



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:36 PM UTC

PDB ID : 3QBJ / pdb_00003qbj
Title : Crystal structure of dipeptidyl peptidase IV in complex with inhibitor
Authors : Liu, S.P.
Deposited on : 2011-01-13
Resolution : 2.21 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

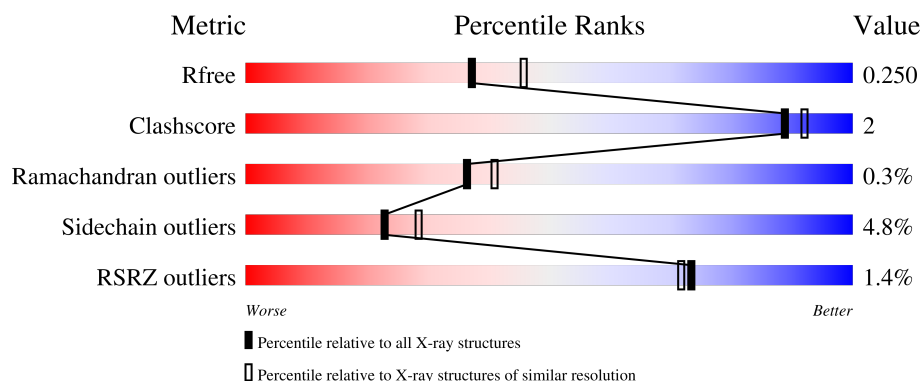
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	748	% 87% 10% ..
1	B	748	% 87% 10% ..
2	C	2	100%
2	E	2	100%
3	D	4	100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12183 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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5957	3825	980	1126	26			
1	B	728	Total	C	N	O	S	0	0	0
			5957	3825	980	1126	26			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	150	ALA	ASN	engineered mutation	UNP P27487
A	520	ALA	ASN	engineered mutation	UNP P27487
A	767	LEU	-	expression tag	UNP P27487
A	768	VAL	-	expression tag	UNP P27487
A	769	PRO	-	expression tag	UNP P27487
A	770	ARG	-	expression tag	UNP P27487
A	771	GLY	-	expression tag	UNP P27487
A	772	SER	-	expression tag	UNP P27487
A	773	HIS	-	expression tag	UNP P27487
A	774	HIS	-	expression tag	UNP P27487
A	775	HIS	-	expression tag	UNP P27487
A	776	HIS	-	expression tag	UNP P27487
A	777	HIS	-	expression tag	UNP P27487
A	778	HIS	-	expression tag	UNP P27487
B	150	ALA	ASN	engineered mutation	UNP P27487
B	520	ALA	ASN	engineered mutation	UNP P27487
B	767	LEU	-	expression tag	UNP P27487
B	768	VAL	-	expression tag	UNP P27487
B	769	PRO	-	expression tag	UNP P27487
B	770	ARG	-	expression tag	UNP P27487
B	771	GLY	-	expression tag	UNP P27487
B	772	SER	-	expression tag	UNP P27487
B	773	HIS	-	expression tag	UNP P27487
B	774	HIS	-	expression tag	UNP P27487
B	775	HIS	-	expression tag	UNP P27487

Continued on next page...

Continued from previous page...

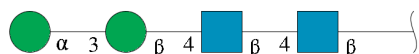
Chain	Residue	Modelled	Actual	Comment	Reference
B	776	HIS	-	expression tag	UNP P27487
B	777	HIS	-	expression tag	UNP P27487
B	778	HIS	-	expression tag	UNP P27487

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



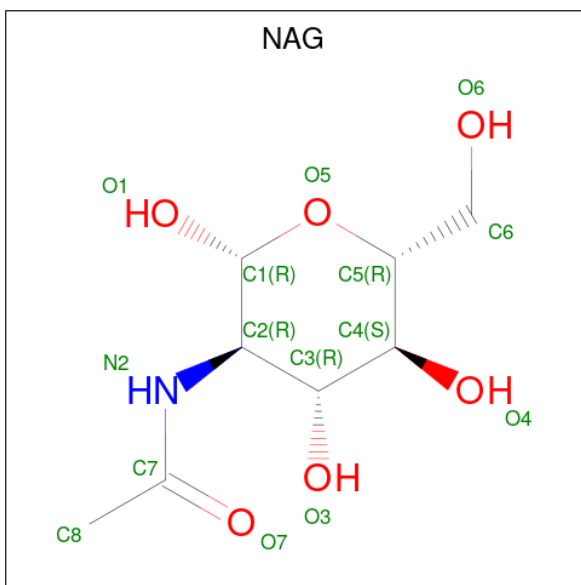
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



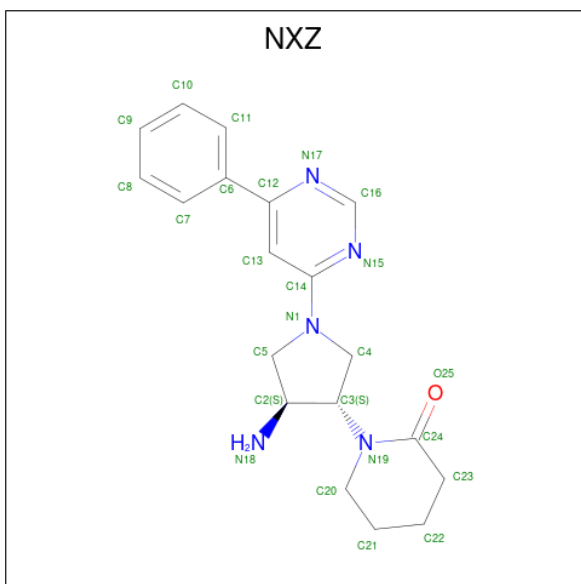
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is 1-[(3S,4S)-4-amino-1-(6-phenylpyrimidin-4-yl)pyrrolidin-3-yl]piperidin-2-one (CCD ID: NXZ) (formula: C₁₉H₂₃N₅O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			25	19	5	1		
5	B	1	Total	C	N	O	0	0
			25	19	5	1		

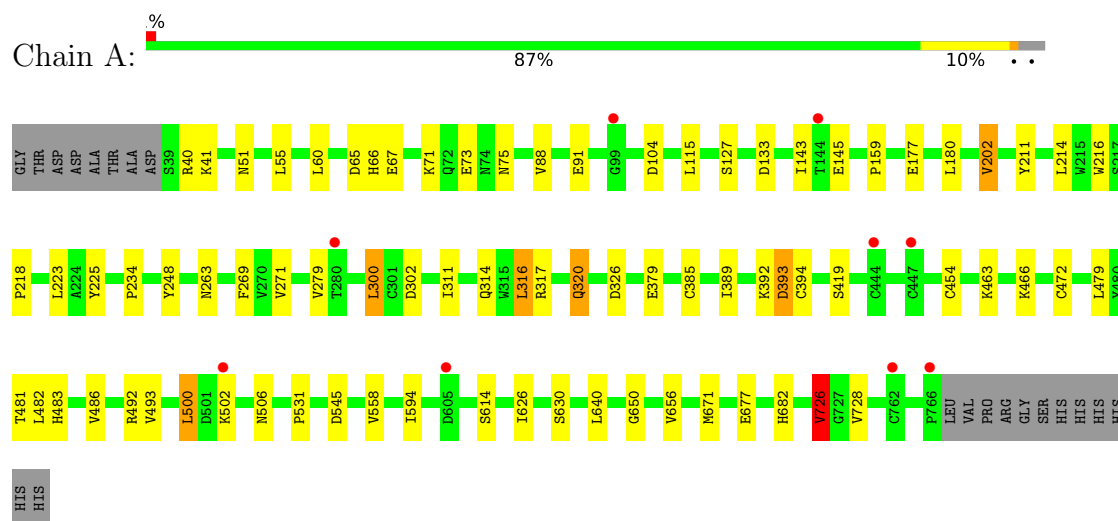
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	28	Total	O	0	0
			28	28		
6	B	43	Total	O	0	0
			43	43		

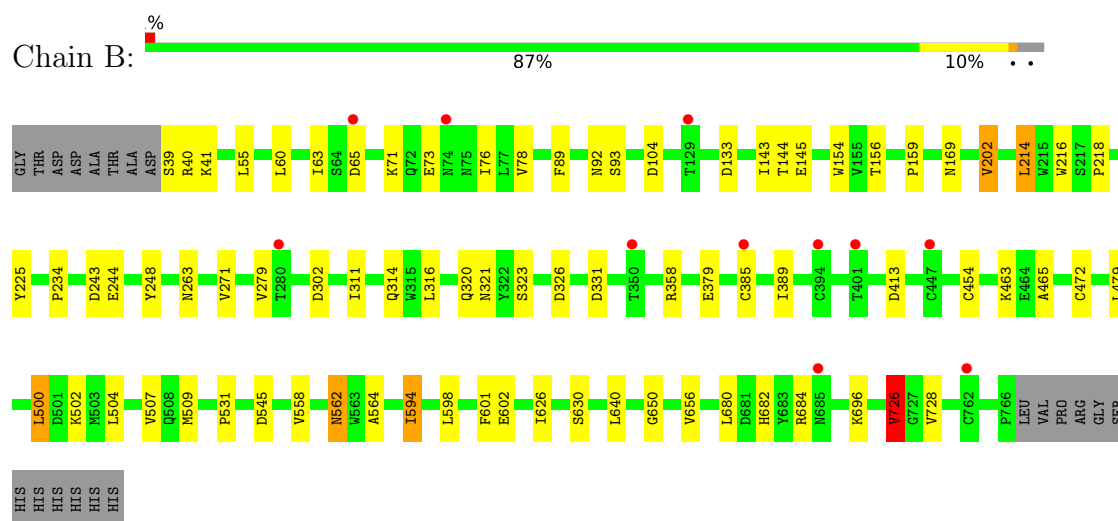
3 Residue-property plots [i](#)

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: Dipeptidyl peptidase 4



• Molecule 1: Dipeptidyl peptidase 4



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



NAG1
NAG2

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

Chain E:  100%NAG1
NAG2

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

Chain D:  100%NAG1
NAG2
BMA3
MAN4

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.75Å 69.08Å 424.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.11 – 2.21 18.11 – 2.21	Depositor EDS
% Data completeness (in resolution range)	80.3 (18.11-2.21) 80.1 (18.11-2.21)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 2.21Å)	Xtriage
Refinement program	BUSTER-TNT, BUSTER 2.9.6	Depositor
R, R_{free}	0.202 , 0.235 0.215 , 0.250	Depositor DCC
R_{free} test set	3918 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	39.7	Xtriage
Anisotropy	0.962	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.024 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12183	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, NXZ, MAN

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	0.84	2/6129 (0.0%)	1.22	16/8336 (0.2%)
1	B	0.84	1/6129 (0.0%)	1.22	22/8336 (0.3%)
All	All	0.84	3/12258 (0.0%)	1.22	38/16672 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	531	PRO	CA-C	5.77	1.55	1.51
1	A	558	VAL	CA-C	5.59	1.59	1.52
1	B	531	PRO	CA-C	5.08	1.54	1.51

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	389	ILE	N-CA-C	9.29	119.90	110.23
1	B	389	ILE	N-CA-C	9.22	119.82	110.23
1	A	656	VAL	N-CA-C	-6.98	99.72	109.21
1	B	41	LYS	N-CA-C	6.88	119.70	110.35
1	A	41	LYS	N-CA-C	6.87	119.17	110.24
1	B	656	VAL	N-CA-C	-6.26	100.70	109.21
1	B	243	ASP	CA-C-N	6.16	128.82	120.38
1	B	243	ASP	C-N-CA	6.16	128.82	120.38
1	B	454	CYS	N-CA-C	6.09	118.68	108.02
1	A	454	CYS	N-CA-C	6.08	118.66	108.02
1	B	76	ILE	N-CA-C	-5.90	99.92	108.36
1	A	614	SER	CA-C-N	5.82	128.66	120.28
1	A	614	SER	C-N-CA	5.82	128.66	120.28
1	A	493	VAL	N-CA-C	-5.76	100.29	108.58
1	B	92	ASN	CA-CB-CG	5.62	118.22	112.60
1	A	726	VAL	CB-CA-C	5.62	117.11	110.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	PRO	CA-C-N	5.61	128.83	120.31
1	A	218	PRO	C-N-CA	5.61	128.83	120.31
1	A	300	LEU	CD1-CG-CD2	5.60	123.13	110.80
1	B	218	PRO	CA-C-N	5.58	128.78	120.31
1	B	218	PRO	C-N-CA	5.58	128.78	120.31
1	B	104	ASP	CA-CB-CG	5.51	118.11	112.60
1	A	104	ASP	CA-CB-CG	5.45	118.05	112.60
1	B	169	ASN	CA-CB-CG	5.33	117.94	112.60
1	B	545	ASP	CA-CB-CG	5.33	117.93	112.60
1	B	39	SER	CA-C-N	5.29	130.53	122.11
1	B	39	SER	C-N-CA	5.29	130.53	122.11
1	B	726	VAL	CB-CA-C	5.25	117.71	111.20
1	A	88	VAL	N-CA-CB	5.18	116.58	110.82
1	B	202	VAL	N-CA-C	5.18	115.91	110.62
1	A	202	VAL	N-CA-C	5.12	115.84	110.62
1	A	300	LEU	N-CA-C	-5.11	100.41	108.73
1	B	465	ALA	N-CA-C	5.08	118.45	111.54
1	A	545	ASP	CA-CB-CG	5.07	117.67	112.60
1	B	331	ASP	CA-CB-CG	5.07	117.67	112.60
1	B	413	ASP	CA-CB-CG	5.05	117.65	112.60
1	B	93	SER	CA-C-N	5.05	127.05	120.28
1	B	93	SER	C-N-CA	5.05	127.05	120.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5957	0	5678	24	0
1	B	5957	0	5681	23	0
2	C	28	0	25	0	0
2	E	28	0	25	0	0
3	D	50	0	43	0	0
4	A	28	0	26	0	0
4	B	14	0	13	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	25	0	23	0	0
5	B	25	0	23	0	0
6	A	28	0	0	0	0
6	B	43	0	0	1	0
All	All	12183	0	11537	45	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 2.

All (45) 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:B:78:VAL:HG23	1:B:89:PHE:HB2	1.73	0.69
1:B:507:VAL:HG13	1:B:509:MET:HG2	1.75	0.69
1:A:225:TYR:CE1	1:A:269:PHE:HD1	2.11	0.68
1:B:504:LEU:HA	1:B:507:VAL:HG12	1.76	0.67
1:B:154:TRP:NE1	1:B:156:THR:OG1	2.29	0.65
1:B:696:LYS:HG2	1:B:728:VAL:HG22	1.78	0.65
1:B:316:LEU:HD13	1:B:323:SER:HB3	1.81	0.62
1:B:562:ASN:HD21	1:B:564:ALA:HB3	1.69	0.58
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.87	0.56
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.88	0.56
1:B:626:ILE:O	1:B:650:GLY:HA2	2.06	0.56
1:B:302:ASP:HB3	1:B:314:GLN:HB2	1.88	0.56
1:A:626:ILE:O	1:A:650:GLY:HA2	2.06	0.55
1:A:214:LEU:HD22	1:A:223:LEU:HD11	1.91	0.51
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.92	0.51
1:B:598:LEU:O	1:B:682:HIS:HE1	1.94	0.51
1:A:316:LEU:HD21	1:A:320:GLN:HA	1.92	0.51
1:A:214:LEU:HD23	1:A:225:TYR:HB3	1.93	0.50
1:A:316:LEU:CD2	1:A:320:GLN:HA	2.43	0.49
1:A:177:GLU:HB2	1:A:180:LEU:HD23	1.95	0.49
1:A:726:VAL:HG13	1:A:728:VAL:HG23	1.95	0.48
1:B:65:ASP:OD1	1:B:463:LYS:O	2.31	0.48
1:B:594:ILE:HD11	1:B:602:GLU:H	1.79	0.47
1:A:65:ASP:HB3	1:A:463:LYS:O	2.15	0.47
1:B:214:LEU:HD12	1:B:225:TYR:HB3	1.97	0.46
1:B:726:VAL:HG13	1:B:728:VAL:HG23	1.96	0.46
1:B:214:LEU:CD1	1:B:225:TYR:HB3	2.47	0.45
1:A:159:PRO:HD3	1:A:216:TRP:HB3	1.98	0.45
1:A:393:ASP:HB2	1:A:394:CYS:H	1.65	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:PRO:HD3	1:B:216:TRP:HB3	1.98	0.44
1:A:316:LEU:HD22	1:A:317:ARG:O	2.19	0.43
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.54	0.43
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.54	0.42
1:A:66:HIS:CD2	1:A:67:GLU:HG3	2.55	0.42
1:B:562:ASN:C	1:B:562:ASN:HD22	2.27	0.42
1:A:177:GLU:CB	1:A:180:LEU:HD23	2.49	0.41
1:A:671:MET:HE1	1:A:682:HIS:CD2	2.56	0.41
1:A:55:LEU:HD23	1:A:500:LEU:HD12	2.01	0.41
1:A:481:THR:OG1	1:A:483:HIS:HE1	2.03	0.41
1:A:66:HIS:HD2	1:A:67:GLU:HG3	1.86	0.41
1:A:75:ASN:HD22	1:A:91:GLU:HA	1.85	0.41
1:A:127:SER:HB3	1:A:211:TYR:CD1	2.56	0.41
1:B:358:ARG:HD2	6:B:802:HOH:O	2.21	0.41
1:B:594:ILE:HD12	1:B:601:PHE:HB2	2.03	0.40
1:B:55:LEU:HD23	1:B:500:LEU:HD12	2.02	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	726/748 (97%)	692 (95%)	31 (4%)	3 (0%)	30	33
1	B	726/748 (97%)	694 (96%)	30 (4%)	2 (0%)	36	41
All	All	1452/1496 (97%)	1386 (96%)	61 (4%)	5 (0%)	36	41

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	GLU
1	B	73	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	320	GLN
1	A	392	LYS
1	B	320	GLN

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	651/667 (98%)	618 (95%)	33 (5%)	21	26
1	B	651/667 (98%)	621 (95%)	30 (5%)	24	30
All	All	1302/1334 (98%)	1239 (95%)	63 (5%)	23	28

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	51	ASN
1	A	60	LEU
1	A	71	LYS
1	A	115	LEU
1	A	133	ASP
1	A	143	ILE
1	A	145	GLU
1	A	202	VAL
1	A	263	ASN
1	A	271	VAL
1	A	279	VAL
1	A	300	LEU
1	A	311	ILE
1	A	316	LEU
1	A	326	ASP
1	A	379	GLU
1	A	385	CYS
1	A	393	ASP
1	A	419	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	466	LYS
1	A	472	CYS
1	A	479	LEU
1	A	482	LEU
1	A	486	VAL
1	A	492	ARG
1	A	500	LEU
1	A	502	LYS
1	A	506	ASN
1	A	594	ILE
1	A	630	SER
1	A	677	GLU
1	A	726	VAL
1	B	40	ARG
1	B	60	LEU
1	B	63	ILE
1	B	71	LYS
1	B	133	ASP
1	B	143	ILE
1	B	144	THR
1	B	145	GLU
1	B	202	VAL
1	B	214	LEU
1	B	244	GLU
1	B	263	ASN
1	B	271	VAL
1	B	279	VAL
1	B	311	ILE
1	B	321	ASN
1	B	326	ASP
1	B	379	GLU
1	B	385	CYS
1	B	472	CYS
1	B	479	LEU
1	B	500	LEU
1	B	502	LYS
1	B	558	VAL
1	B	562	ASN
1	B	594	ILE
1	B	630	SER
1	B	680	LEU
1	B	684	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	726	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	75	ASN
1	A	227	GLN
1	A	247	GLN
1	A	263	ASN
1	A	363	HIS
1	A	435	GLN
1	A	483	HIS
1	A	533	HIS
1	A	731	GLN
1	B	141	GLN
1	B	263	ASN
1	B	298	HIS
1	B	321	ASN
1	B	383	HIS
1	B	562	ASN
1	B	586	GLN
1	B	682	HIS
1	B	697	GLN
1	B	731	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

8 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	1.52	2 (14%)	17,19,21	1.68	4 (23%)
2	NAG	C	2	2	14,14,15	1.86	2 (14%)	17,19,21	2.24	4 (23%)
3	NAG	D	1	1,3	14,14,15	1.03	1 (7%)	17,19,21	1.72	3 (17%)
3	NAG	D	2	3	14,14,15	2.12	5 (35%)	17,19,21	1.72	3 (17%)
3	BMA	D	3	3	11,11,12	1.96	4 (36%)	15,15,17	2.13	6 (40%)
3	MAN	D	4	3	11,11,12	1.71	2 (18%)	15,15,17	1.36	2 (13%)
2	NAG	E	1	2,1	14,14,15	1.52	4 (28%)	17,19,21	1.19	1 (5%)
2	NAG	E	2	2	14,14,15	1.49	3 (21%)	17,19,21	2.15	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	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	2/2/19/22	0/1/1/1
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	NAG	C1-C2	4.71	1.58	1.52
3	D	2	NAG	C3-C2	4.21	1.61	1.52
2	C	1	NAG	C1-C2	3.60	1.57	1.52
3	D	2	NAG	C1-C2	3.42	1.57	1.52
3	D	3	BMA	C2-C3	3.42	1.57	1.52
3	D	2	NAG	C4-C3	3.23	1.60	1.52
3	D	4	MAN	C1-C2	3.15	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3	BMA	C4-C5	3.07	1.59	1.53
3	D	4	MAN	C2-C3	3.02	1.57	1.52
3	D	2	NAG	C2-N2	2.95	1.51	1.46
2	C	1	NAG	C2-N2	-2.74	1.41	1.46
2	C	2	NAG	O5-C5	2.71	1.48	1.43
2	E	1	NAG	C1-C2	2.50	1.55	1.52
2	E	1	NAG	O5-C1	-2.44	1.39	1.43
3	D	3	BMA	C4-C3	2.33	1.58	1.52
2	E	2	NAG	C1-C2	2.32	1.55	1.52
2	E	2	NAG	O4-C4	2.26	1.48	1.43
2	E	2	NAG	C3-C2	2.23	1.57	1.52
3	D	1	NAG	C1-C2	2.11	1.55	1.52
2	E	1	NAG	C4-C5	2.05	1.57	1.53
3	D	2	NAG	O5-C5	2.03	1.47	1.43
2	E	1	NAG	C3-C2	2.01	1.56	1.52
3	D	3	BMA	C6-C5	2.01	1.58	1.51

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C1-O5-C5	6.88	121.41	112.19
2	E	2	NAG	C1-O5-C5	6.56	120.98	112.19
3	D	2	NAG	C4-C3-C2	5.05	118.41	111.02
3	D	1	NAG	C1-C2-N2	4.37	117.33	110.43
3	D	3	BMA	C2-C3-C4	4.32	118.46	110.86
3	D	3	BMA	C1-C2-C3	-3.52	104.52	109.64
3	D	3	BMA	O2-C2-C3	3.47	117.33	110.15
2	C	2	NAG	O5-C1-C2	3.37	116.50	111.29
3	D	2	NAG	C3-C4-C5	3.34	116.29	110.23
2	C	1	NAG	C8-C7-N2	-3.29	110.66	116.12
2	E	2	NAG	O5-C1-C2	3.15	116.17	111.29
2	E	1	NAG	O5-C1-C2	-3.11	106.48	111.29
2	C	1	NAG	C3-C4-C5	-3.06	104.68	110.23
2	C	2	NAG	O5-C5-C4	2.93	117.94	110.83
2	E	2	NAG	O5-C5-C4	2.91	117.90	110.83
2	E	2	NAG	C8-C7-N2	-2.63	111.75	116.12
3	D	4	MAN	O4-C4-C3	-2.60	104.25	110.38
3	D	3	BMA	O3-C3-C2	2.35	114.86	110.05
3	D	3	BMA	C3-C4-C5	2.34	114.48	110.23
2	C	1	NAG	C2-N2-C7	2.34	126.03	122.90
3	D	2	NAG	O4-C4-C3	-2.32	104.90	110.38
2	C	2	NAG	C8-C7-N2	-2.29	112.32	116.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	O5-C1-C2	-2.28	107.76	111.29
3	D	3	BMA	O4-C4-C3	-2.25	105.08	110.38
3	D	1	NAG	C4-C3-C2	2.24	114.30	111.02
3	D	4	MAN	C2-C3-C4	2.24	114.80	110.86
3	D	1	NAG	O4-C4-C3	-2.23	105.12	110.38
2	E	2	NAG	O5-C5-C6	2.08	111.71	107.66

There are no chirality outliers.

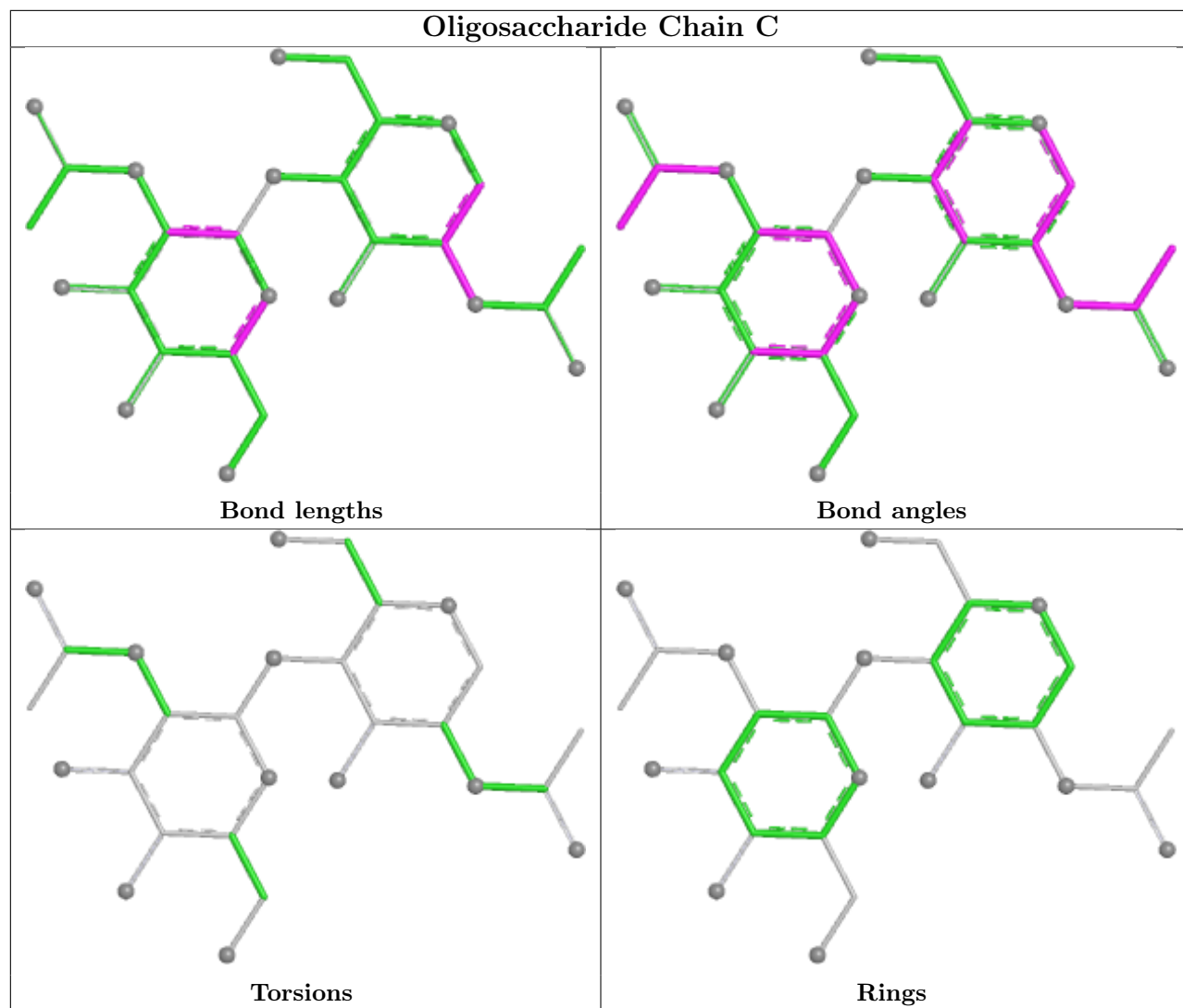
All (4) torsion outliers are listed below:

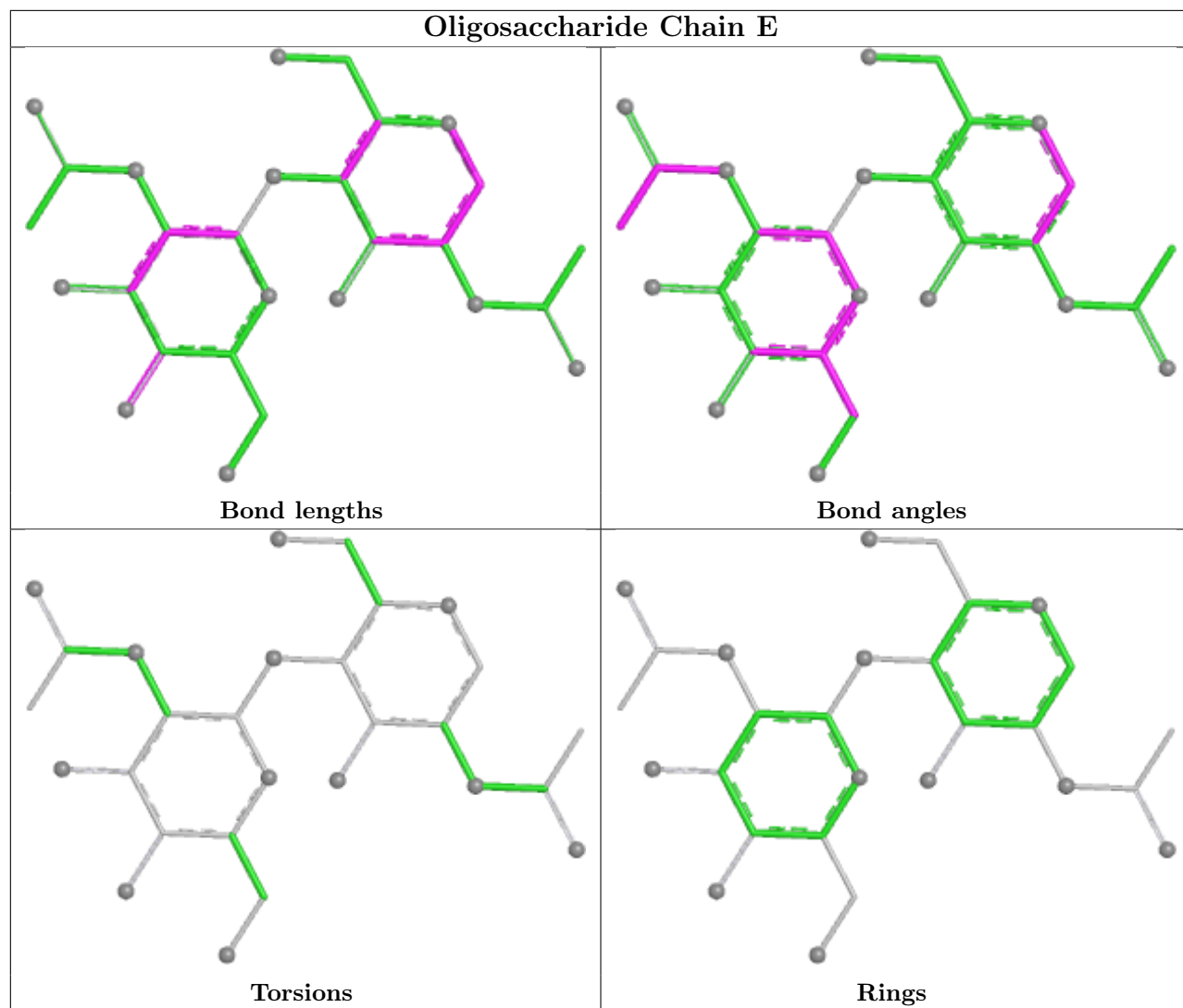
Mol	Chain	Res	Type	Atoms
3	D	4	MAN	O5-C5-C6-O6
3	D	4	MAN	C4-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6

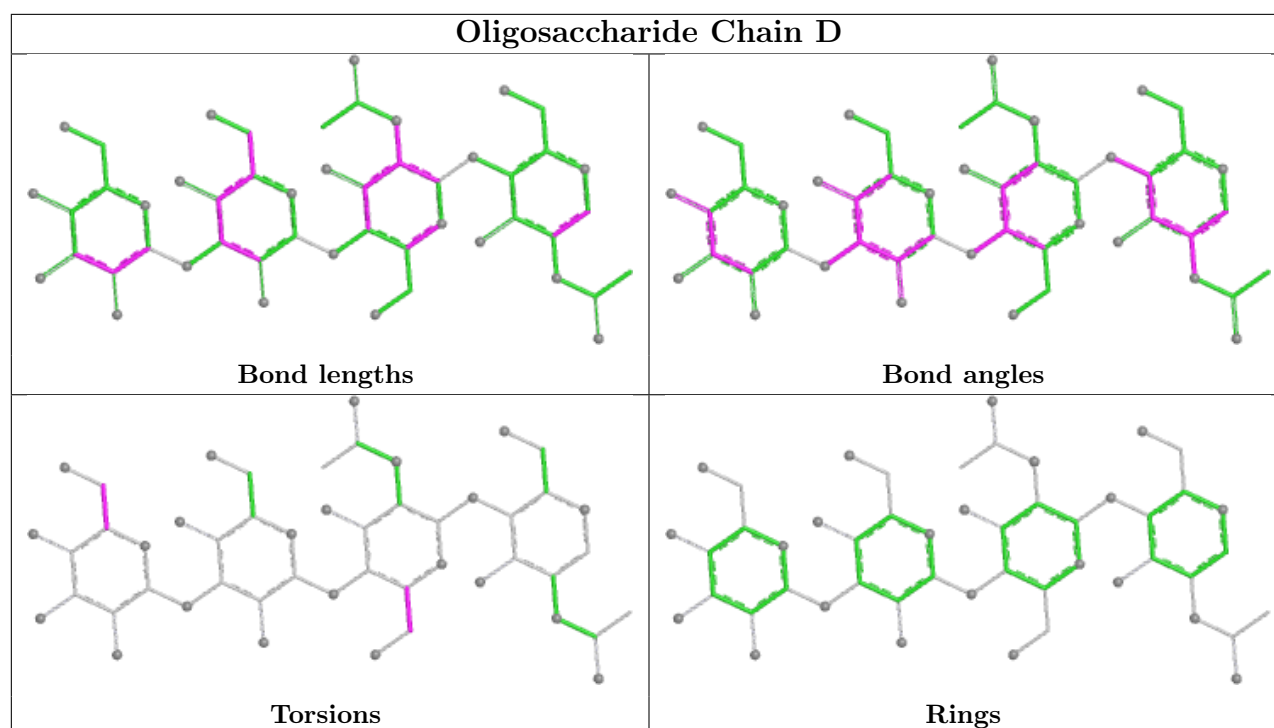
There are no ring outliers.

No monomer is involved in short contacts.

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







5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	800	1	14,14,15	2.28	5 (35%)	17,19,21	1.61	3 (17%)
4	NAG	B	796	1	14,14,15	1.24	2 (14%)	17,19,21	1.43	2 (11%)
4	NAG	A	799	1	14,14,15	1.90	4 (28%)	17,19,21	2.65	7 (41%)
5	NXZ	A	900	-	28,28,28	2.25	13 (46%)	30,39,39	3.60	11 (36%)
5	NXZ	B	900	-	28,28,28	2.45	15 (53%)	30,39,39	3.47	11 (36%)

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
4	NAG	A	800	1	-	0/6/23/26	0/1/1/1
4	NAG	B	796	1	-	0/6/23/26	0/1/1/1
4	NAG	A	799	1	-	4/6/23/26	0/1/1/1
5	NXZ	A	900	-	-	0/12/35/35	0/4/4/4
5	NXZ	B	900	-	-	0/12/35/35	0/4/4/4

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	900	NXZ	C7-C6	4.96	1.49	1.39
4	A	800	NAG	C1-C2	4.94	1.59	1.52
5	B	900	NXZ	C7-C6	4.62	1.48	1.39
5	B	900	NXZ	C14-N15	4.44	1.43	1.34
4	A	799	NAG	C1-C2	3.81	1.57	1.52
5	B	900	NXZ	C10-C9	3.81	1.46	1.38
4	A	800	NAG	C3-C2	3.67	1.60	1.52
5	A	900	NXZ	C11-C6	3.62	1.46	1.39
5	A	900	NXZ	C14-N15	3.58	1.42	1.34
5	B	900	NXZ	C12-N17	3.47	1.42	1.35
5	B	900	NXZ	C11-C6	3.42	1.46	1.39
5	A	900	NXZ	C10-C11	3.39	1.44	1.38
5	B	900	NXZ	C24-N19	3.39	1.40	1.35
5	A	900	NXZ	C9-C8	3.29	1.45	1.38
5	B	900	NXZ	C10-C11	3.27	1.44	1.38
4	A	800	NAG	C4-C3	3.25	1.60	1.52
5	B	900	NXZ	C20-N19	3.24	1.52	1.47
5	B	900	NXZ	C8-C7	3.06	1.44	1.38
5	A	900	NXZ	C8-C7	3.02	1.44	1.38
4	B	796	NAG	C1-C2	2.91	1.56	1.52
5	B	900	NXZ	C13-C12	2.89	1.44	1.39
5	A	900	NXZ	C12-N17	2.79	1.40	1.35
5	A	900	NXZ	C10-C9	2.66	1.44	1.38
5	B	900	NXZ	C4-N1	2.56	1.50	1.46
5	A	900	NXZ	C5-N1	2.56	1.50	1.46
5	A	900	NXZ	C13-C12	2.45	1.43	1.39
4	A	800	NAG	O4-C4	2.42	1.48	1.43
5	B	900	NXZ	C5-C2	2.41	1.57	1.52
4	B	796	NAG	C3-C2	2.39	1.57	1.52
4	A	799	NAG	C4-C5	2.39	1.58	1.53
4	A	800	NAG	C2-N2	2.37	1.50	1.46
5	B	900	NXZ	C23-C24	2.34	1.55	1.51
5	B	900	NXZ	C22-C21	2.33	1.60	1.51
5	A	900	NXZ	C24-N19	2.29	1.38	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	799	NAG	C7-N2	2.21	1.41	1.34
4	A	799	NAG	O5-C5	2.20	1.47	1.43
5	B	900	NXZ	C9-C8	2.16	1.43	1.38
5	A	900	NXZ	C20-N19	2.13	1.50	1.47
5	A	900	NXZ	C23-C24	2.02	1.55	1.51

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	900	NXZ	C16-N15-C14	13.07	125.92	114.95
5	B	900	NXZ	C16-N15-C14	12.21	125.19	114.95
5	A	900	NXZ	N17-C16-N15	-8.47	115.76	128.58
5	B	900	NXZ	N17-C16-N15	-7.77	116.81	128.58
4	A	799	NAG	C1-O5-C5	6.83	121.34	112.19
5	A	900	NXZ	C16-N17-C12	5.90	124.11	115.89
5	B	900	NXZ	C4-N1-C14	-5.45	116.98	123.58
5	B	900	NXZ	C16-N17-C12	5.03	122.90	115.89
5	B	900	NXZ	C5-N1-C4	4.78	118.57	111.64
4	A	800	NAG	C1-O5-C5	4.58	118.33	112.19
5	A	900	NXZ	C4-N1-C14	-4.58	118.04	123.58
5	A	900	NXZ	C3-N19-C24	-4.23	114.95	119.33
5	B	900	NXZ	C3-N19-C24	-4.22	114.96	119.33
4	A	799	NAG	C4-C3-C2	-4.09	105.03	111.02
5	A	900	NXZ	C5-N1-C4	4.06	117.53	111.64
4	A	799	NAG	O5-C1-C2	3.84	117.22	111.29
4	B	796	NAG	C1-C2-N2	3.72	116.29	110.43
5	B	900	NXZ	C21-C20-N19	3.28	115.72	110.65
4	A	799	NAG	C1-C2-N2	3.13	115.36	110.43
4	A	799	NAG	O3-C3-C4	3.06	117.59	110.38
5	B	900	NXZ	C10-C9-C8	2.96	123.92	119.87
4	A	799	NAG	O5-C5-C4	2.91	117.91	110.83
5	B	900	NXZ	C13-C14-N15	-2.87	118.05	122.82
5	A	900	NXZ	C13-C14-N15	-2.77	118.20	122.82
5	A	900	NXZ	C21-C20-N19	2.76	114.91	110.65
5	A	900	NXZ	C10-C9-C8	2.55	123.36	119.87
4	B	796	NAG	C4-C3-C2	2.41	114.55	111.02
5	A	900	NXZ	C8-C7-C6	-2.39	117.81	120.54
4	A	800	NAG	C8-C7-N2	-2.28	112.33	116.12
5	A	900	NXZ	C22-C21-C20	2.26	115.37	111.19
4	A	800	NAG	O4-C4-C3	2.25	115.67	110.38
5	B	900	NXZ	N15-C14-N1	2.13	119.80	116.76
5	B	900	NXZ	C9-C10-C11	-2.02	117.75	120.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	799	NAG	O3-C3-C2	2.02	113.59	109.40

There are no chirality outliers.

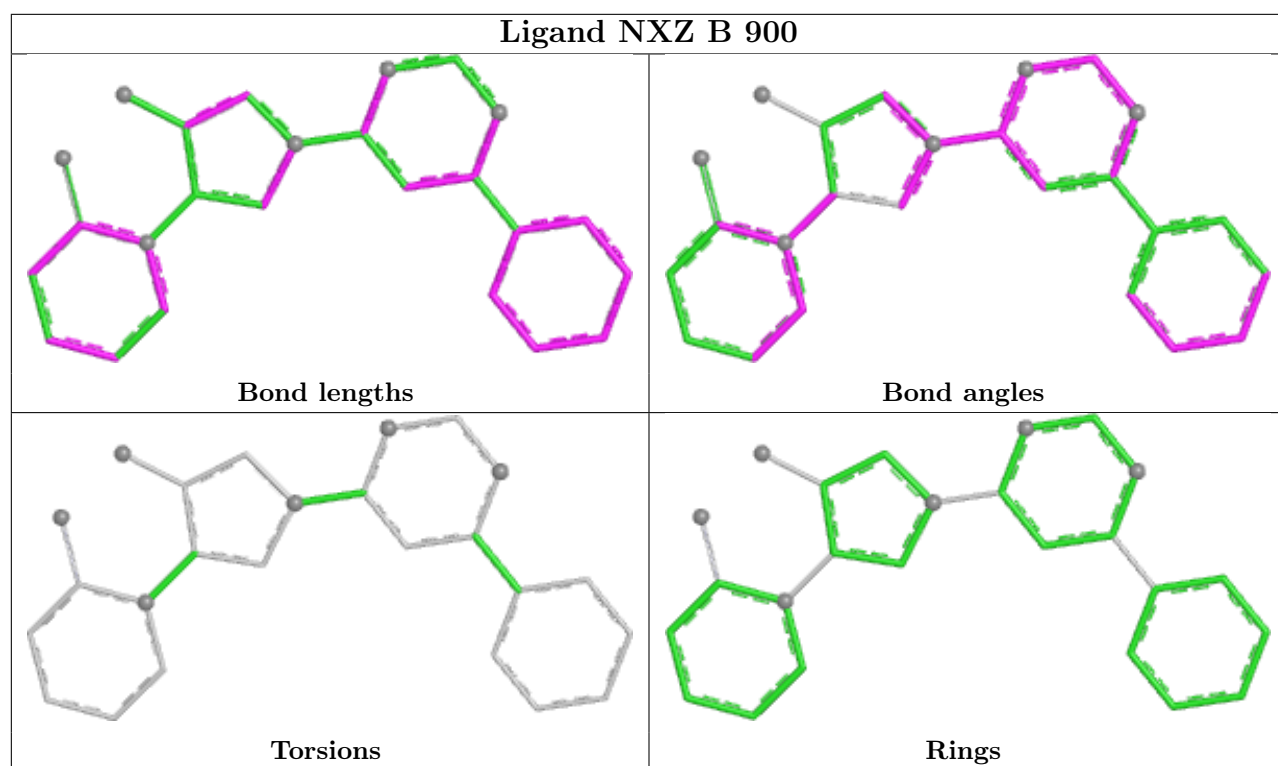
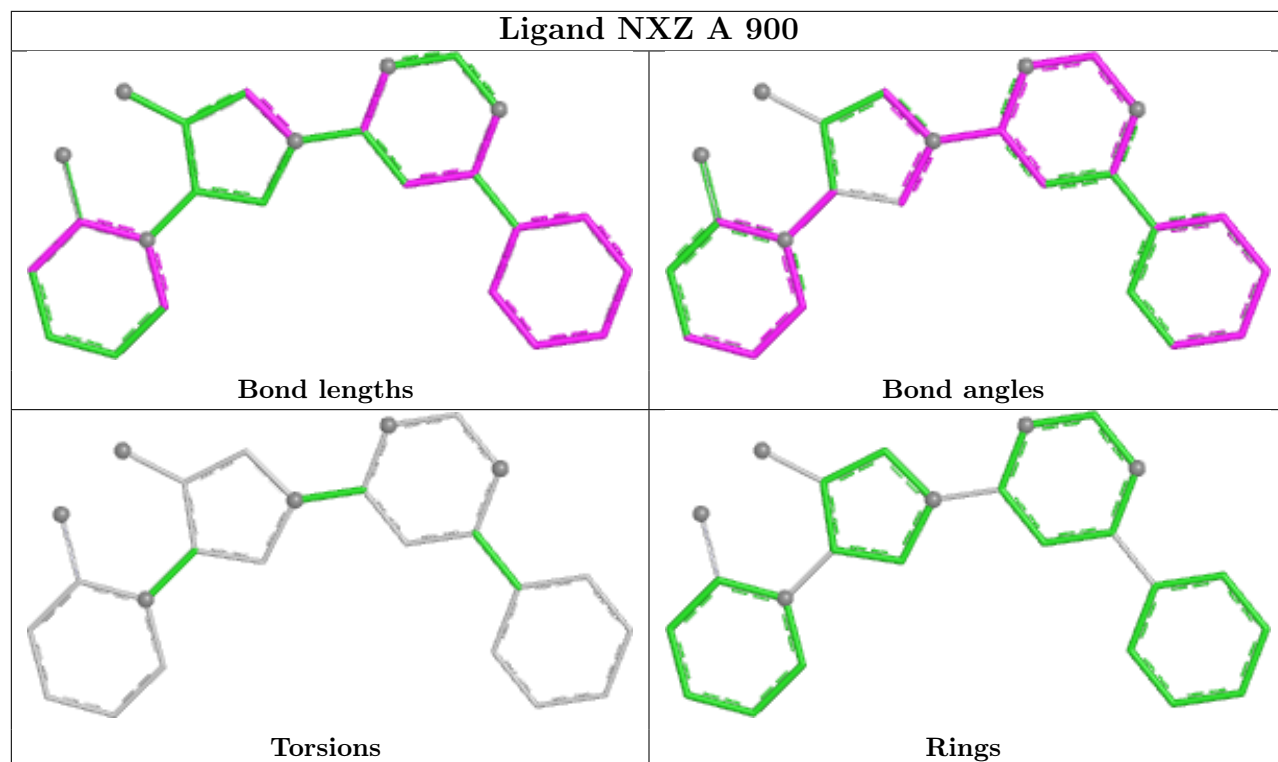
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	799	NAG	O5-C5-C6-O6
4	A	799	NAG	C8-C7-N2-C2
4	A	799	NAG	O7-C7-N2-C2
4	A	799	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 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 ⓘ

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	728/748 (97%)	0.14	9 (1%) 76 75	50, 72, 105, 128	0
1	B	728/748 (97%)	0.14	11 (1%) 72 70	46, 66, 99, 124	0
All	All	1456/1496 (97%)	0.14	20 (1%) 73 72	46, 69, 102, 128	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	762	CYS	4.5
1	B	280	THR	3.3
1	A	502	LYS	2.4
1	B	762	CYS	2.4
1	B	685	ASN	2.4
1	A	280	THR	2.4
1	A	766	PRO	2.4
1	B	65	ASP	2.3
1	A	605	ASP	2.3
1	A	444	CYS	2.3
1	A	99	GLY	2.3
1	B	394	CYS	2.2
1	B	385	CYS	2.2
1	B	350	THR	2.2
1	B	129	THR	2.2
1	B	401	THR	2.2
1	B	447	CYS	2.1
1	A	144	THR	2.1
1	A	447	CYS	2.0
1	B	74	ASN	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](#)

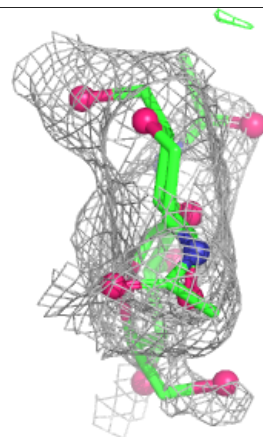
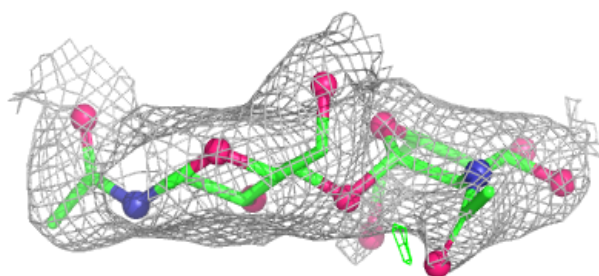
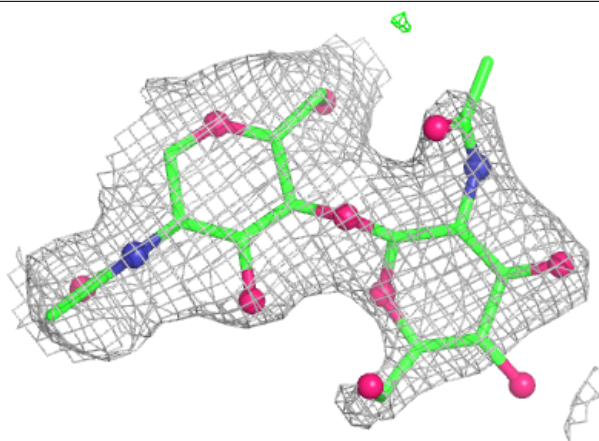
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	BMA	D	3	11/12	0.75	0.11	96,99,101,102	0
3	MAN	D	4	11/12	0.76	0.12	106,108,111,112	0
3	NAG	D	2	14/15	0.78	0.13	77,81,83,83	0
2	NAG	E	2	14/15	0.80	0.12	94,98,101,101	0
2	NAG	C	2	14/15	0.87	0.12	87,91,94,94	0
2	NAG	E	1	14/15	0.92	0.08	63,66,72,72	0
3	NAG	D	1	14/15	0.93	0.10	68,74,77,78	0
2	NAG	C	1	14/15	0.93	0.08	75,79,84,85	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.

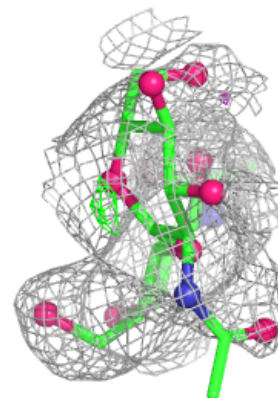
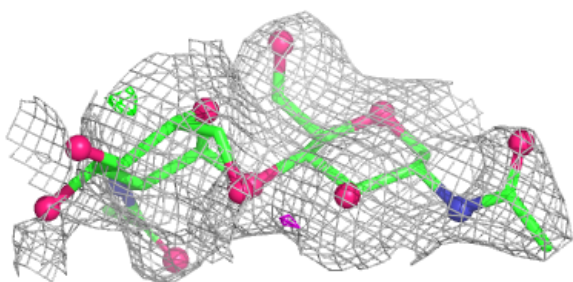
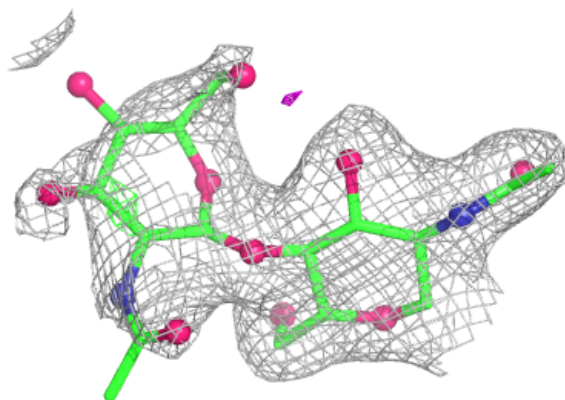
Electron density around Chain C:

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

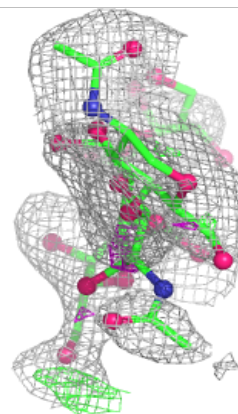
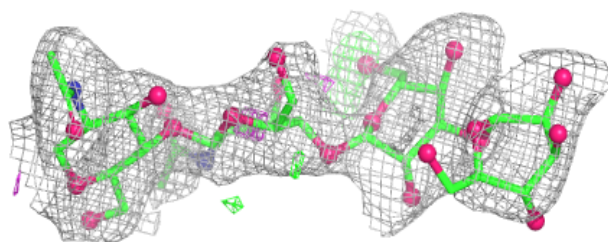
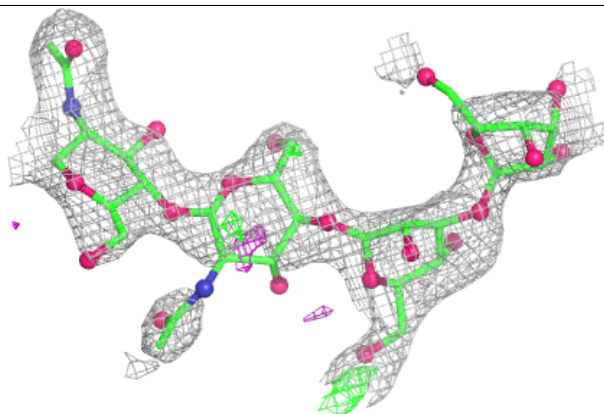


Electron density around Chain E:

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

**Electron density around Chain D:**

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

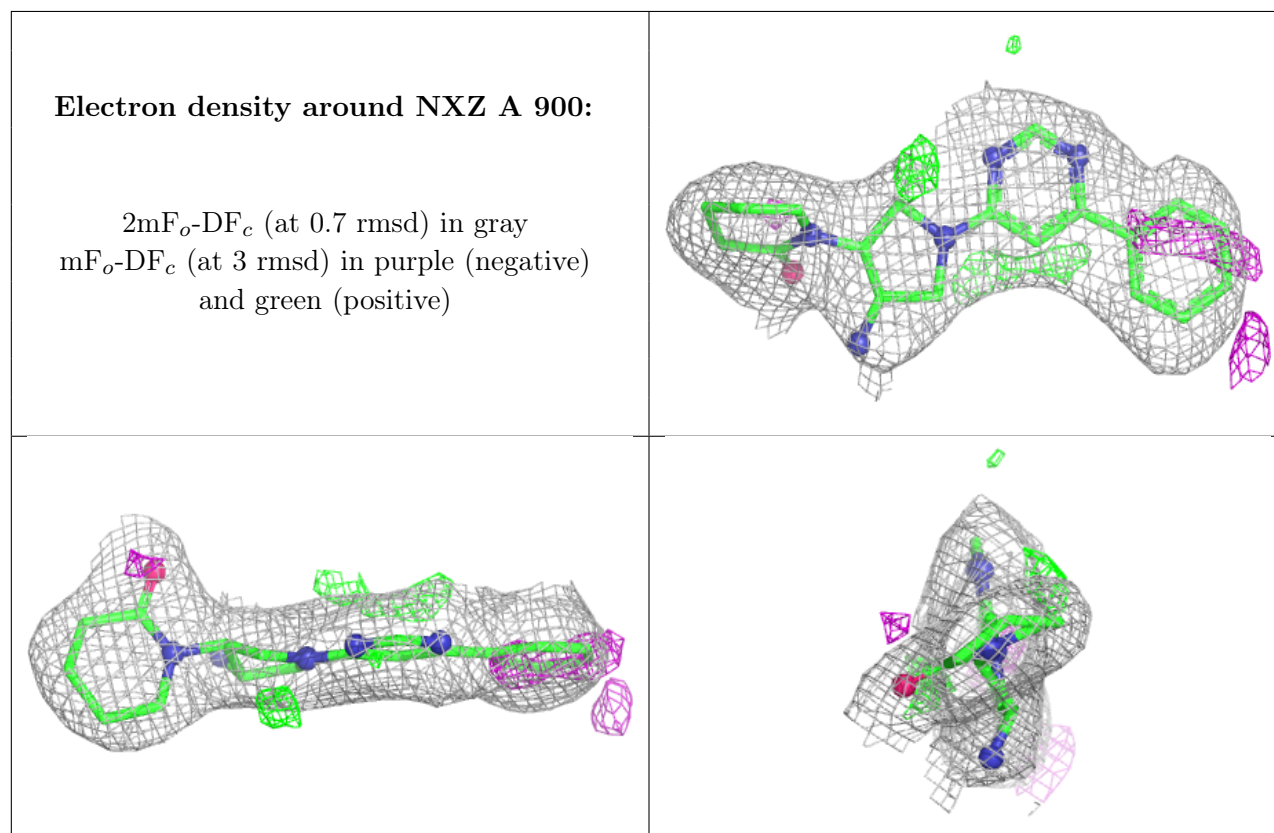


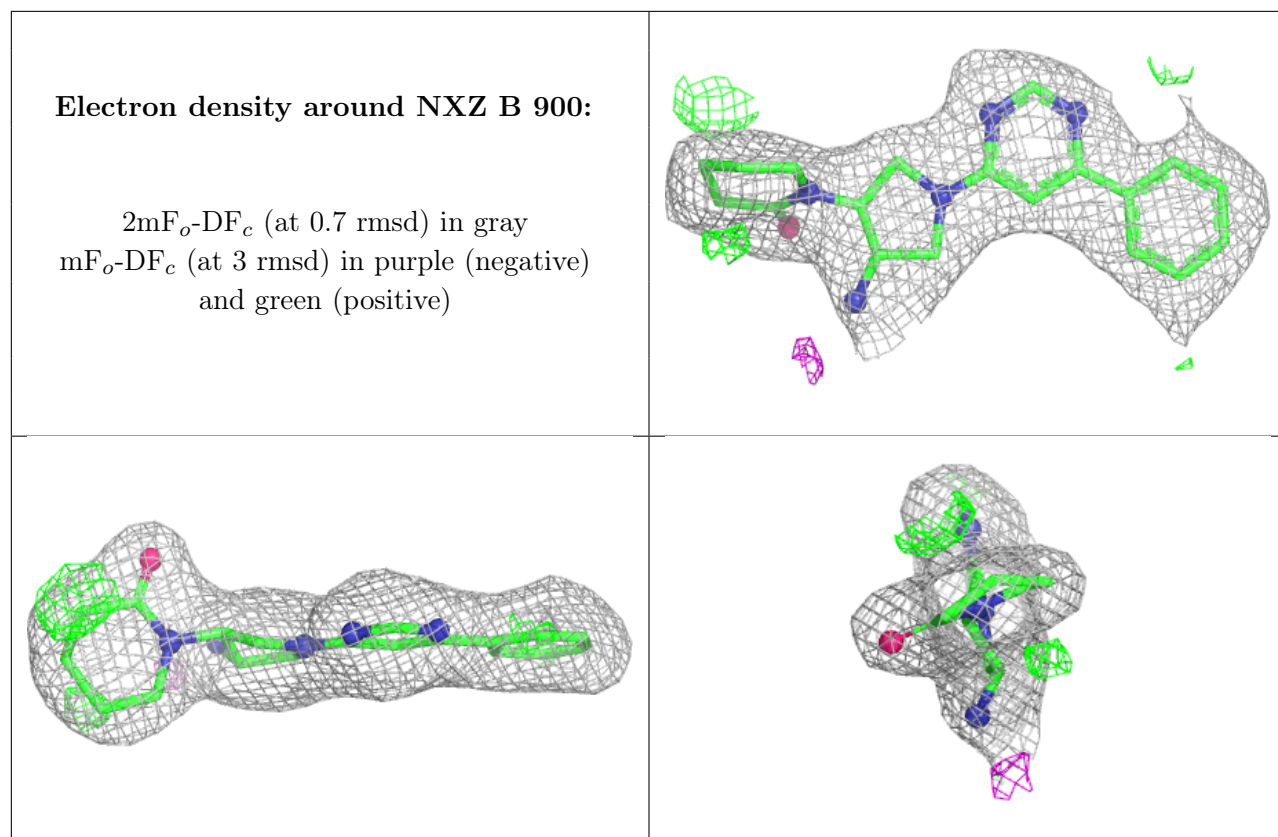
6.4 Ligands [i](#)

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
4	NAG	A	799	14/15	0.77	0.11	99,103,105,106	0
4	NAG	A	800	14/15	0.80	0.10	89,93,95,95	0
4	NAG	B	796	14/15	0.87	0.10	70,76,80,81	0
5	NXZ	A	900	25/25	0.87	0.09	46,54,76,78	0
5	NXZ	B	900	25/25	0.92	0.07	41,49,69,70	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.