



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:37 AM UTC

PDB ID : 4Z64 / pdb_00004z64
Title : the plant peptide hormone receptor complex in arabidopsis
Authors : Chai, J.; Wang, J.; Han, Z.
Deposited on : 2015-04-03
Resolution : 2.66 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
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

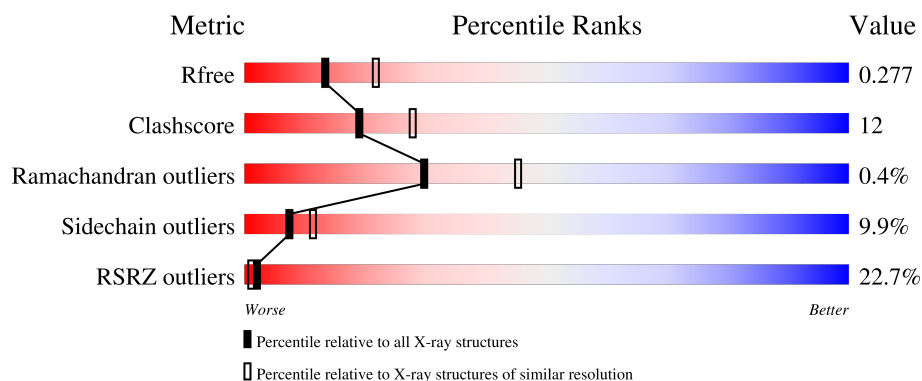
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.66 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	631	16% 74% 19% . .
2	C	219	36% 62% 17% 5% 15%
3	P	5	20% 40% 40%
4	B	2	100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6364 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 Phytosulfokine receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	605	Total	C	N	O	S	0	0	0
			4715	2986	822	888	19			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	649	HIS	-	expression tag	UNP Q9ZVR7
A	650	HIS	-	expression tag	UNP Q9ZVR7
A	651	HIS	-	expression tag	UNP Q9ZVR7
A	652	HIS	-	expression tag	UNP Q9ZVR7
A	653	HIS	-	expression tag	UNP Q9ZVR7
A	654	HIS	-	expression tag	UNP Q9ZVR7

- Molecule 2 is a protein called Somatic embryogenesis receptor kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	186	Total	C	N	O	S	0	0	0
			1418	895	240	278	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	115	ASP	ASN	engineered mutation	UNP Q94AG2
C	163	GLN	ASN	engineered mutation	UNP Q94AG2
C	214	HIS	-	expression tag	UNP Q94AG2
C	215	HIS	-	expression tag	UNP Q94AG2
C	216	HIS	-	expression tag	UNP Q94AG2
C	217	HIS	-	expression tag	UNP Q94AG2
C	218	HIS	-	expression tag	UNP Q94AG2
C	219	HIS	-	expression tag	UNP Q94AG2

- Molecule 3 is a protein called Phytosulfokine.

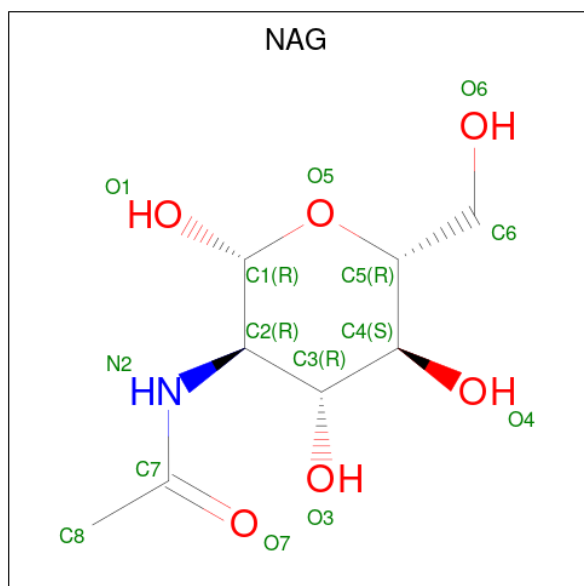
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	5	Total	C	N	O	S	0	0	0
			57	33	6	16	2			

- Molecule 4 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
4	B	2	Total	C	N	O		0	0	0
			28	16	2	10				

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



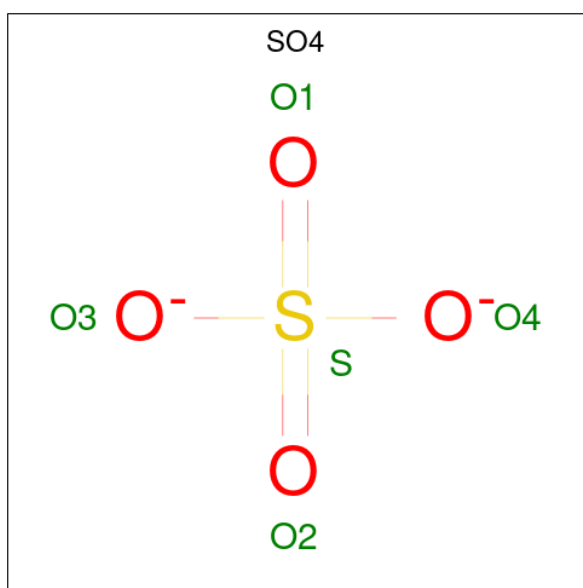
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O		0	0
			14	8	1	5			
5	A	1	Total	C	N	O		0	0
			14	8	1	5			
5	A	1	Total	C	N	O		0	0
			14	8	1	5			
5	A	1	Total	C	N	O		0	0
			14	8	1	5			

Continued on next page...

Continued from previous page...

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

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



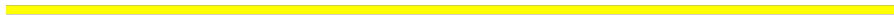
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O S	0	0
			5	4 1		
6	A	1	Total	O S	0	0
			5	4 1		
6	A	1	Total	O S	0	0
			5	4 1		
6	C	1	Total	O S	0	0
			5	4 1		

- Molecule 3: Phytosulfokine

Chain P:  20% 40% 40%


Y28
Y29
Y30
T31
Q32

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

Chain B:  100%


MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	152.54Å 220.89Å 105.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.91 – 2.66 48.91 – 2.66	Depositor EDS
% Data completeness (in resolution range)	95.7 (48.91-2.66) 95.6 (48.91-2.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.60 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.200 , 0.246 0.247 , 0.277	Depositor DCC
R_{free} test set	2516 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	50.0	Xtriage
Anisotropy	0.868	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6364	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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: NAG, TYS, SO4

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	0.72	3/4816 (0.1%)	0.90	5/6524 (0.1%)
2	C	0.69	1/1448 (0.1%)	0.92	0/1986
3	P	0.42	0/23	0.94	0/27
All	All	0.71	4/6287 (0.1%)	0.90	5/8537 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	251	VAL	CA-CB	-6.59	1.47	1.54
1	A	243	LEU	CA-C	-5.59	1.47	1.53
1	A	406	LEU	CA-C	-5.49	1.47	1.53
2	C	109	ILE	CA-C	-5.11	1.49	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	512	SER	N-CA-C	6.71	118.67	111.36
1	A	617	PHE	N-CA-C	6.00	118.78	111.82
1	A	336	LEU	CA-C-N	-5.63	114.01	119.87
1	A	336	LEU	C-N-CA	-5.63	114.01	119.87
1	A	247	VAL	N-CA-C	-5.46	107.50	112.96

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	4715	0	4680	80	2
2	C	1418	0	1405	68	0
3	P	57	0	44	5	0
4	B	28	0	25	0	0
5	A	112	0	104	0	0
5	C	14	0	13	0	0
6	A	15	0	0	1	0
6	C	5	0	0	0	0
All	All	6364	0	6271	148	2

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 12.

All (148) 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)
2:C:208:HIS:ND1	2:C:209:PRO:HD2	1.02	1.32
2:C:208:HIS:ND1	2:C:209:PRO:CD	1.98	1.25
1:A:583:LEU:HD12	1:A:605:ASN:ND2	1.60	1.15
2:C:178:SER:OG	2:C:199:LEU:CD2	1.97	1.13
2:C:198:ASN:HD22	2:C:201:LEU:CD1	1.65	1.09
1:A:583:LEU:HB2	1:A:605:ASN:HD22	1.15	1.09
2:C:208:HIS:CE1	2:C:209:PRO:HD2	1.91	1.06
2:C:39:THR:HG21	2:C:86:VAL:CG1	1.88	1.03
2:C:198:ASN:CB	2:C:201:LEU:HD12	1.93	0.98
1:A:583:LEU:HD12	1:A:605:ASN:HD21	1.17	0.97
2:C:202:CYS:HA	2:C:206:THR:HG21	1.46	0.95
2:C:138:GLY:HA3	2:C:160:SER:HB3	1.48	0.95
2:C:198:ASN:ND2	2:C:201:LEU:CD1	2.30	0.94
1:A:583:LEU:CD1	1:A:605:ASN:HD21	1.83	0.92
2:C:181:VAL:CG2	2:C:201:LEU:HD22	2.01	0.91
1:A:300:ARG:NH1	6:A:712:SO4:O3	2.03	0.91
1:A:160:ASN:HD22	1:A:161:GLY:H	1.18	0.90
2:C:198:ASN:HB2	2:C:201:LEU:HD12	1.54	0.89
2:C:178:SER:OG	2:C:199:LEU:HD23	1.72	0.89
1:A:583:LEU:HB2	1:A:605:ASN:ND2	1.90	0.86
2:C:39:THR:HG21	2:C:86:VAL:HG11	1.56	0.86
2:C:181:VAL:HG22	2:C:201:LEU:HD22	1.56	0.86
1:A:583:LEU:CD1	1:A:605:ASN:ND2	2.38	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:HIS:CD2	1:A:402:HIS:H	1.94	0.84
1:A:160:ASN:HD22	1:A:161:GLY:N	1.74	0.83
2:C:181:VAL:HG22	2:C:201:LEU:CD2	2.08	0.83
1:A:583:LEU:CB	1:A:605:ASN:HD22	1.92	0.82
2:C:195:PHE:CD2	2:C:205:VAL:HG11	2.16	0.81
2:C:208:HIS:CG	2:C:209:PRO:HD2	2.14	0.81
1:A:251:VAL:CG1	1:A:251:VAL:O	2.30	0.80
1:A:160:ASN:ND2	1:A:161:GLY:N	2.30	0.79
2:C:198:ASN:HD22	2:C:201:LEU:HD12	1.48	0.77
2:C:205:VAL:CG1	2:C:205:VAL:O	2.33	0.77
1:A:160:ASN:ND2	1:A:161:GLY:H	1.82	0.77
2:C:198:ASN:ND2	2:C:201:LEU:HD12	1.99	0.76
1:A:583:LEU:CB	1:A:605:ASN:ND2	2.49	0.75
2:C:178:SER:OG	2:C:199:LEU:HD21	1.83	0.75
2:C:203:GLY:O	2:C:206:THR:HG22	1.86	0.75
1:A:140:ILE:HG13	1:A:164:PRO:HG3	1.67	0.74
1:A:409:ASP:OD1	1:A:409:ASP:C	2.29	0.74
1:A:251:VAL:O	1:A:251:VAL:HG12	1.88	0.74
2:C:205:VAL:O	2:C:205:VAL:HG12	1.89	0.72
1:A:597:LEU:O	1:A:616:GLN:HG2	1.88	0.72
1:A:488:SER:HA	1:A:494:ILE:HG21	1.72	0.71
1:A:371:LEU:HD13	1:A:376:LEU:HD11	1.73	0.71
2:C:35:THR:O	2:C:39:THR:HG22	1.90	0.71
1:A:406:LEU:HD13	1:A:427:LEU:HD13	1.76	0.67
1:A:409:ASP:OD1	1:A:411:SER:N	2.28	0.67
1:A:583:LEU:CG	1:A:605:ASN:ND2	2.58	0.66
2:C:206:THR:HG23	2:C:208:HIS:O	1.95	0.66
2:C:198:ASN:ND2	2:C:201:LEU:HD11	2.09	0.66
2:C:34:HIS:O	2:C:38:VAL:HG22	1.97	0.65
1:A:510:ASN:OD1	1:A:512:SER:N	2.30	0.65
2:C:181:VAL:CG2	2:C:201:LEU:CD2	2.71	0.65
2:C:198:ASN:CG	2:C:201:LEU:HD12	2.23	0.64
1:A:583:LEU:CG	1:A:605:ASN:HD21	2.09	0.64
1:A:510:ASN:OD1	1:A:510:ASN:C	2.40	0.64
2:C:202:CYS:CA	2:C:206:THR:HG21	2.25	0.64
1:A:175:ARG:NH1	1:A:199:GLU:OE1	2.33	0.61
1:A:580:ASN:C	1:A:581:ASN:HD22	2.08	0.61
2:C:178:SER:HG	2:C:199:LEU:HD21	1.66	0.59
1:A:498:GLU:HB2	1:A:522:PHE:CE2	2.38	0.59
2:C:178:SER:HG	2:C:199:LEU:CD2	2.11	0.59
2:C:195:PHE:HD2	2:C:205:VAL:HG11	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:203:GLY:N	2:C:206:THR:CG2	2.67	0.57
2:C:203:GLY:O	2:C:206:THR:CG2	2.51	0.57
2:C:198:ASN:HD22	2:C:201:LEU:HD13	1.66	0.57
1:A:570:MET:HE3	1:A:573:LEU:HD22	1.87	0.57
2:C:39:THR:HG21	2:C:86:VAL:HG13	1.83	0.56
1:A:476:THR:HA	1:A:534:ASN:O	2.05	0.56
1:A:419:VAL:HG13	1:A:443:LEU:HD22	1.88	0.55
1:A:620:PHE:O	1:A:635:ARG:NH1	2.38	0.55
1:A:583:LEU:H	1:A:605:ASN:ND2	2.04	0.55
1:A:632:GLY:HA3	1:A:635:ARG:O	2.07	0.55
1:A:117:PRO:HD2	1:A:120:ILE:HD12	1.88	0.55
1:A:481:LYS:O	1:A:484:THR:OG1	2.24	0.54
2:C:31:ASP:O	2:C:35:THR:HG23	2.07	0.54
2:C:36:LEU:HD22	2:C:89:LEU:HD21	1.90	0.54
2:C:112:ASN:O	2:C:113:LEU:C	2.52	0.53
1:A:358:GLU:H	1:A:358:GLU:CD	2.16	0.52
1:A:478:GLU:HA	1:A:536:SER:O	2.09	0.52
1:A:369:PHE:CE2	1:A:371:LEU:HD12	2.45	0.51
1:A:370:SER:OG	3:P:31:THR:HG21	2.10	0.51
1:A:127:GLN:HA	1:A:149:LEU:HA	1.93	0.50
1:A:421:VAL:HG13	1:A:445:ASP:HB3	1.93	0.49
1:A:251:VAL:O	1:A:251:VAL:HG13	2.12	0.49
2:C:112:ASN:O	2:C:114:GLY:N	2.46	0.49
1:A:532:HIS:CE1	1:A:556:TRP:CD1	3.01	0.49
2:C:203:GLY:N	2:C:206:THR:HG22	2.27	0.49
2:C:197:ASN:O	2:C:197:ASN:OD1	2.30	0.49
2:C:72:ILE:HG13	2:C:73:ARG:HG3	1.93	0.48
2:C:35:THR:O	2:C:38:VAL:HG23	2.14	0.48
2:C:206:THR:OG1	2:C:207:SER:N	2.44	0.48
1:A:77:ARG:HA	1:A:77:ARG:HD2	1.57	0.48
1:A:431:MET:HG3	1:A:456:PRO:HD3	1.95	0.47
1:A:424:ASN:ND2	3:P:28:TYS:O3	2.47	0.47
1:A:319:ASN:HA	1:A:342:LEU:HA	1.95	0.47
1:A:455:ILE:O	1:A:480:PRO:HG3	2.14	0.47
1:A:506:PHE:CE2	3:P:32:GLN:HG2	2.50	0.46
1:A:409:ASP:OD1	1:A:410:SER:N	2.47	0.46
1:A:217:PHE:HA	1:A:243:LEU:HD21	1.97	0.46
1:A:370:SER:CB	3:P:31:THR:HG21	2.45	0.46
1:A:431:MET:HE2	1:A:459:ILE:HD13	1.98	0.46
2:C:208:HIS:CE1	2:C:209:PRO:CD	2.78	0.45
1:A:62:CYS:HA	1:A:65:TRP:CE2	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:193:ILE:H	2:C:193:ILE:HG13	1.51	0.45
1:A:265:ASP:OD1	1:A:265:ASP:N	2.43	0.44
2:C:112:ASN:C	2:C:114:GLY:N	2.75	0.44
2:C:39:THR:CG2	2:C:86:VAL:HG11	2.37	0.44
2:C:181:VAL:HG21	2:C:201:LEU:HD22	1.93	0.44
2:C:41:VAL:HB	2:C:82:SER:OG	2.18	0.44
2:C:203:GLY:H	2:C:206:THR:CG2	2.31	0.44
1:A:165:SER:OG	1:A:191:GLY:HA3	2.18	0.43
1:A:553:ASP:OD1	1:A:577:ASP:HB3	2.18	0.43
1:A:541:GLU:HG2	1:A:564:PRO:HB3	1.99	0.43
1:A:77:ARG:HG3	1:A:101:GLU:HG3	1.99	0.43
1:A:581:ASN:HD22	1:A:581:ASN:N	2.16	0.43
2:C:204:PRO:C	2:C:206:THR:H	2.25	0.43
1:A:62:CYS:HA	1:A:65:TRP:CD2	2.54	0.43
1:A:181:VAL:HG22	1:A:205:MET:CG	2.49	0.43
1:A:401:PHE:O	1:A:404:GLU:HG3	2.19	0.43
1:A:370:SER:HB2	3:P:31:THR:HG21	2.01	0.42
2:C:195:PHE:HD2	2:C:205:VAL:CG1	2.30	0.42
2:C:64:THR:HB	2:C:73:ARG:HB2	2.00	0.42
2:C:202:CYS:SG	2:C:210:CYS:HA	2.59	0.42
2:C:203:GLY:C	2:C:206:THR:HG22	2.45	0.42
1:A:45:HIS:O	1:A:90:GLY:HA3	2.20	0.42
1:A:241:ARG:HB3	1:A:263:VAL:HB	2.01	0.42
2:C:197:ASN:O	2:C:197:ASN:CG	2.60	0.42
1:A:545:ASN:O	1:A:547:LYS:N	2.53	0.41
2:C:195:PHE:CD2	2:C:205:VAL:CG1	2.97	0.41
2:C:197:ASN:OD1	2:C:197:ASN:C	2.61	0.41
2:C:204:PRO:C	2:C:206:THR:N	2.78	0.41
2:C:124:LEU:HB3	2:C:129:PHE:CE2	2.55	0.41
1:A:124:LYS:HE2	1:A:145:ASN:ND2	2.35	0.41
2:C:106:THR:HG22	2:C:128:SER:HB2	2.02	0.41
1:A:46:LEU:HA	1:A:89:SER:O	2.21	0.41
2:C:191:THR:O	2:C:194:SER:OG	2.39	0.41
1:A:498:GLU:HB2	1:A:522:PHE:CZ	2.56	0.41
2:C:199:LEU:HD23	2:C:200:ASP:N	2.36	0.41
2:C:205:VAL:O	2:C:205:VAL:HG13	2.17	0.41
1:A:97:GLY:HA3	1:A:119:SER:HB2	2.03	0.41
1:A:230:ASN:HB3	1:A:231:ARG:H	1.73	0.41
1:A:483:LEU:HD23	1:A:483:LEU:HA	1.90	0.41
1:A:605:ASN:HB3	1:A:606:ASN:H	1.78	0.41
1:A:163:LEU:HA	1:A:164:PRO:HD3	1.89	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:ASN:HB3	1:A:474:SER:H	1.77	0.40
1:A:581:ASN:HB3	1:A:582:ARG:H	1.75	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:SER:OG	1:A:305:SER:OG[4_555]	1.64	0.56
1:A:309:MET:CG	1:A:309:MET:SD[4_555]	1.83	0.37

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	601/631 (95%)	546 (91%)	53 (9%)	2 (0%)	36	52
2	C	184/219 (84%)	169 (92%)	14 (8%)	1 (0%)	24	39
3	P	2/5 (40%)	2 (100%)	0	0	100	100
All	All	787/855 (92%)	717 (91%)	67 (8%)	3 (0%)	30	45

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	PRO
1	A	546	LEU
2	C	113	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	544/567 (96%)	495 (91%)	49 (9%)	9	14
2	C	170/201 (85%)	149 (88%)	21 (12%)	4	6
3	P	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	717/771 (93%)	646 (90%)	71 (10%)	7	11

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	SER
1	A	77	ARG
1	A	96	LEU
1	A	105	LEU
1	A	113	LYS
1	A	128	THR
1	A	158	LYS
1	A	162	SER
1	A	165	SER
1	A	173	GLN
1	A	175	ARG
1	A	179	LEU
1	A	196	VAL
1	A	205	MET
1	A	216	LEU
1	A	220	LYS
1	A	238	ARG
1	A	240	ILE
1	A	241	ARG
1	A	251	VAL
1	A	265	ASP
1	A	294	LEU
1	A	305	SER
1	A	309	MET
1	A	310	LEU
1	A	363	PHE
1	A	374	SER
1	A	394	THR
1	A	402	HIS
1	A	409	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	410	SER
1	A	411	SER
1	A	436	SER
1	A	494	ILE
1	A	500	SER
1	A	508	LYS
1	A	510	ASN
1	A	511	GLU
1	A	520	GLN
1	A	529	GLU
1	A	548	LYS
1	A	572	SER
1	A	589	VAL
1	A	607	LEU
1	A	610	VAL
1	A	613	SER
1	A	633	GLU
1	A	635	ARG
1	A	638	CYS
2	C	35	THR
2	C	38	VAL
2	C	39	THR
2	C	54	LEU
2	C	67	ASN
2	C	102	SER
2	C	113	LEU
2	C	120	VAL
2	C	128	SER
2	C	130	SER
2	C	159	MET
2	C	160	SER
2	C	163	GLN
2	C	192	PRO
2	C	193	ILE
2	C	199	LEU
2	C	200	ASP
2	C	201	LEU
2	C	205	VAL
2	C	207	SER
2	C	210	CYS
3	P	31	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	160	ASN
1	A	200	HIS
1	A	269	GLN
1	A	295	ASN
1	A	388	HIS
1	A	402	HIS
1	A	424	ASN
1	A	493	ASN
1	A	532	HIS
1	A	605	ASN
2	C	45	ASN
2	C	62	HIS
2	C	94	ASN
2	C	198	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	TYS	P	30	3	15,16,17	2.04	3 (20%)	15,22,24	0.42	0
3	TYS	P	28	3	15,16,17	1.95	2 (13%)	15,22,24	0.64	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TYS	P	30	3	-	0/10/11/13	0/1/1/1
3	TYS	P	28	3	-	0/10/11/13	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	30	TYS	OH-CZ	-7.05	1.31	1.42
3	P	28	TYS	OH-CZ	-6.88	1.31	1.42
3	P	30	TYS	O1-S	2.24	1.55	1.45
3	P	28	TYS	O2-S	2.18	1.54	1.45
3	P	30	TYS	O2-S	2.01	1.54	1.45

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	28	TYS	1	0

5.5 Carbohydrates

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	$\# Z > 2$
4	NAG	B	1	1,4	14,14,15	0.57	0	17,19,21	0.99	1 (5%)
4	NAG	B	2	4	14,14,15	0.53	0	17,19,21	0.82	1 (5%)

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	B	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	B	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1	NAG	C1-O5-C5	2.54	115.59	112.19
4	B	2	NAG	C2-N2-C7	-2.05	120.15	122.90

There are no chirality outliers.

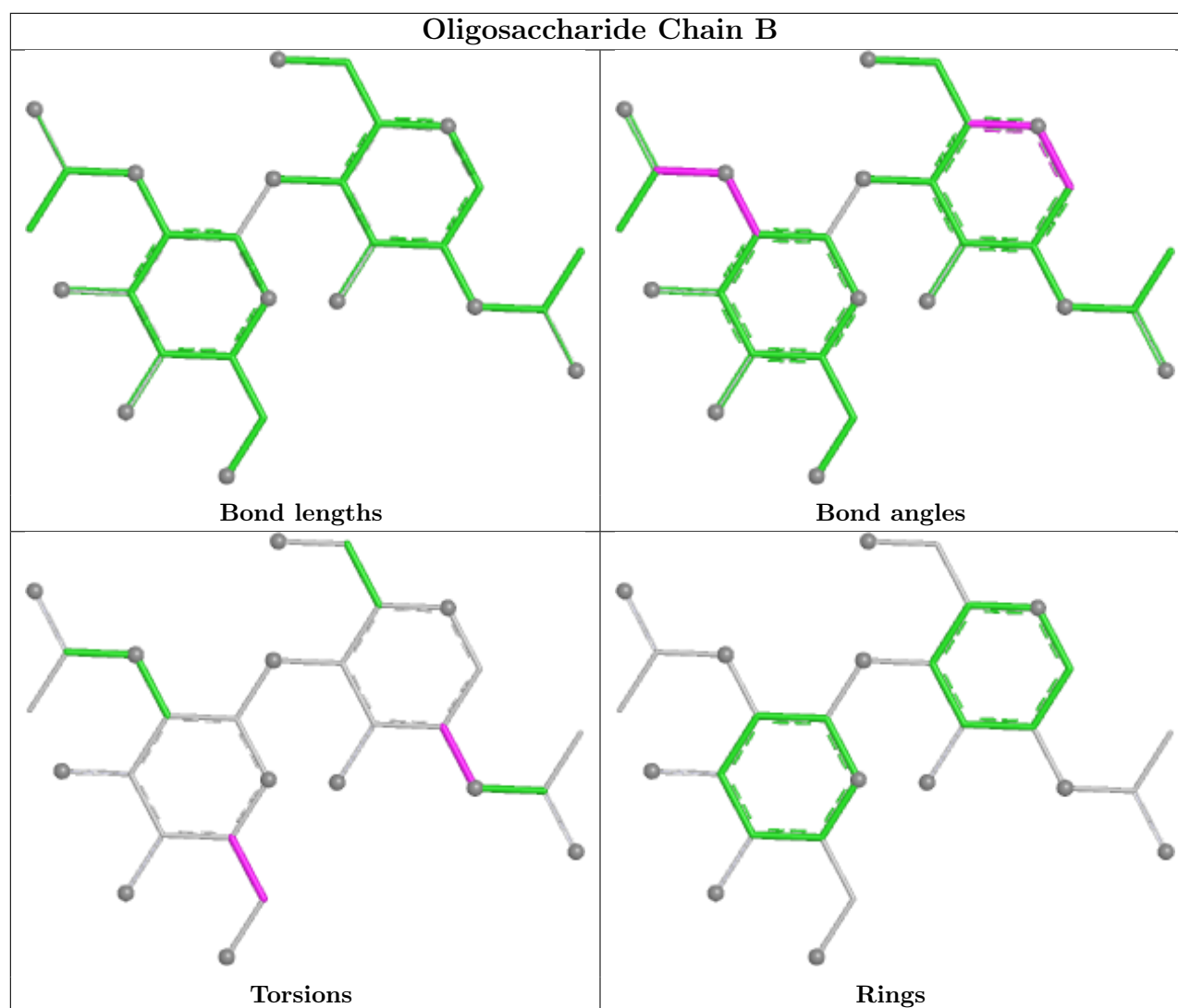
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	2	NAG	O5-C5-C6-O6
4	B	2	NAG	C4-C5-C6-O6
4	B	1	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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



5.6 Ligand geometry [i](#)

13 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	$\# Z > 2$
5	NAG	A	708	1	14,14,15	0.50	0	17,19,21	1.19	1 (5%)
6	SO4	A	711	-	4,4,4	0.28	0	6,6,6	0.14	0
5	NAG	A	702	1	14,14,15	0.52	0	17,19,21	1.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	705	1	14,14,15	0.65	0	17,19,21	2.14	7 (41%)
5	NAG	A	701	1	14,14,15	0.54	0	17,19,21	1.01	1 (5%)
6	SO4	A	712	-	4,4,4	0.26	0	6,6,6	0.20	0
5	NAG	A	707	1	14,14,15	0.49	0	17,19,21	1.24	3 (17%)
5	NAG	A	710	1	14,14,15	0.46	0	17,19,21	1.30	1 (5%)
6	SO4	A	713	-	4,4,4	0.26	0	6,6,6	0.06	0
5	NAG	C	1501	2	14,14,15	0.45	0	17,19,21	1.34	2 (11%)
6	SO4	C	1502	-	4,4,4	0.26	0	6,6,6	0.23	0
5	NAG	A	706	1	14,14,15	0.60	0	17,19,21	0.89	0
5	NAG	A	709	1	14,14,15	0.47	0	17,19,21	1.75	3 (17%)

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
5	NAG	A	708	1	-	2/6/23/26	0/1/1/1
5	NAG	A	702	1	-	4/6/23/26	0/1/1/1
5	NAG	A	705	1	-	2/6/23/26	0/1/1/1
5	NAG	A	701	1	-	2/6/23/26	0/1/1/1
5	NAG	A	707	1	-	4/6/23/26	0/1/1/1
5	NAG	A	710	1	-	4/6/23/26	0/1/1/1
5	NAG	C	1501	2	-	2/6/23/26	0/1/1/1
5	NAG	A	706	1	-	0/6/23/26	0/1/1/1
5	NAG	A	709	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	709	NAG	C2-N2-C7	4.52	128.96	122.90
5	A	705	NAG	C1-O5-C5	4.44	118.14	112.19
5	A	709	NAG	C1-O5-C5	4.11	117.69	112.19
5	A	708	NAG	C1-O5-C5	4.10	117.68	112.19
5	A	710	NAG	C1-O5-C5	4.06	117.63	112.19
5	C	1501	NAG	C1-O5-C5	3.96	117.50	112.19
5	A	705	NAG	O4-C4-C3	3.90	119.56	110.38
5	A	705	NAG	C4-C3-C2	-2.92	106.73	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	707	NAG	C2-N2-C7	-2.92	118.99	122.90
5	A	705	NAG	C3-C4-C5	-2.52	105.67	110.23
5	A	705	NAG	O3-C3-C4	2.43	116.11	110.38
5	A	707	NAG	C1-O5-C5	2.40	115.40	112.19
5	C	1501	NAG	O5-C5-C6	2.38	112.29	107.66
5	A	705	NAG	O7-C7-C8	-2.32	117.92	122.05
5	A	709	NAG	O7-C7-N2	2.24	125.94	121.98
5	A	705	NAG	O7-C7-N2	2.17	125.82	121.98
5	A	701	NAG	C3-C4-C5	-2.09	106.45	110.23
5	A	707	NAG	C4-C3-C2	-2.02	108.05	111.02

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	702	NAG	C8-C7-N2-C2
5	A	710	NAG	C8-C7-N2-C2
5	A	710	NAG	C4-C5-C6-O6
5	A	701	NAG	C4-C5-C6-O6
5	A	707	NAG	C4-C5-C6-O6
5	A	702	NAG	O7-C7-N2-C2
5	A	710	NAG	O7-C7-N2-C2
5	A	702	NAG	O5-C5-C6-O6
5	A	710	NAG	O5-C5-C6-O6
5	A	701	NAG	O5-C5-C6-O6
5	C	1501	NAG	C4-C5-C6-O6
5	A	707	NAG	O5-C5-C6-O6
5	A	707	NAG	C8-C7-N2-C2
5	A	708	NAG	C8-C7-N2-C2
5	C	1501	NAG	O5-C5-C6-O6
5	A	708	NAG	O7-C7-N2-C2
5	A	705	NAG	C4-C5-C6-O6
5	A	707	NAG	O7-C7-N2-C2
5	A	705	NAG	O5-C5-C6-O6
5	A	702	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	712	SO4	1	0

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	605/631 (95%)	1.06	102 (16%) 4 3	31, 60, 96, 142	1 (0%)
2	C	186/219 (84%)	1.96	78 (41%) 0 0	38, 74, 98, 139	0
3	P	3/5 (60%)	0.60	0 100 100	44, 44, 47, 52	0
All	All	794/855 (92%)	1.27	180 (22%) 2 1	31, 65, 96, 142	1 (0%)

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	208	HIS	6.8
1	A	613	SER	6.0
1	A	614	GLY	6.0
2	C	211	PRO	5.9
2	C	163	GLN	5.8
1	A	402	HIS	5.5
1	A	71	ASN	5.4
2	C	135	GLU	5.2
2	C	115	ASP	5.1
1	A	509	ARG	5.0
2	C	39	THR	4.8
2	C	184	ASN	4.4
2	C	199	LEU	4.3
2	C	165	THR	4.3
1	A	52	GLY	4.3
1	A	633	GLU	4.3
2	C	80	GLU	4.3
1	A	513	ALA	4.3
2	C	205	VAL	4.3
1	A	615	GLY	4.2
1	A	627	SER	4.2
1	A	639	SER	4.1
1	A	30	ARG	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	51	ASP	4.1
1	A	538	PRO	4.0
1	A	634	HIS	4.0
1	A	608	SER	4.0
2	C	130	SER	4.0
1	A	426	ARG	3.9
2	C	169	VAL	3.8
2	C	147	ARG	3.8
1	A	492	ARG	3.8
1	A	33	PRO	3.8
1	A	582	ARG	3.7
1	A	638	CYS	3.7
2	C	183	ASP	3.7
1	A	610	VAL	3.7
2	C	204	PRO	3.7
2	C	189	LEU	3.7
2	C	190	PHE	3.7
2	C	193	ILE	3.6
1	A	558	ALA	3.6
1	A	585	GLY	3.6
1	A	440	GLU	3.6
2	C	210	CYS	3.6
2	C	207	SER	3.6
2	C	182	PRO	3.6
2	C	209	PRO	3.6
1	A	31	CYS	3.5
1	A	494	ILE	3.5
2	C	152	SER	3.4
2	C	160	SER	3.4
2	C	129	PHE	3.4
2	C	38	VAL	3.4
2	C	195	PHE	3.4
1	A	59	SER	3.3
2	C	187	PHE	3.3
1	A	57	SER	3.3
2	C	35	THR	3.2
2	C	106	THR	3.2
1	A	93	SER	3.2
1	A	609	GLY	3.2
2	C	200	ASP	3.2
2	C	125	TYR	3.2
1	A	101	GLU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	176	ARG	3.1
1	A	61	ASP	3.1
2	C	202	CYS	3.1
1	A	491	SER	3.1
1	A	433	ARG	3.1
1	A	511	GLU	3.0
2	C	93	LYS	3.0
2	C	84	HIS	3.0
1	A	41	ASP	3.0
2	C	192	PRO	3.0
1	A	358	GLU	2.9
2	C	146	LEU	2.9
1	A	548	LYS	2.9
2	C	157	ILE	2.9
1	A	115	SER	2.9
2	C	117	THR	2.9
1	A	630	LEU	2.9
1	A	63	CYS	2.8
2	C	141	SER	2.8
1	A	185	ALA	2.8
1	A	589	VAL	2.8
1	A	77	ARG	2.8
2	C	107	GLY	2.8
2	C	201	LEU	2.8
2	C	112	ASN	2.7
1	A	632	GLY	2.7
2	C	82	SER	2.7
2	C	145	PHE	2.7
2	C	153	LEU	2.7
1	A	66	THR	2.7
2	C	155	GLY	2.7
2	C	197	ASN	2.6
2	C	44	ASN	2.6
1	A	601	SER	2.6
1	A	484	THR	2.6
2	C	162	THR	2.6
1	A	70	CYS	2.6
1	A	621	PRO	2.6
1	A	160	ASN	2.6
2	C	26	ALA	2.6
2	C	164	ILE	2.5
1	A	391	ASN	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	89	SER	2.5
1	A	118	LEU	2.5
1	A	547	LYS	2.5
2	C	128	SER	2.5
1	A	37	GLU	2.5
2	C	131	GLY	2.5
1	A	510	ASN	2.5
1	A	631	CYS	2.5
2	C	42	ASP	2.5
1	A	602	VAL	2.5
1	A	162	SER	2.4
1	A	569	GLY	2.4
1	A	91	LYS	2.4
1	A	592	GLN	2.4
1	A	629	HIS	2.4
1	A	410	SER	2.4
1	A	625	PHE	2.4
1	A	361	LYS	2.4
2	C	196	ALA	2.4
1	A	54	ILE	2.3
1	A	493	ASN	2.3
2	C	188	SER	2.3
1	A	606	ASN	2.3
1	A	47	GLU	2.3
1	A	45	HIS	2.3
1	A	604	TYR	2.3
1	A	50	PRO	2.3
2	C	109	ILE	2.3
1	A	637	PRO	2.3
2	C	168	GLN	2.3
1	A	99	LEU	2.3
2	C	161	LEU	2.3
2	C	75	ASP	2.2
1	A	537	GLY	2.2
1	A	62	CYS	2.2
1	A	574	GLU	2.2
2	C	132	PRO	2.2
1	A	562	SER	2.2
1	A	571	THR	2.2
1	A	575	ALA	2.2
1	A	207	ASP	2.2
2	C	178	SER	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	180	SER	2.2
1	A	540	TRP	2.1
1	A	564	PRO	2.1
1	A	411	SER	2.1
1	A	568	SER	2.1
1	A	450	ARG	2.1
1	A	189	THR	2.1
1	A	32	HIS	2.1
1	A	78	VAL	2.1
1	A	611	ILE	2.1
2	C	194	SER	2.1
1	A	588	PRO	2.1
2	C	113	LEU	2.1
2	C	170	LEU	2.1
2	C	185	GLY	2.1
1	A	617	PHE	2.1
1	A	457	SER	2.1
2	C	156	SER	2.1
2	C	85	LEU	2.1
1	A	35	ASP	2.0
1	A	49	LYS	2.0
1	A	113	LYS	2.0
2	C	87	PRO	2.0
1	A	67	GLY	2.0
2	C	179	GLY	2.0
2	C	186	SER	2.0
1	A	146	LEU	2.0
2	C	81	LEU	2.0
1	A	400	ASN	2.0
2	C	27	ASN	2.0
2	C	86	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.

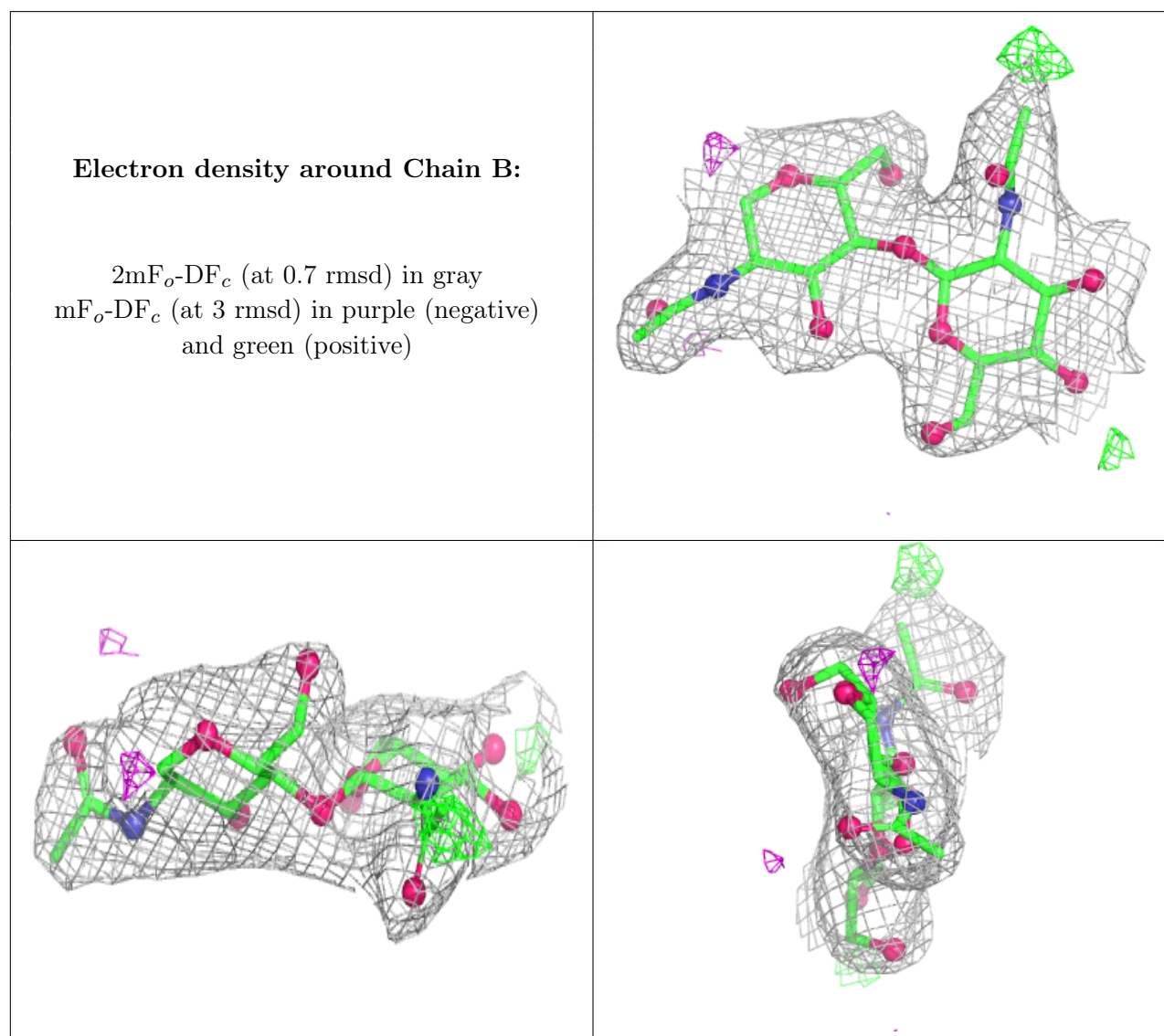
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	TYS	P	30	16/17	0.94	0.10	35,49,62,76	0
3	TYS	P	28	16/17	0.95	0.12	40,57,75,92	0

6.3 Carbohydrates ⓘ

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	B	1	14/15	-	-	44,57,73,77	0
4	NAG	B	2	14/15	-	-	73,81,88,95	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

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
5	NAG	A	709	14/15	0.54	0.28	94,106,113,114	0
5	NAG	A	707	14/15	0.62	0.20	72,82,93,96	0
6	SO4	A	713	5/5	0.64	0.19	127,131,132,132	0
5	NAG	A	710	14/15	0.70	0.20	94,99,103,104	0
6	SO4	A	711	5/5	0.73	0.14	108,112,114,121	0
5	NAG	C	1501	14/15	0.73	0.20	86,95,99,99	0
6	SO4	A	712	5/5	0.76	0.19	90,106,109,115	0
6	SO4	C	1502	5/5	0.79	0.17	147,148,149,150	0
5	NAG	A	701	14/15	0.85	0.14	44,61,70,78	0
5	NAG	A	702	14/15	0.86	0.13	42,62,69,75	0
5	NAG	A	708	14/15	0.88	0.16	66,81,88,92	0
5	NAG	A	706	14/15	0.90	0.13	51,58,68,71	0
5	NAG	A	705	14/15	0.90	0.14	37,51,67,73	0

6.5 Other polymers

There are no such residues in this entry.