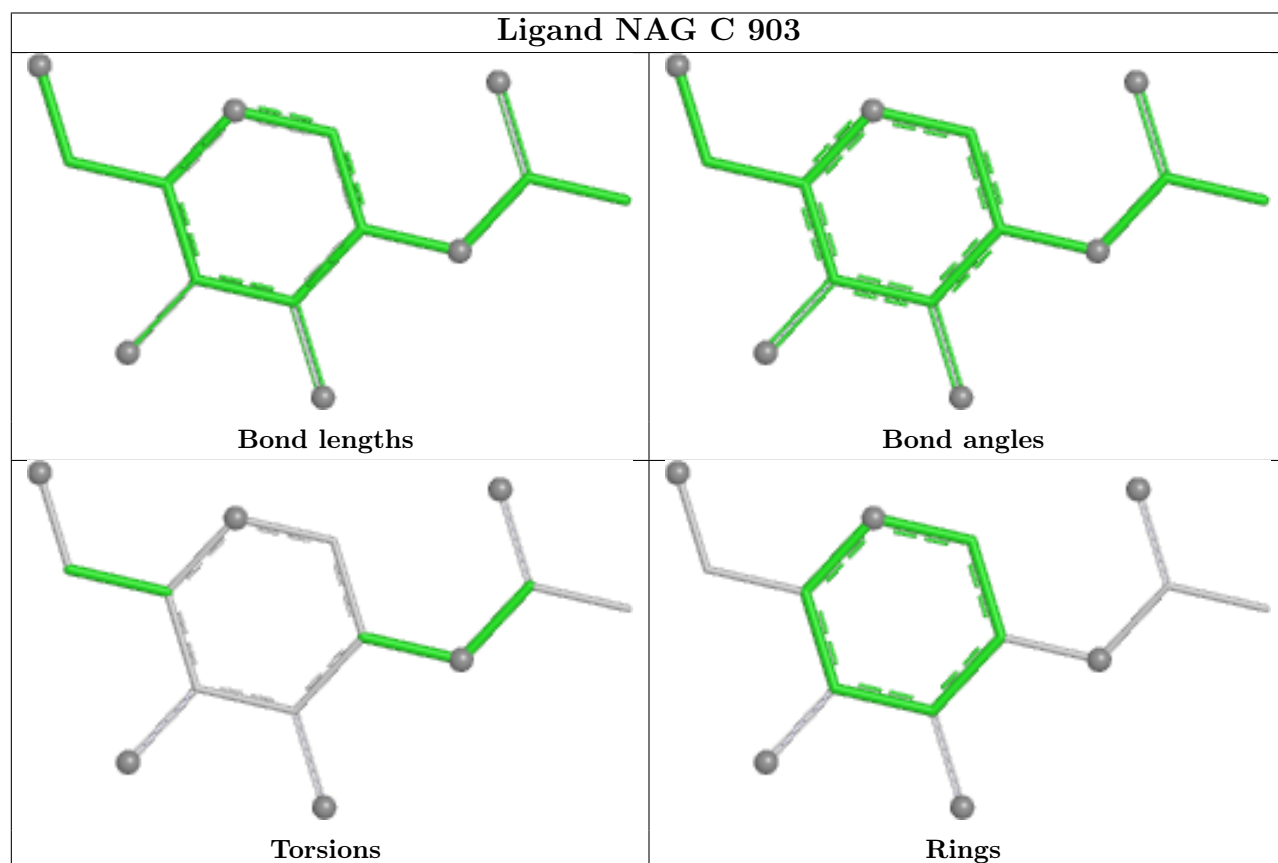
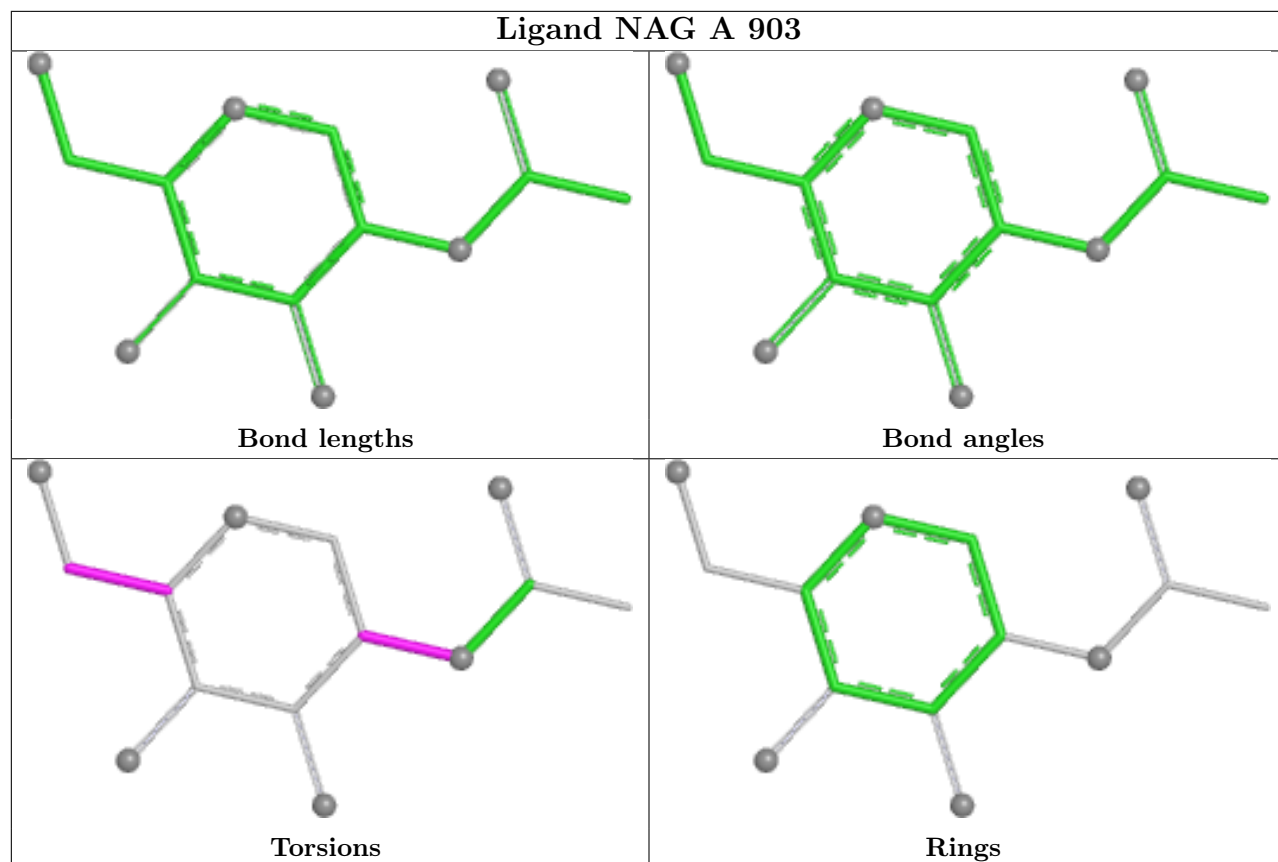
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	902	NAG	1	0

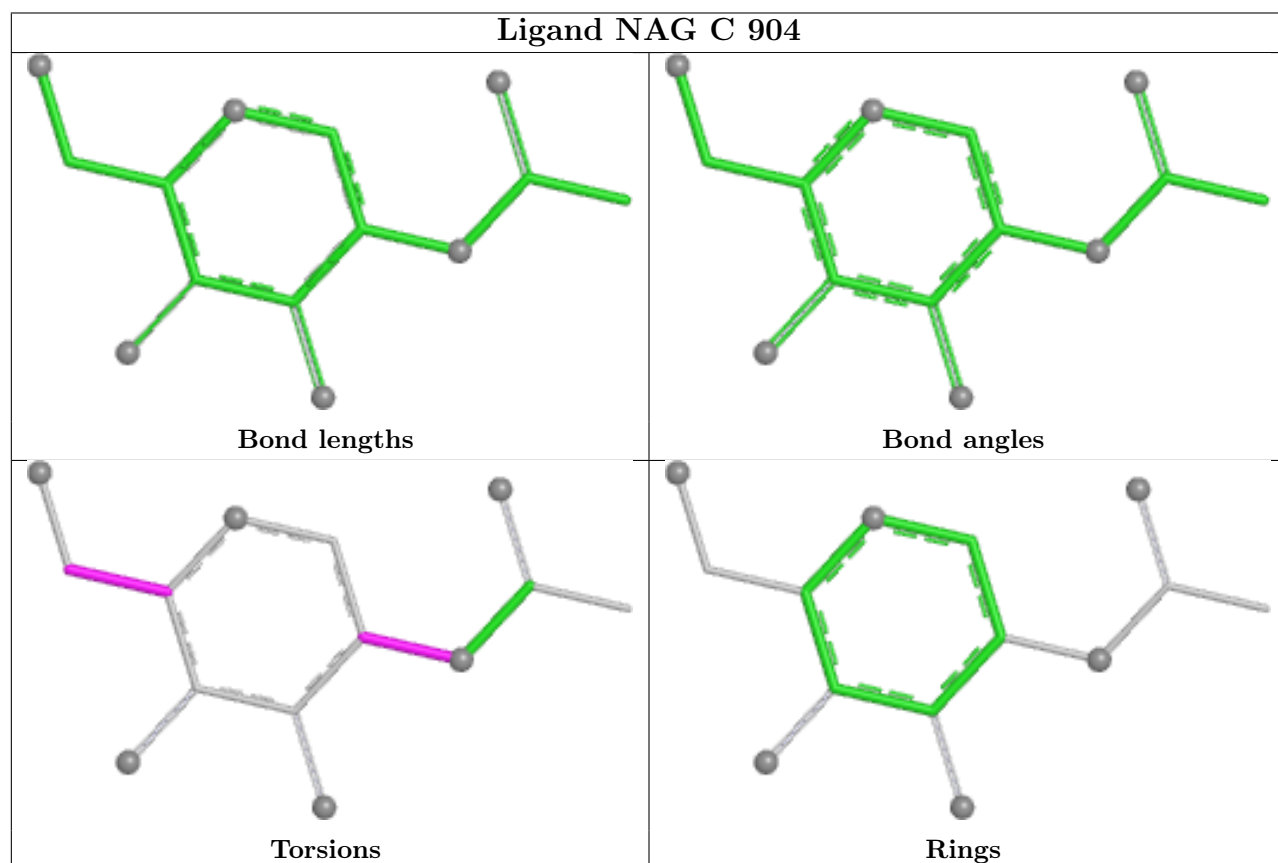
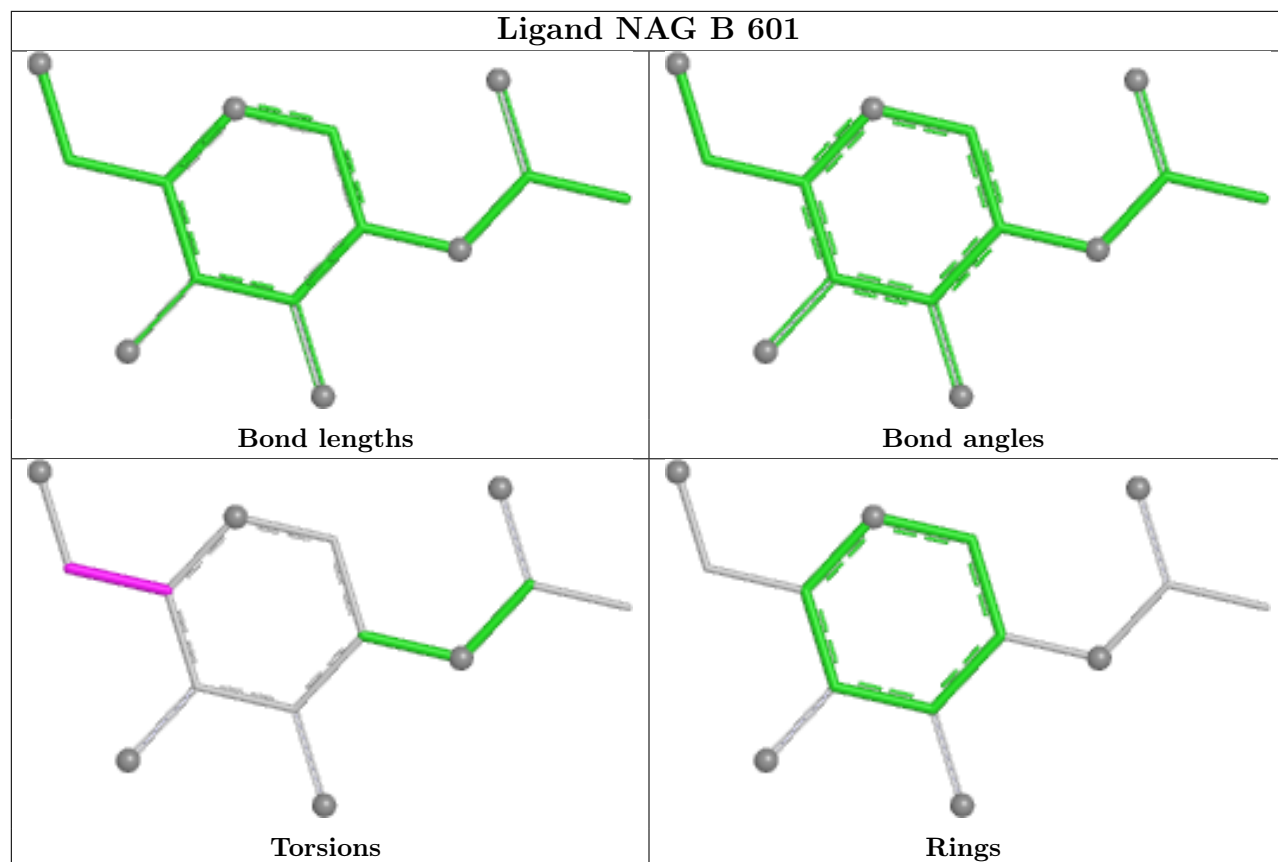
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	596/805 (74%)	0.16	11 (1%) 67 53	23, 48, 101, 189	1 (0%)
1	C	596/805 (74%)	0.54	73 (12%) 8 9	24, 54, 136, 236	1 (0%)
2	B	195/247 (78%)	0.73	23 (11%) 9 10	31, 73, 181, 224	1 (0%)
2	D	195/247 (78%)	0.79	25 (12%) 7 9	32, 66, 175, 222	1 (0%)
All	All	1582/2104 (75%)	0.45	132 (8%) 17 15	23, 56, 148, 236	4 (0%)

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	142	LEU	5.7
1	C	478	TRP	5.6
2	B	527	PRO	5.5
1	C	148	LEU	5.4
1	C	498	CYS	5.0
2	D	392	PHE	4.8
2	B	365	TYR	4.7
2	D	365	TYR	4.7
1	C	474	MET	4.7
2	B	372	ALA	4.6
1	C	144	LEU	4.5
1	C	264	ALA	4.5
1	C	254	SER	4.4
2	D	396	TYR	4.4
1	C	141	CYS	4.2
1	C	613	TYR	4.2
1	C	168	TRP	3.8
1	C	610	TRP	3.8
1	C	612	PRO	3.8
1	C	164	ALA	3.7
1	C	270	MET	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	156	LEU	3.6
1	C	138	PRO	3.6
2	D	384	PRO	3.6
1	C	491	VAL	3.6
2	D	517	LEU	3.6
1	C	149	ASN	3.5
1	C	146	PRO	3.5
2	B	373	PRO	3.5
1	C	473	TRP	3.5
2	D	368	LEU	3.4
2	D	515	PHE	3.4
2	D	372	ALA	3.4
2	D	346	THR	3.4
1	C	104	GLY	3.3
1	C	132	VAL	3.3
1	C	501	ALA	3.3
2	D	484	ALA	3.3
2	B	384	PRO	3.2
2	D	394	ASN	3.2
1	C	427	ASP	3.2
2	D	527	PRO	3.2
1	C	134	ASN	3.2
1	C	267	LEU	3.1
1	C	133	CYS	3.1
2	B	390	LEU	3.0
1	C	137	ASN	3.0
2	D	395	VAL	3.0
1	C	163	TRP	3.0
2	D	387	LEU	3.0
2	B	341	VAL	3.0
2	D	374	PHE	3.0
1	A	143	LEU	2.9
2	D	373	PRO	2.9
1	C	158	TYR	2.9
2	B	392	PHE	2.9
1	C	91	LEU	2.9
1	C	497	TYR	2.9
1	C	255	TYR	2.9
1	C	151	ILE	2.8
1	C	256	ILE	2.8
1	C	186	LEU	2.8
1	C	262	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	135	PRO	2.8
1	A	156	LEU	2.8
1	C	603	PHE	2.7
1	C	191	ALA	2.7
1	C	490	PRO	2.7
1	C	248	LEU	2.7
1	C	157	ASP	2.7
2	D	425	LEU	2.6
2	B	337	PRO	2.6
2	D	520	ALA	2.6
2	D	371	PHE	2.6
2	B	471	GLU	2.6
1	C	428	PHE	2.5
1	A	19	SER	2.5
2	B	493[A]	GLN	2.5
1	C	499	ASP	2.5
1	C	508	ASN	2.5
2	D	514	SER	2.5
1	A	160	GLU	2.5
1	C	172	VAL	2.5
1	C	614	ALA	2.4
1	C	143	LEU	2.4
1	C	500	PRO	2.4
1	C	271	TRP	2.4
2	B	371	PHE	2.4
1	C	263	PRO	2.4
2	D	333	THR	2.4
1	A	429	GLN	2.4
1	C	339	VAL	2.4
2	D	481	ASN	2.3
1	C	477	TRP	2.3
2	B	517	LEU	2.3
1	A	430	GLU	2.3
2	B	387	LEU	2.3
2	D	393	THR	2.3
1	C	257	SER	2.3
1	A	21	ILE	2.2
1	C	118	THR	2.2
1	C	265	HIS	2.2
1	C	199	TYR	2.2
1	C	268	GLY	2.2
2	B	374	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	369	TYR	2.2
1	C	266	LEU	2.2
1	A	614	ALA	2.2
1	C	25	ALA	2.2
1	C	206	ASP	2.2
2	B	453	TYR	2.2
2	B	482	GLY	2.2
2	B	515	PHE	2.2
1	C	475	LYS	2.1
1	C	153	ALA	2.1
1	A	133	CYS	2.1
1	C	136	ASP	2.1
1	C	152	MET	2.1
2	B	395	VAL	2.1
1	A	435	GLU	2.1
2	B	388	ASN	2.1
1	C	494	ASP	2.1
1	C	468	ILE	2.1
1	C	425	SER	2.0
1	C	108	LEU	2.0
2	D	390	LEU	2.0
2	D	424	LYS	2.0
1	C	155	SER	2.0
1	A	332	MET	2.0
2	B	481	ASN	2.0
1	C	179	LEU	2.0
2	B	518	LEU	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](#)

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.

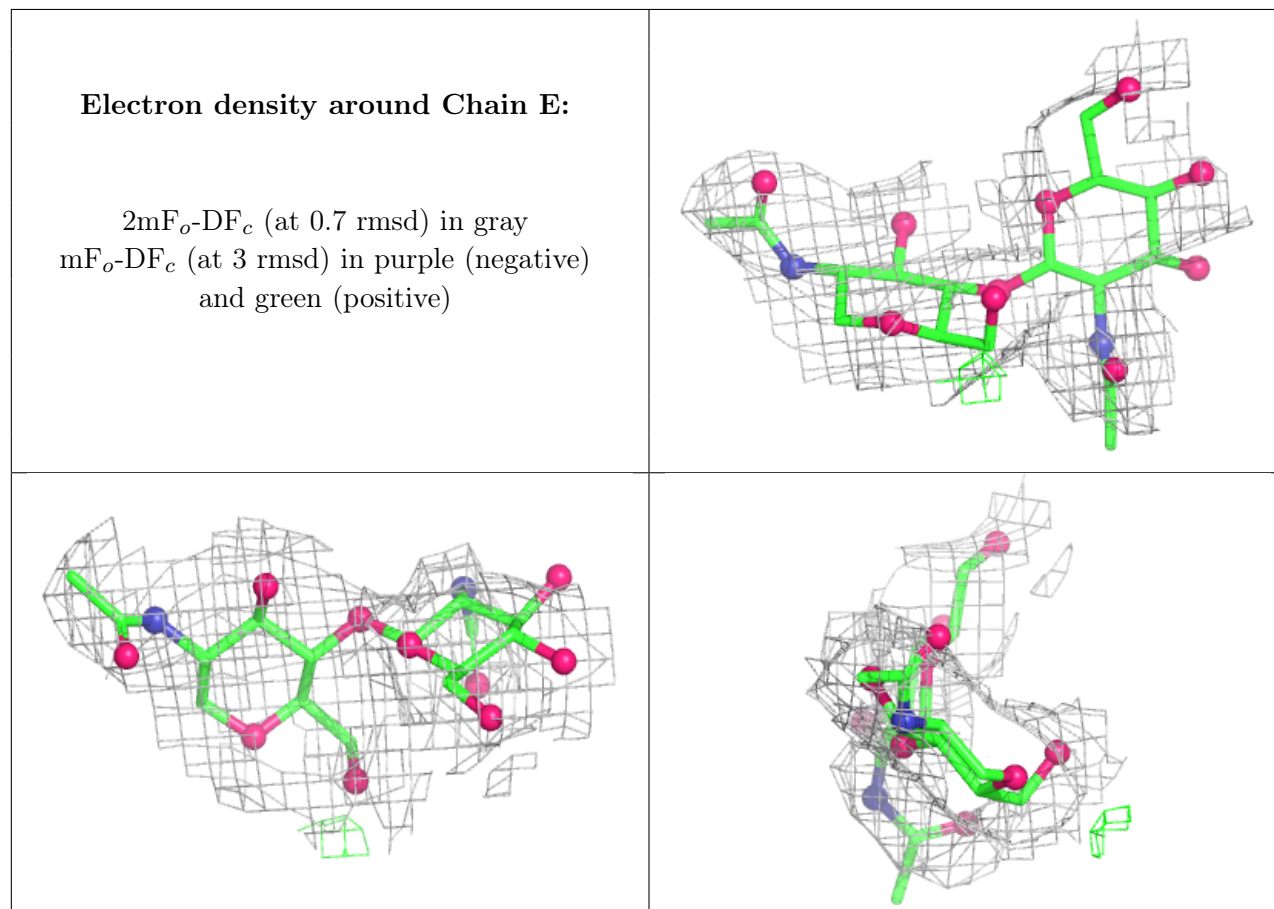
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	F	2	14/15	0.63	0.10	112,118,127,130	0

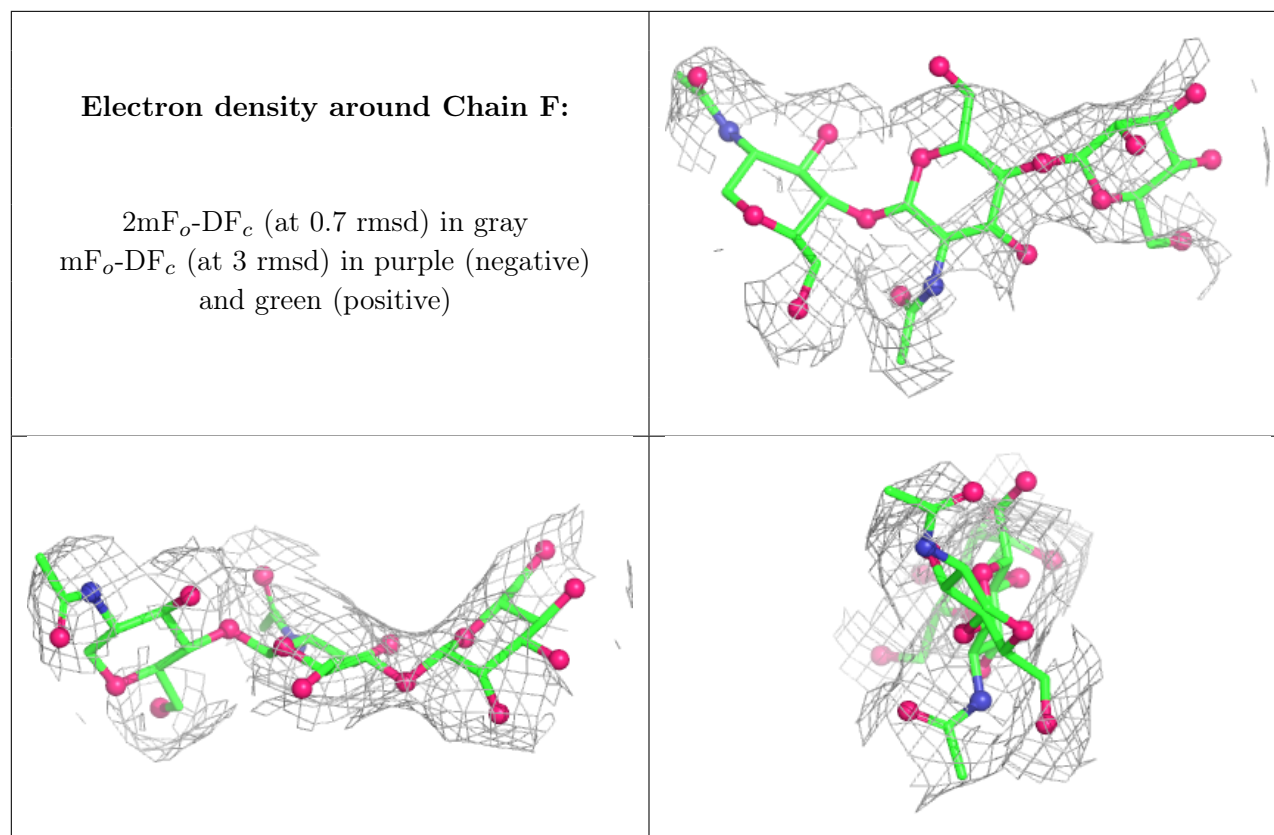
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	E	2	14/15	0.67	0.14	88,97,105,106	0
4	BMA	F	3	11/12	0.70	0.10	104,108,115,117	0
3	NAG	E	1	14/15	0.81	0.13	52,58,64,74	0
4	NAG	F	1	14/15	0.88	0.09	61,76,84,89	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





6.4 Ligands [i](#)

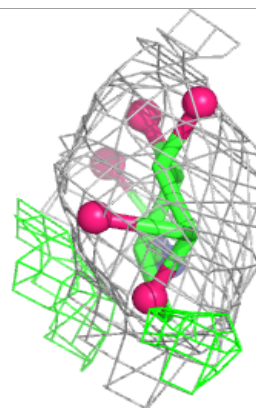
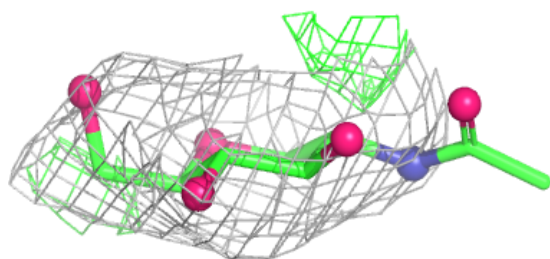
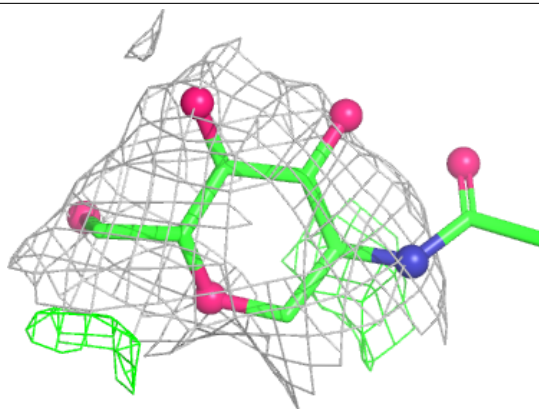
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	C	902	14/15	0.48	0.18	119,123,126,127	0
6	NAG	C	905	14/15	0.62	0.17	62,80,95,110	0
6	NAG	A	903	14/15	0.66	0.14	108,121,130,134	0
6	NAG	A	902	14/15	0.67	0.14	83,88,97,104	0
6	NAG	C	903	14/15	0.71	0.16	87,101,106,107	0
6	NAG	B	601	14/15	0.73	0.15	143,151,154,155	0
6	NAG	C	904	14/15	0.84	0.14	71,78,85,91	0
5	ZN	A	901	1/1	0.98	0.03	40,40,40,40	0
5	ZN	C	901	1/1	0.99	0.04	36,36,36,36	0

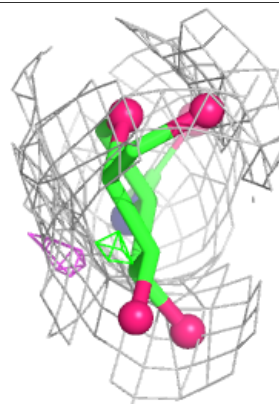
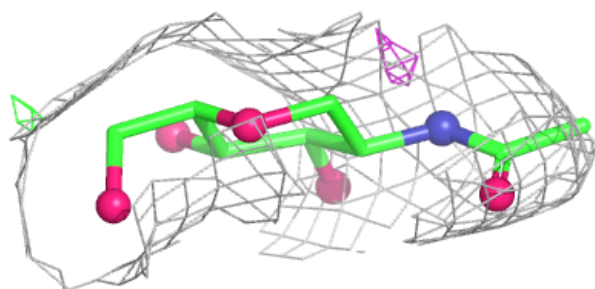
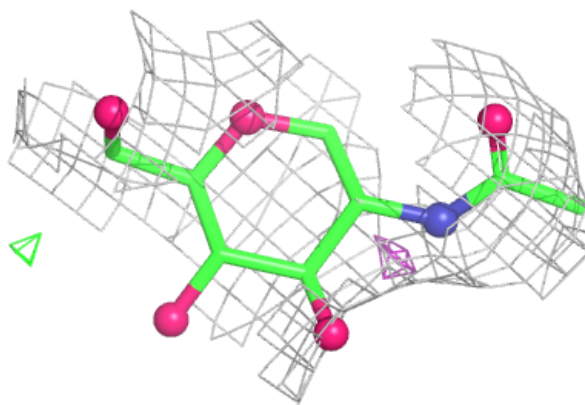
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAG C 902:

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

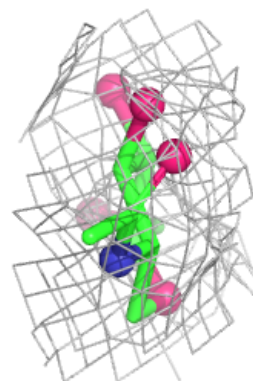
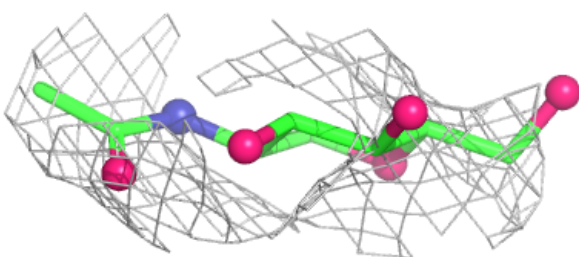
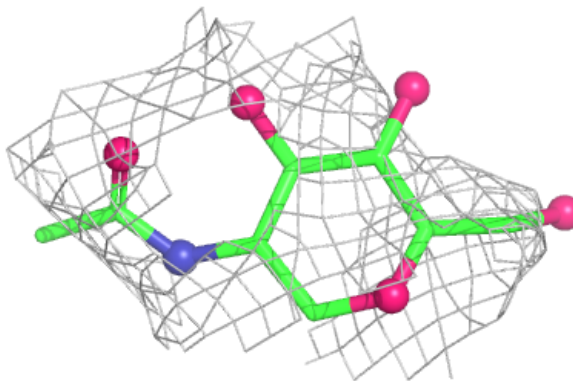
**Electron density around NAG C 905:**

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

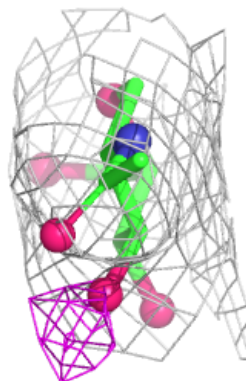
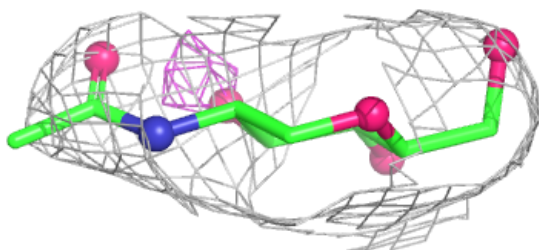
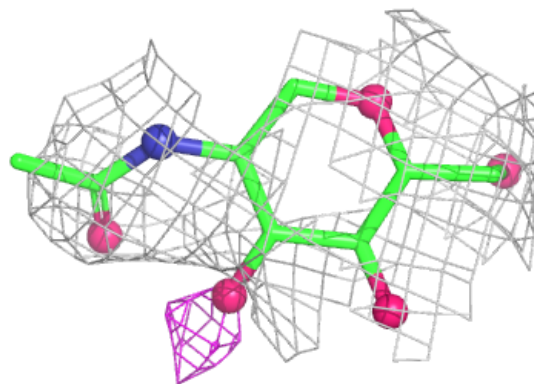


Electron density around NAG A 903:

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

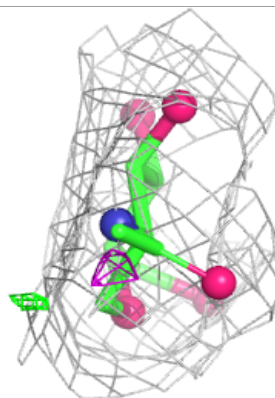
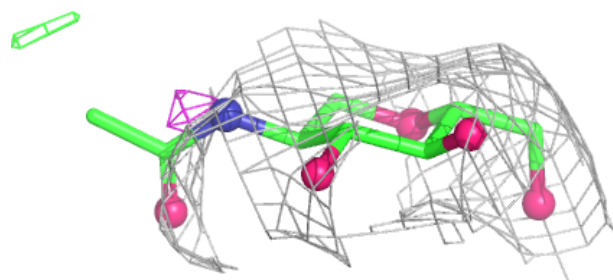
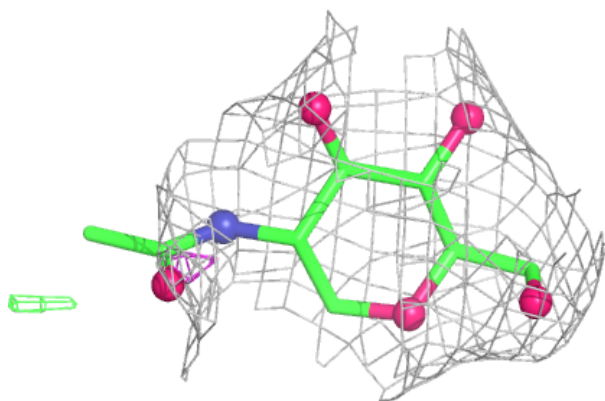
**Electron density around NAG A 902:**

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

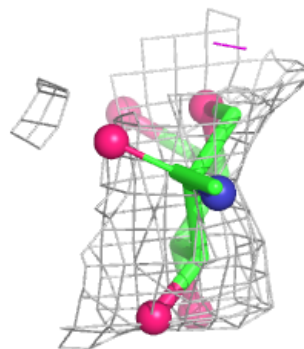
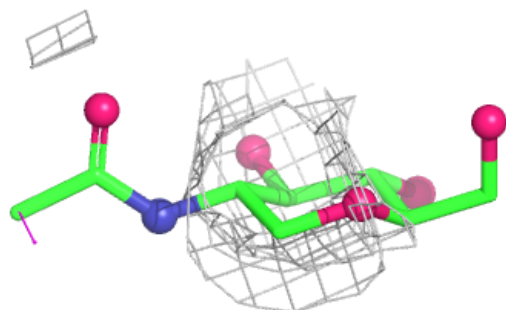
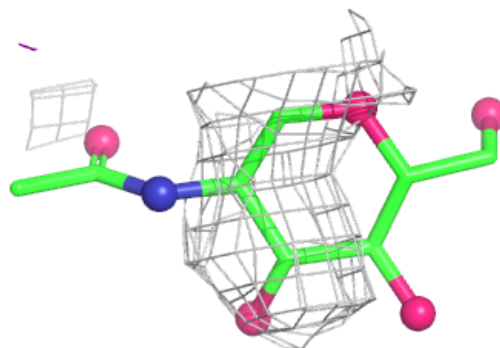


Electron density around NAG C 903:

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

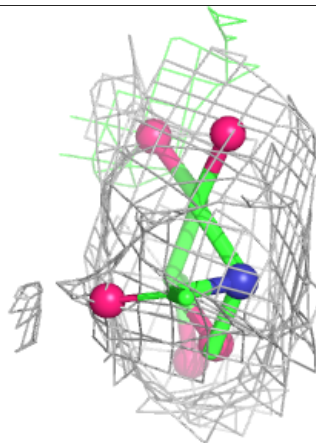
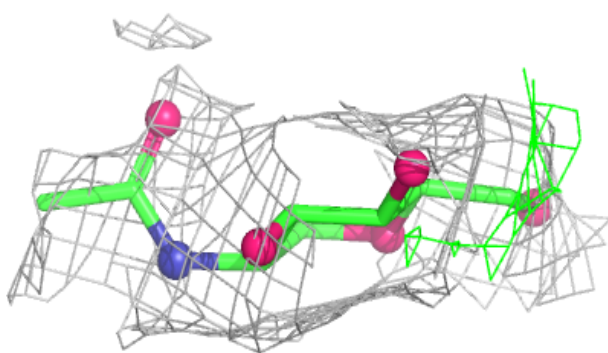
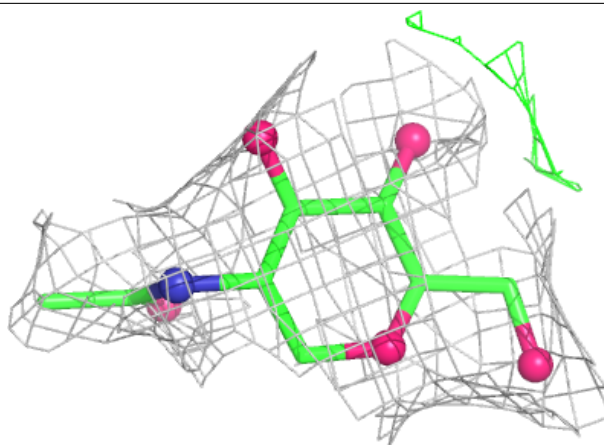
**Electron density around NAG B 601:**

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



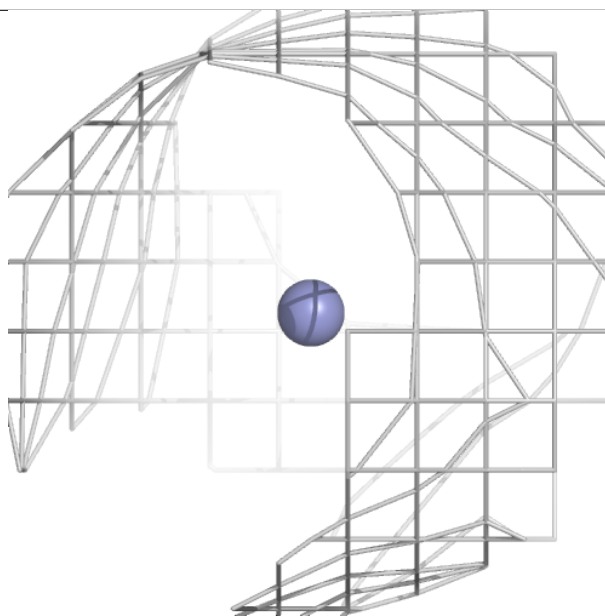
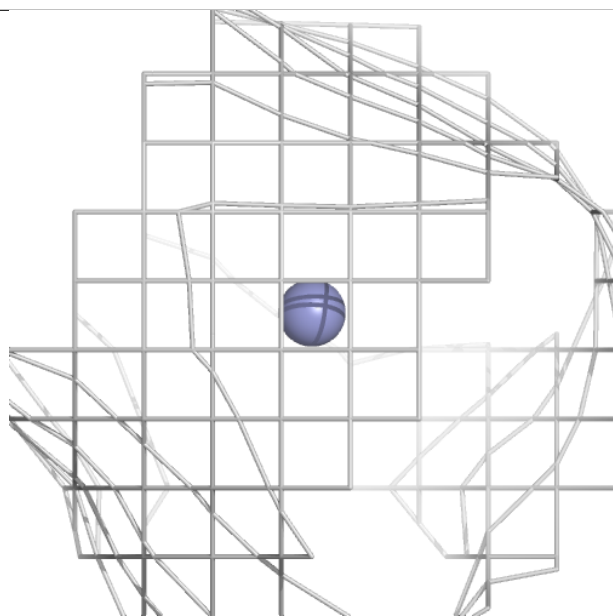
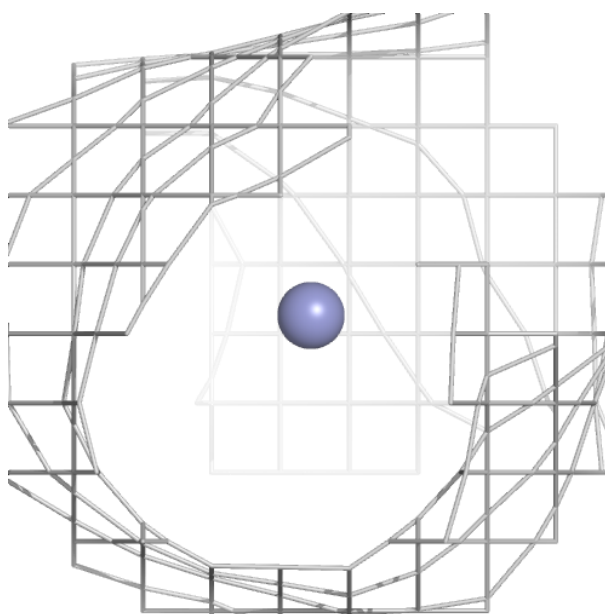
Electron density around NAG C 904:

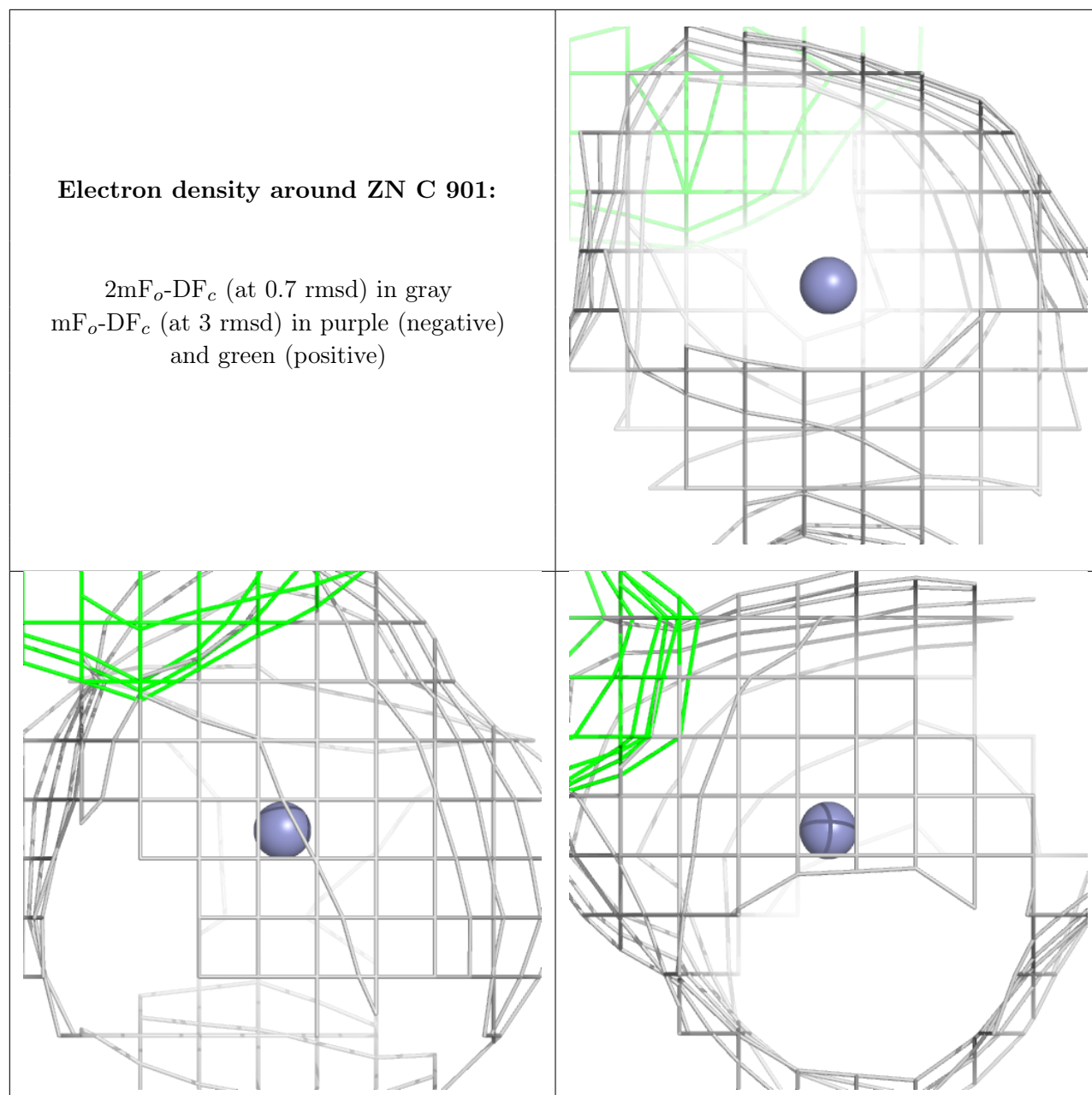
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN A 901:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.