



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2024 – 06:17 pm GMT

PDB ID : 8P3E
Title : Crystal structure of glucocerebrosidase in complex with allosteric activator
Authors : Schulze, M.-S.
Deposited on : 2023-05-17
Resolution : 1.75 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 : 1.8.4, 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

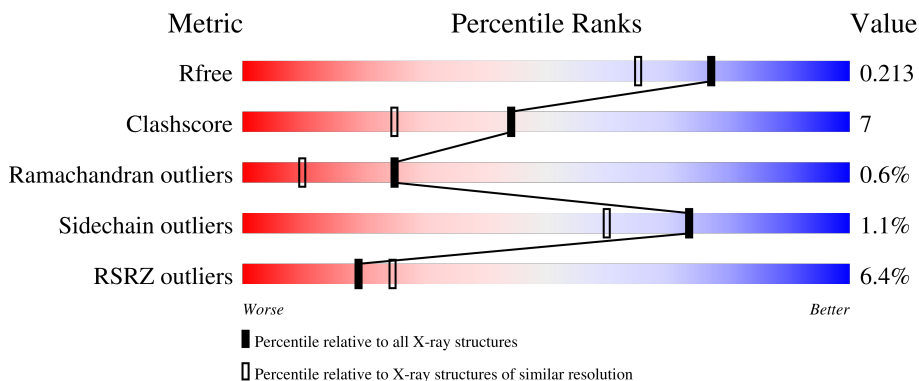
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

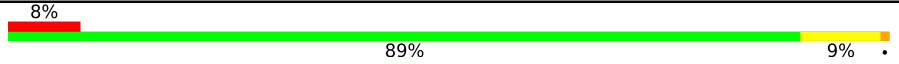
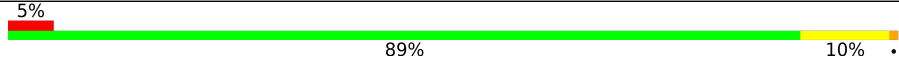

The reported resolution of this entry is 1.75 Å.

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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	497	
1	B	497	
2	C	2	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8452 atoms, of which 55 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 Glucosylceramidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	497	3929	2532	671	710	16	0	0	0
1	B	497	3929	2532	671	710	16	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	495	HIS	ARG	conflict	UNP P04062
B	495	HIS	ARG	conflict	UNP P04062

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



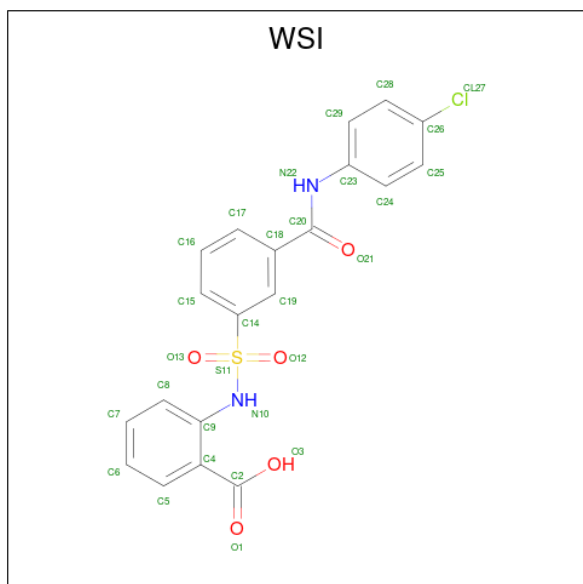
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	C	2	55	16	27	2	10	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
3	A	1	28	8	14	1	5	0	0
3	A	1	28	8	14	1	5	0	0

- Molecule 4 is 2-[[3-[(4-chlorophenyl)carbamoyl]phenyl]sulfonylamino]benzoic acid (three-letter code: WSI) (formula: $C_{20}H_{15}ClN_2O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	N	O	S		
4	B	1	29	20	1	2	5	1	0	0

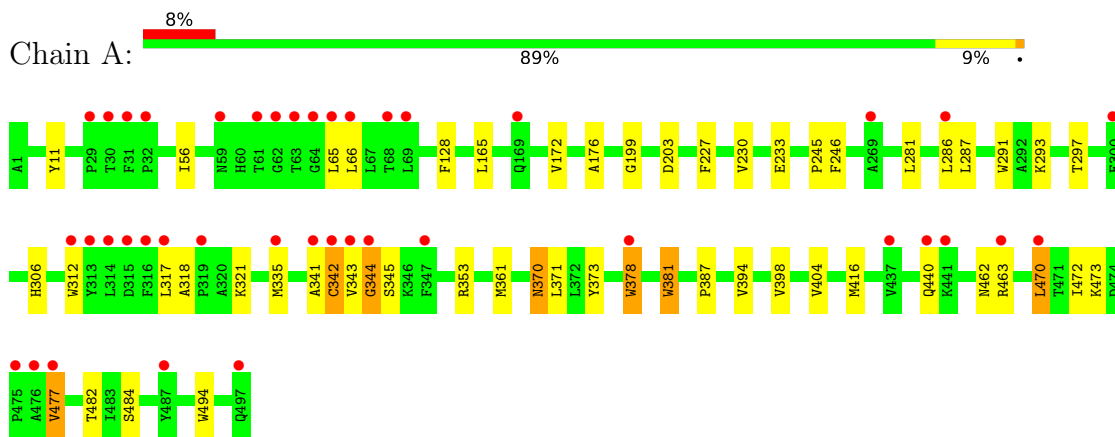
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	198	Total 198	O 198	0	0
5	B	256	Total 256	O 256	0	0

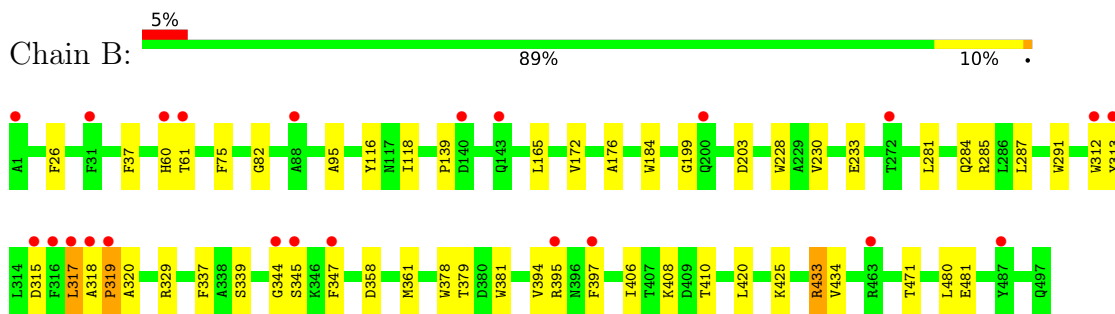
3 Residue-property plots [i](#)

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: Glucosylceramidase



- Molecule 1: Glucosylceramidase



- 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	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	110.31Å 285.64Å 91.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.61 – 1.75 47.61 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.61-1.75) 99.5 (47.61-1.75)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 1.75Å)	Xtrriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.190 , 0.214 0.189 , 0.213	Depositor DCC
R_{free} test set	7233 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	27.8	Xtrriage
Anisotropy	0.736	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8452	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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, WSI

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	0.50	1/4050 (0.0%)	0.63	0/5523
1	B	0.49	0/4050	0.64	0/5523
All	All	0.49	1/8100 (0.0%)	0.63	0/11046

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	378	TRP	CB-CG	-6.35	1.38	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3929	0	3843	43	0
1	B	3929	0	3843	61	0
2	C	28	27	25	0	0
3	A	28	28	26	3	0
4	B	29	0	0	1	0
5	A	198	0	0	1	0
5	B	256	0	0	0	0
All	All	8397	55	7737	104	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 (104) 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:286:LEU:HD13	1:A:318:ALA:HB2	1.54	0.89
1:B:60:HIS:HE1	1:B:471:THR:OG1	1.57	0.86
1:A:246:PHE:CD1	1:A:394:VAL:HG21	2.12	0.85
3:A:501:NAG:O4	3:A:502:NAG:C1	2.28	0.82
1:B:284:GLN:CD	1:B:313:TYR:HE2	1.86	0.79
1:B:285:ARG:HH11	1:B:312:TRP:HH2	1.29	0.77
1:A:312:TRP:CE3	1:A:341:ALA:HB1	2.21	0.76
1:B:60:HIS:CE1	1:B:471:THR:HG21	2.25	0.71
1:B:284:GLN:CD	1:B:313:TYR:CE2	2.66	0.69
1:A:470:LEU:HD21	1:A:472:ILE:HG13	1.73	0.69
1:A:371:LEU:HG	1:A:378:TRP:CH2	2.28	0.69
1:B:408:LYS:O	1:B:410:THR:HG23	1.93	0.67
4:B:501:WSI:N10	4:B:501:WSI:O3	2.26	0.67
1:A:246:PHE:HD1	1:A:394:VAL:HG21	1.58	0.66
1:B:60:HIS:ND1	1:B:471:THR:HG21	2.10	0.66
1:A:343:VAL:O	1:A:345:SER:N	2.28	0.66
1:A:165:LEU:HD22	1:A:172:VAL:HB	1.77	0.66
1:B:285:ARG:HH21	1:B:318:ALA:C	1.98	0.65
1:B:285:ARG:HH21	1:B:318:ALA:HB3	1.60	0.65
1:A:286:LEU:CD1	1:A:318:ALA:HB2	2.24	0.65
3:A:501:NAG:C4	3:A:502:NAG:C1	2.75	0.65
1:B:284:GLN:NE2	1:B:313:TYR:CE2	2.67	0.62
1:B:284:GLN:NE2	1:B:313:TYR:HE2	1.96	0.62
1:B:165:LEU:HD22	1:B:172:VAL:HB	1.82	0.62
1:B:285:ARG:NH1	1:B:312:TRP:CH2	2.67	0.61
1:B:394:VAL:O	1:B:395:ARG:HG3	2.01	0.61
1:B:95:ALA:HB1	1:B:406:ILE:HD12	1.83	0.61
1:B:60:HIS:CE1	1:B:471:THR:OG1	2.47	0.60
1:B:60:HIS:HE1	1:B:471:THR:CB	2.14	0.60
1:B:358:ASP:HA	1:B:361:MET:HE2	1.84	0.59
1:A:293:LYS:O	1:A:297:THR:HG23	2.01	0.59
1:A:342:CYS:SG	1:A:381:TRP:HB3	2.44	0.57
1:B:285:ARG:HH21	1:B:318:ALA:CB	2.18	0.57
1:B:287:LEU:HB3	1:B:291:TRP:CD1	2.40	0.57
1:A:312:TRP:CE3	1:A:341:ALA:CB	2.88	0.56
1:A:317:LEU:HD13	1:B:317:LEU:O	2.06	0.55
1:B:61:THR:HG22	1:B:481:GLU:HG3	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:LEU:C	1:A:470:LEU:HD23	2.27	0.54
1:A:343:VAL:HG22	5:A:613:HOH:O	2.07	0.54
1:B:284:GLN:OE1	1:B:313:TYR:CE2	2.61	0.53
1:A:470:LEU:HD22	1:A:482:THR:CG2	2.38	0.53
1:B:285:ARG:NH2	1:B:318:ALA:HB3	2.24	0.53
1:A:246:PHE:CE1	1:A:394:VAL:HG21	2.44	0.52
1:B:285:ARG:HD3	1:B:312:TRP:CH2	2.45	0.52
1:A:287:LEU:HB3	1:A:291:TRP:CD1	2.45	0.51
1:B:285:ARG:NH2	1:B:318:ALA:C	2.64	0.50
1:A:56:ILE:HD13	1:A:477:VAL:HG11	1.93	0.50
1:B:60:HIS:CE1	1:B:471:THR:CB	2.94	0.50
1:B:285:ARG:NH1	1:B:312:TRP:HH2	2.03	0.50
1:B:60:HIS:CE1	1:B:471:THR:CG2	2.94	0.50
3:A:501:NAG:H4	3:A:502:NAG:C1	2.41	0.50
1:A:286:LEU:HD21	1:B:317:LEU:HB3	1.92	0.49
1:A:343:VAL:HG21	1:A:416:MET:SD	2.53	0.49
1:A:462:ASN:HB2	1:A:484:SER:OG	2.12	0.49
1:A:387:PRO:HD3	1:A:404:VAL:O	2.13	0.49
1:B:345:SER:O	1:B:397:PHE:CZ	2.66	0.49
1:B:285:ARG:NH1	1:B:312:TRP:CZ3	2.82	0.48
1:A:371:LEU:CD2	1:A:378:TRP:HH2	2.27	0.48
1:A:321:LYS:HD3	1:A:373:TYR:HE1	1.79	0.48
1:A:361:MET:CE	1:A:463:ARG:HA	2.44	0.48
1:B:116:TYR:OH	1:B:420:LEU:HD13	2.13	0.48
1:B:378:TRP:CZ3	1:B:420:LEU:HD21	2.50	0.47
1:A:66:LEU:HD11	1:A:473:LYS:HB2	1.97	0.46
1:B:176:ALA:HB3	1:B:230:VAL:HG12	1.97	0.46
1:B:339:SER:O	1:B:379:THR:OG1	2.33	0.46
1:B:199:GLY:HA3	1:B:203:ASP:OD2	2.15	0.46
1:B:75:PHE:HB2	1:B:433:ARG:HG2	1.97	0.46
1:B:315:ASP:OD2	1:B:344:GLY:C	2.54	0.45
1:A:370:ASN:HB3	1:A:378:TRP:HZ2	1.82	0.45
1:B:285:ARG:HH21	1:B:318:ALA:CA	2.28	0.45
1:B:318:ALA:HB1	1:B:319:PRO:CD	2.47	0.45
1:A:245:PRO:HG3	1:B:347:PHE:CZ	2.52	0.45
1:B:329:ARG:HG2	1:B:329:ARG:HH11	1.82	0.45
1:A:176:ALA:HB3	1:A:230:VAL:HG12	1.98	0.45
1:B:26:PHE:CG	1:B:425:LYS:HE2	2.51	0.44
1:B:285:ARG:HD3	1:B:312:TRP:CZ3	2.53	0.44
1:A:306:HIS:NE2	1:A:335:MET:SD	2.91	0.43
1:A:65:LEU:HD13	1:A:440:GLN:HG3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:LEU:HD13	1:B:317:LEU:HA	1.76	0.43
1:B:344:GLY:HA3	1:B:397:PHE:CE2	2.53	0.43
1:B:329:ARG:HG2	1:B:329:ARG:NH1	2.33	0.43
1:B:337:PHE:CZ	1:B:379:THR:CG2	3.02	0.43
1:B:315:ASP:OD2	1:B:344:GLY:O	2.36	0.43
1:B:394:VAL:O	1:B:395:ARG:CG	2.66	0.43
1:A:199:GLY:HA3	1:A:203:ASP:OD2	2.18	0.43
1:B:82:GLY:HA3	1:B:118:ILE:O	2.18	0.43
1:A:381:TRP:HA	1:A:381:TRP:CE3	2.54	0.42
1:A:381:TRP:HA	1:A:381:TRP:HE3	1.85	0.42
1:B:139:PRO:HA	1:B:184:TRP:CD1	2.54	0.42
1:B:284:GLN:OE1	1:B:313:TYR:CD2	2.73	0.42
1:A:176:ALA:HB2	1:A:227:PHE:CE2	2.55	0.42
1:A:317:LEU:HB3	1:B:317:LEU:O	2.19	0.41
1:A:128:PHE:CZ	1:A:398:VAL:HG22	2.55	0.41
1:B:37:PHE:CD2	1:B:480:LEU:HG	2.55	0.41
1:B:433:ARG:HG3	1:B:434:VAL:N	2.32	0.41
1:A:11:TYR:CZ	1:A:353:ARG:HG2	2.54	0.41
1:A:370:ASN:HB3	1:A:378:TRP:CZ2	2.55	0.41
1:B:344:GLY:HA3	1:B:397:PHE:HE2	1.86	0.41
1:B:165:LEU:CD2	1:B:172:VAL:HB	2.47	0.41
1:A:477:VAL:HG21	1:A:494:TRP:CD1	2.55	0.41
1:B:285:ARG:HE	1:B:318:ALA:HB3	1.86	0.41
1:A:343:VAL:O	1:A:344:GLY:C	2.59	0.40
1:A:312:TRP:HZ2	1:A:378:TRP:CD1	2.39	0.40
1:B:285:ARG:NH1	1:B:320:ALA:HB2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	495/497 (100%)	477 (96%)	15 (3%)	3 (1%)	25	10
1	B	495/497 (100%)	474 (96%)	18 (4%)	3 (1%)	25	10
All	All	990/994 (100%)	951 (96%)	33 (3%)	6 (1%)	25	10

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	344	GLY
1	B	319	PRO
1	A	233	GLU
1	B	233	GLU
1	B	281	LEU
1	A	281	LEU

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	424/424 (100%)	419 (99%)	5 (1%)	71	56
1	B	424/424 (100%)	420 (99%)	4 (1%)	78	67
All	All	848/848 (100%)	839 (99%)	9 (1%)	73	60

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	342	CYS
1	A	370	ASN
1	A	381	TRP
1	A	470	LEU
1	A	477	VAL
1	B	228	TRP
1	B	317	LEU
1	B	381	TRP
1	B	433	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	60	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](#)

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	C	1	2,1	14,14,15	0.97	1 (7%)	17,19,21	0.48	0
2	NAG	C	2	2	14,14,15	0.43	0	17,19,21	0.39	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
2	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	NAG	O5-C1	-3.49	1.38	1.43

There are no bond angle outliers.

There are no chirality outliers.

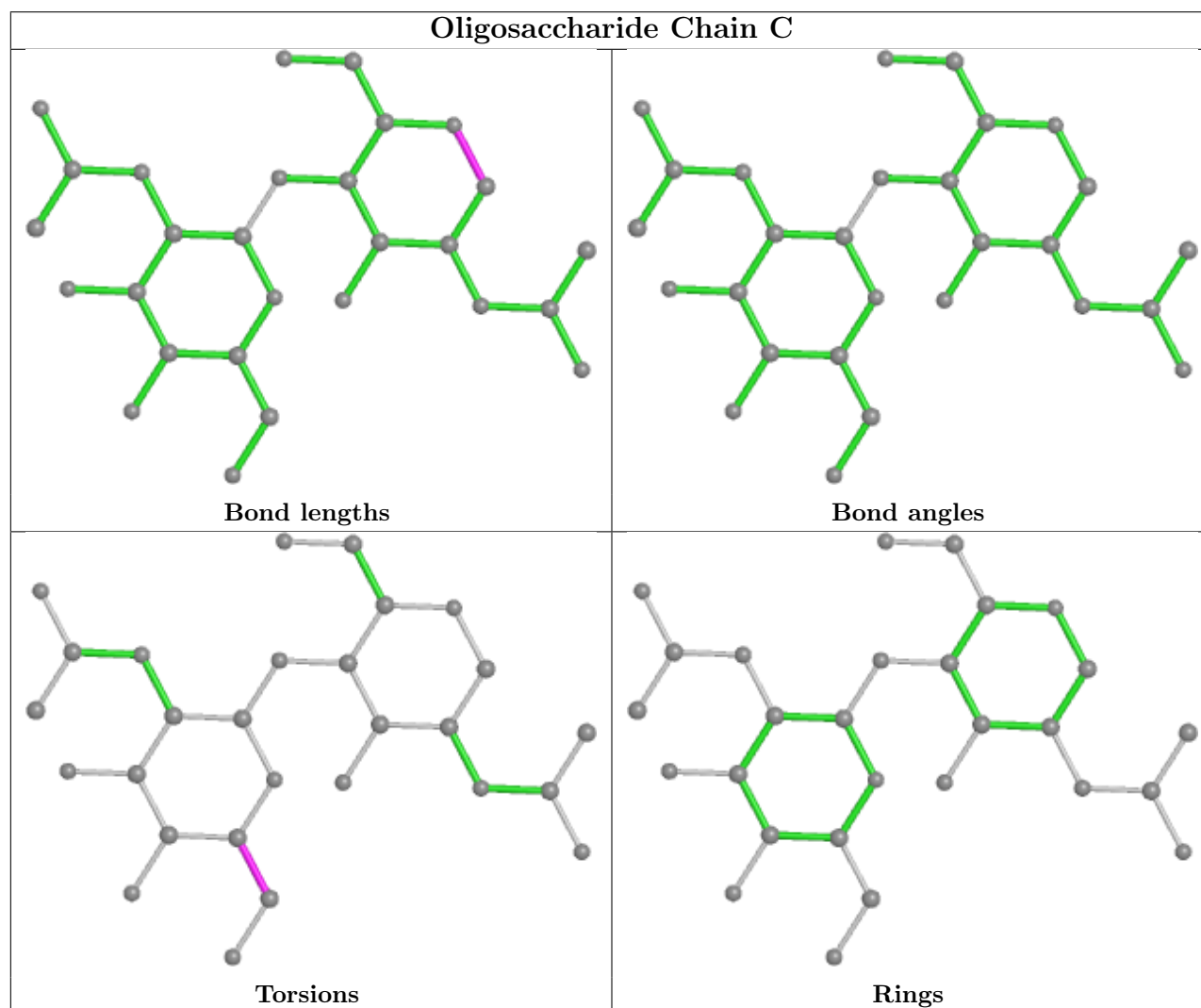
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6

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](#)

3 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
3	NAG	A	501	1	14,14,15	1.02	1 (7%)	17,19,21	1.00	2 (11%)
3	NAG	A	502	-	14,14,15	1.51	2 (14%)	17,19,21	0.96	1 (5%)
4	WSI	B	501	-	31,31,31	1.19	2 (6%)	44,44,44	1.35	6 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	501	1	-	0/6/23/26	0/1/1/1
3	NAG	A	502	-	-	2/6/23/26	0/1/1/1
4	WSI	B	501	-	-	2/23/23/23	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	WSI	S11-N10	4.66	1.71	1.63
3	A	502	NAG	O5-C1	-4.64	1.36	1.43
3	A	501	NAG	O5-C1	-3.51	1.38	1.43
3	A	502	NAG	C1-C2	-2.83	1.48	1.52
4	B	501	WSI	C4-C9	-2.25	1.37	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	WSI	O12-S11-N10	3.36	115.15	106.73
4	B	501	WSI	C23-N22-C20	-3.26	118.11	126.58
3	A	501	NAG	C3-C4-C5	2.78	115.20	110.24
4	B	501	WSI	O1-C2-C4	-2.58	115.67	121.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	NAG	C1-O5-C5	-2.55	108.73	112.19
4	B	501	WSI	C14-S11-N10	-2.34	103.89	106.83
4	B	501	WSI	C9-C4-C2	-2.33	118.97	121.72
3	A	501	NAG	O4-C4-C3	-2.21	105.24	110.35
4	B	501	WSI	O13-S11-O12	-2.20	116.85	119.55

There are no chirality outliers.

All (4) torsion outliers are listed below:

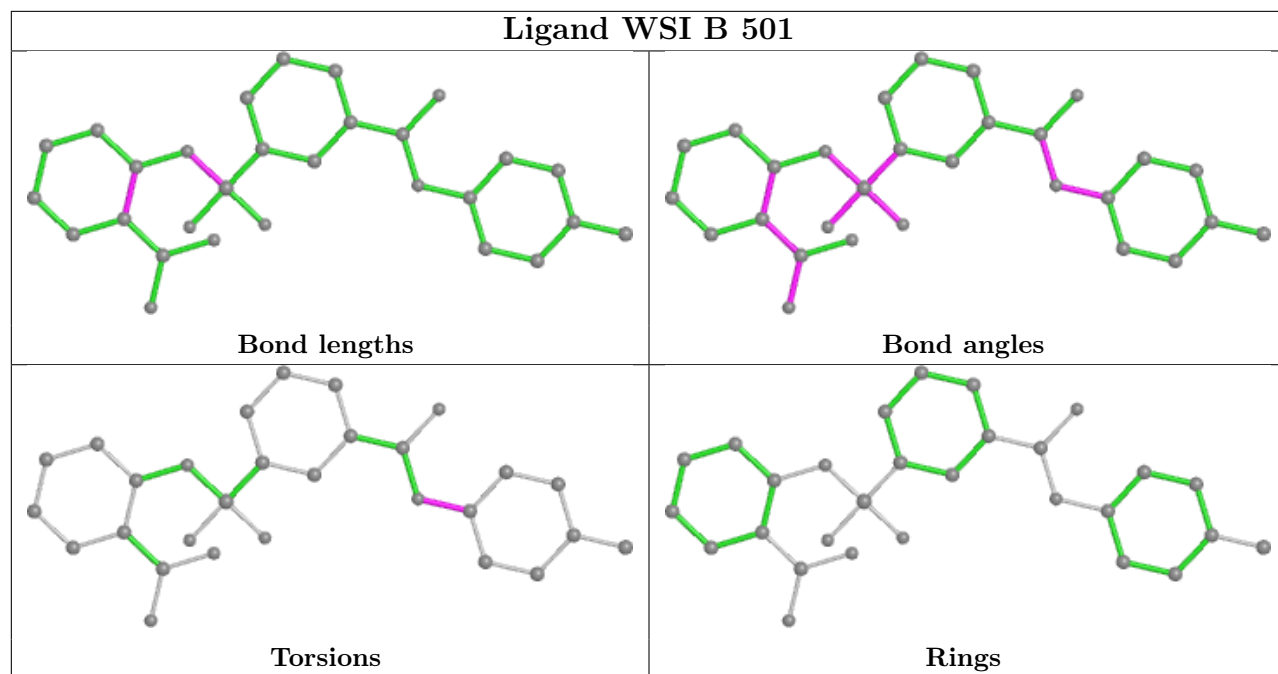
Mol	Chain	Res	Type	Atoms
3	A	502	NAG	O5-C5-C6-O6
3	A	502	NAG	C4-C5-C6-O6
4	B	501	WSI	C29-C23-N22-C20
4	B	501	WSI	C24-C23-N22-C20

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	NAG	3	0
3	A	502	NAG	3	0
4	B	501	WSI	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	497/497 (100%)	0.44	41 (8%) 11 15	21, 31, 52, 65	0
1	B	497/497 (100%)	0.34	23 (4%) 32 38	21, 29, 49, 71	0
All	All	994/994 (100%)	0.39	64 (6%) 19 25	21, 30, 52, 71	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	318	ALA	12.2
1	B	317	LEU	11.7
1	B	313	TYR	9.6
1	B	316	PHE	8.5
1	A	63	THR	8.3
1	A	477	VAL	7.6
1	B	397	PHE	7.6
1	A	344	GLY	6.7
1	A	31	PHE	5.9
1	B	319	PRO	5.3
1	B	344	GLY	5.2
1	A	312	TRP	5.1
1	A	313	TYR	5.0
1	B	312	TRP	5.0
1	A	476	ALA	5.0
1	A	316	PHE	4.9
1	A	342	CYS	4.7
1	A	378	TRP	4.5
1	A	441	LYS	4.5
1	A	30	THR	4.3
1	A	59	ASN	4.0
1	A	32	PRO	3.9
1	A	475	PRO	3.8
1	A	61	THR	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	64	GLY	3.7
1	A	317	LEU	3.7
1	B	315	ASP	3.6
1	A	343	VAL	3.5
1	A	29	PRO	3.5
1	B	345	SER	3.3
1	B	347	PHE	3.3
1	A	65	LEU	3.3
1	A	69	LEU	3.2
1	B	395	ARG	3.1
1	A	497	GLN	3.1
1	B	140	ASP	2.9
1	A	319	PRO	2.8
1	A	314	LEU	2.8
1	B	272	THR	2.8
1	B	60	HIS	2.7
1	A	315	ASP	2.6
1	B	31	PHE	2.5
1	A	341	ALA	2.5
1	A	286	LEU	2.5
1	A	300	GLU	2.5
1	B	487	TYR	2.4
1	B	143	GLN	2.4
1	B	463	ARG	2.4
1	A	470	LEU	2.4
1	A	487	TYR	2.4
1	B	88	ALA	2.4
1	A	68	THR	2.3
1	A	347	PHE	2.3
1	A	335	MET	2.3
1	A	463	ARG	2.2
1	A	169	GLN	2.2
1	B	1	ALA	2.2
1	A	66	LEU	2.2
1	B	61	THR	2.2
1	A	62	GLY	2.2
1	A	440	GLN	2.2
1	A	437	VAL	2.1
1	B	200	GLN	2.1
1	A	269	ALA	2.1

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

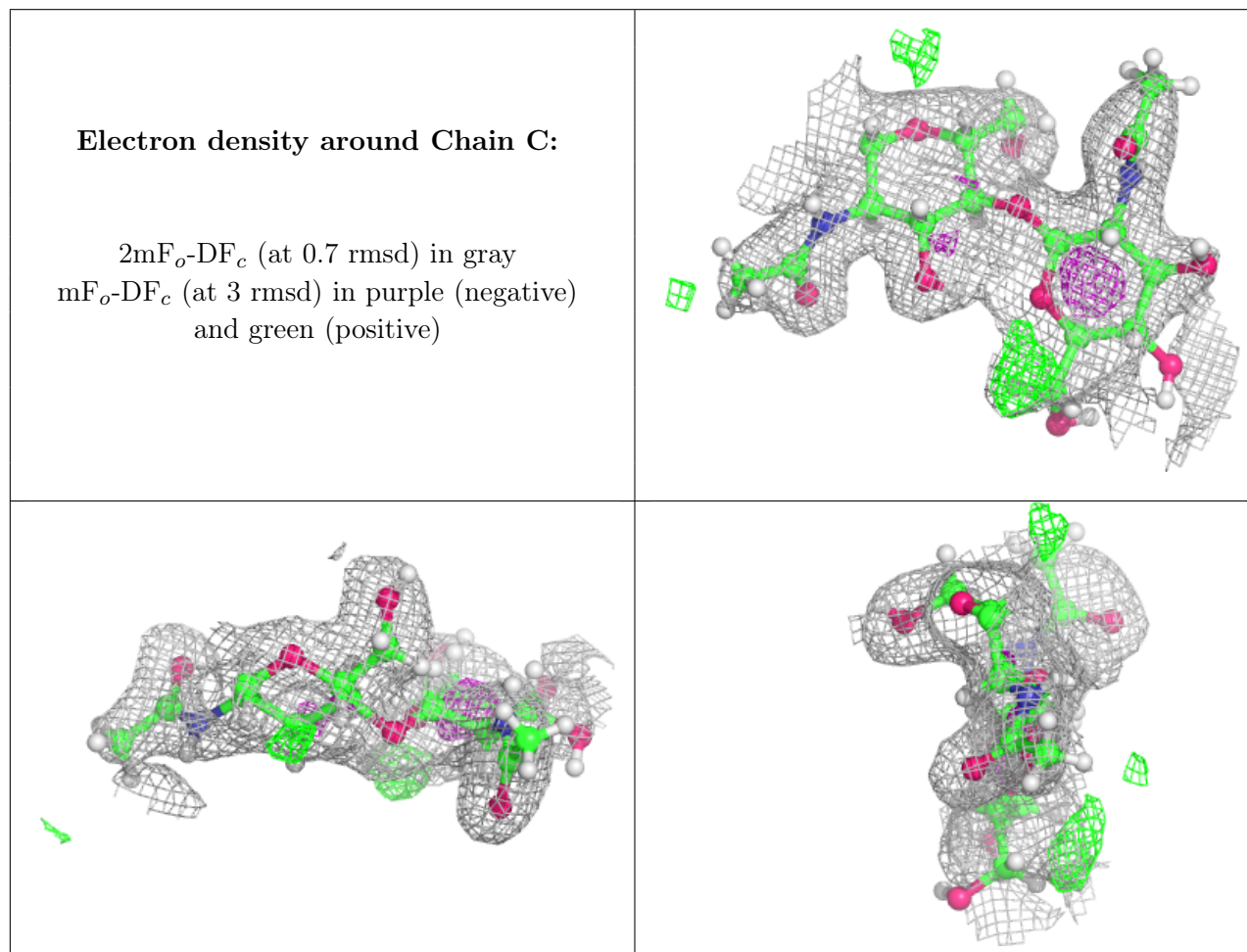
There are no non-standard protein/DNA/RNA residues in this entry.

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	NAG	C	2	14/15	0.83	0.32	47,64,80,95	0
2	NAG	C	1	14/15	0.90	0.17	34,44,52,53	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.

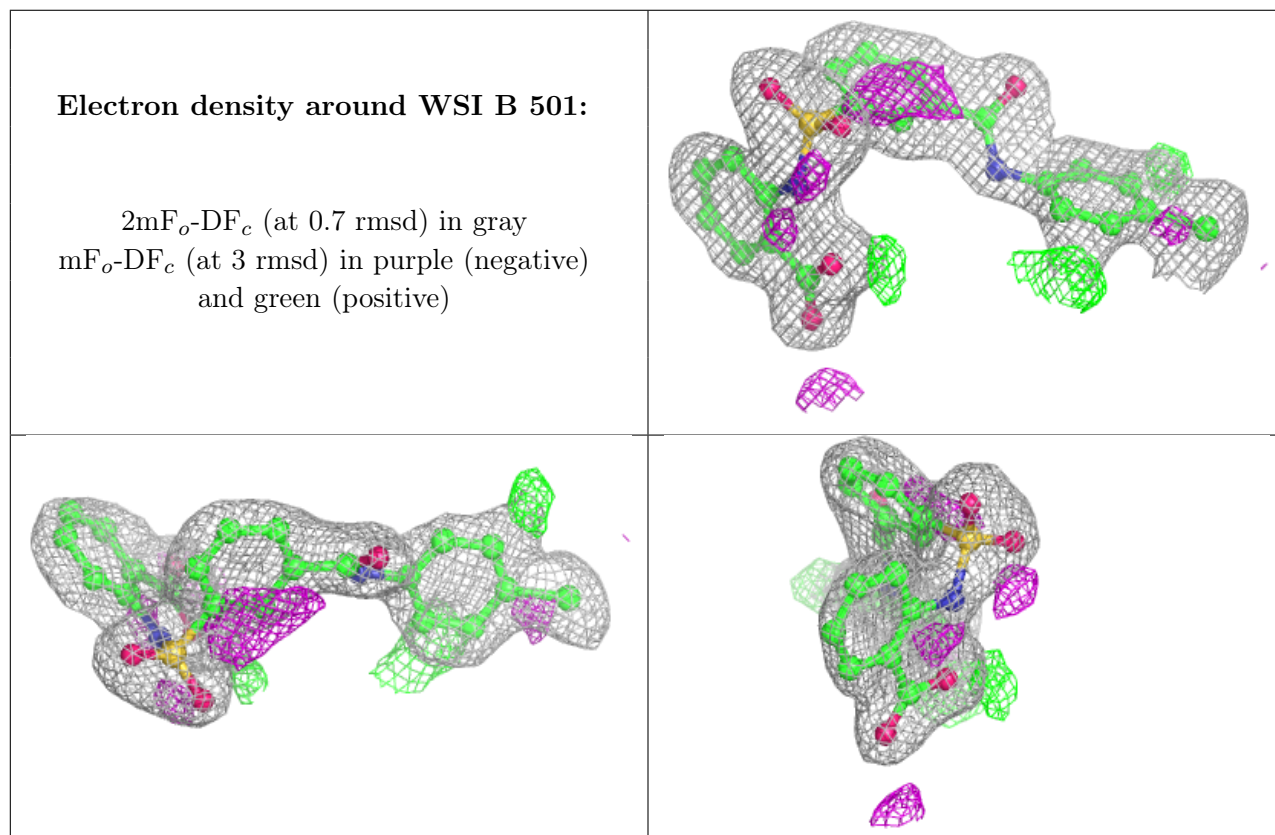


6.4 Ligands [i](#)

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
3	NAG	A	502	14/15	0.75	0.30	50,72,88,93	0
3	NAG	A	501	14/15	0.90	0.14	32,43,53,59	0
4	WSI	B	501	29/29	0.92	0.16	31,45,54,59	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.