



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 11:15 PM JST

PDB ID : 7Y3U
Title : Crystal structure of the complex of Lactoperoxidase with Nitric oxide at 2.50Å resolution
Authors : Singh, P.K.; Viswanathan, V.; Ahmad, N.; Rani, C.; Sharma, P.; Sharma, S.; Singh, T.P.
Deposited on : 2022-06-13
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

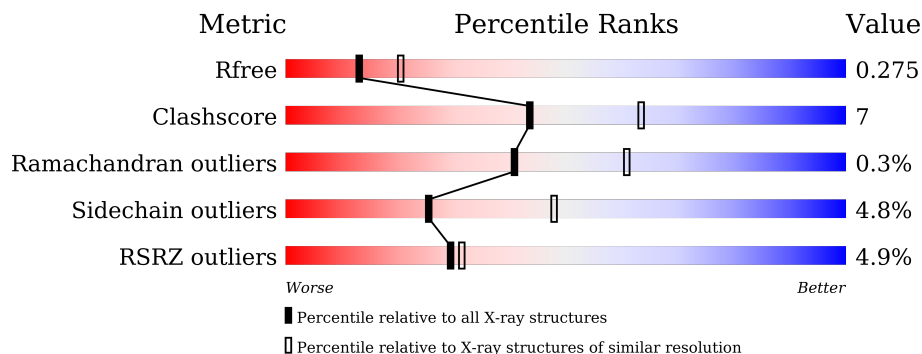
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

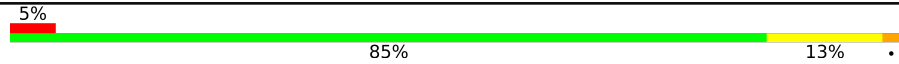

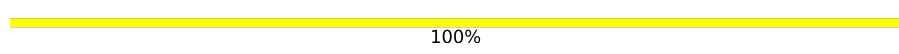

The reported resolution of this entry is 2.50 Å.

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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	595	 5% 85% 13% .
1	B	595	 5% 86% 12% .
2	C	3	 100%
2	D	3	 33% 67%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 9986 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 Lactoperoxidase.

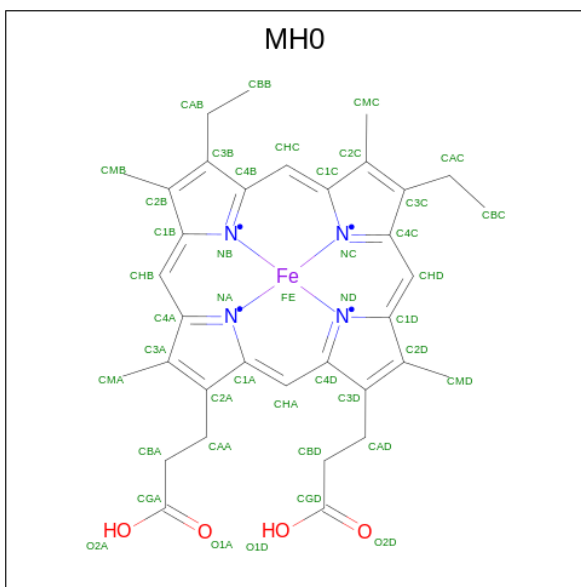
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	595	4771	3037	847	861	26	0	0	0
1	B	595	4771	3037	847	861	26	0	0	0

- Molecule 2 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
			Total	C	N	O			
2	C	3	39	22	2	15	0	0	0
2	D	3	39	22	2	15	0	0	0

- Molecule 3 is MesoHEME (three-letter code: MH0) (formula: $C_{34}H_{36}FeN_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

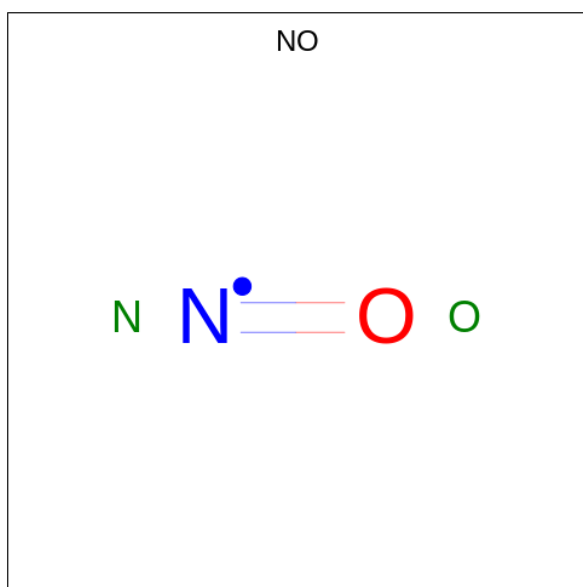
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



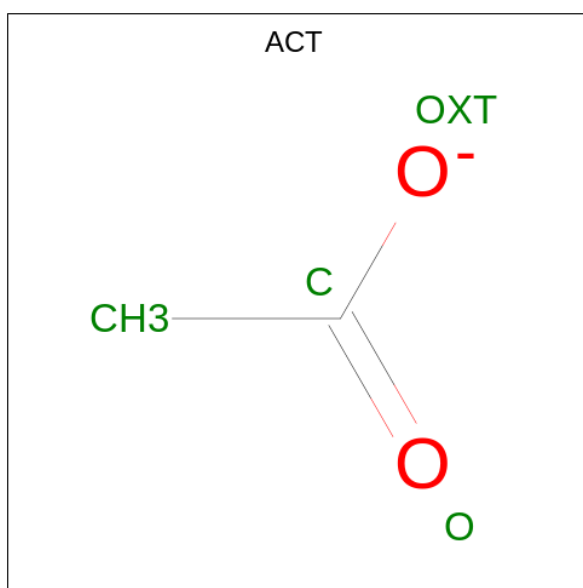
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	14	8	1	5	0	0
6	A	1	14	8	1	5	0	0
6	A	1	14	8	1	5	0	0
6	B	1	14	8	1	5	0	0
6	B	1	14	8	1	5	0	0
6	B	1	14	8	1	5	0	0

- Molecule 7 is NITRIC OXIDE (three-letter code: NO) (formula: NO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	N	O	0	0
			2	1	1		
7	B	1	Total	N	O	0	0
			2	1	1		

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			4	2	2		

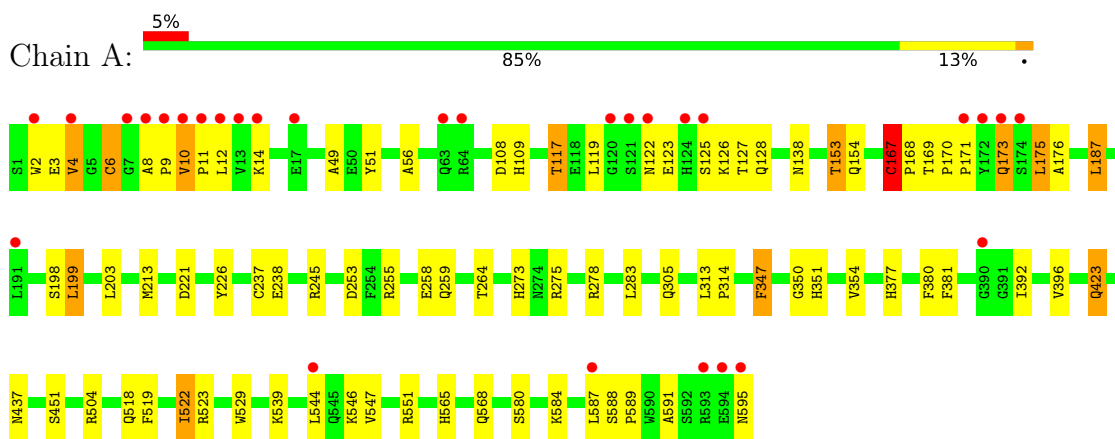
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	101	Total 101	O 101	0	0
9	B	84	Total 84	O 84	0	0

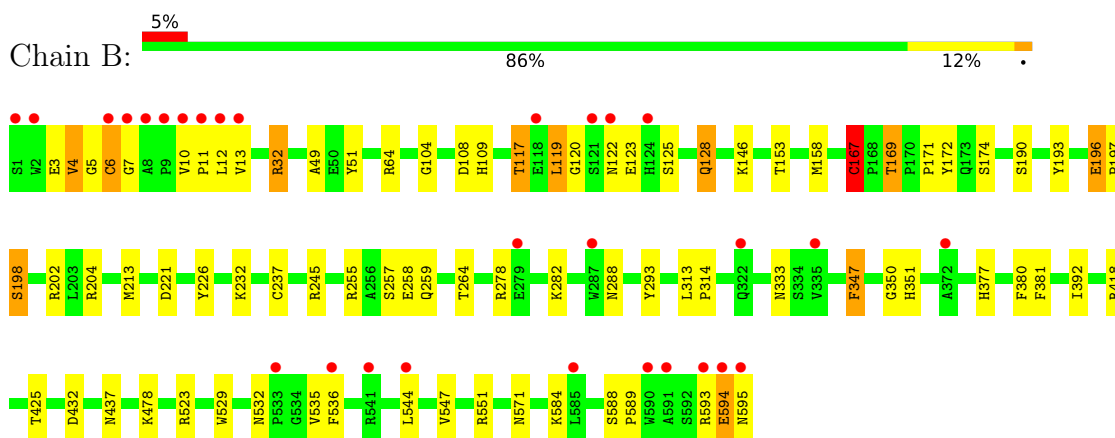
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Lactoperoxidase



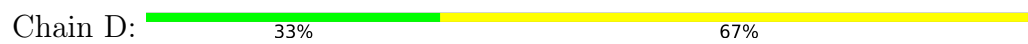
- Molecule 1: Lactoperoxidase



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



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



MAG1
MAG2
BMA3

4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.73Å 93.17Å 82.32Å 90.00° 91.20° 90.00°	Depositor
Resolution (Å)	48.86 – 2.50 48.86 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.86-2.50) 98.9 (48.86-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.219 , 0.277 0.219 , 0.275	Depositor DCC
R_{free} test set	2105 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	48.7	Xtrriage
Anisotropy	0.005	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 35.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.000 for l,k,-h 0.035 for h,-k,-l 0.021 for l,-k,h	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9986	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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: CL, BMA, CA, NO, ACT, NAG, MH0

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	0.66	0/4899	0.77	0/6645
1	B	0.65	0/4899	0.77	0/6645
All	All	0.65	0/9798	0.77	0/13290

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	119	LEU	Peptide
1	B	167	CYS	Peptide

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	4771	0	4687	72	0
1	B	4771	0	4688	62	0
2	C	39	0	33	0	0
2	D	39	0	34	0	0
3	A	43	0	34	16	0
3	B	43	0	34	13	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
6	A	42	0	38	0	0
6	B	42	0	39	0	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
8	B	4	0	3	0	0
9	A	101	0	0	3	0
9	B	84	0	0	2	0
All	All	9986	0	9590	130	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 7.

All (130) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:GLU:OE2	3:A:601:MH0:H15	1.21	1.38
1:B:258:GLU:OE2	3:B:602:MH0:H15	1.24	1.37
1:A:108:ASP:OD2	3:A:601:MH0:H31	1.07	1.24
1:B:5:GLY:O	1:B:167:CYS:HA	1.35	1.22
1:B:108:ASP:OD2	3:B:602:MH0:H31	1.05	1.19
1:A:108:ASP:OD2	3:A:601:MH0:CMD	1.93	1.17
1:B:108:ASP:OD2	3:B:602:MH0:CMD	1.95	1.12
1:A:108:ASP:CG	3:A:601:MH0:H31	1.79	1.02
1:A:170:PRO:HD3	1:B:197:PRO:HG2	1.40	1.02
1:B:108:ASP:CG	3:B:602:MH0:H31	1.80	1.00
1:A:258:GLU:OE2	3:A:601:MH0:CMB	2.11	0.97
1:B:258:GLU:OE2	3:B:602:MH0:CMB	2.15	0.94
1:B:5:GLY:O	1:B:167:CYS:CA	2.17	0.90
1:A:259:GLN:HG2	3:A:601:MH0:H20	1.56	0.87
1:B:258:GLU:CD	3:B:602:MH0:H15	1.96	0.86
1:A:258:GLU:CD	3:A:601:MH0:H15	1.95	0.85
1:B:351:HIS:HD1	1:B:437:ASN:HD21	1.31	0.78
1:A:351:HIS:HD1	1:A:437:ASN:HD21	1.31	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:CYS:HB2	1:A:168:PRO:CD	2.16	0.76
1:A:170:PRO:CD	1:B:197:PRO:HG2	2.17	0.75
1:A:2:TRP:CE3	1:A:6:CYS:HA	2.22	0.75
1:A:8:ALA:HB2	1:A:167:CYS:N	2.02	0.74
1:B:169:THR:HG23	1:B:171:PRO:HD2	1.74	0.70
1:A:167:CYS:HB2	1:A:168:PRO:HD3	1.75	0.67
1:B:122:ASN:O	9:B:901:HOH:O	2.13	0.66
1:B:532:ASN:O	1:B:535:VAL:HG22	1.95	0.66
9:A:1069:HOH:O	1:B:12:LEU:HD21	1.95	0.66
1:A:519:PHE:HA	1:A:522:ILE:CD1	2.26	0.65
1:A:350:GLY:HA3	3:A:601:MH0:H27	1.79	0.64
3:A:601:MH0:H28	3:A:601:MH0:H21	1.78	0.64
1:A:8:ALA:HB2	1:A:167:CYS:H	1.62	0.64
1:B:588:SER:OG	1:B:589:PRO:HD3	1.99	0.63
1:A:588:SER:OG	1:A:589:PRO:HD3	1.99	0.62
1:A:8:ALA:HB1	1:A:9:PRO:HD2	1.82	0.62
3:A:601:MH0:H21	3:A:601:MH0:CBC	2.30	0.61
1:A:168:PRO:HB3	1:B:198:SER:HB3	1.84	0.60
1:A:2:TRP:O	1:A:6:CYS:N	2.34	0.60
3:B:602:MH0:H13	3:B:602:MH0:CBB	2.31	0.60
1:B:196:GLU:OE1	1:B:198:SER:OG	2.15	0.59
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.84	0.59
1:A:170:PRO:HG3	1:B:197:PRO:HD2	1.85	0.58
1:B:120:GLY:O	1:B:123:GLU:HB2	2.03	0.58
1:B:204:ARG:HD2	1:B:293:TYR:CE2	2.39	0.58
1:B:32:ARG:NH2	1:B:333:ASN:HB2	2.19	0.58
1:A:123:GLU:OE2	1:B:13:VAL:HG22	2.04	0.58
1:A:167:CYS:CB	1:A:168:PRO:CD	2.81	0.57
1:A:354:VAL:HG21	3:A:601:MH0:H17	1.86	0.57
1:B:5:GLY:O	1:B:167:CYS:N	2.37	0.57
1:B:593:ARG:O	1:B:594:GLU:HG2	2.04	0.57
1:B:551:ARG:HD3	1:B:584:LYS:HA	1.86	0.57
3:B:602:MH0:H13	3:B:602:MH0:H20	1.87	0.57
1:B:259:GLN:HG2	3:B:602:MH0:H20	1.86	0.57
1:A:171:PRO:HD2	1:B:10:VAL:HG13	1.87	0.56
1:A:519:PHE:O	1:A:522:ILE:HD13	2.06	0.55
1:A:171:PRO:HD2	1:B:10:VAL:CG1	2.36	0.55
1:A:3:GLU:HG3	1:A:4:VAL:HG23	1.89	0.54
1:A:126:LYS:HG3	1:A:127:THR:N	2.23	0.54
1:B:3:GLU:HG3	1:B:4:VAL:HG23	1.90	0.53
1:A:565:HIS:O	1:A:568:GLN:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:THR:N	1:A:170:PRO:HD2	2.24	0.53
1:A:283:LEU:HD12	1:A:591:ALA:HB2	1.92	0.52
1:A:199:LEU:HD22	1:A:203:LEU:CD1	2.41	0.51
1:A:2:TRP:HB2	1:B:202:ARG:HE	1.76	0.51
1:A:168:PRO:HA	1:B:198:SER:HA	1.93	0.51
1:A:237:CYS:HA	1:A:381:PHE:O	2.11	0.50
1:A:56:ALA:HB2	1:A:173:GLN:HG2	1.92	0.50
1:B:237:CYS:HA	1:B:381:PHE:O	2.12	0.49
1:B:125:SER:HA	1:B:128:GLN:HB2	1.94	0.49
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.48	0.49
1:B:193:TYR:HD1	1:B:213:MET:HE1	1.77	0.49
1:B:529:TRP:O	1:B:535:VAL:HG21	2.13	0.49
1:B:3:GLU:HB3	1:B:117:THR:HG22	1.94	0.49
1:A:10:VAL:HG23	1:A:12:LEU:HD12	1.94	0.48
1:A:169:THR:N	1:A:170:PRO:CD	2.77	0.48
1:B:221:ASP:HB2	1:B:226:TYR:CZ	2.47	0.48
1:A:167:CYS:SG	1:A:168:PRO:HD2	2.53	0.48
1:A:350:GLY:CA	3:A:601:MH0:H27	2.43	0.48
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.48	0.48
1:A:264:THR:HG23	1:A:392:ILE:HB	1.96	0.48
1:B:347:PHE:O	3:B:602:MH0:H25	2.14	0.47
1:A:3:GLU:O	1:A:4:VAL:HB	2.15	0.47
1:A:125:SER:HA	1:A:128:GLN:HB3	1.97	0.47
1:B:350:GLY:HA3	3:B:602:MH0:H27	1.96	0.46
1:A:519:PHE:HA	1:A:522:ILE:HD13	1.98	0.46
1:B:158:MET:SD	9:B:951:HOH:O	2.61	0.46
1:B:535:VAL:HG23	1:B:536:PHE:N	2.29	0.46
1:B:377:HIS:HA	1:B:380:PHE:CE2	2.50	0.46
1:B:104:GLY:HA3	3:B:602:MH0:H28	1.97	0.46
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.51	0.46
1:B:120:GLY:O	1:B:123:GLU:CB	2.64	0.46
1:B:523:ARG:HG3	1:B:529:TRP:CE2	2.51	0.46
1:B:544:LEU:O	1:B:547:VAL:HG22	2.16	0.46
1:A:8:ALA:HA	1:A:167:CYS:HA	1.98	0.46
1:B:213:MET:CE	1:B:293:TYR:CE2	2.99	0.46
1:B:264:THR:HG23	1:B:392:ILE:HB	1.97	0.45
1:A:8:ALA:HB1	1:A:9:PRO:CD	2.46	0.45
1:B:109:HIS:HA	1:B:255:ARG:NH2	2.31	0.45
3:B:602:MH0:H21	3:B:602:MH0:CBC	2.47	0.45
1:A:109:HIS:HA	1:A:255:ARG:NH2	2.31	0.45
1:A:544:LEU:O	1:A:547:VAL:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:THR:HB	1:B:12:LEU:HD22	1.98	0.45
1:B:169:THR:CG2	1:B:171:PRO:HD2	2.44	0.45
1:A:253:ASP:HA	9:A:1021:HOH:O	2.16	0.44
1:B:213:MET:HE2	1:B:293:TYR:CE2	2.52	0.44
1:A:313:LEU:N	1:A:314:PRO:CD	2.80	0.44
1:A:4:VAL:O	1:A:4:VAL:HG12	2.17	0.44
3:A:601:MH0:H13	3:A:601:MH0:CBB	2.48	0.44
1:B:49:ALA:HB1	1:B:51:TYR:CE2	2.53	0.43
1:A:49:ALA:HB1	1:A:51:TYR:CE2	2.54	0.43
1:B:10:VAL:HB	1:B:11:PRO:HD3	2.01	0.43
1:B:313:LEU:N	1:B:314:PRO:CD	2.81	0.43
1:B:123:GLU:OE1	1:B:125:SER:HB2	2.19	0.43
1:B:5:GLY:C	1:B:167:CYS:HA	2.25	0.43
1:A:167:CYS:CB	1:A:168:PRO:HD2	2.49	0.43
1:A:347:PHE:O	3:A:601:MH0:H25	2.19	0.42
1:B:6:CYS:SG	1:B:7:GLY:HA3	2.59	0.42
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.55	0.42
1:A:153:THR:HG22	1:A:154:GLN:HG3	2.01	0.42
1:A:187:LEU:HD13	1:A:305:GLN:HA	2.00	0.42
1:A:175:LEU:HD23	1:A:176:ALA:H	1.84	0.42
1:A:238:GLU:HB2	1:A:245:ARG:HA	2.01	0.42
1:B:418:ARG:O	1:B:432:ASP:HA	2.20	0.41
1:A:11:PRO:O	1:B:288:ASN:ND2	2.53	0.41
1:A:138:ASN:HB2	9:A:1047:HOH:O	2.20	0.41
1:B:257:SER:O	1:B:381:PHE:HA	2.21	0.41
1:A:423:GLN:HE21	1:A:423:GLN:HA	1.85	0.41
1:A:392:ILE:O	1:A:396:VAL:HG23	2.21	0.41
1:A:518:GLN:O	1:A:522:ILE:HG23	2.21	0.40
1:A:108:ASP:OD1	3:A:601:MH0:H31	2.15	0.40
3:A:601:MH0:H13	3:A:601:MH0:H19	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	593/595 (100%)	558 (94%)	33 (6%)	2 (0%)	41	61
1	B	593/595 (100%)	565 (95%)	27 (5%)	1 (0%)	47	68
All	All	1186/1190 (100%)	1123 (95%)	60 (5%)	3 (0%)	41	61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
1	A	167	CYS
1	B	4	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	518/518 (100%)	493 (95%)	25 (5%)	25	48
1	B	518/518 (100%)	493 (95%)	25 (5%)	25	48
All	All	1036/1036 (100%)	986 (95%)	50 (5%)	25	48

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	CYS
1	A	10	VAL
1	A	14	LYS
1	A	117	THR
1	A	119	LEU
1	A	122	ASN
1	A	153	THR
1	A	167	CYS
1	A	173	GLN
1	A	175	LEU

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Mol	Chain	Res	Type
1	A	187	LEU
1	A	198	SER
1	A	199	LEU
1	A	275	ARG
1	A	278	ARG
1	A	347	PHE
1	A	423	GLN
1	A	451	SER
1	A	504	ARG
1	A	522	ILE
1	A	539	LYS
1	A	546	LYS
1	A	580	SER
1	A	587	LEU
1	A	595	ASN
1	B	6	CYS
1	B	32	ARG
1	B	64	ARG
1	B	117	THR
1	B	119	LEU
1	B	128	GLN
1	B	146	LYS
1	B	153	THR
1	B	167	CYS
1	B	169	THR
1	B	172	TYR
1	B	174	SER
1	B	190	SER
1	B	196	GLU
1	B	198	SER
1	B	232	LYS
1	B	245	ARG
1	B	278	ARG
1	B	282	LYS
1	B	347	PHE
1	B	425	THR
1	B	478	LYS
1	B	571	ASN
1	B	594	GLU
1	B	595	ASN

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

Mol	Chain	Res	Type
1	A	423	GLN
1	A	595	ASN
1	B	63	GLN
1	B	138	ASN
1	B	273	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

6 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	$\# Z > 2$
2	NAG	C	1	2,1	14,14,15	0.48	0	17,19,21	1.79	2 (11%)
2	NAG	C	2	2	14,14,15	0.67	0	17,19,21	1.63	5 (29%)
2	BMA	C	3	2	11,11,12	0.60	0	15,15,17	1.16	1 (6%)
2	NAG	D	1	2,1	14,14,15	0.43	0	17,19,21	0.98	0
2	NAG	D	2	2	14,14,15	0.78	0	17,19,21	1.54	4 (23%)
2	BMA	D	3	2	11,11,12	1.01	0	15,15,17	1.74	3 (20%)

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	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C3-C4-C5	4.87	118.94	110.24
2	D	2	NAG	C4-C3-C2	4.41	117.48	111.02
2	C	1	NAG	C1-O5-C5	4.28	117.98	112.19
2	D	3	BMA	C1-C2-C3	3.68	114.19	109.67
2	C	3	BMA	C3-C4-C5	3.32	116.16	110.24
2	D	3	BMA	O4-C4-C3	-3.04	103.32	110.35
2	D	3	BMA	C3-C4-C5	3.03	115.64	110.24
2	C	2	NAG	O5-C5-C4	-3.02	103.49	110.83
2	C	2	NAG	O5-C5-C6	2.71	111.46	107.20
2	C	2	NAG	C3-C4-C5	2.60	114.87	110.24
2	C	2	NAG	C4-C3-C2	2.44	114.59	111.02
2	D	2	NAG	O5-C5-C6	-2.10	103.91	107.20
2	D	2	NAG	C3-C4-C5	2.06	113.91	110.24
2	C	2	NAG	C1-O5-C5	-2.05	109.42	112.19
2	D	2	NAG	O5-C1-C2	2.03	114.49	111.29

There are no chirality outliers.

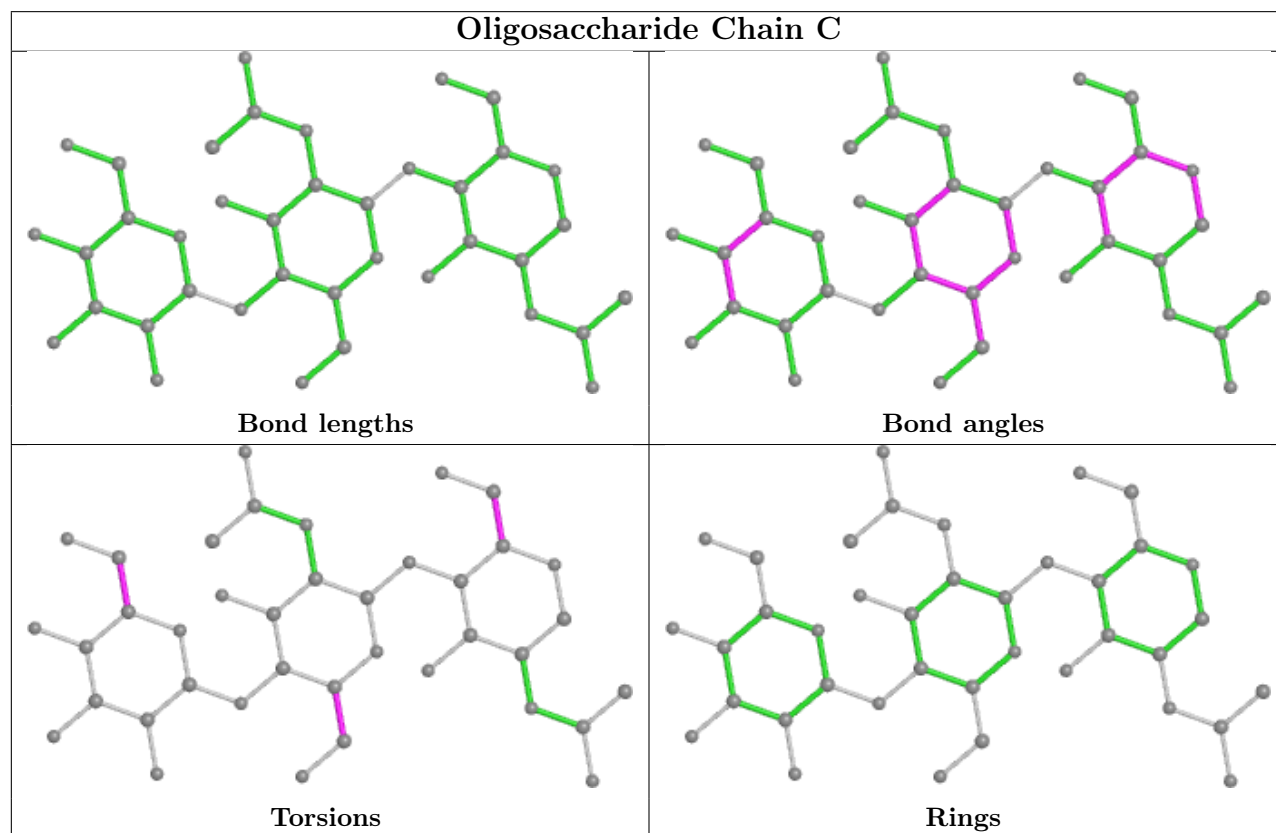
All (8) torsion outliers are listed below:

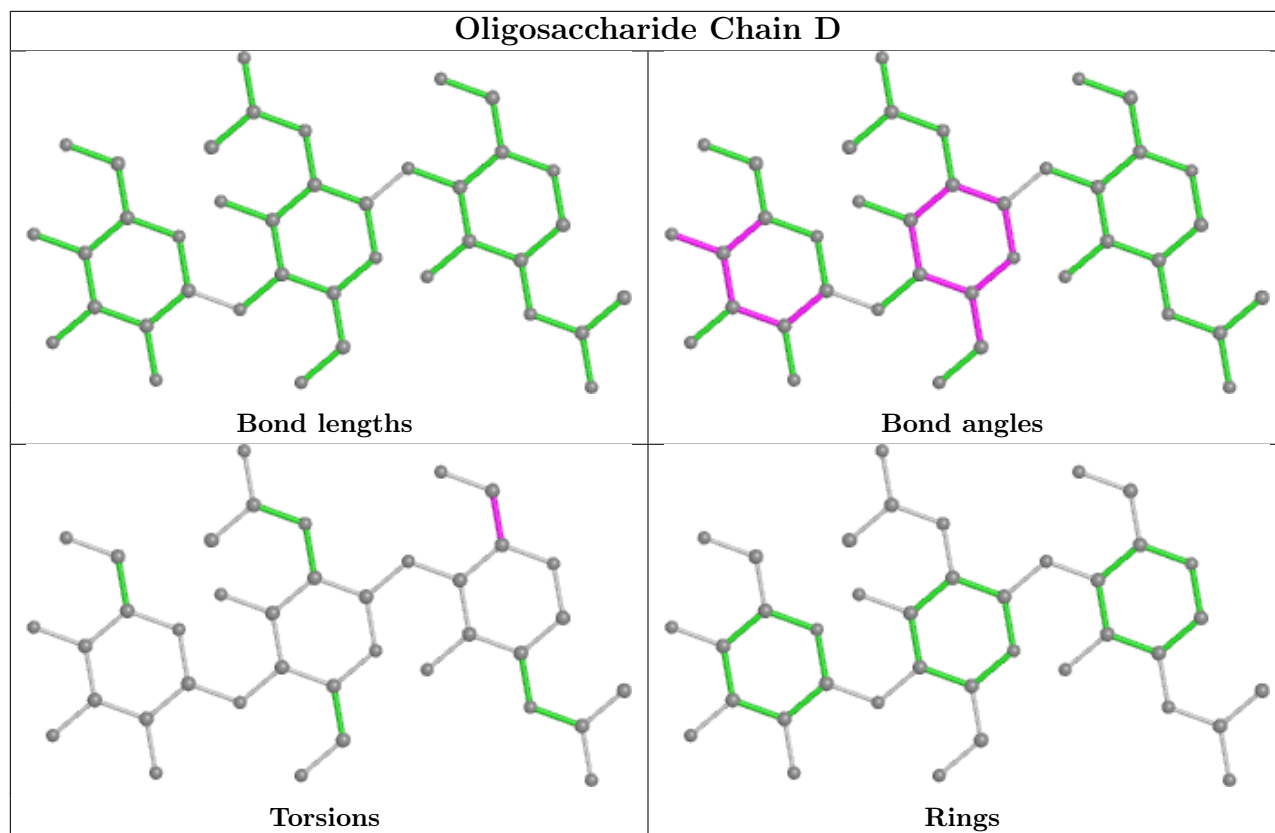
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 3 are monoatomic - leaving 11 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	A	606	1	14,14,15	1.52	1 (7%)	17,19,21	1.58	3 (17%)
3	MH0	A	601	1,7	50,50,50	1.70	11 (22%)	68,82,82	1.83	20 (29%)
6	NAG	A	605	1	14,14,15	0.71	0	17,19,21	2.06	3 (17%)
6	NAG	B	605	1	14,14,15	0.72	0	17,19,21	1.28	1 (5%)
7	NO	B	607	3	0,1,1	-	-	-		
8	ACT	B	601	-	3,3,3	1.01	0	3,3,3	0.73	0
3	MH0	B	602	1,7	50,50,50	1.70	10 (20%)	68,82,82	1.75	15 (22%)
6	NAG	B	604	1	14,14,15	0.44	0	17,19,21	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	604	1	14,14,15	0.70	0	17,19,21	1.93	3 (17%)
7	NO	A	607	3	0,1,1	-	-	-		
6	NAG	B	606	1	14,14,15	0.34	0	17,19,21	0.93	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	A	606	1	-	2/6/23/26	0/1/1/1
3	MH0	A	601	1,7	-	8/14/54/54	-
6	NAG	A	605	1	-	0/6/23/26	0/1/1/1
6	NAG	B	605	1	-	2/6/23/26	0/1/1/1
3	MH0	B	602	1,7	-	8/14/54/54	-
6	NAG	B	604	1	-	2/6/23/26	0/1/1/1
6	NAG	A	604	1	-	1/6/23/26	0/1/1/1
6	NAG	B	606	1	-	0/6/23/26	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	606	NAG	C1-C2	-5.04	1.44	1.52
3	B	602	MH0	C1B-NB	-4.56	1.32	1.40
3	A	601	MH0	CBC-CAC	-4.31	1.32	1.51
3	A	601	MH0	CBB-CAB	-4.10	1.33	1.51
3	A	601	MH0	C1B-NB	-4.10	1.33	1.40
3	B	602	MH0	CBB-CAB	-4.06	1.33	1.51
3	B	602	MH0	CBC-CAC	-3.91	1.34	1.51
3	A	601	MH0	C1C-NC	-3.71	1.33	1.40
3	B	602	MH0	C1A-C2A	-3.44	1.39	1.45
3	B	602	MH0	FE-NB	3.12	2.12	1.96
3	B	602	MH0	C1D-ND	-3.03	1.35	1.40
3	A	601	MH0	FE-NB	2.70	2.10	1.96
3	B	602	MH0	C1C-C2C	-2.60	1.39	1.44
3	A	601	MH0	C4B-NB	-2.53	1.33	1.38
3	A	601	MH0	FE-NC	2.45	2.09	1.96
3	A	601	MH0	C4D-C3D	2.44	1.49	1.45
3	B	602	MH0	C1C-NC	-2.42	1.36	1.40
3	A	601	MH0	C1C-C2C	-2.40	1.39	1.44
3	B	602	MH0	FE-NC	2.36	2.08	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	MH0	C1A-C2A	-2.30	1.41	1.45
3	A	601	MH0	C1D-ND	-2.23	1.36	1.40
3	B	602	MH0	C4B-NB	-2.21	1.34	1.38

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	604	NAG	C1-O5-C5	5.97	120.27	112.19
6	A	605	NAG	C1-O5-C5	5.93	120.23	112.19
3	B	602	MH0	CBB-CAB-C3B	4.52	124.89	112.43
3	A	601	MH0	CHC-C4B-NB	4.46	129.27	124.42
3	A	601	MH0	CBB-CAB-C3B	4.36	124.45	112.43
3	B	602	MH0	CBC-CAC-C3C	4.25	124.15	112.43
3	B	602	MH0	CHC-C4B-NB	4.15	128.93	124.42
3	A	601	MH0	C1B-NB-C4B	3.83	109.03	105.07
6	A	606	NAG	O5-C1-C2	3.77	117.24	111.29
3	A	601	MH0	CBC-CAC-C3C	3.76	122.79	112.43
3	A	601	MH0	CMD-C2D-C1D	3.70	130.67	125.04
3	B	602	MH0	CMD-C2D-C1D	3.48	130.34	125.04
6	B	605	NAG	C1-O5-C5	3.42	116.83	112.19
3	B	602	MH0	CHA-C4D-ND	3.36	128.07	124.42
6	A	606	NAG	C4-C3-C2	3.34	115.91	111.02
6	A	605	NAG	C3-C4-C5	-3.33	104.30	110.24
6	A	604	NAG	O5-C5-C4	3.28	118.82	110.83
3	A	601	MH0	CAD-C3D-C4D	3.20	130.26	124.66
3	A	601	MH0	CAB-C3B-C2B	3.16	132.94	127.53
3	B	602	MH0	C1B-NB-C4B	3.03	108.21	105.07
3	A	601	MH0	CHA-C4D-C3D	-2.98	120.46	124.84
3	A	601	MH0	CHA-C4D-ND	2.96	127.63	124.42
3	A	601	MH0	CHC-C4B-C3B	-2.93	120.53	124.84
3	B	602	MH0	CHC-C4B-C3B	-2.89	120.58	124.84
3	B	602	MH0	CAD-C3D-C4D	2.82	129.58	124.66
3	A	601	MH0	C1C-NC-C4C	2.73	107.90	105.07
3	B	602	MH0	CHD-C1D-ND	2.64	127.64	124.37
3	A	601	MH0	CHD-C4C-NC	2.59	127.23	124.42
6	A	604	NAG	C6-C5-C4	-2.55	107.02	113.00
3	B	602	MH0	C1C-NC-C4C	2.50	107.66	105.07
6	A	606	NAG	C1-O5-C5	2.49	115.57	112.19
3	B	602	MH0	CAB-C3B-C2B	2.47	131.75	127.53
3	B	602	MH0	CHA-C4D-C3D	-2.46	121.22	124.84
6	A	605	NAG	O7-C7-N2	2.36	126.28	121.95
3	A	601	MH0	CBA-CAA-C2A	-2.29	106.26	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	MH0	CBD-CAD-C3D	-2.18	106.58	112.63
3	A	601	MH0	CHD-C1D-ND	2.18	127.06	124.37
3	B	602	MH0	CHA-C1A-NA	2.14	127.01	124.37
3	B	602	MH0	C4B-C3B-C2B	-2.13	103.80	106.90
3	A	601	MH0	O1D-CGD-O2D	-2.11	118.04	123.30
3	A	601	MH0	C4B-C3B-C2B	-2.08	103.86	106.90
3	A	601	MH0	C3C-C4C-NC	-2.08	108.34	110.36
3	A	601	MH0	CHA-C1A-NA	2.06	126.91	124.37
3	A	601	MH0	O1D-CGD-CBD	2.03	120.54	114.03
3	A	601	MH0	O2A-CGA-O1A	-2.01	118.28	123.30

There are no chirality outliers.

All (23) torsion outliers are listed below:

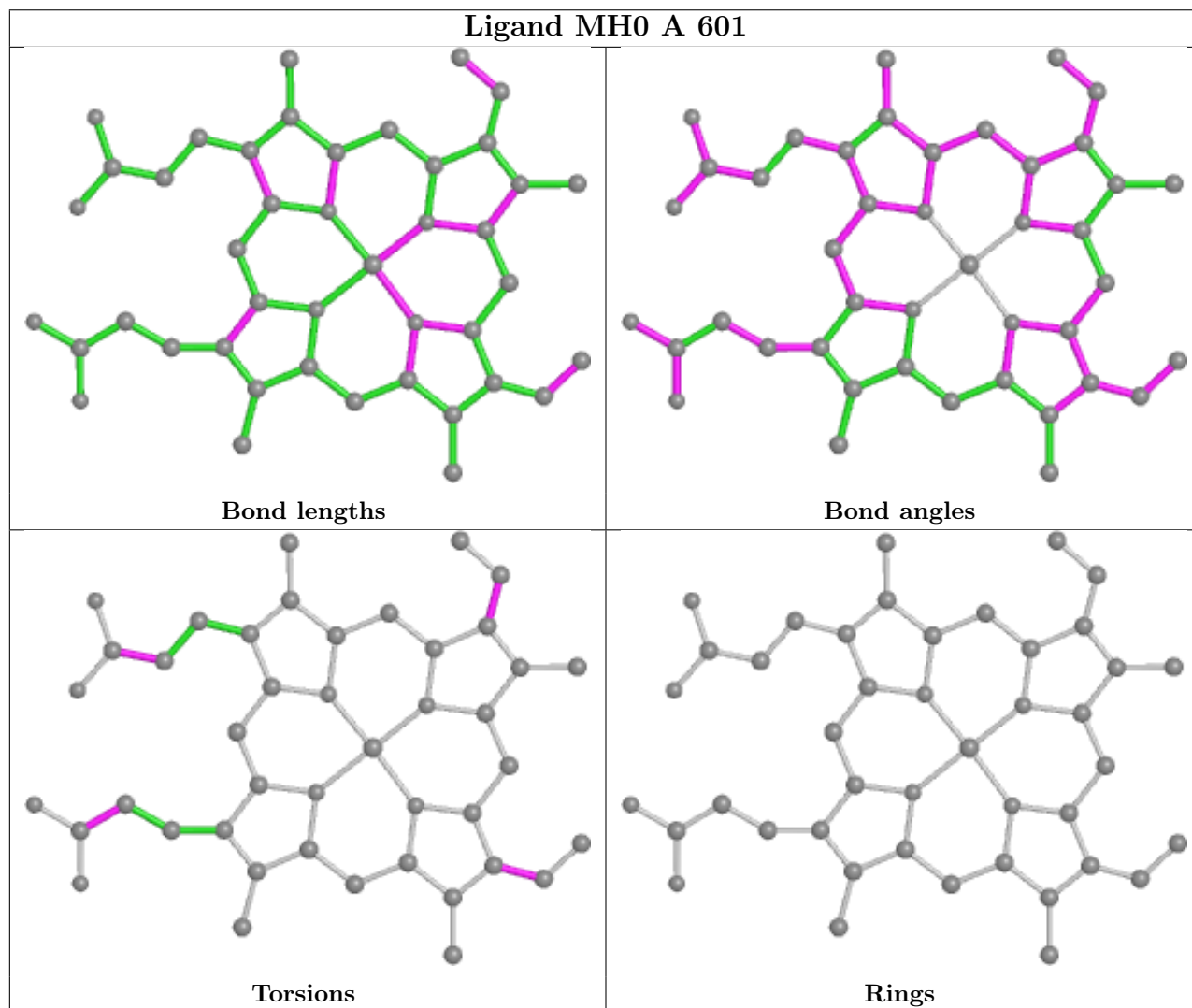
Mol	Chain	Res	Type	Atoms
3	A	601	MH0	C4C-C3C-CAC-CBC
3	B	602	MH0	C2C-C3C-CAC-CBC
3	B	602	MH0	C4C-C3C-CAC-CBC
3	A	601	MH0	C2B-C3B-CAB-CBB
3	B	602	MH0	C2B-C3B-CAB-CBB
6	B	604	NAG	O5-C5-C6-O6
3	A	601	MH0	C4B-C3B-CAB-CBB
3	A	601	MH0	C2C-C3C-CAC-CBC
3	B	602	MH0	C4B-C3B-CAB-CBB
6	A	606	NAG	O5-C5-C6-O6
6	B	604	NAG	C4-C5-C6-O6
6	A	606	NAG	C4-C5-C6-O6
6	B	605	NAG	O5-C5-C6-O6
6	A	604	NAG	C4-C5-C6-O6
6	B	605	NAG	C4-C5-C6-O6
3	B	602	MH0	CAA-CBA-CGA-O1A
3	A	601	MH0	CAA-CBA-CGA-O1A
3	A	601	MH0	CAA-CBA-CGA-O2A
3	A	601	MH0	CAD-CBD-CGD-O2D
3	B	602	MH0	CAA-CBA-CGA-O2A
3	A	601	MH0	CAD-CBD-CGD-O1D
3	B	602	MH0	CAD-CBD-CGD-O1D
3	B	602	MH0	CAD-CBD-CGD-O2D

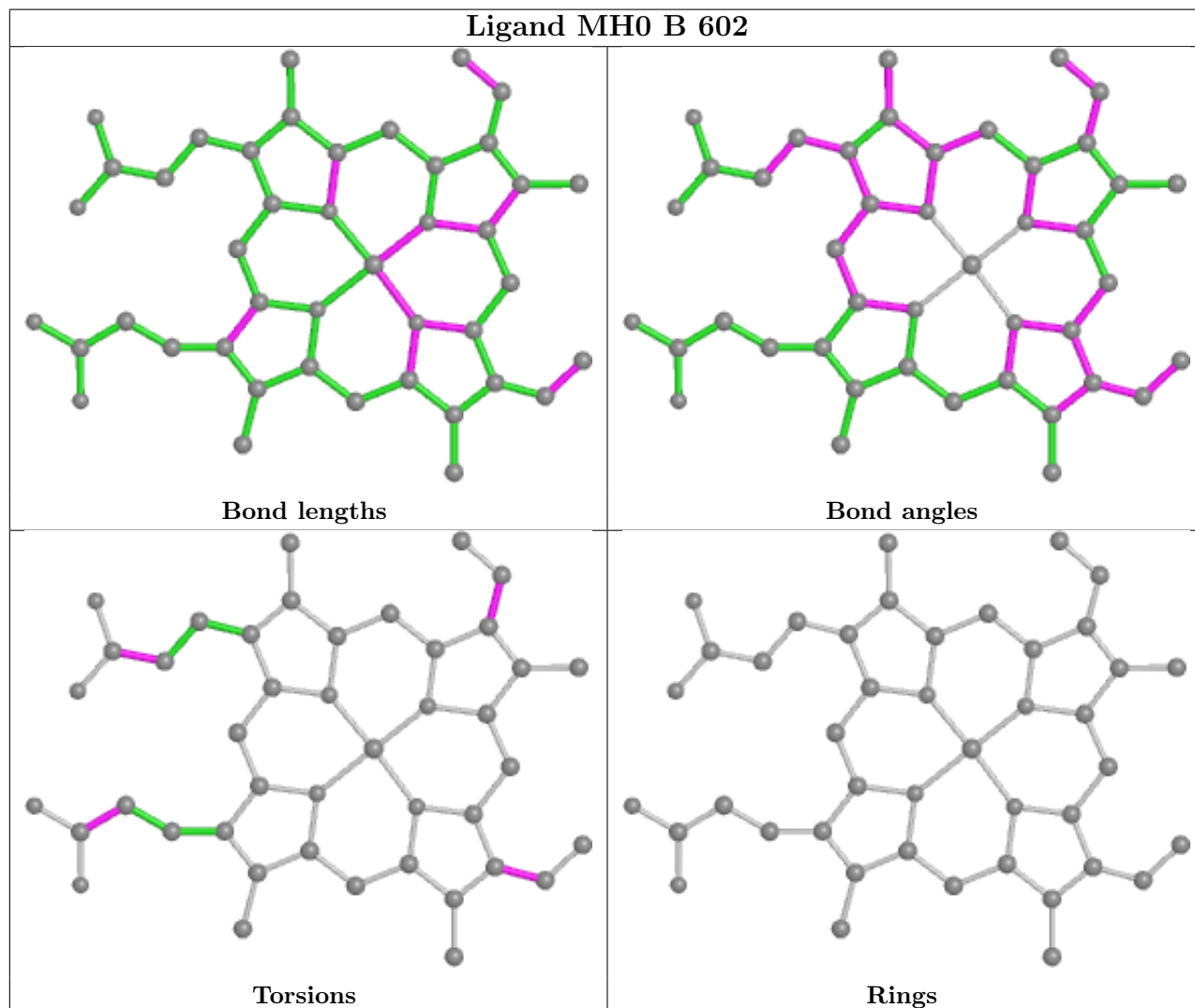
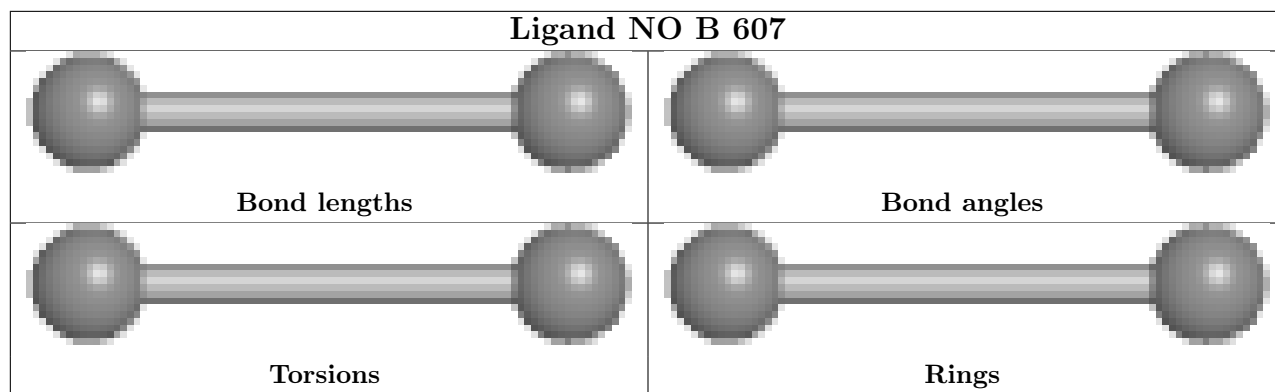
There are no ring outliers.





2 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	MH0	16	0
3	B	602	MH0	13	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 NO A 607	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

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	595/595 (100%)	0.14	29 (4%) 29 31	32, 56, 117, 190	0
1	B	595/595 (100%)	0.17	29 (4%) 29 31	33, 57, 107, 199	0
All	All	1190/1190 (100%)	0.15	58 (4%) 29 31	32, 56, 115, 199	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	13	VAL	11.8
1	A	122	ASN	11.3
1	B	124	HIS	9.0
1	B	11	PRO	8.0
1	B	1	SER	7.8
1	B	10	VAL	7.4
1	A	174	SER	7.2
1	A	595	ASN	6.9
1	B	595	ASN	6.8
1	A	12	LEU	6.7
1	A	594	GLU	6.2
1	B	6	CYS	6.0
1	B	9	PRO	5.8
1	B	121	SER	4.8
1	A	9	PRO	4.7
1	B	7	GLY	4.5
1	A	593	ARG	4.4
1	A	172	TYR	4.4
1	A	173	GLN	4.3
1	B	12	LEU	4.2
1	B	335	VAL	4.2
1	A	7	GLY	4.2
1	A	14	LYS	4.0
1	A	171	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	2	TRP	3.3
1	B	541	ARG	3.2
1	B	13	VAL	3.1
1	A	124	HIS	3.1
1	B	594	GLU	3.1
1	B	591	ALA	3.1
1	A	11	PRO	3.1
1	A	17	GLU	3.0
1	B	8	ALA	3.0
1	B	593	ARG	3.0
1	B	585	LEU	3.0
1	A	64	ARG	3.0
1	B	536	PHE	2.9
1	A	120	GLY	2.7
1	A	10	VAL	2.7
1	A	544	LEU	2.7
1	A	2	TRP	2.6
1	A	8	ALA	2.5
1	B	287	TRP	2.5
1	A	587	LEU	2.5
1	A	63	GLN	2.4
1	A	390	GLY	2.4
1	A	191	LEU	2.3
1	A	125	SER	2.3
1	B	533	PRO	2.3
1	B	122	ASN	2.3
1	B	544	LEU	2.3
1	A	4	VAL	2.2
1	B	279	GLU	2.2
1	B	322	GLN	2.2
1	B	372	ALA	2.2
1	B	118	GLU	2.1
1	A	121	SER	2.1
1	B	590	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

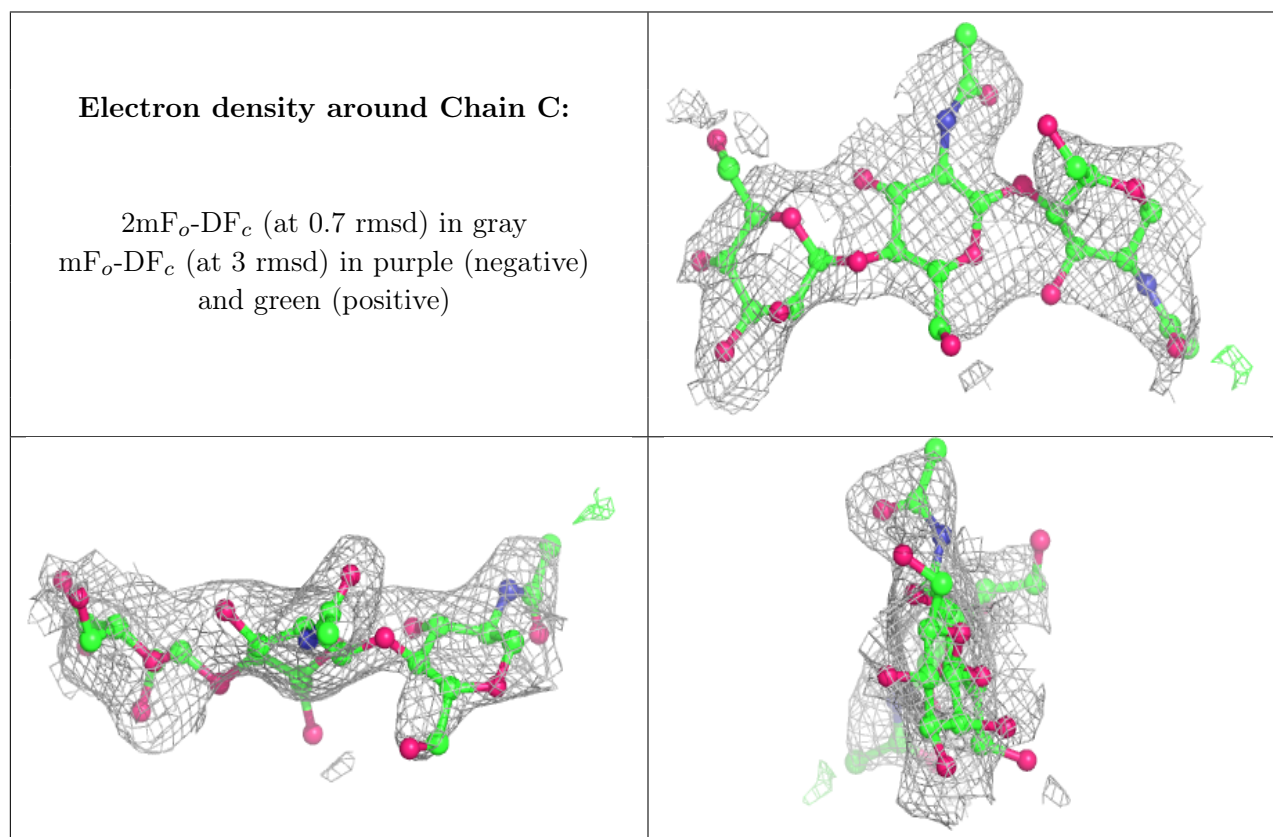
There are no non-standard protein/DNA/RNA residues in this entry.

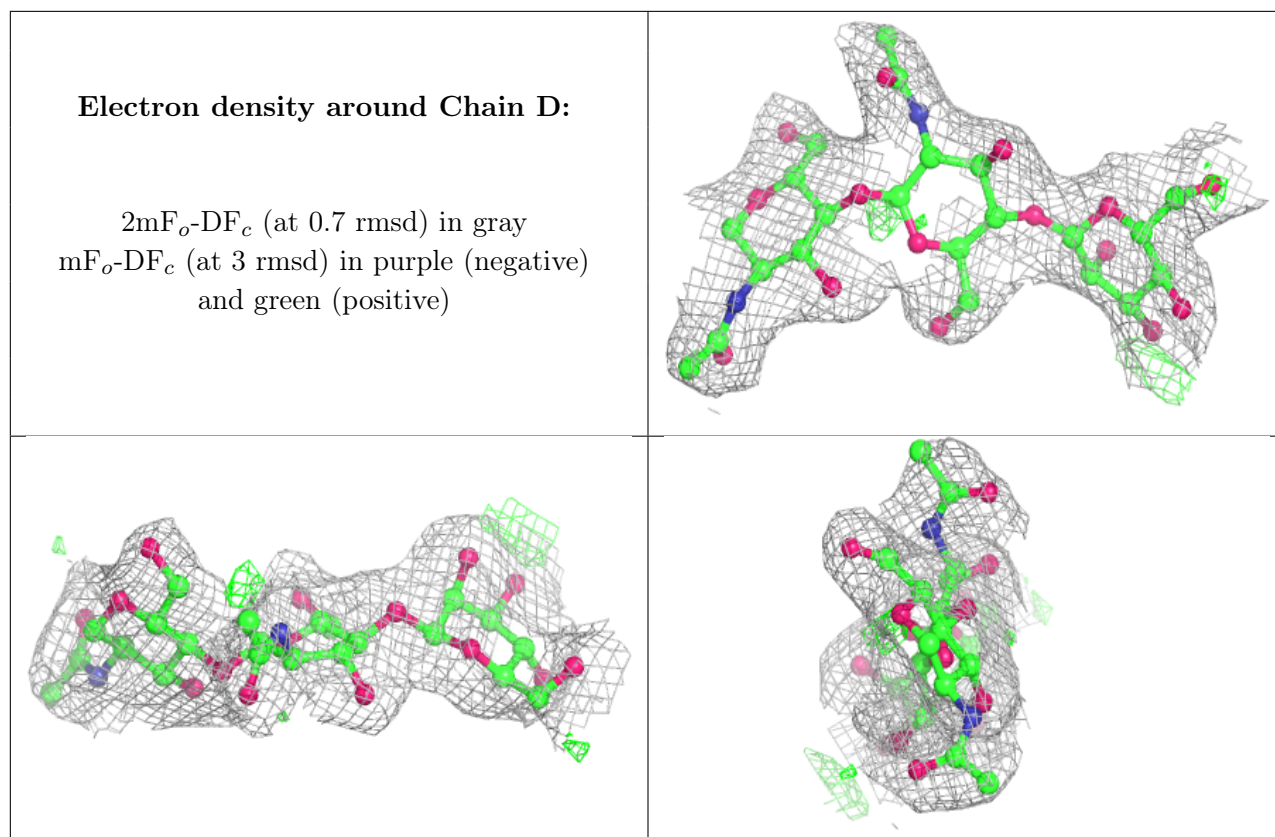
6.3 Carbohydrates [i](#)

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(Å ²)	Q<0.9
2	BMA	C	3	11/12	0.76	0.19	96,113,123,124	0
2	NAG	C	2	14/15	0.77	0.17	82,109,121,129	0
2	NAG	C	1	14/15	0.79	0.18	90,104,116,119	0
2	BMA	D	3	11/12	0.81	0.13	76,85,87,88	0
2	NAG	D	2	14/15	0.85	0.14	81,92,99,102	0
2	NAG	D	1	14/15	0.93	0.09	67,78,82,88	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.



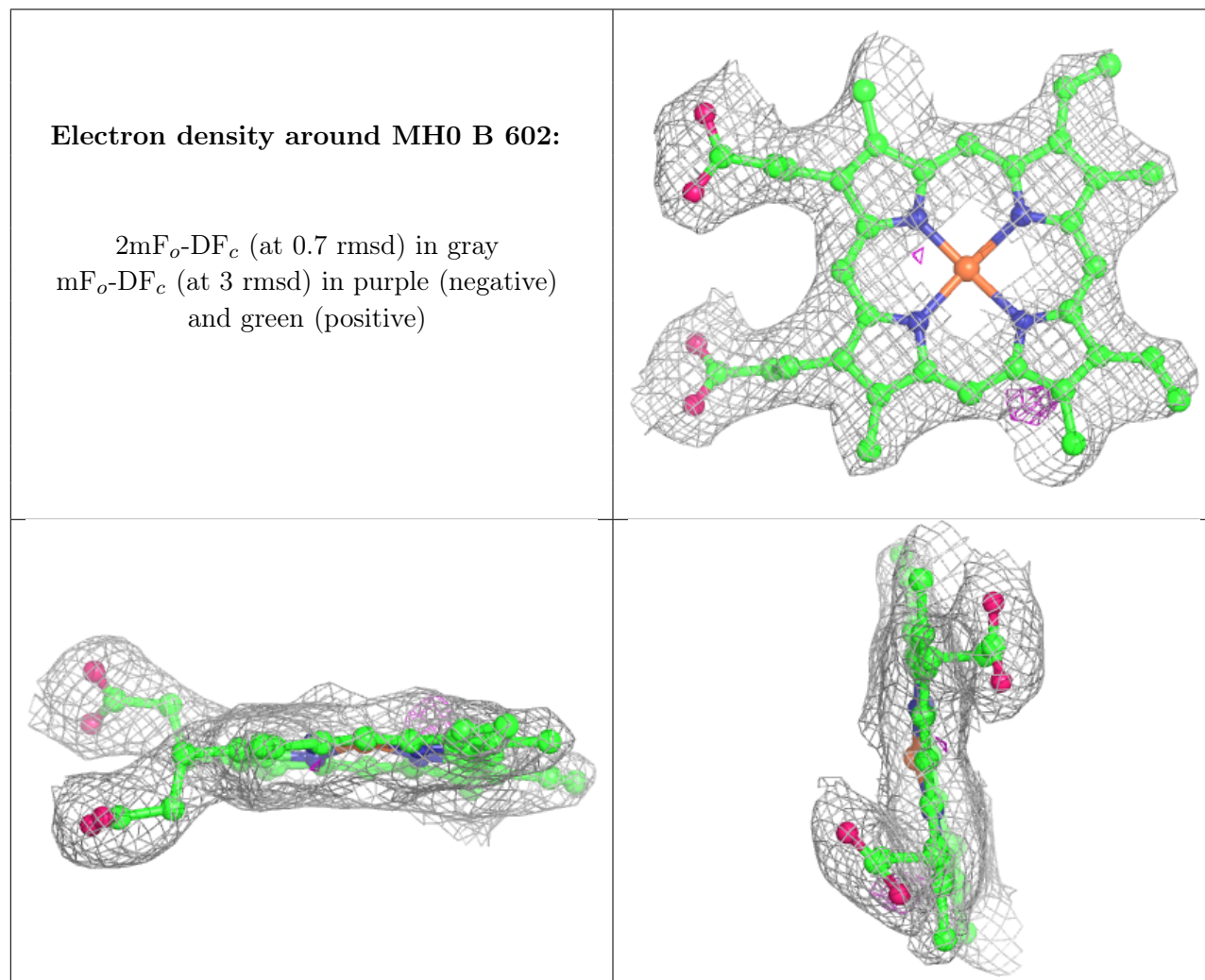


6.4 Ligands [i](#)

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.

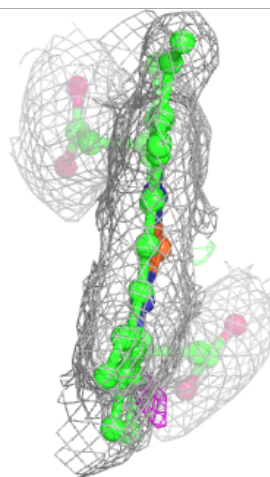
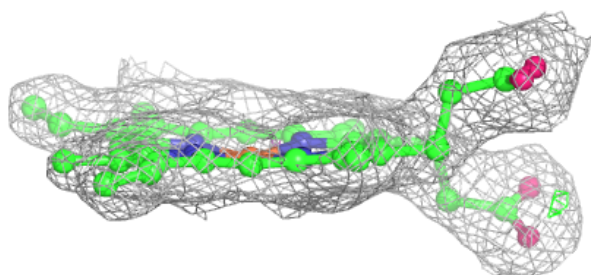
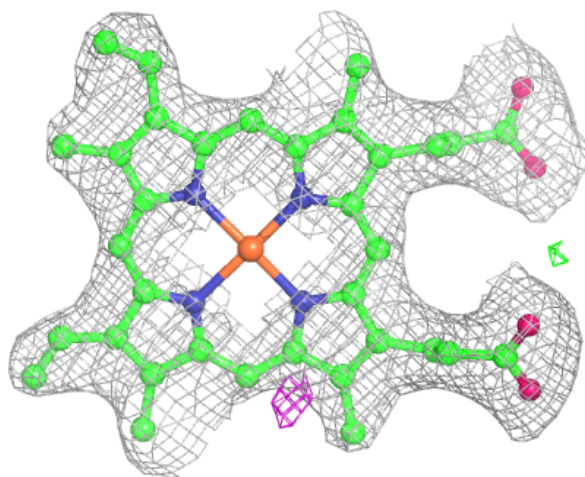
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	A	604	14/15	0.75	0.27	76,87,95,97	0
6	NAG	A	606	14/15	0.78	0.18	73,95,104,105	0
6	NAG	B	604	14/15	0.85	0.16	92,101,106,108	0
6	NAG	B	606	14/15	0.87	0.24	94,111,119,122	0
6	NAG	B	605	14/15	0.88	0.14	60,65,74,80	0
8	ACT	B	601	4/4	0.93	0.21	58,63,64,66	0
6	NAG	A	605	14/15	0.95	0.12	45,49,55,56	0
4	CA	A	602	1/1	0.95	0.10	43,43,43,43	0
5	CL	A	603	1/1	0.98	0.07	48,48,48,48	0
3	MH0	B	602	43/43	0.98	0.14	32,38,42,44	0
3	MH0	A	601	43/43	0.98	0.15	27,37,41,43	0
4	CA	B	603	1/1	0.98	0.08	45,45,45,45	0
7	NO	B	607	2/2	0.99	0.09	55,55,55,60	0
7	NO	A	607	2/2	0.99	0.11	53,53,53,54	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.



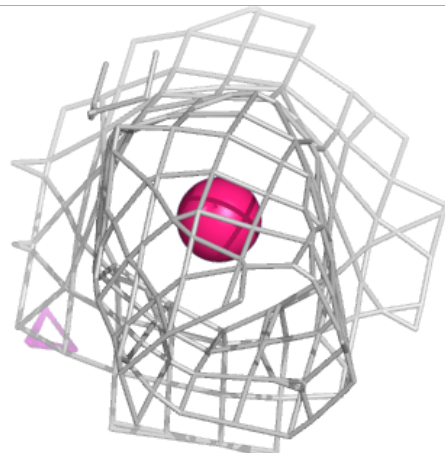
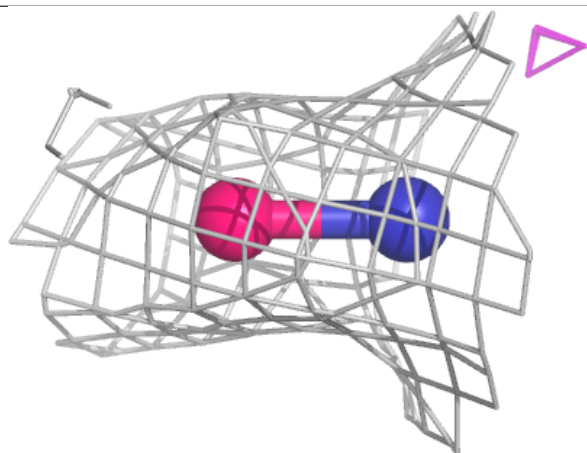
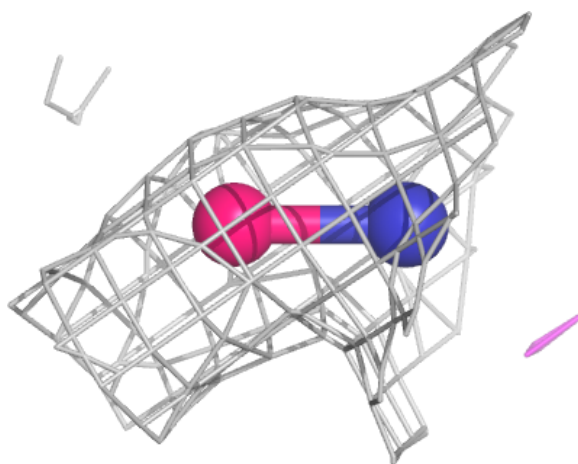
Electron density around MH0 A 601:

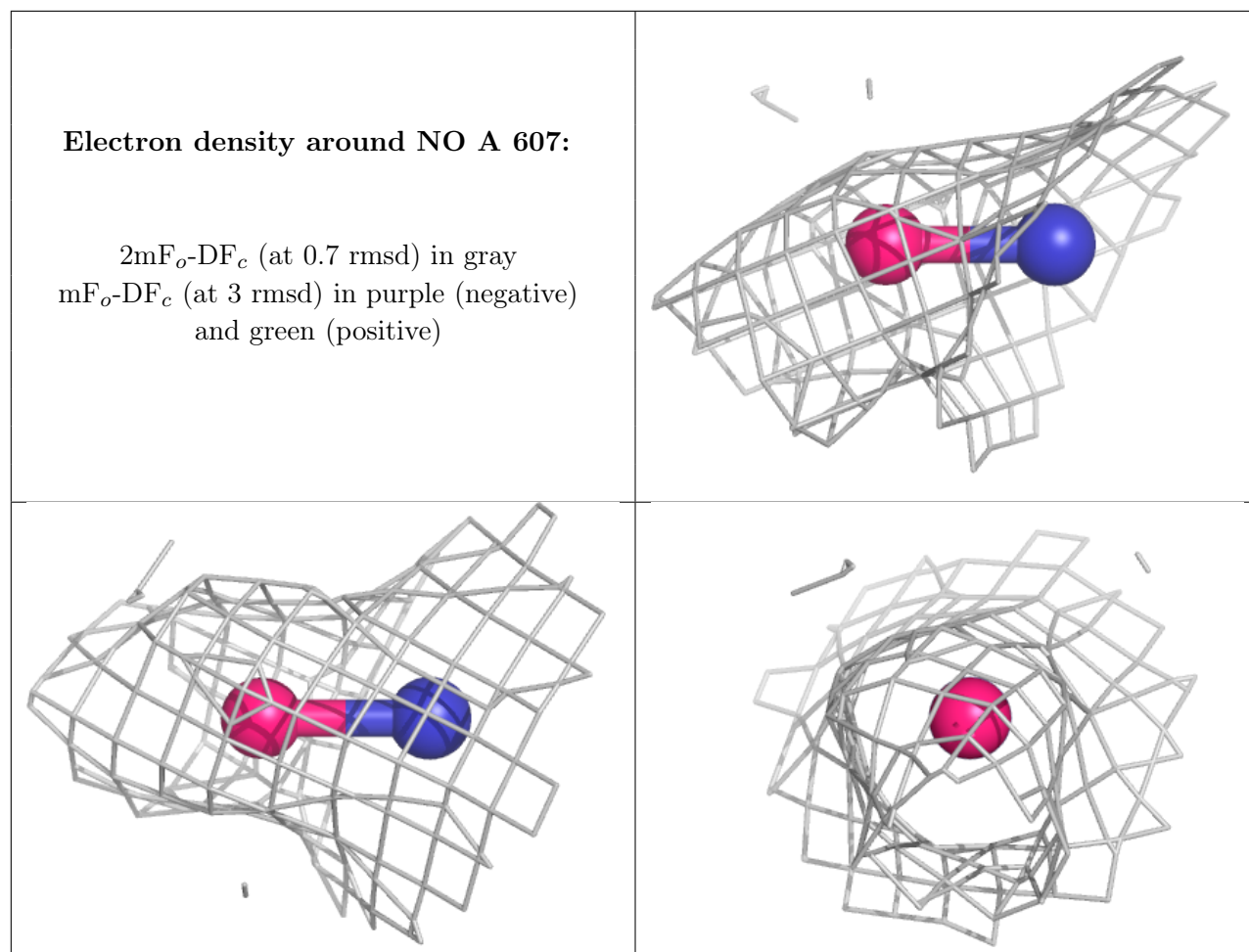
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NO B 607:

$2mF_o-DF_c$ (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.