



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:59 AM UTC

PDB ID : 8ING / pdb_00008ing
Title : Structure of the ternary complex of lactoperoxidase with substrate nitric oxide (NO) and product nitrite ion (NO₂) at 1.98 Å resolution
Authors : Ahmad, M.I.; Viswanathan, V.; Kumar, M.; Singh, R.P.; Singh, A.K.; Sinha, M.; Kaur, P.; Sharma, P.; Sharma, S.; Singh, T.P.
Deposited on : 2023-03-09
Resolution : 1.98 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

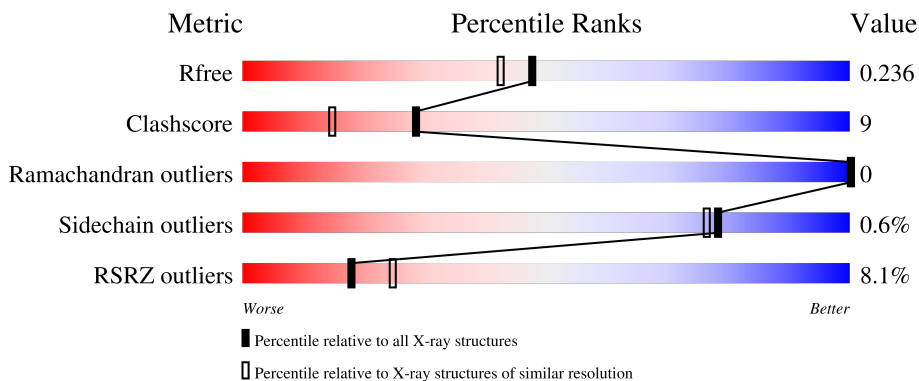
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

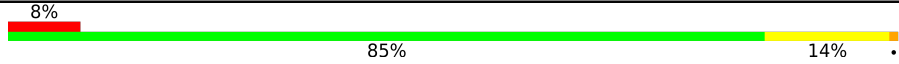
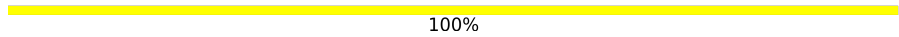
The reported resolution of this entry is 1.98 Å.

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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	 8% 85% 14% .
2	B	2	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	OSM	A	632	-	-	X	-
4	NO	A	604	-	-	X	-
9	IOD	A	619	-	-	X	-

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 5333 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.

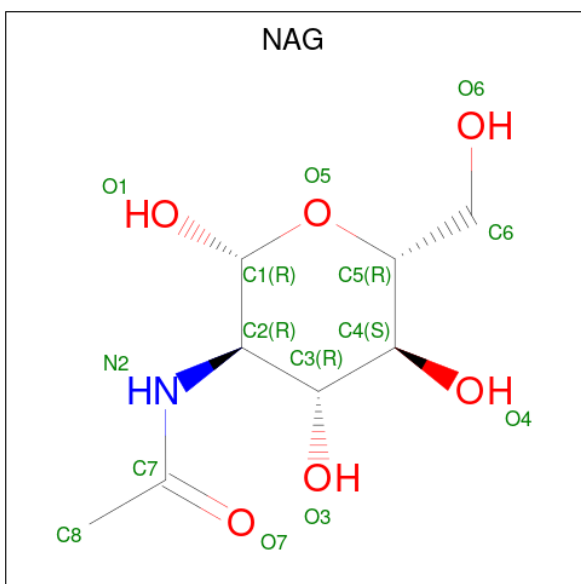
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	595	4774	3035	849	863	1	26	0	2	0

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



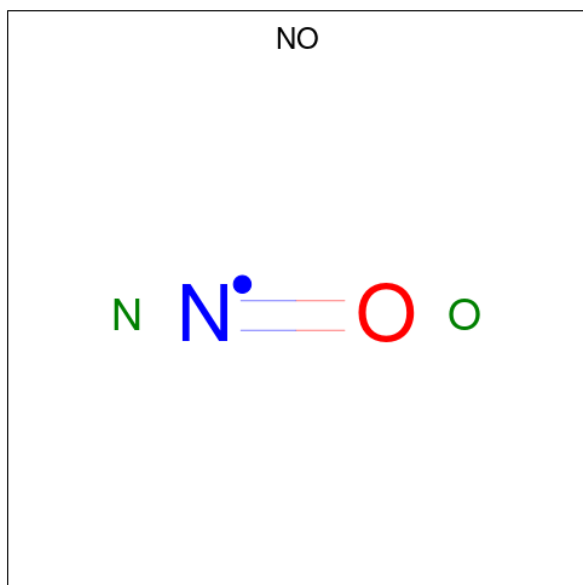
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	2	28	16	2	10	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



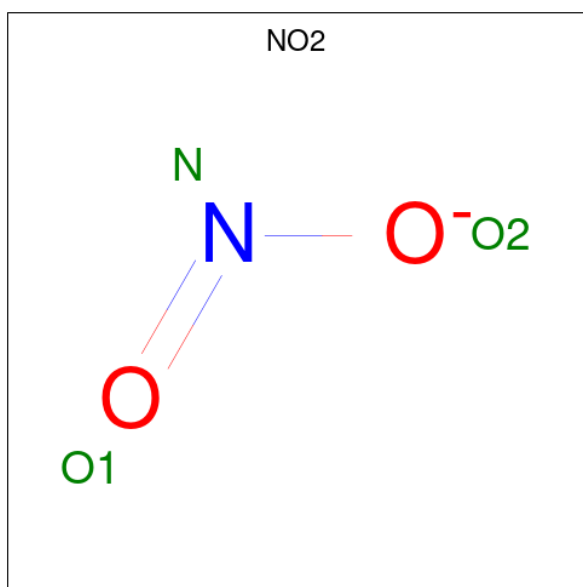
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is NITRIC OXIDE (CCD ID: NO) (formula: NO) (labeled as "Ligand of Interest" by depositor).



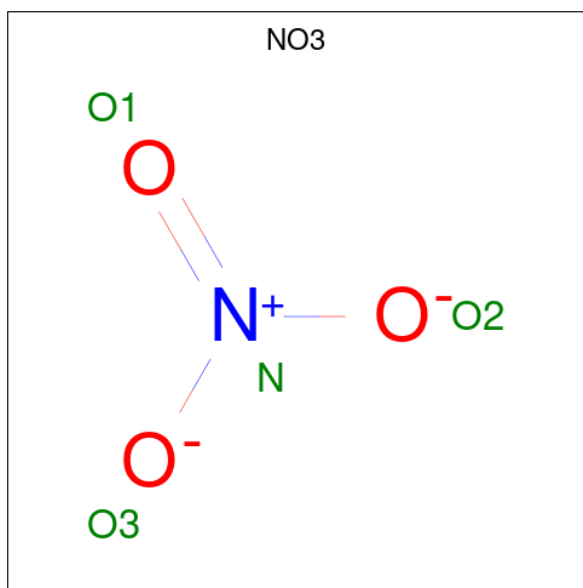
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
4	A	1	Total	N	O	0	0
			2	1	1		
4	A	1	Total	N	O	0	0
			2	1	1		

- Molecule 5 is NITRITE ION (CCD ID: NO₂) (formula: NO₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	O		
5	A	1	3	1	2	0	0

- Molecule 6 is NITRATE ION (CCD ID: NO3) (formula: NO₃).



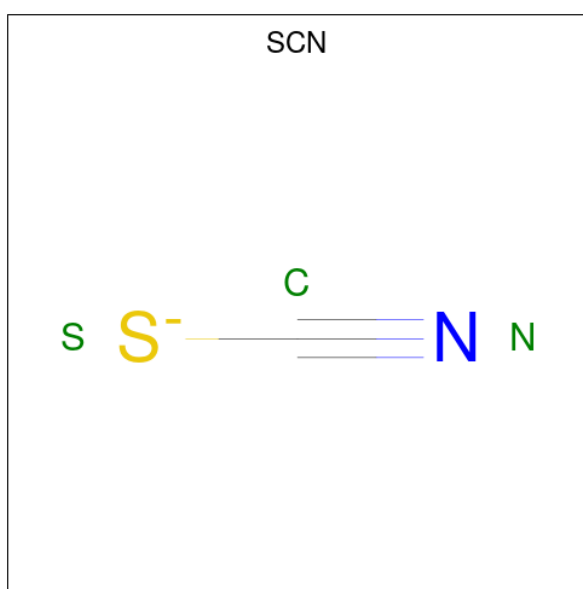
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	O		
6	A	1	4	1	3	0	0
6	A	1	4	1	3	0	0
6	A	1	4	1	3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	N	O	0	0
			4	1	3		
6	A	1	Total	N	O	0	0
			4	1	3		
6	A	1	Total	N	O	0	0
			4	1	3		
6	A	1	Total	N	O	0	0
			4	1	3		

- Molecule 7 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	S	0	0
			3	1	1	1		
7	A	1	Total	C	N	S	0	0
			3	1	1	1		
7	A	1	Total	C	N	S	0	0
			3	1	1	1		
7	A	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).

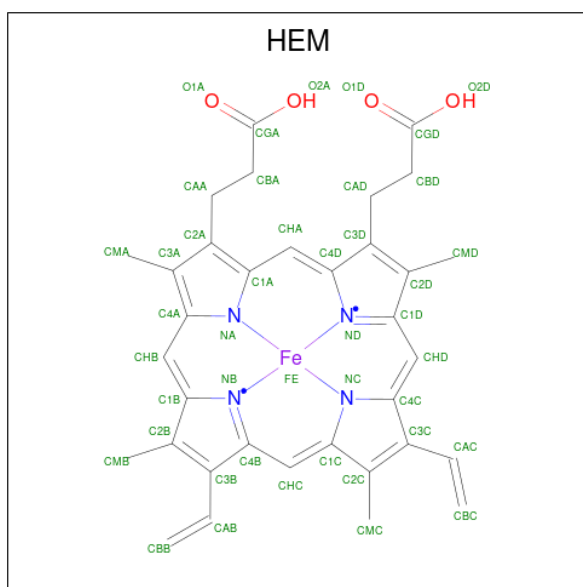


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0

- Molecule 9 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	13	Total I 13 13	0	0

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄) (labeled as "Ligand of Interest" by depositor).

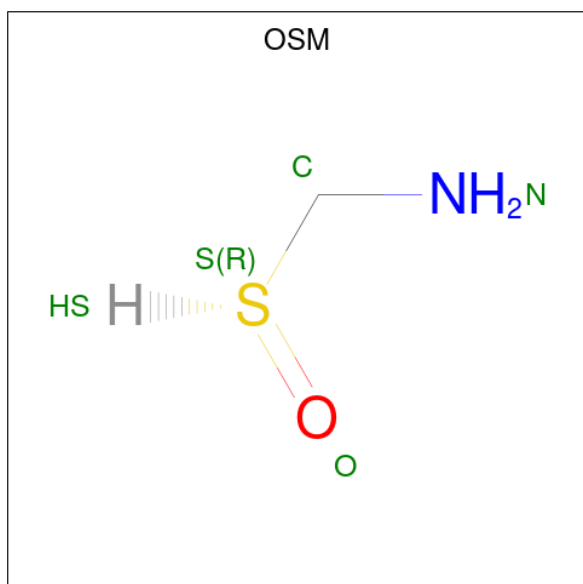


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
10	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 11 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1	Total	Ca	0	0
			1	1		

- Molecule 12 is 1-(OXIDOSULFANYL)METHANAMINE (CCD ID: OSM) (formula: CH₅NOS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
12	A	1	4	1	1	1	1	0	0

- Molecule 13 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
13	A	2	2	2	0	0

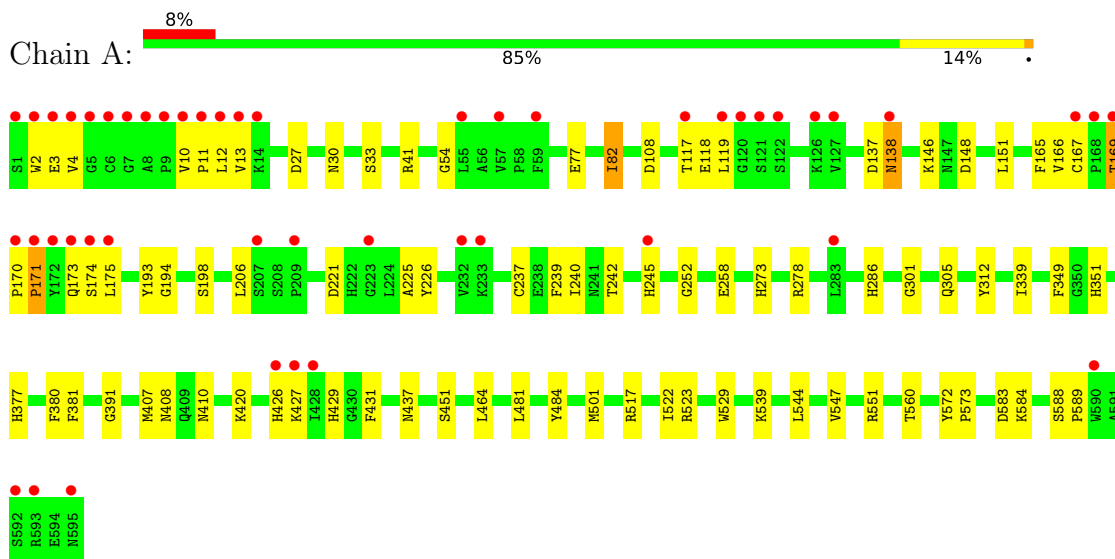
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
14	A	366	367	367	0	1

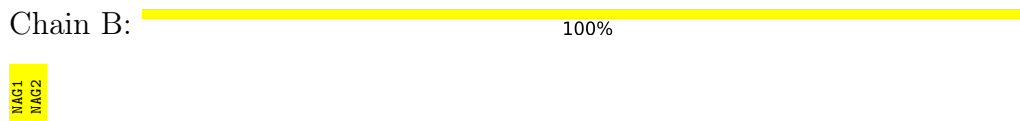
3 Residue-property plots [i](#)

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.05Å 80.34Å 76.12Å 90.00° 102.82° 90.00°	Depositor
Resolution (Å)	35.33 – 1.98 35.33 – 1.98	Depositor EDS
% Data completeness (in resolution range)	98.3 (35.33-1.98) 98.3 (35.33-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 1.98Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.183 , 0.234 0.189 , 0.236	Depositor DCC
R_{free} test set	2188 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	29.9	Xtrriage
Anisotropy	0.139	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5333	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% 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, NO, OSM, SCN, NO₂, HEM, EDO, SEP, IOD, NO₃, CA, NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.07	3/4898 (0.1%)	1.33	8/6647 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	171	PRO	C-N	-9.34	1.20	1.33
1	A	339	ILE	C-O	5.97	1.30	1.24
1	A	312	TYR	C-O	5.64	1.30	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	349	PHE	CA-C-O	-7.30	111.85	120.10
1	A	82	ILE	CB-CA-C	-6.86	105.02	111.06
1	A	169	THR	N-CA-C	5.45	121.85	109.81
1	A	391	GLY	CA-C-N	5.32	129.06	120.55
1	A	391	GLY	C-N-CA	5.32	129.06	120.55
1	A	137	ASP	N-CA-C	-5.20	100.29	109.02
1	A	138	ASN	N-CA-C	5.15	118.34	111.75
1	A	206	LEU	N-CA-C	-5.07	107.15	113.38

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	4774	0	4683	73	0
2	B	28	0	25	0	0
3	A	42	0	39	2	0
4	A	4	0	0	2	0
5	A	3	0	0	1	0
6	A	28	0	0	3	0
7	A	12	0	0	1	0
8	A	12	0	18	1	0
9	A	13	0	0	5	0
10	A	43	0	30	12	0
11	A	1	0	0	0	0
12	A	4	0	5	4	0
13	A	2	0	0	0	0
14	A	367	0	0	12	0
All	All	5333	0	4800	86	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 9.

All (86) 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:108:ASP:OD2	10:A:626:HEM:CMD	1.64	1.44
1:A:258:GLU:OE2	10:A:626:HEM:CMB	1.74	1.33
1:A:108:ASP:CG	10:A:626:HEM:HMD1	1.73	1.12
1:A:410:ASN:OD1	9:A:619:IOD:I	2.39	1.10
1:A:10:VAL:HA	1:A:41[A]:ARG:HH12	1.11	1.07
1:A:258:GLU:OE2	10:A:626:HEM:HMB1	0.87	1.03
3:A:602:NAG:O4	14:A:701:HOH:O	1.80	0.98
1:A:560:THR:N	6:A:612:NO3:O2	1.99	0.95
9:A:636:IOD:I	14:A:943:HOH:O	2.56	0.92
1:A:10:VAL:HA	1:A:41[A]:ARG:NH1	1.88	0.87
1:A:108:ASP:OD2	10:A:626:HEM:HMD1	0.70	0.87
1:A:10:VAL:CA	1:A:41[A]:ARG:HH12	1.89	0.86
1:A:2:TRP:HB3	1:A:175:LEU:HB2	1.57	0.86
1:A:258:GLU:CD	10:A:626:HEM:HMB1	1.99	0.85
1:A:165:PHE:CZ	1:A:169:THR:HG23	2.16	0.81
1:A:242:THR:O	1:A:245:HIS:CE1	2.36	0.79
1:A:239:PHE:CZ	1:A:427:LYS:HB2	2.19	0.78
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:THR:HB	1:A:170:PRO:HD3	1.72	0.70
1:A:258:GLU:CD	10:A:626:HEM:CMB	2.62	0.68
4:A:604:NO:O	9:A:617:IOD:I	2.83	0.67
6:A:615:NO3:O2	14:A:703:HOH:O	2.09	0.66
1:A:117:THR:HG21	1:A:138:ASN:HB3	1.78	0.66
1:A:108:ASP:CG	10:A:626:HEM:CMD	2.50	0.65
1:A:2:TRP:CZ3	1:A:173:GLN:HB2	2.33	0.63
1:A:2:TRP:HZ3	1:A:173:GLN:HB2	1.62	0.63
1:A:2:TRP:CZ2	1:A:174:SER:HB3	2.34	0.62
1:A:551:ARG:HD3	1:A:583:ASP:O	2.01	0.61
10:A:626:HEM:HMC2	10:A:626:HEM:HBC2	1.84	0.59
1:A:464:LEU:HA	1:A:481:LEU:HD12	1.84	0.59
1:A:481:LEU:HA	1:A:484:TYR:O	2.03	0.58
1:A:117:THR:HG23	1:A:119:LEU:HD23	1.85	0.57
1:A:351:HIS:HD1	1:A:437:ASN:HD21	1.53	0.57
4:A:604:NO:O	5:A:605:NO2:O1	2.22	0.57
1:A:77:GLU:HG3	6:A:614:NO3:O2	2.05	0.56
1:A:237:CYS:HA	1:A:381:PHE:O	2.05	0.56
1:A:239:PHE:HZ	1:A:427:LYS:HB2	1.70	0.56
1:A:523:ARG:HG3	1:A:529:TRP:CE2	2.42	0.55
1:A:551:ARG:CD	1:A:583:ASP:O	2.56	0.54
1:A:225:ALA:N	12:A:632:OSM:O	2.40	0.54
1:A:146:LYS:O	14:A:704:HOH:O	2.18	0.54
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.45	0.52
1:A:11:PRO:O	1:A:12:LEU:HB2	2.11	0.51
12:A:632:OSM:H1	14:A:877:HOH:O	2.10	0.50
1:A:170:PRO:HD2	1:A:171:PRO:HD3	1.94	0.49
1:A:30:ASN:HB3	1:A:33:SER:O	2.12	0.49
1:A:3:GLU:OE2	1:A:4:VAL:O	2.30	0.48
1:A:221:ASP:HB2	1:A:226:TYR:CZ	2.49	0.47
1:A:278:ARG:HH12	12:A:632:OSM:H1	1.78	0.47
9:A:633:IOD:I	14:A:1045:HOH:O	1.18	0.47
1:A:464:LEU:HA	1:A:481:LEU:CD1	2.45	0.47
1:A:10:VAL:N	1:A:11:PRO:CD	2.78	0.47
1:A:10:VAL:HG12	1:A:11:PRO:HD3	1.97	0.47
1:A:239:PHE:CZ	1:A:427:LYS:CB	2.94	0.47
1:A:410:ASN:CG	9:A:619:IOD:I	3.25	0.47
1:A:517:ARG:NH1	14:A:716:HOH:O	2.47	0.47
1:A:118:GLU:C	1:A:119:LEU:HD22	2.40	0.47
1:A:13:VAL:CG1	1:A:27:ASP:HB3	2.45	0.46
1:A:407:MET:HB3	1:A:501:MET:CE	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:610:EDO:O1	14:A:705:HOH:O	2.21	0.46
1:A:170:PRO:N	1:A:171:PRO:CD	2.79	0.45
1:A:165:PHE:HZ	1:A:169:THR:HG23	1.75	0.45
1:A:407:MET:HB3	1:A:501:MET:HE2	1.97	0.45
1:A:451:SER:HA	14:A:909:HOH:O	2.16	0.45
10:A:626:HEM:HBC2	10:A:626:HEM:CMC	2.46	0.44
1:A:170:PRO:CD	1:A:171:PRO:HD3	2.47	0.43
1:A:54:GLY:HA2	14:A:954:HOH:O	2.18	0.43
10:A:626:HEM:HBB2	10:A:626:HEM:HMB2	1.99	0.43
1:A:193:TYR:OH	1:A:273:HIS:HD2	2.02	0.43
1:A:420:LYS:HA	1:A:429:HIS:O	2.19	0.43
1:A:544:LEU:O	1:A:547:VAL:HG22	2.19	0.43
1:A:194:GLY:HA2	1:A:252:GLY:O	2.19	0.42
1:A:258:GLU:OE2	10:A:626:HEM:C2B	2.62	0.41
1:A:301:GLY:O	1:A:305:GLN:HG3	2.20	0.41
1:A:166:VAL:O	1:A:167:CYS:HB2	2.20	0.41
1:A:539:LYS:HD3	1:A:539:LYS:HA	1.95	0.41
1:A:82:ILE:O	1:A:82:ILE:HG22	2.19	0.41
1:A:408:ASN:HB2	14:A:952:HOH:O	2.18	0.41
3:A:601:NAG:O6	7:A:631:SCN:N	2.47	0.41
1:A:148:ASP:O	1:A:151:LEU:HB2	2.20	0.41
1:A:426:HIS:HB3	1:A:431:PHE:CE1	2.56	0.41
1:A:13:VAL:HG11	1:A:27:ASP:HB3	2.02	0.41
12:A:632:OSM:N	14:A:702:HOH:O	2.08	0.41
1:A:572:TYR:CD1	1:A:573:PRO:HA	2.56	0.40
1:A:117:THR:HG21	1:A:138:ASN:CB	2.46	0.40
1:A:588:SER:N	1:A:589:PRO:CD	2.85	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	594/595 (100%)	581 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	518/516 (100%)	514 (99%)	4 (1%)	73	71

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

Mol	Chain	Res	Type
1	A	240	ILE
1	A	286	HIS
1	A	522[A]	ILE
1	A	522[B]	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	245	HIS
1	A	273	HIS
1	A	489	ASN
1	A	545	GLN
1	A	556	ASN
1	A	558	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](#)

1 non-standard protein/DNA/RNA residue is 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
1	SEP	A	198	13,1	8,9,10	1.36	1 (12%)	7,12,14	2.04	2 (28%)

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
1	SEP	A	198	13,1	-	5/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	P-OG	2.60	1.68	1.60

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	O2P-P-OG	-4.06	96.09	106.67
1	A	198	SEP	O3P-P-O2P	2.45	116.97	107.80

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	198	SEP	N-CA-CB-OG
1	A	198	SEP	CA-CB-OG-P
1	A	198	SEP	CB-OG-P-O2P
1	A	198	SEP	CB-OG-P-O3P
1	A	198	SEP	CB-OG-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

2 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	B	1	2,1	14,14,15	0.75	0	17,19,21	1.63	4 (23%)
2	NAG	B	2	2	14,14,15	0.43	0	17,19,21	1.70	5 (29%)

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	B	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C1-O5-C5	4.17	117.77	112.19
2	B	1	NAG	C6-C5-C4	3.09	120.61	113.02
2	B	1	NAG	O5-C5-C4	-2.87	103.86	110.83
2	B	1	NAG	O5-C1-C2	-2.80	106.97	111.29
2	B	1	NAG	C1-O5-C5	-2.50	108.84	112.19
2	B	2	NAG	O5-C5-C6	2.38	112.30	107.66
2	B	2	NAG	C4-C3-C2	-2.34	107.59	111.02
2	B	2	NAG	C2-N2-C7	-2.29	119.83	122.90
2	B	2	NAG	C3-C4-C5	2.01	113.88	110.23

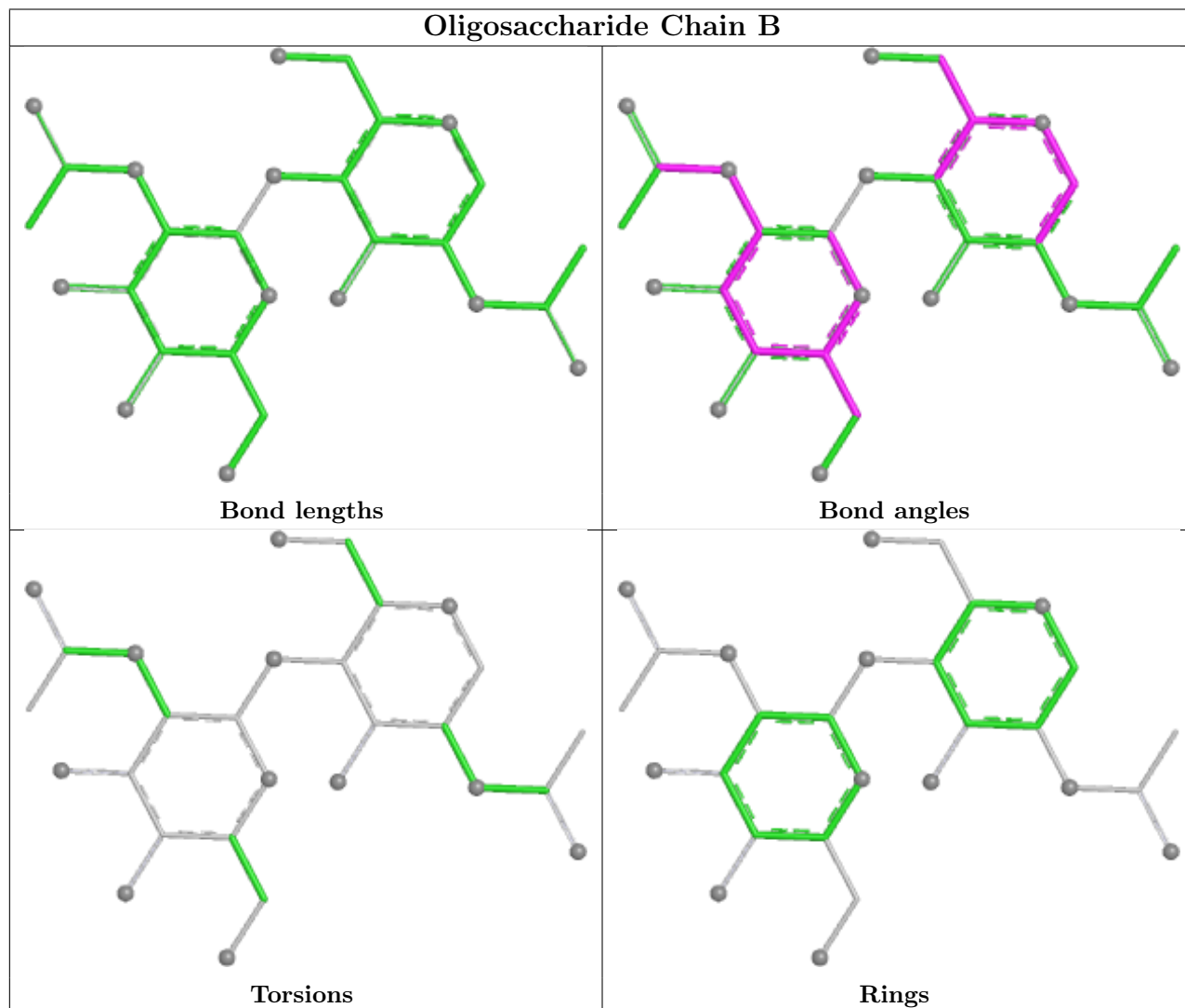
There are no chirality outliers.

There are no torsion outliers.

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 38 ligands modelled in this entry, 16 are monoatomic - leaving 22 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	NO3	A	612	-	1,3,3	0.12	0	0,3,3	-	-
5	NO2	A	605	-	1,2,2	0.68	0	0,1,1	-	-
7	SCN	A	631	-	1,2,2	2.42	1 (100%)	0,1,1	-	-
7	SCN	A	608	-	1,2,2	0.82	0	0,1,1	-	-
12	OSM	A	632	-	1,3,3	0.23	0	0,2,2	-	-
4	NO	A	630	13	0,1,1	-	-	-	-	-
4	NO	A	604	10	0,1,1	-	-	-	-	-
3	NAG	A	601	1	14,14,15	0.83	0	17,19,21	1.06	0
10	HEM	A	626	4,1	50,50,50	1.78	10 (20%)	67,82,82	1.42	11 (16%)
8	EDO	A	629	-	3,3,3	0.07	0	2,2,2	0.22	0
3	NAG	A	602	1	14,14,15	0.69	0	17,19,21	0.99	0
6	NO3	A	613	-	1,3,3	0.32	0	0,3,3	-	-
6	NO3	A	607	-	1,3,3	0.44	0	0,3,3	-	-
6	NO3	A	606	-	1,3,3	0.54	0	0,3,3	-	-
6	NO3	A	614	-	1,3,3	0.05	0	0,3,3	-	-
7	SCN	A	611	-	1,2,2	1.60	0	0,1,1	-	-
8	EDO	A	610	-	3,3,3	0.12	0	2,2,2	0.26	0
7	SCN	A	609	-	1,2,2	1.59	0	0,1,1	-	-
6	NO3	A	616	-	1,3,3	1.00	0	0,3,3	-	-
6	NO3	A	615	-	1,3,3	0.16	0	0,3,3	-	-
3	NAG	A	603	1	14,14,15	0.41	0	17,19,21	1.24	2 (11%)
8	EDO	A	627	-	3,3,3	0.29	0	2,2,2	0.12	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
12	OSM	A	632	-	-	0/0/1/1	-
8	EDO	A	610	-	-	1/1/1/1	-
8	EDO	A	629	-	-	0/1/1/1	-
3	NAG	A	602	1	-	0/6/23/26	0/1/1/1
10	HEM	A	626	4,1	-	4/14/54/54	-
3	NAG	A	603	1	-	2/6/23/26	0/1/1/1
3	NAG	A	601	1	-	0/6/23/26	0/1/1/1
8	EDO	A	627	-	-	1/1/1/1	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	626	HEM	FE-NB	5.51	2.11	1.94
10	A	626	HEM	FE-NC	4.42	2.09	1.95
10	A	626	HEM	C4D-ND	-4.35	1.32	1.40
10	A	626	HEM	C4C-NC	-3.35	1.33	1.39
10	A	626	HEM	FE-NA	2.66	2.03	1.95
7	A	631	SCN	C-N	2.42	1.23	1.15
10	A	626	HEM	C4D-C3D	2.36	1.49	1.45
10	A	626	HEM	C1C-C2C	-2.27	1.40	1.45
10	A	626	HEM	C3D-C2D	-2.11	1.32	1.36
10	A	626	HEM	C1C-NC	-2.04	1.35	1.39
10	A	626	HEM	C1D-ND	-2.03	1.34	1.38

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	626	HEM	C4B-C3B-C2B	-3.29	104.25	107.28
10	A	626	HEM	CAD-C3D-C4D	3.14	130.18	124.70
3	A	603	NAG	C1-O5-C5	3.03	116.24	112.19
10	A	626	HEM	CMD-C2D-C1D	2.86	129.50	125.03
10	A	626	HEM	C3B-C2B-C1B	2.84	108.54	106.41
10	A	626	HEM	CBD-CAD-C3D	-2.58	105.40	112.53
10	A	626	HEM	CHC-C4B-NB	2.57	127.19	124.42
3	A	603	NAG	O5-C5-C4	-2.47	104.81	110.83
10	A	626	HEM	CHA-C4D-C3D	-2.47	120.67	125.23
10	A	626	HEM	C3D-C4D-ND	2.19	112.57	110.17
10	A	626	HEM	C4D-C3D-C2D	-2.11	103.82	106.89
10	A	626	HEM	C4A-C3A-C2A	2.07	109.19	106.82
10	A	626	HEM	C1A-CHA-C4D	-2.01	121.53	126.25

There are no chirality outliers.

All (8) torsion outliers are listed below:

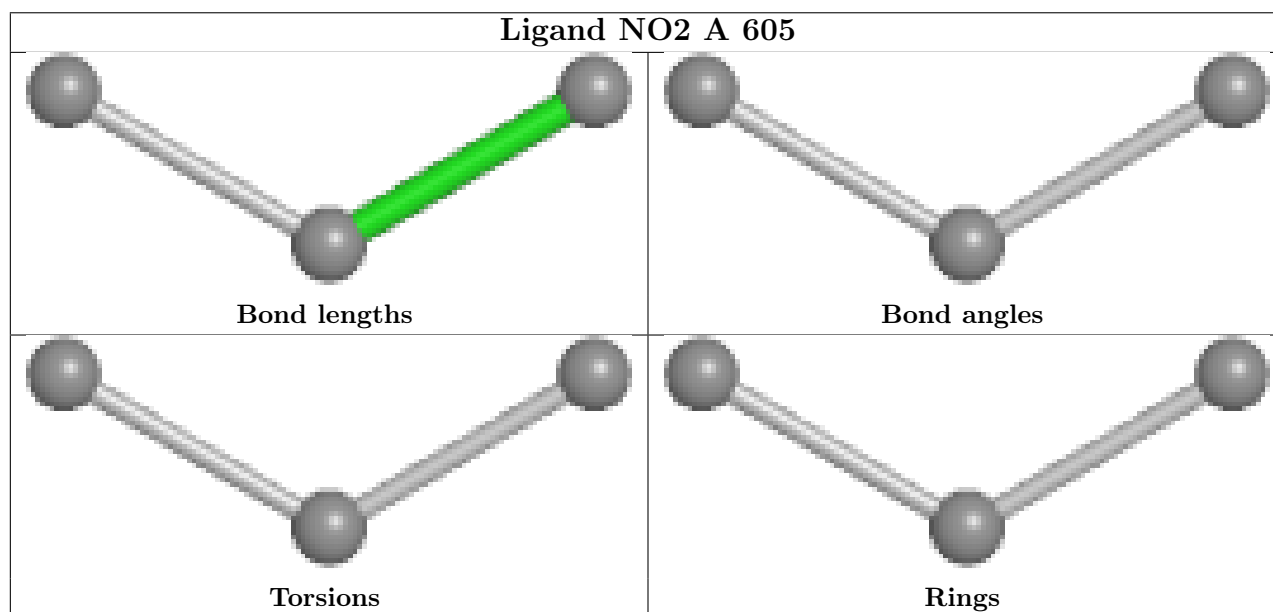
Mol	Chain	Res	Type	Atoms
3	A	603	NAG	C4-C5-C6-O6
3	A	603	NAG	O5-C5-C6-O6
8	A	610	EDO	O1-C1-C2-O2
8	A	627	EDO	O1-C1-C2-O2
10	A	626	HEM	CAA-CBA-CGA-O1A
10	A	626	HEM	CAA-CBA-CGA-O2A
10	A	626	HEM	CAD-CBD-CGD-O1D
10	A	626	HEM	CAD-CBD-CGD-O2D

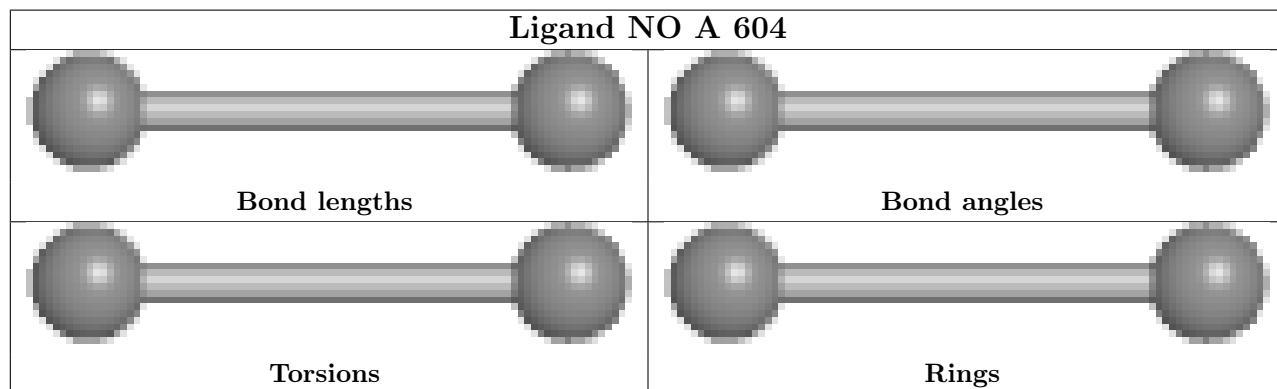
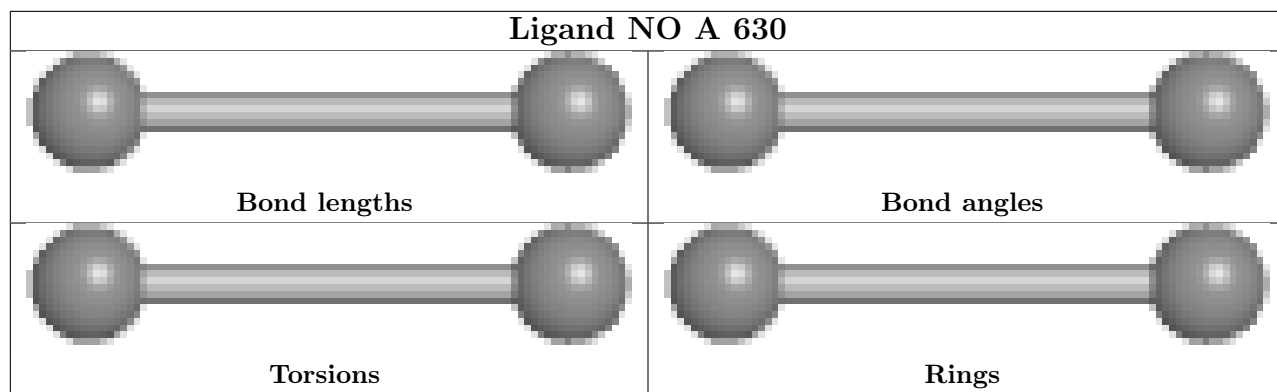
There are no ring outliers.

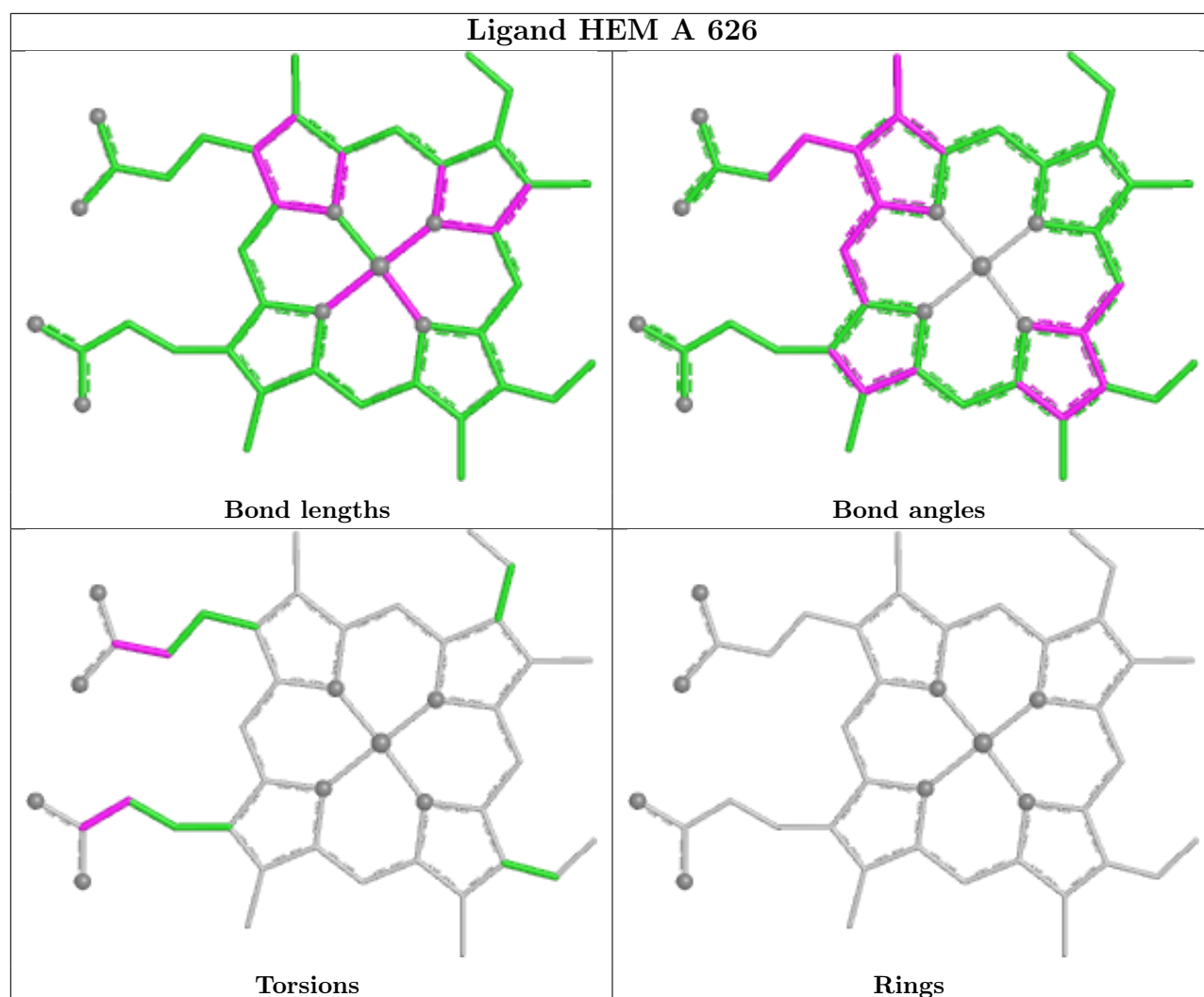
11 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	612	NO3	1	0
5	A	605	NO2	1	0
7	A	631	SCN	1	0
12	A	632	OSM	4	0
4	A	604	NO	2	0
3	A	601	NAG	1	0
10	A	626	HEM	12	0
3	A	602	NAG	1	0
6	A	614	NO3	1	0
8	A	610	EDO	1	0
6	A	615	NO3	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	594/595 (99%)	0.53	48 (8%) 18 25	18, 35, 98, 178	2 (0%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	172	TYR	8.7
1	A	169	THR	7.3
1	A	2	TRP	7.2
1	A	8	ALA	7.2
1	A	173	GLN	7.2
1	A	10	VAL	5.5
1	A	5	GLY	5.5
1	A	9	PRO	5.4
1	A	7	GLY	5.4
1	A	426	HIS	5.2
1	A	168	PRO	4.9
1	A	119	LEU	4.7
1	A	6	CYS	4.6
1	A	13	VAL	4.4
1	A	245	HIS	4.3
1	A	4	VAL	4.2
1	A	12	LEU	4.1
1	A	11	PRO	3.9
1	A	1	SER	3.8
1	A	170	PRO	3.8
1	A	117	THR	3.8
1	A	126	LYS	3.4
1	A	174	SER	3.3
1	A	171	PRO	3.2
1	A	428	ILE	3.1
1	A	232	VAL	3.1
1	A	167	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	14	LYS	3.0
1	A	122	SER	3.0
1	A	121	SER	2.9
1	A	593	ARG	2.9
1	A	209	PRO	2.9
1	A	120	GLY	2.8
1	A	175	LEU	2.8
1	A	223	GLY	2.7
1	A	207	SER	2.6
1	A	283	LEU	2.4
1	A	59	PHE	2.3
1	A	427	LYS	2.3
1	A	3	GLU	2.2
1	A	595	ASN	2.1
1	A	592	SER	2.1
1	A	57	VAL	2.1
1	A	138	ASN	2.1
1	A	233	LYS	2.1
1	A	55	LEU	2.1
1	A	590	TRP	2.0
1	A	127	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	SEP	A	198	10/11	0.83	0.16	35,43,61,61	0

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.

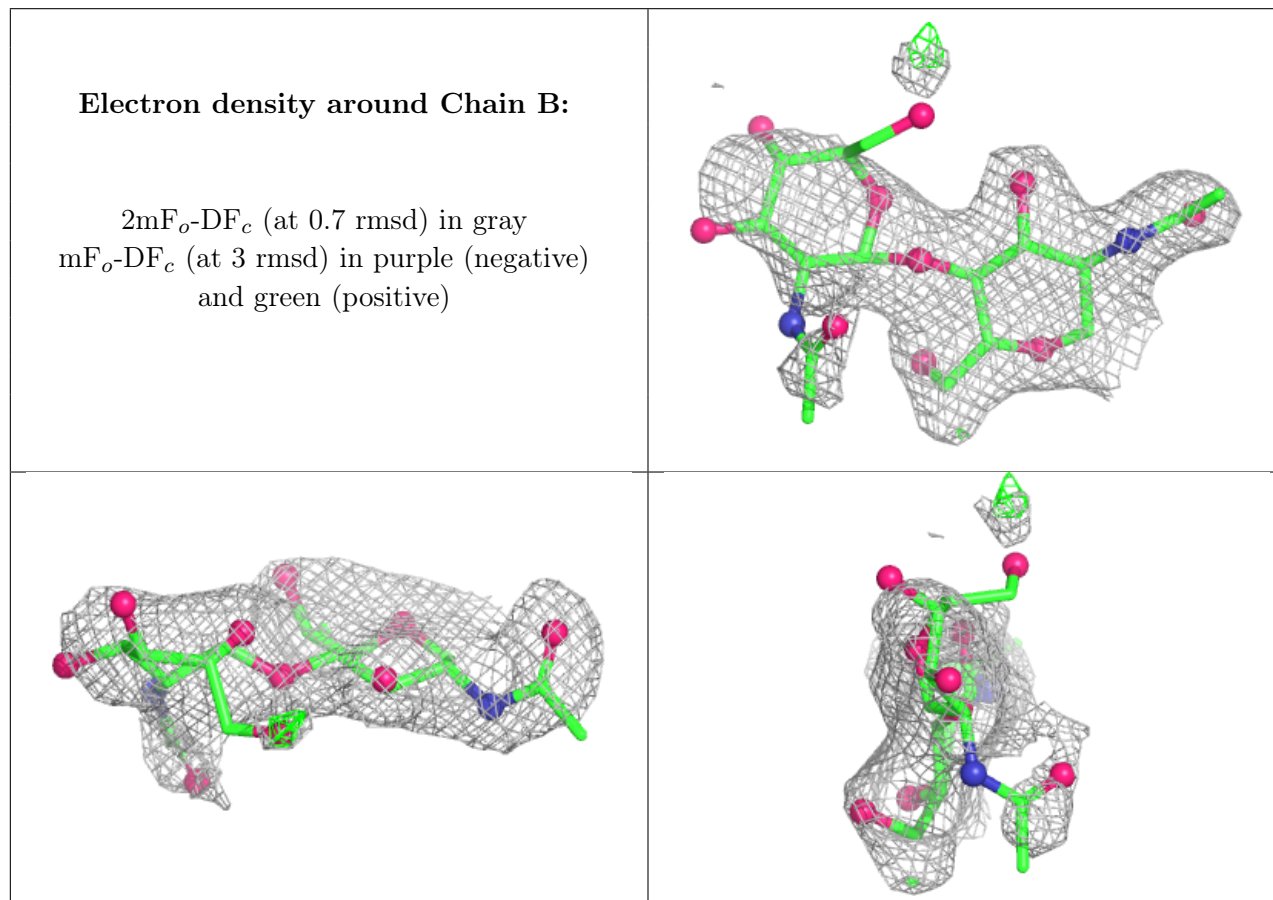
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	B	2	14/15	0.67	0.16	66,72,80,81	14

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	B	1	14/15	0.91	0.09	38,46,54,55	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(\AA^2)	Q<0.9
3	NAG	A	601	14/15	0.72	0.15	47,60,69,75	0
3	NAG	A	603	14/15	0.74	0.17	59,71,78,86	14
8	EDO	A	629	4/4	0.80	0.17	44,44,45,47	0
8	EDO	A	627	4/4	0.88	0.14	32,34,40,52	0
3	NAG	A	602	14/15	0.88	0.10	44,50,53,53	0
8	EDO	A	610	4/4	0.89	0.14	50,50,52,53	0

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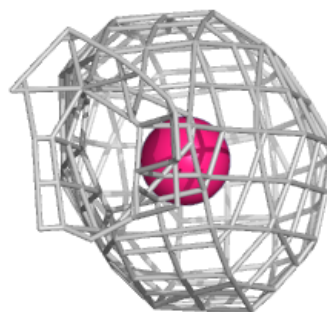
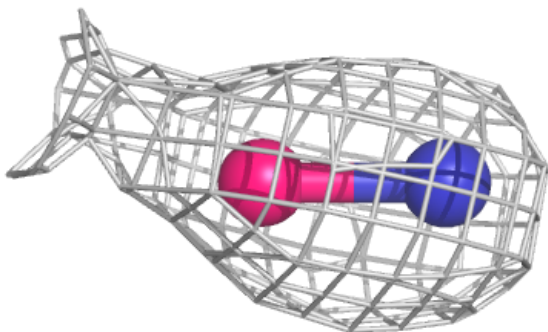
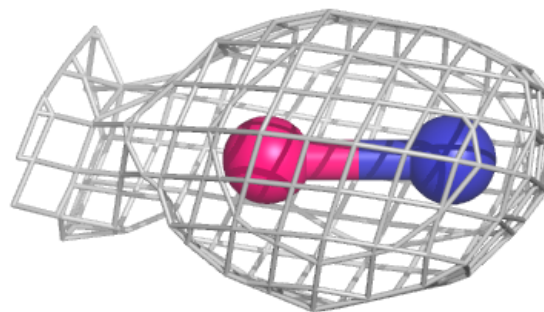
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	SCN	A	608	3/3	0.91	0.12	37,37,41,44	3
12	OSM	A	632	4/4	0.91	0.16	33,37,38,43	4
13	NA	A	638	1/1	0.91	0.12	40,40,40,40	0
7	SCN	A	611	3/3	0.92	0.09	25,25,26,34	0
6	NO3	A	612	4/4	0.93	0.08	19,19,20,22	4
6	NO3	A	613	4/4	0.94	0.07	20,21,22,23	4
6	NO3	A	615	4/4	0.94	0.07	27,28,33,35	4
6	NO3	A	606	4/4	0.94	0.12	31,32,42,49	0
4	NO	A	630	2/2	0.94	0.09	42,42,42,46	0
7	SCN	A	631	3/3	0.94	0.09	39,39,39,44	0
6	NO3	A	607	4/4	0.95	0.08	30,30,33,43	4
6	NO3	A	614	4/4	0.95	0.09	15,16,17,22	4
4	NO	A	604	2/2	0.95	0.08	32,32,32,40	0
6	NO3	A	616	4/4	0.95	0.12	27,33,35,56	0
9	IOD	A	635	1/1	0.96	0.07	60,60,60,60	1
13	NA	A	637	1/1	0.96	0.07	37,37,37,37	0
9	IOD	A	636	1/1	0.96	0.07	55,55,55,55	1
9	IOD	A	619	1/1	0.97	0.13	56,56,56,56	1
7	SCN	A	609	3/3	0.97	0.08	38,38,45,47	0
9	IOD	A	618	1/1	0.98	0.06	51,51,51,51	1
5	NO2	A	605	3/3	0.98	0.05	15,15,16,19	3
10	HEM	A	626	43/43	0.98	0.07	18,21,26,29	0
9	IOD	A	617	1/1	0.99	0.02	25,25,25,25	1
9	IOD	A	621	1/1	0.99	0.05	43,43,43,43	1
9	IOD	A	622	1/1	0.99	0.03	33,33,33,33	1
11	CA	A	628	1/1	0.99	0.03	25,25,25,25	0
9	IOD	A	624	1/1	0.99	0.03	30,30,30,30	1
9	IOD	A	633	1/1	0.99	0.03	37,37,37,37	1
9	IOD	A	634	1/1	0.99	0.04	37,37,37,37	1
9	IOD	A	623	1/1	1.00	0.02	35,35,35,35	1
9	IOD	A	620	1/1	1.00	0.01	26,26,26,26	0
9	IOD	A	625	1/1	1.00	0.05	40,40,40,40	1

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.

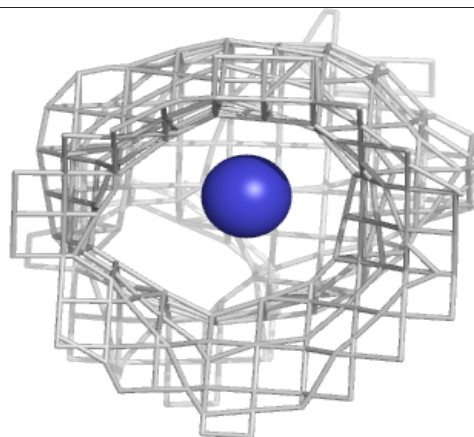
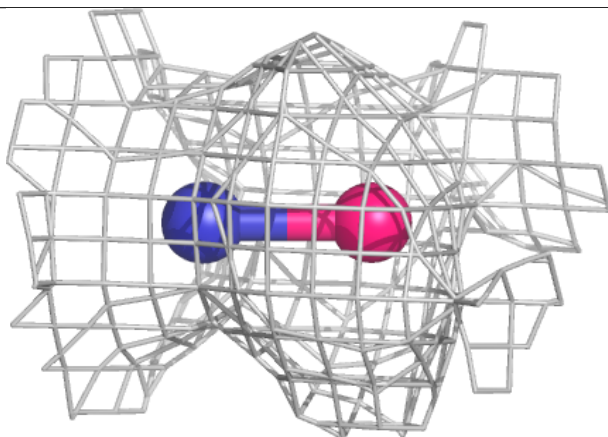
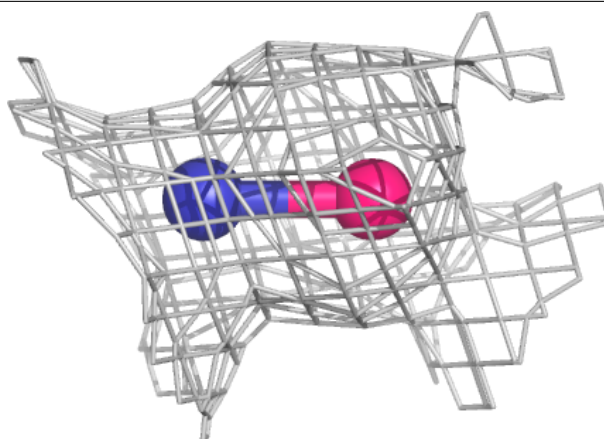
Electron density around NO A 630:

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

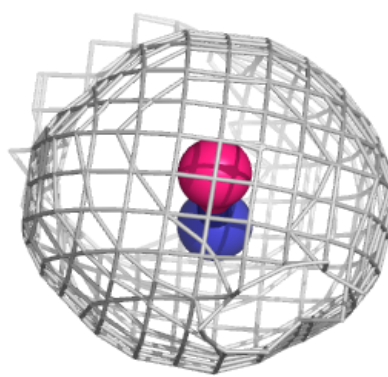
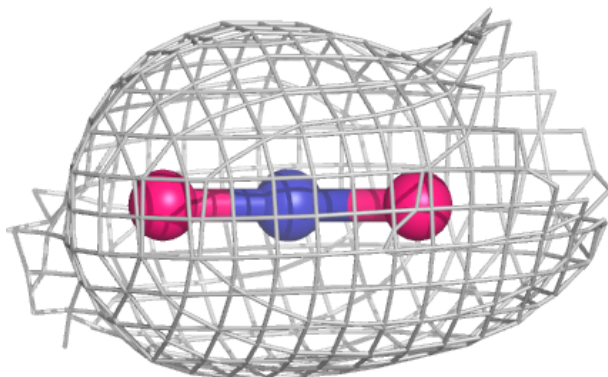
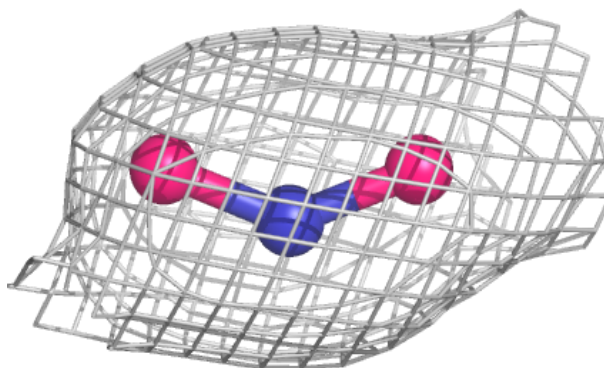


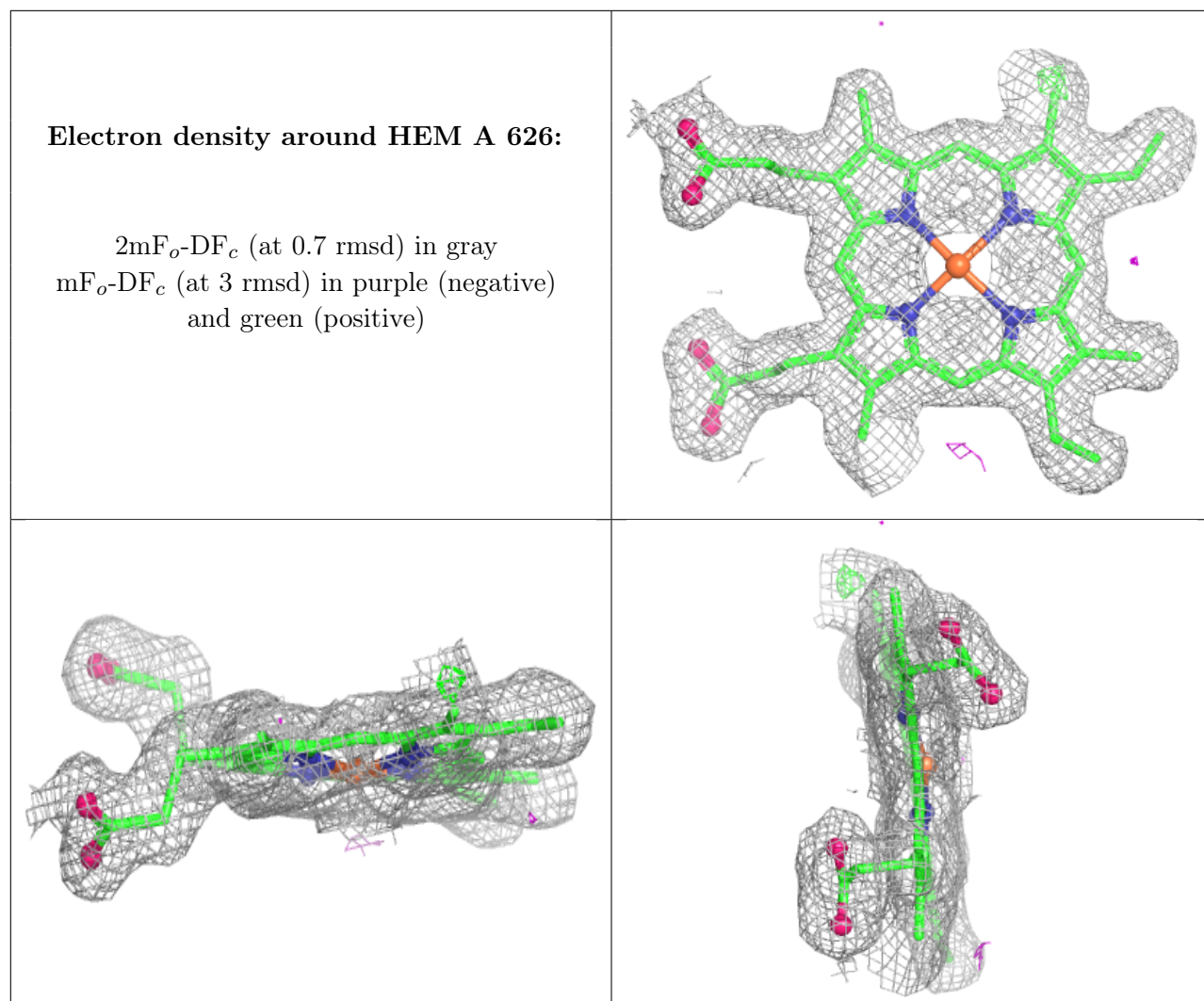
Electron density around NO A 604:

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

**Electron density around NO2 A 605:**

$2mF_o-DF_c$ (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.