



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:03 AM UTC

PDB ID : 1M6B / pdb_00001m6b
Title : Structure of the HER3 (ERBB3) Extracellular Domain
Authors : Leahy, D.J.; Cho, H.-S.
Deposited on : 2002-07-15
Resolution : 2.60 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

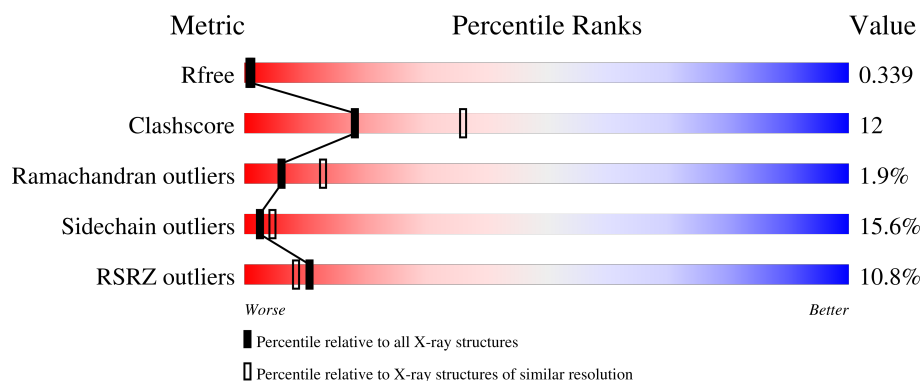
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	621	8% 57% 27% 5% 12%
1	B	621	12% 64% 24% 5% 6%
2	C	2	50% 50%
2	D	2	50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	626	X	-	-	-
3	NAG	A	628	X	-	-	-
3	NAG	B	626	X	-	-	-
3	NAG	B	627	X	-	-	-
3	NAG	B	628	X	-	-	-
4	SO4	B	5001	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9012 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 Receptor protein-tyrosine kinase erbB-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	0	0	0
			4206	2603	765	784	54			
1	B	584	Total	C	N	O	S	0	0	0
			4478	2766	813	840	59			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	VAL	ILE	engineered mutation	UNP P21860
B	61	VAL	ILE	engineered mutation	UNP P21860

- 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	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		

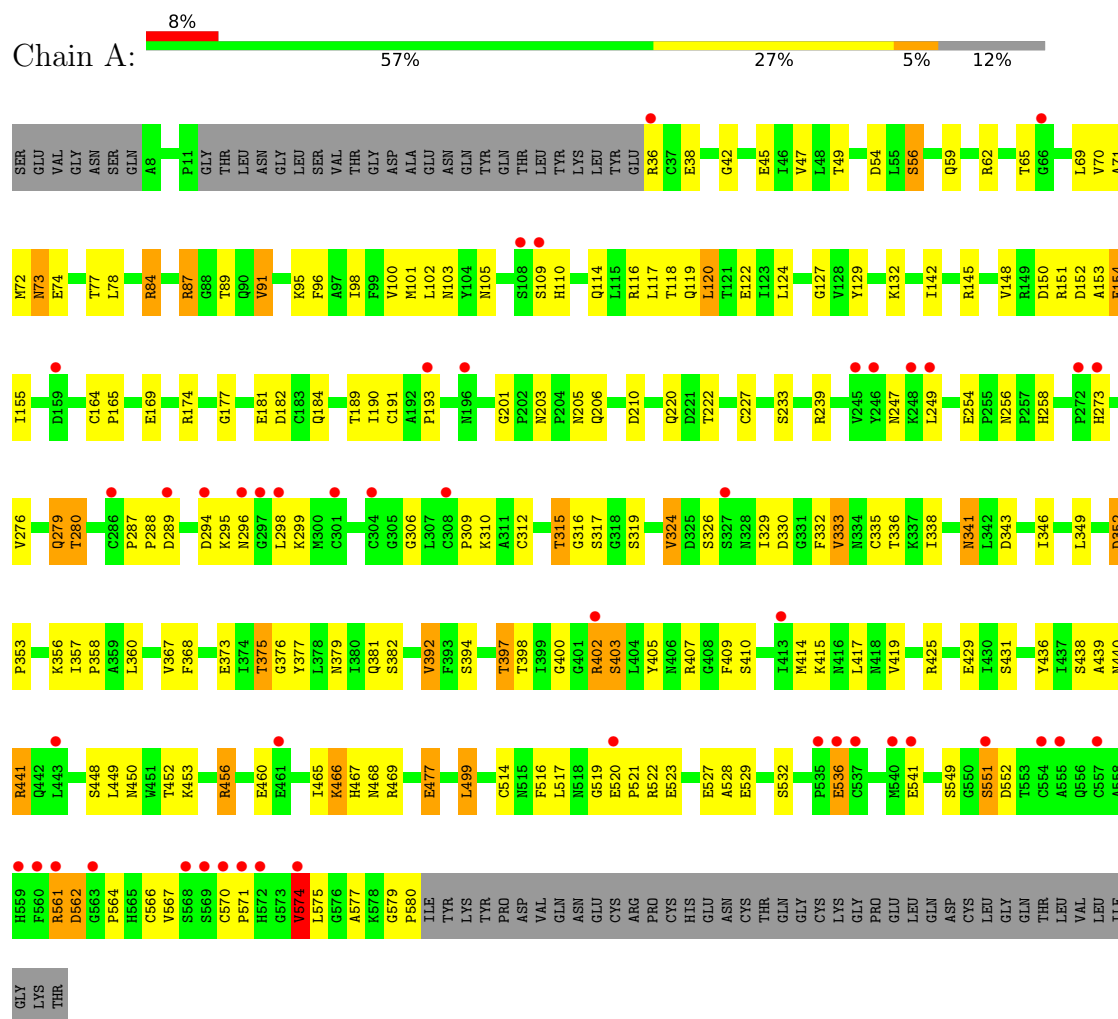
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	20	Total	O	0	0
			20	20		
5	B	65	Total	O	0	0
			65	65		

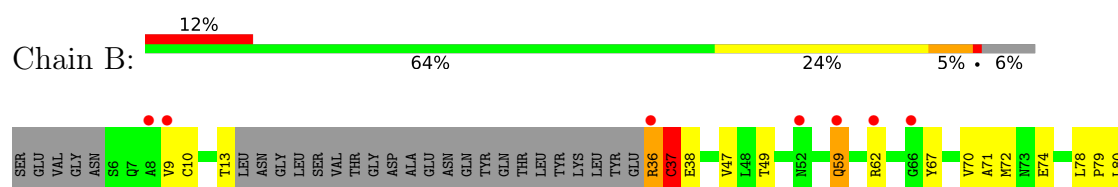
3 Residue-property plots [i](#)

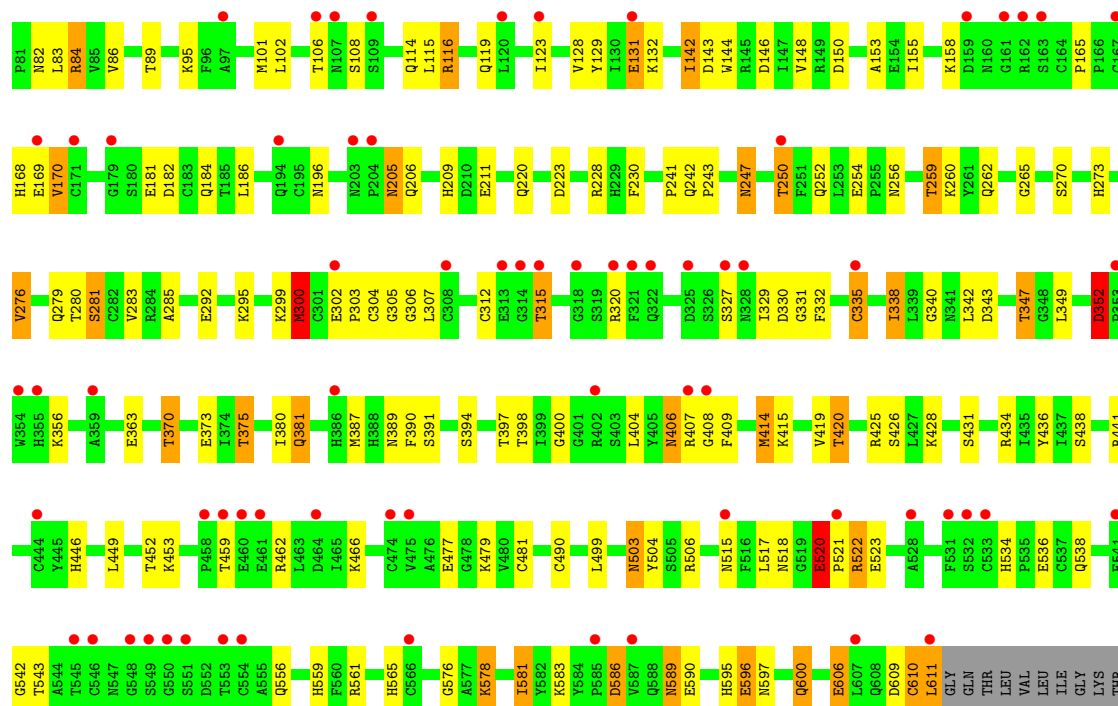
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Receptor protein-tyrosine kinase erbB-3



• Molecule 1: Receptor protein-tyrosine kinase erbB-3





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

Chain C: 50% 50%

MAG1
MAG2

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

Chain D: 50% 50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	236.26Å 49.62Å 190.86Å 90.00° 125.56° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 20.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.5 (20.00-2.60) 91.0 (20.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.235 , 0.294 0.299 , 0.339	Depositor DCC
R_{free} test set	2754 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	48.1	Xtriage
Anisotropy	0.756	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 23.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	9012	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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, 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	0.71	1/4308 (0.0%)	1.04	11/5845 (0.2%)
1	B	0.78	1/4586 (0.0%)	1.06	6/6222 (0.1%)
All	All	0.75	2/8894 (0.0%)	1.05	17/12067 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	300	MET	SD-CE	11.40	2.08	1.79
1	A	324	VAL	CA-CB	5.68	1.60	1.54

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	CYS	N-CA-C	7.99	122.13	109.50
1	B	37	CYS	N-CA-C	7.23	121.34	110.64
1	A	405	TYR	N-CA-C	7.16	121.88	112.72
1	B	165	PRO	O-C-N	6.78	124.43	121.31
1	A	122	GLU	N-CA-C	6.41	119.16	109.23
1	B	281	SER	N-CA-C	6.27	118.60	109.07
1	A	346	ILE	N-CA-C	5.93	116.67	110.62
1	A	164	CYS	N-CA-C	5.63	117.67	109.84
1	B	59	GLN	N-CA-C	5.53	118.83	111.75
1	A	528	ALA	N-CA-C	5.47	119.24	112.24
1	A	477	GLU	N-CA-C	-5.44	106.01	113.30
1	A	429	GLU	N-CA-C	5.40	117.22	108.26
1	B	352	ASP	CB-CA-C	5.16	118.92	111.02
1	A	254	GLU	N-CA-C	5.12	112.63	108.07
1	A	165	PRO	O-C-N	5.08	123.54	121.15
1	A	536	GLU	N-CA-C	5.03	116.44	109.54
1	B	589	ASN	N-CA-C	5.00	119.33	113.23

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	4206	0	3996	83	0
1	B	4478	0	4242	127	0
2	C	28	0	25	1	0
2	D	28	0	25	1	0
3	A	98	0	91	0	0
3	B	84	0	78	2	0
4	B	5	0	0	4	0
5	A	20	0	0	3	0
5	B	65	0	0	7	0
All	All	9012	0	8457	210	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 12.

All (210) 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:300:MET:CE	1:B:300:MET:SD	2.08	1.42
1:B:116:ARG:HG3	1:B:116:ARG:HH11	1.11	1.11
1:B:335:CYS:O	1:B:370:THR:HG22	1.56	1.03
1:B:452:THR:HG22	1:B:459:THR:HG21	1.42	1.00
1:B:578:LYS:HE2	1:B:578:LYS:H	1.31	0.96
1:B:247:ASN:ND2	5:B:1072:HOH:O	2.01	0.91
1:B:520:GLU:HB2	1:B:521:PRO:CD	2.00	0.90
1:B:452:THR:CG2	1:B:459:THR:HG21	2.03	0.87
1:B:168:HIS:HD2	1:B:170:VAL:HB	1.41	0.86
1:B:250:THR:HG21	1:B:254:GLU:OE2	1.75	0.86
1:B:534:HIS:HD2	1:B:536:GLU:H	1.26	0.84
1:A:330:ASP:O	1:A:333:VAL:HG23	1.77	0.83
1:A:145:ARG:HE	1:A:155:ILE:HD13	1.44	0.83
1:B:335:CYS:O	1:B:370:THR:CG2	2.28	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:TYR:CE2	1:B:438:SER:HB2	2.18	0.79
1:A:315:THR:HG21	1:A:343:ASP:HB2	1.65	0.79
1:B:452:THR:HG22	1:B:459:THR:CG2	2.12	0.78
1:A:469:ARG:NH2	1:A:477:GLU:OE2	2.16	0.76
1:A:551:SER:HB2	1:A:566:CYS:H	1.51	0.75
1:B:36:ARG:HD3	1:B:37:CYS:H	1.50	0.75
1:B:434:ARG:HG2	1:B:462:ARG:HB2	1.69	0.75
1:B:520:GLU:HB2	1:B:521:PRO:HD3	1.68	0.75
1:B:116:ARG:HG3	1:B:116:ARG:NH1	1.92	0.75
1:B:559:HIS:NE2	4:B:5001:SO4:O2	2.21	0.74
1:B:565:HIS:HD2	5:B:1058:HOH:O	1.72	0.73
1:A:87:ARG:HG2	1:A:124:LEU:HD12	1.69	0.73
1:B:247:ASN:CG	5:B:1072:HOH:O	2.27	0.73
1:A:456:ARG:HH11	1:A:456:ARG:HB2	1.54	0.72
1:B:534:HIS:CD2	1:B:536:GLU:H	2.08	0.72
1:B:420:THR:HG22	1:B:479:LYS:NZ	2.04	0.72
1:B:559:HIS:NE2	4:B:5001:SO4:O4	2.25	0.70
1:A:73:ASN:ND2	1:A:103:ASN:OD1	2.25	0.69
1:B:414:MET:O	1:B:415:LYS:HG2	1.92	0.68
1:B:243:PRO:HA	1:B:259:THR:HG23	1.77	0.67
1:B:315:THR:HG22	1:B:343:ASP:OD2	1.94	0.67
1:A:150:ASP:HB3	1:A:153:ALA:HB2	1.77	0.67
1:B:381:GLN:HG2	1:B:415:LYS:HE2	1.77	0.67
1:B:116:ARG:HH11	1:B:116:ARG:CG	1.97	0.66
1:B:586:ASP:HB2	1:B:590:GLU:H	1.60	0.66
1:A:375:THR:HA	1:A:402:ARG:HH11	1.61	0.65
1:B:209:HIS:HD2	1:B:211:GLU:H	1.41	0.65
1:B:534:HIS:CD2	1:B:536:GLU:HB2	2.32	0.65
1:B:520:GLU:CB	1:B:521:PRO:CD	2.74	0.64
1:B:150:ASP:HB3	1:B:153:ALA:HB2	1.80	0.64
1:B:520:GLU:HB2	1:B:521:PRO:HD2	1.77	0.64
1:A:552:ASP:HA	1:A:564:PRO:O	1.99	0.63
1:B:36:ARG:CB	1:B:36:ARG:HH11	2.12	0.62
1:B:559:HIS:NE2	4:B:5001:SO4:S	2.69	0.62
1:B:220:GLN:HB2	1:B:223:ASP:OD2	2.00	0.62
1:A:551:SER:HB2	1:A:566:CYS:N	2.15	0.61
1:A:70:VAL:HB	1:A:100:VAL:HG22	1.83	0.60
5:A:1045:HOH:O	2:C:1:NAG:H81	2.00	0.60
1:A:117:LEU:HD13	1:A:120:LEU:HD22	1.83	0.60
1:A:440:ASN:HD22	1:A:468:ASN:ND2	1.99	0.60
1:B:243:PRO:HA	1:B:259:THR:CG2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:MET:HE1	1:A:102:LEU:HB2	1.83	0.59
1:B:302:GLU:HG3	1:B:303:PRO:HD2	1.84	0.58
1:A:101:MET:HE3	1:A:102:LEU:HD12	1.86	0.58
1:A:315:THR:CG2	1:A:343:ASP:HB2	2.34	0.58
1:A:440:ASN:H	1:A:468:ASN:HD22	1.52	0.58
1:B:578:LYS:HE2	1:B:578:LYS:N	2.11	0.58
1:A:436:TYR:CE2	1:A:438:SER:HB2	2.40	0.57
1:B:586:ASP:HB2	1:B:590:GLU:N	2.19	0.57
1:A:341:ASN:HD22	1:A:377:TYR:H	1.52	0.57
1:B:283:VAL:HG12	1:B:285:ALA:H	1.69	0.56
1:A:332:PHE:O	1:A:335:CYS:HB2	2.06	0.56
1:B:36:ARG:HD3	1:B:37:CYS:HB2	1.87	0.56
1:B:373:GLU:HG3	1:B:398:THR:HB	1.87	0.56
1:B:304:CYS:O	1:B:306:GLY:N	2.38	0.56
1:B:129:TYR:CE2	1:B:131:GLU:HB2	2.41	0.55
1:B:101:MET:HE3	1:B:102:LEU:HD12	1.87	0.55
1:B:114:GLN:OE1	1:B:116:ARG:HD3	2.07	0.55
1:B:606:GLU:HB2	1:B:609:ASP:OD2	2.06	0.55
1:B:241:PRO:HG2	1:B:260:LYS:HG3	1.89	0.55
1:B:420:THR:HG22	1:B:479:LYS:HZ3	1.72	0.55
1:A:256:ASN:HD21	1:A:258:HIS:HB2	1.72	0.55
1:B:565:HIS:CD2	5:B:1058:HOH:O	2.55	0.55
1:A:84:ARG:HD3	1:A:119:GLN:HG3	1.88	0.54
1:A:466:LYS:HG3	1:A:467:HIS:CD2	2.42	0.54
1:A:574:VAL:O	1:A:580:PRO:HA	2.07	0.54
1:B:247:ASN:OD1	1:B:247:ASN:C	2.50	0.54
1:B:520:GLU:CB	1:B:521:PRO:HD3	2.34	0.54
1:B:610:CYS:O	1:B:611:LEU:O	2.25	0.54
1:A:456:ARG:HB2	1:A:456:ARG:NH1	2.20	0.54
1:B:534:HIS:HD2	1:B:536:GLU:HB2	1.73	0.54
1:B:438:SER:OG	1:B:466:LYS:HG3	2.08	0.54
1:B:330:ASP:C	1:B:332:PHE:H	2.16	0.53
1:B:36:ARG:CD	1:B:37:CYS:H	2.19	0.53
1:A:397:THR:HG22	1:A:398:THR:OG1	2.09	0.53
1:B:36:ARG:HH11	1:B:36:ARG:HB2	1.73	0.53
1:A:87:ARG:NH2	1:A:227:CYS:O	2.27	0.53
1:B:420:THR:HG22	1:B:479:LYS:HZ1	1.72	0.53
1:A:425:ARG:NH1	5:A:1025:HOH:O	2.41	0.52
1:A:415:LYS:HA	1:A:439:ALA:O	2.10	0.52
1:B:228:ARG:HG2	1:B:228:ARG:HH11	1.75	0.52
1:B:262:GLN:HB2	1:B:281:SER:CB	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:GLY:O	1:B:431:SER:HB2	2.09	0.52
1:A:449:LEU:HD12	1:A:499:LEU:HD12	1.92	0.51
1:A:349:LEU:HD12	1:A:382:SER:OG	2.10	0.51
1:A:341:ASN:HD22	1:A:376:GLY:HA3	1.75	0.51
1:A:201:GLY:HA3	1:A:206:GLN:OE1	2.11	0.51
1:B:80:LEU:HD13	1:B:83:LEU:HD22	1.92	0.50
1:B:146:ASP:OD1	1:B:186:LEU:HA	2.11	0.50
1:B:518:ASN:HA	1:B:522:ARG:CZ	2.40	0.50
1:B:209:HIS:CD2	1:B:211:GLU:H	2.25	0.50
1:A:440:ASN:H	1:A:468:ASN:ND2	2.09	0.50
1:A:519:GLY:O	1:A:522:ARG:HD3	2.12	0.50
1:B:47:VAL:HA	1:B:71:ALA:O	2.12	0.50
1:B:595:HIS:C	1:B:597:ASN:H	2.19	0.50
1:A:222:THR:HG22	1:A:222:THR:O	2.12	0.50
1:B:168:HIS:CD2	1:B:170:VAL:HB	2.32	0.50
1:B:609:ASP:O	1:B:610:CYS:SG	2.70	0.50
1:A:54:ASP:OD1	1:A:56:SER:HB3	2.12	0.49
1:A:469:ARG:HD3	5:A:1022:HOH:O	2.11	0.49
1:B:243:PRO:HD2	5:B:1065:HOH:O	2.13	0.48
1:B:446:HIS:HA	5:B:1042:HOH:O	2.14	0.48
1:A:279:GLN:CG	1:A:280:THR:H	2.25	0.48
1:A:520:GLU:HB2	1:A:521:PRO:HD3	1.96	0.48
1:A:127:GLY:HA3	1:A:154:GLU:O	2.14	0.48
1:B:143:ASP:H	1:B:184:GLN:HE22	1.61	0.48
1:A:71:ALA:C	1:A:72:MET:HG2	2.39	0.48
1:A:341:ASN:ND2	1:A:376:GLY:HA3	2.28	0.48
1:B:409:PHE:CE2	1:B:436:TYR:HB2	2.49	0.48
1:A:42:GLY:H	1:A:65:THR:HG1	1.61	0.48
1:A:38:GLU:OE1	1:A:62:ARG:NH1	2.47	0.47
1:A:174:ARG:HB3	1:A:184:GLN:HB3	1.96	0.47
1:A:409:PHE:CD2	1:A:436:TYR:HB2	2.49	0.47
1:B:404:LEU:HD13	1:B:408:GLY:HA2	1.96	0.47
1:B:515:ASN:HB3	1:B:518:ASN:O	2.14	0.47
1:B:583:LYS:NZ	5:B:1069:HOH:O	2.47	0.47
1:A:450:ASN:ND2	1:A:453:LYS:HD2	2.29	0.47
1:B:397:THR:HA	1:B:426:SER:O	2.13	0.47
1:B:409:PHE:CD2	1:B:436:TYR:HB2	2.49	0.47
1:B:205:ASN:ND2	1:B:206:GLN:HG3	2.29	0.47
1:B:78:LEU:HD23	1:B:115:LEU:HD22	1.98	0.46
1:B:499:LEU:HD23	1:B:499:LEU:HA	1.78	0.46
1:A:373:GLU:HG3	1:A:398:THR:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:ASN:HD21	1:A:381:GLN:HG3	1.81	0.46
1:A:394:SER:HB2	1:A:425:ARG:HD3	1.97	0.46
1:B:72:MET:HE1	1:B:102:LEU:HB2	1.96	0.46
1:B:453:LYS:HE2	3:B:627:NAG:O6	2.15	0.46
1:A:381:GLN:HG2	1:A:414:MET:HE2	1.97	0.46
1:A:72:MET:CE	1:A:102:LEU:HB2	2.46	0.46
1:B:406:ASN:HB3	1:B:407:ARG:H	1.49	0.46
1:A:449:LEU:CD1	1:A:499:LEU:HD12	2.46	0.45
1:B:506:ARG:HD3	1:B:523:GLU:OE1	2.16	0.45
1:A:368:PHE:HB2	1:A:392:VAL:CG1	2.46	0.45
1:A:376:GLY:HA2	1:A:403:SER:H	1.81	0.45
1:B:576:GLY:HA3	1:B:581:ILE:CD1	2.47	0.45
1:B:262:GLN:HB2	1:B:281:SER:HB3	1.99	0.45
1:B:205:ASN:HD22	1:B:206:GLN:HG3	1.81	0.45
1:B:380:ILE:HG21	1:B:390:PHE:CE2	2.51	0.45
1:A:309:PRO:HA	1:A:336:THR:OG1	2.17	0.45
1:B:230:PHE:HA	1:B:265:GLY:O	2.17	0.45
1:A:514:CYS:HB2	1:A:516:PHE:CE1	2.52	0.45
1:B:243:PRO:CA	1:B:259:THR:HG23	2.46	0.45
1:B:559:HIS:CD2	4:B:5001:SO4:O2	2.70	0.45
1:A:417:LEU:HD22	1:A:441:ARG:HG3	1.98	0.44
1:A:356:LYS:O	1:A:358:PRO:HD3	2.17	0.44
1:B:72:MET:CE	1:B:102:LEU:HB2	2.47	0.44
1:A:222:THR:O	1:A:222:THR:CG2	2.65	0.44
1:A:375:THR:HA	1:A:402:ARG:NH1	2.27	0.44
1:A:349:LEU:HD23	1:A:360:LEU:HD12	1.99	0.44
1:A:96:PHE:CD2	1:A:129:TYR:HB2	2.52	0.44
1:A:352:ASP:HA	1:A:353:PRO:HD3	1.76	0.44
1:A:74:GLU:HB3	1:A:110:HIS:HB3	2.00	0.44
1:B:59:GLN:O	1:B:82:ASN:ND2	2.39	0.44
1:B:116:ARG:NH1	1:B:116:ARG:CG	2.65	0.43
1:A:440:ASN:HD22	1:A:468:ASN:HD21	1.62	0.43
1:B:340:GLY:H	1:B:375:THR:HB	1.83	0.43
1:B:242:GLN:O	1:B:259:THR:HG23	2.17	0.43
1:B:128:VAL:HG21	1:B:144:TRP:CE3	2.54	0.43
1:A:400:GLY:HA3	1:A:402:ARG:CZ	2.48	0.43
1:B:589:ASN:HD22	1:B:589:ASN:HA	1.62	0.43
1:B:148:VAL:HG21	1:B:155:ILE:HD11	2.00	0.43
1:A:91:VAL:O	1:A:91:VAL:CG1	2.66	0.43
1:A:287:PRO:C	1:A:289:ASP:H	2.27	0.43
1:A:315:THR:CG2	1:A:316:GLY:N	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:ASN:HB2	1:B:504:TYR:H	1.62	0.43
1:B:347:THR:HG22	1:B:352:ASP:HB2	2.00	0.43
1:B:452:THR:OG1	3:B:627:NAG:H5	2.19	0.43
1:A:45:GLU:HG2	1:A:69:LEU:HD23	2.00	0.42
1:A:169:GLU:OE2	1:B:62:ARG:NH2	2.53	0.42
1:A:47:VAL:HA	1:A:71:ALA:O	2.18	0.42
1:B:70:VAL:HG21	1:B:78:LEU:HD22	2.01	0.42
1:B:67:TYR:CD1	1:B:67:TYR:C	2.97	0.42
1:B:506:ARG:HH11	1:B:523:GLU:CD	2.28	0.42
1:B:115:LEU:HD23	1:B:115:LEU:HA	1.81	0.42
1:A:579:GLY:HA2	1:A:580:PRO:HD2	1.87	0.42
1:B:262:GLN:HB2	1:B:281:SER:HB2	2.02	0.42
1:B:338:ILE:HD13	1:B:342:LEU:HD11	2.00	0.42
1:B:506:ARG:NH1	1:B:523:GLU:OE2	2.53	0.42
1:B:375:THR:O	1:B:400:GLY:HA3	2.20	0.42
1:B:143:ASP:N	1:B:184:GLN:HE22	2.17	0.41
1:B:538:GLN:HB3	1:B:556:GLN:HB3	2.01	0.41
1:A:177:GLY:HA3	1:A:182:ASP:CB	2.51	0.41
1:B:256:ASN:O	1:B:259:THR:OG1	2.38	0.41
1:B:389:ASN:OD1	1:B:391:SER:HB3	2.21	0.41
1:B:517:LEU:HD13	1:B:542:GLY:O	2.20	0.41
1:B:142:ILE:O	1:B:142:ILE:HG22	2.20	0.41
1:A:561:ARG:HG2	1:A:562:ASP:N	2.36	0.41
1:A:101:MET:CE	1:A:102:LEU:HD12	2.51	0.41
1:B:387:MET:HA	2:D:1:NAG:O6	2.20	0.41
1:B:481:CYS:SG	1:B:490:CYS:N	2.93	0.41
1:A:78:LEU:O	1:A:116:ARG:HB2	2.21	0.40
1:A:203:ASN:HB2	1:A:206:GLN:HG3	2.02	0.40
1:A:521:PRO:O	1:A:523:GLU:HG3	2.21	0.40
1:B:86:VAL:O	1:B:123:ILE:HA	2.21	0.40
1:B:276:VAL:HG21	1:B:292:GLU:HG3	2.02	0.40
1:B:84:ARG:NH2	1:B:119:GLN:HG3	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	545/621 (88%)	482 (88%)	52 (10%)	11 (2%)	6	12
1	B	580/621 (93%)	525 (90%)	45 (8%)	10 (2%)	7	15
All	All	1125/1242 (91%)	1007 (90%)	97 (9%)	21 (2%)	6	13

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	317	SER
1	A	460	GLU
1	B	520	GLU
1	B	586	ASP
1	A	296	ASN
1	B	305	GLY
1	B	596	GLU
1	B	600	GLN
1	B	610	CYS
1	A	279	GLN
1	A	577	ALA
1	A	120	LEU
1	A	193	PRO
1	A	288	PRO
1	B	279	GLN
1	B	406	ASN
1	A	306	GLY
1	A	571	PRO
1	B	331	GLY
1	A	574	VAL
1	B	79	PRO

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	474/537 (88%)	392 (83%)	82 (17%)	2	3
1	B	506/537 (94%)	435 (86%)	71 (14%)	3	6
All	All	980/1074 (91%)	827 (84%)	153 (16%)	2	4

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ARG
1	A	49	THR
1	A	56	SER
1	A	59	GLN
1	A	73	ASN
1	A	77	THR
1	A	84	ARG
1	A	87	ARG
1	A	89	THR
1	A	91	VAL
1	A	95	LYS
1	A	98	ILE
1	A	105	ASN
1	A	109	SER
1	A	114	GLN
1	A	118	THR
1	A	132	LYS
1	A	142	ILE
1	A	148	VAL
1	A	151	ARG
1	A	152	ASP
1	A	154	GLU
1	A	181	GLU
1	A	189	THR
1	A	190	ILE
1	A	205	ASN
1	A	210	ASP
1	A	220	GLN
1	A	233	SER
1	A	239	ARG
1	A	247	ASN
1	A	249	LEU
1	A	273	HIS
1	A	276	VAL
1	A	280	THR

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Mol	Chain	Res	Type
1	A	294	ASP
1	A	295	LYS
1	A	298	LEU
1	A	299	LYS
1	A	310	LYS
1	A	312	CYS
1	A	315	THR
1	A	319	SER
1	A	324	VAL
1	A	326	SER
1	A	329	ILE
1	A	333	VAL
1	A	338	ILE
1	A	341	ASN
1	A	352	ASP
1	A	357	ILE
1	A	367	VAL
1	A	375	THR
1	A	392	VAL
1	A	397	THR
1	A	402	ARG
1	A	403	SER
1	A	407	ARG
1	A	410	SER
1	A	419	VAL
1	A	431	SER
1	A	441	ARG
1	A	448	SER
1	A	452	THR
1	A	456	ARG
1	A	465	ILE
1	A	466	LYS
1	A	499	LEU
1	A	517	LEU
1	A	527	GLU
1	A	529	GLU
1	A	532	SER
1	A	536	GLU
1	A	541	GLU
1	A	549	SER
1	A	551	SER
1	A	561	ARG

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Mol	Chain	Res	Type
1	A	562	ASP
1	A	567	VAL
1	A	570	CYS
1	A	574	VAL
1	A	575	LEU
1	B	9	VAL
1	B	10	CYS
1	B	13	THR
1	B	36	ARG
1	B	37	CYS
1	B	38	GLU
1	B	49	THR
1	B	74	GLU
1	B	84	ARG
1	B	89	THR
1	B	95	LYS
1	B	106	THR
1	B	108	SER
1	B	116	ARG
1	B	131	GLU
1	B	132	LYS
1	B	142	ILE
1	B	158	LYS
1	B	169	GLU
1	B	170	VAL
1	B	181	GLU
1	B	182	ASP
1	B	196	ASN
1	B	205	ASN
1	B	247	ASN
1	B	250	THR
1	B	252	GLN
1	B	259	THR
1	B	270	SER
1	B	273	HIS
1	B	276	VAL
1	B	280	THR
1	B	295	LYS
1	B	299	LYS
1	B	300	MET
1	B	307	LEU
1	B	312	CYS

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Mol	Chain	Res	Type
1	B	315	THR
1	B	320	ARG
1	B	327	SER
1	B	329	ILE
1	B	335	CYS
1	B	338	ILE
1	B	347	THR
1	B	349	LEU
1	B	352	ASP
1	B	356	LYS
1	B	363	GLU
1	B	370	THR
1	B	375	THR
1	B	381	GLN
1	B	394	SER
1	B	414	MET
1	B	419	VAL
1	B	420	THR
1	B	425	ARG
1	B	428	LYS
1	B	441	ARG
1	B	449	LEU
1	B	477	GLU
1	B	503	ASN
1	B	520	GLU
1	B	522	ARG
1	B	543	THR
1	B	561	ARG
1	B	578	LYS
1	B	581	ILE
1	B	596	GLU
1	B	600	GLN
1	B	606	GLU
1	B	611	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	59	GLN
1	A	119	GLN
1	A	138	HIS

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Mol	Chain	Res	Type
1	A	168	HIS
1	A	198	HIS
1	A	242	GLN
1	A	256	ASN
1	A	341	ASN
1	A	379	ASN
1	A	381	GLN
1	A	442	GLN
1	A	467	HIS
1	A	468	ASN
1	A	538	GLN
1	A	565	HIS
1	B	105	ASN
1	B	138	HIS
1	B	168	HIS
1	B	184	GLN
1	B	205	ASN
1	B	209	HIS
1	B	229	HIS
1	B	381	GLN
1	B	467	HIS
1	B	534	HIS
1	B	589	ASN

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 ⓘ

4 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	1,2	14,14,15	0.84	0	17,19,21	1.62	4 (23%)
2	NAG	C	2	2	14,14,15	0.43	0	17,19,21	1.59	3 (17%)
2	NAG	D	1	1,2	14,14,15	0.45	0	17,19,21	1.23	1 (5%)
2	NAG	D	2	2	14,14,15	0.57	0	17,19,21	0.83	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	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	5/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	5/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C1-O5-C5	4.08	117.66	112.19
2	D	1	NAG	C1-O5-C5	3.42	116.77	112.19
2	C	1	NAG	C2-N2-C7	-3.11	118.73	122.90
2	C	2	NAG	C2-N2-C7	2.60	126.39	122.90
2	C	1	NAG	C4-C3-C2	2.39	114.51	111.02
2	C	1	NAG	O5-C1-C2	-2.34	107.67	111.29
2	C	2	NAG	C3-C4-C5	-2.16	106.31	110.23
2	C	1	NAG	O3-C3-C2	-2.05	105.13	109.40

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2

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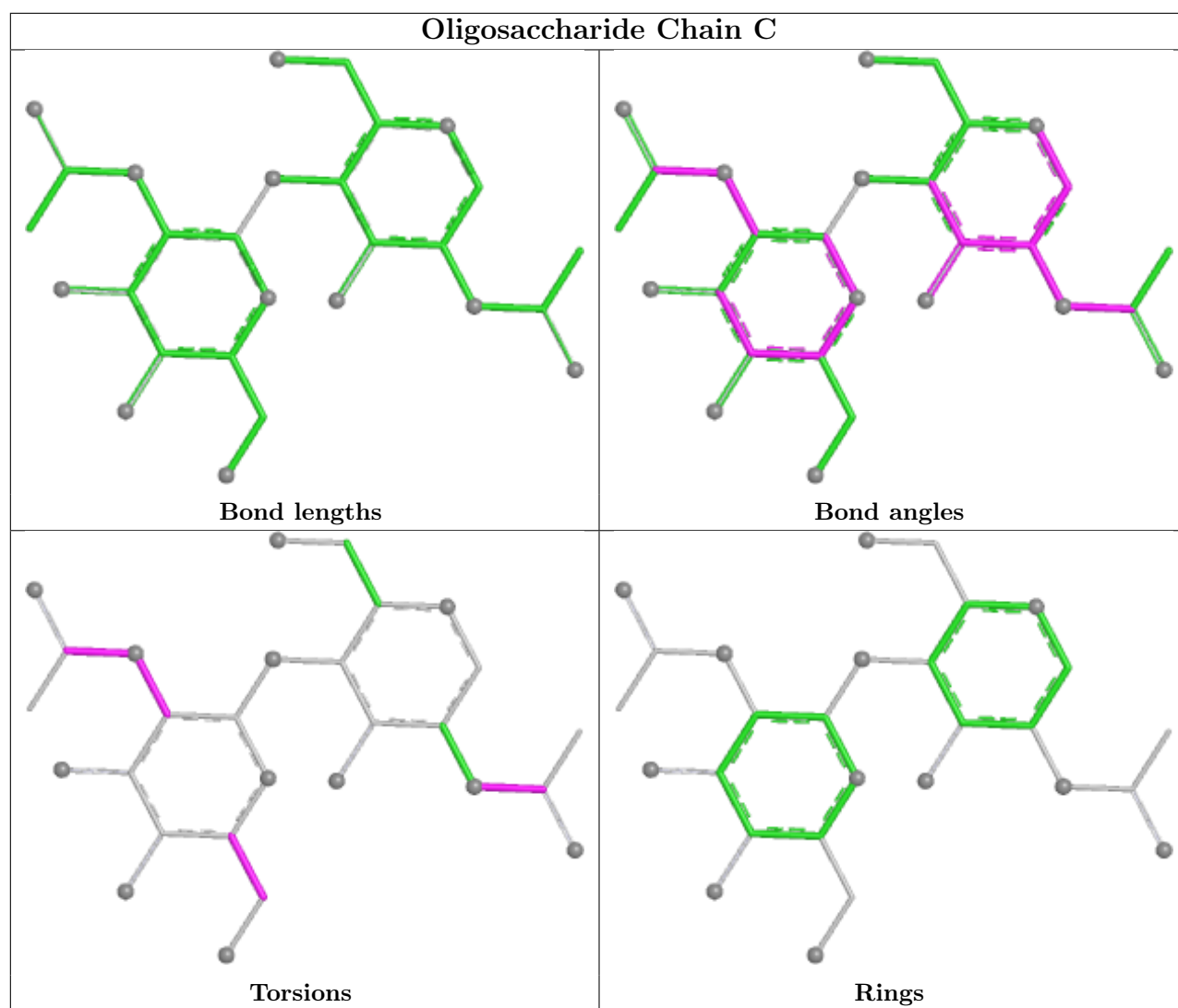
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O7-C7-N2-C2
2	C	2	NAG	C8-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	C	2	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C1-C2-N2-C7
2	D	2	NAG	C1-C2-N2-C7
2	C	2	NAG	O5-C5-C6-O6

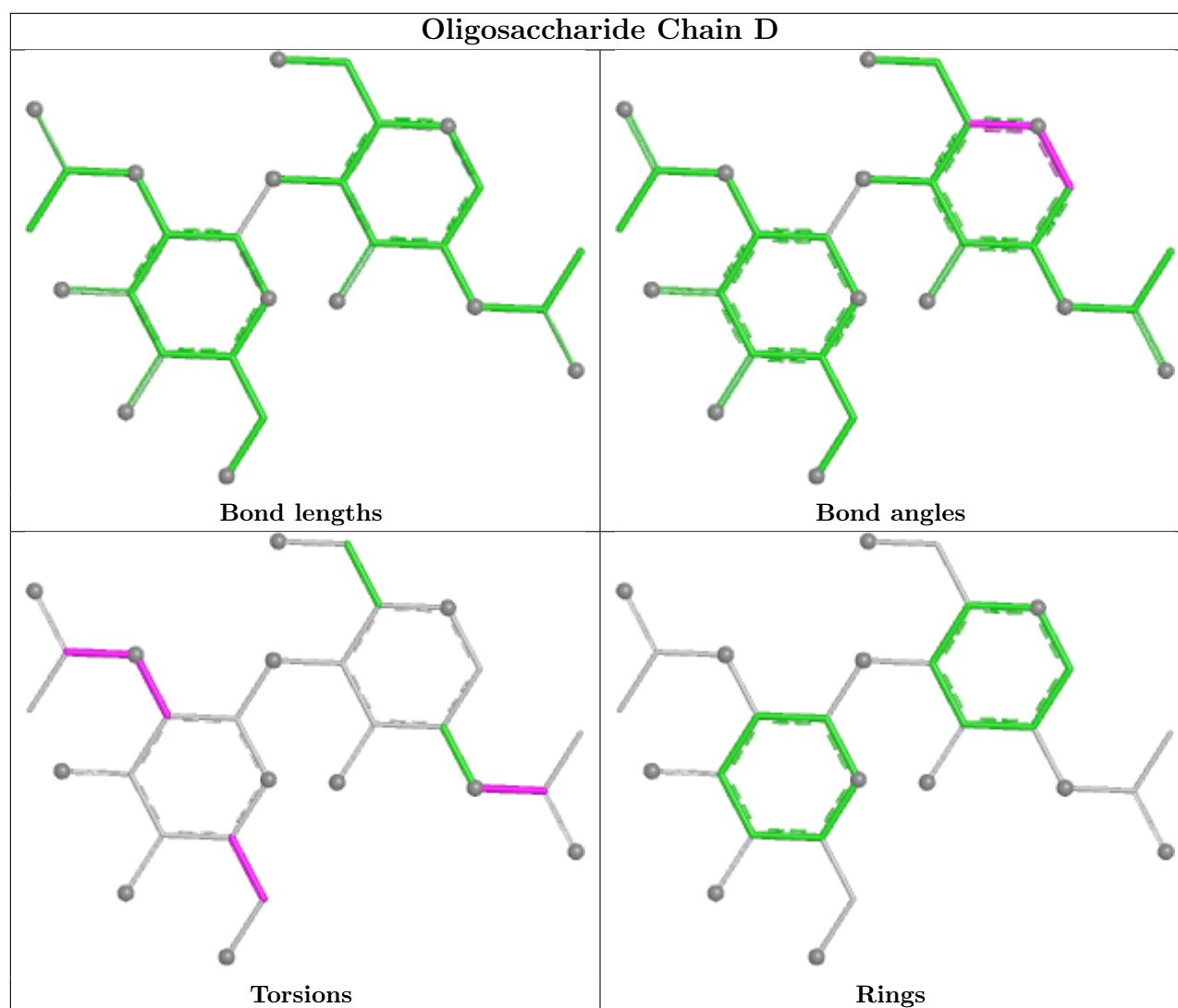
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	1	0
2	D	1	NAG	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 oligosaccharide.





5.6 Ligand geometry [i](#)

14 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	629	1	14,14,15	0.84	1 (7%)	17,19,21	1.61	4 (23%)
3	NAG	B	629	1	14,14,15	1.09	1 (7%)	17,19,21	1.59	3 (17%)
3	NAG	A	630	1	14,14,15	0.69	0	17,19,21	1.66	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	627	1	14,14,15	0.64	0	17,19,21	1.53	4 (23%)
3	NAG	A	622	1	14,14,15	0.43	0	17,19,21	2.26	2 (11%)
3	NAG	B	628	1	14,14,15	0.68	0	17,19,21	1.69	2 (11%)
3	NAG	B	623	1	14,14,15	0.72	0	17,19,21	1.61	4 (23%)
3	NAG	A	628	1	14,14,15	0.76	1 (7%)	17,19,21	1.75	4 (23%)
3	NAG	B	622	1	14,14,15	0.69	0	17,19,21	3.13	7 (41%)
3	NAG	B	627	1	14,14,15	0.57	0	17,19,21	1.54	2 (11%)
4	SO4	B	5001	-	4,4,4	0.30	0	6,6,6	0.26	0
3	NAG	A	626	1	14,14,15	0.62	0	17,19,21	1.18	2 (11%)
3	NAG	B	626	1	14,14,15	0.71	0	17,19,21	1.83	6 (35%)
3	NAG	A	623	1	14,14,15	0.72	0	17,19,21	1.26	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
3	NAG	A	629	1	-	0/6/23/26	0/1/1/1
3	NAG	B	629	1	-	5/6/23/26	0/1/1/1
3	NAG	A	630	1	-	4/6/23/26	0/1/1/1
3	NAG	A	627	1	-	4/6/23/26	0/1/1/1
3	NAG	A	622	1	-	3/6/23/26	0/1/1/1
3	NAG	B	628	1	1/1/5/7	3/6/23/26	0/1/1/1
3	NAG	B	623	1	-	4/6/23/26	0/1/1/1
3	NAG	A	628	1	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	B	627	1	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	B	622	1	-	4/6/23/26	0/1/1/1
3	NAG	A	626	1	1/1/5/7	1/6/23/26	0/1/1/1
3	NAG	B	626	1	1/1/5/7	5/6/23/26	0/1/1/1
3	NAG	A	623	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	629	NAG	C1-C2	3.28	1.56	1.52
3	A	629	NAG	C1-C2	2.66	1.56	1.52
3	A	628	NAG	C1-C2	2.05	1.55	1.52

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	622	NAG	C2-N2-C7	-8.75	111.17	122.90
3	A	622	NAG	C1-O5-C5	8.02	122.93	112.19
3	A	630	NAG	C1-O5-C5	5.66	119.78	112.19
3	B	622	NAG	C1-O5-C5	5.65	119.76	112.19
3	B	628	NAG	C2-N2-C7	-5.22	115.91	122.90
3	A	628	NAG	O5-C1-C2	-5.09	103.42	111.29
3	B	626	NAG	C1-O5-C5	4.28	117.92	112.19
3	B	622	NAG	C4-C3-C2	3.92	116.77	111.02
3	B	627	NAG	O5-C1-C2	-3.91	105.23	111.29
3	B	629	NAG	C1-O5-C5	3.84	117.33	112.19
3	A	629	NAG	C1-O5-C5	3.61	117.02	112.19
3	B	622	NAG	O7-C7-N2	-3.58	115.66	121.98
3	B	623	NAG	C4-C3-C2	3.58	116.26	111.02
3	B	627	NAG	C1-O5-C5	3.41	116.76	112.19
3	A	629	NAG	C2-N2-C7	-3.16	118.67	122.90
3	B	626	NAG	C4-C3-C2	-3.08	106.50	111.02
3	B	629	NAG	C1-C2-N2	2.93	115.05	110.43
3	A	623	NAG	C4-C3-C2	2.92	115.30	111.02
3	B	626	NAG	O5-C5-C6	2.91	113.32	107.66
3	B	622	NAG	C3-C4-C5	2.80	115.31	110.23
3	B	626	NAG	C3-C4-C5	-2.70	105.34	110.23
3	A	628	NAG	C4-C3-C2	2.68	114.94	111.02
3	A	623	NAG	O5-C1-C2	-2.67	107.17	111.29
3	A	627	NAG	C1-O5-C5	2.59	115.66	112.19
3	A	627	NAG	O5-C1-C2	-2.56	107.33	111.29
3	A	627	NAG	C1-C2-N2	2.48	114.34	110.43
3	A	626	NAG	C3-C4-C5	2.44	114.66	110.23
3	A	626	NAG	O5-C1-C2	-2.40	107.57	111.29
3	B	628	NAG	C1-C2-N2	-2.36	106.71	110.43
3	B	629	NAG	C2-N2-C7	2.34	126.03	122.90
3	A	629	NAG	C3-C4-C5	-2.33	106.01	110.23
3	B	623	NAG	C3-C4-C5	2.33	114.45	110.23
3	B	623	NAG	C2-N2-C7	2.31	126.00	122.90
3	B	626	NAG	O3-C3-C2	2.28	114.14	109.40
3	A	622	NAG	O4-C4-C5	2.28	114.93	109.32
3	A	630	NAG	C3-C4-C5	2.25	114.31	110.23
3	A	628	NAG	C1-O5-C5	2.22	115.16	112.19
3	A	629	NAG	C1-C2-N2	2.15	113.82	110.43
3	B	623	NAG	C1-O5-C5	2.15	115.06	112.19
3	B	622	NAG	C6-C5-C4	-2.15	107.75	113.02
3	B	626	NAG	O4-C4-C5	2.08	114.44	109.32
3	A	623	NAG	C2-N2-C7	-2.05	120.15	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	627	NAG	C2-N2-C7	-2.05	120.16	122.90
3	A	628	NAG	C2-N2-C7	-2.02	120.19	122.90
3	A	630	NAG	O5-C5-C4	2.02	115.74	110.83
3	B	622	NAG	C8-C7-N2	2.00	119.44	116.12

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	626	NAG	C1
3	A	628	NAG	C1
3	B	626	NAG	C1
3	B	627	NAG	C1
3	B	628	NAG	C1

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	622	NAG	C8-C7-N2-C2
3	A	622	NAG	O7-C7-N2-C2
3	A	628	NAG	C8-C7-N2-C2
3	A	628	NAG	O7-C7-N2-C2
3	A	630	NAG	C8-C7-N2-C2
3	A	630	NAG	O7-C7-N2-C2
3	B	629	NAG	C1-C2-N2-C7
3	B	629	NAG	C8-C7-N2-C2
3	B	629	NAG	O7-C7-N2-C2
3	B	626	NAG	O5-C5-C6-O6
3	A	628	NAG	O5-C5-C6-O6
3	A	630	NAG	O5-C5-C6-O6
3	A	628	NAG	C4-C5-C6-O6
3	B	626	NAG	C4-C5-C6-O6
3	A	630	NAG	C4-C5-C6-O6
3	B	623	NAG	O5-C5-C6-O6
3	B	626	NAG	C8-C7-N2-C2
3	B	626	NAG	O7-C7-N2-C2
3	B	629	NAG	O5-C5-C6-O6
3	B	622	NAG	O5-C5-C6-O6
3	B	622	NAG	C4-C5-C6-O6
3	A	627	NAG	C8-C7-N2-C2
3	B	622	NAG	C8-C7-N2-C2
3	B	623	NAG	C8-C7-N2-C2
3	B	623	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	A	627	NAG	O7-C7-N2-C2
3	A	627	NAG	O5-C5-C6-O6
3	B	622	NAG	O7-C7-N2-C2
3	B	627	NAG	C4-C5-C6-O6
3	A	626	NAG	O5-C5-C6-O6
3	A	627	NAG	C4-C5-C6-O6
3	A	622	NAG	O5-C5-C6-O6
3	B	629	NAG	C4-C5-C6-O6
3	B	627	NAG	O5-C5-C6-O6
3	B	623	NAG	C4-C5-C6-O6
3	B	627	NAG	C8-C7-N2-C2
3	B	628	NAG	C8-C7-N2-C2
3	B	626	NAG	C3-C2-N2-C7
3	B	627	NAG	O7-C7-N2-C2
3	B	628	NAG	O5-C5-C6-O6
3	B	628	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	627	NAG	2	0
4	B	5001	SO4	4	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	549/621 (88%)	0.74	47 (8%) 16 12	4, 13, 23, 57	0
1	B	584/621 (94%)	0.96	75 (12%) 7 6	6, 17, 28, 66	0
All	All	1133/1242 (91%)	0.86	122 (10%) 11 8	4, 15, 26, 66	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	354	TRP	6.3
1	B	611	LEU	6.2
1	B	320	ARG	5.0
1	B	460	GLU	4.2
1	A	560	PHE	4.1
1	A	561	ARG	4.1
1	A	557	CYS	4.1
1	B	52	ASN	4.0
1	B	407	ARG	4.0
1	A	568	SER	3.9
1	A	248	LYS	3.9
1	B	162	ARG	3.8
1	B	167	CYS	3.7
1	A	245	VAL	3.7
1	A	569	SER	3.6
1	B	203	ASN	3.6
1	B	194	GLN	3.5
1	A	572	HIS	3.5
1	B	359	ALA	3.5
1	A	551	SER	3.5
1	B	607	LEU	3.5
1	B	314	GLY	3.4
1	B	464	ASP	3.4
1	B	408	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	9	VAL	3.3
1	A	294	ASP	3.3
1	B	302	GLU	3.3
1	B	313	GLU	3.3
1	B	444	CYS	3.2
1	B	318	GLY	3.2
1	A	193	PRO	3.1
1	A	535	PRO	3.1
1	A	308	CYS	3.1
1	B	545	THR	3.1
1	A	246	TYR	3.0
1	A	297	GLY	3.0
1	A	296	ASN	3.0
1	A	36	ARG	3.0
1	B	161	GLY	3.0
1	A	571	PRO	2.9
1	B	549	SER	2.9
1	B	171	CYS	2.9
1	A	541	GLU	2.8
1	B	458	PRO	2.8
1	A	443	LEU	2.8
1	A	563	GLY	2.8
1	A	109	SER	2.7
1	B	321	PHE	2.7
1	A	298	LEU	2.7
1	A	108	SER	2.7
1	B	159	ASP	2.7
1	A	520	GLU	2.7
1	B	461	GLU	2.6
1	A	196	ASN	2.6
1	B	8	ALA	2.6
1	A	301	CYS	2.6
1	A	574	VAL	2.6
1	B	325	ASP	2.6
1	B	402	ARG	2.6
1	B	541	GLU	2.6
1	B	353	PRO	2.5
1	A	555	ALA	2.5
1	B	250	THR	2.5
1	A	327	SER	2.5
1	A	249	LEU	2.5
1	A	540	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	570	CYS	2.5
1	B	36	ARG	2.5
1	A	66	GLY	2.5
1	B	308	CYS	2.5
1	B	532	SER	2.5
1	B	109	SER	2.4
1	B	335	CYS	2.4
1	B	474	CYS	2.4
1	A	273	HIS	2.4
1	B	355	HIS	2.4
1	A	536	GLU	2.4
1	B	131	GLU	2.4
1	B	521	PRO	2.4
1	A	461	GLU	2.4
1	B	475	VAL	2.4
1	B	548	GLY	2.4
1	A	537	CYS	2.3
1	B	59	GLN	2.3
1	B	179	GLY	2.3
1	B	315	THR	2.3
1	B	459	THR	2.3
1	B	328	ASN	2.3
1	B	515	ASN	2.3
1	B	120	LEU	2.3
1	A	413	ILE	2.2
1	B	97	ALA	2.2
1	B	62	ARG	2.2
1	B	551	SER	2.2
1	B	587	VAL	2.2
1	B	386	HIS	2.2
1	B	554	CYS	2.2
1	A	159	ASP	2.2
1	A	286	CYS	2.2
1	B	169	GLU	2.2
1	B	553	THR	2.2
1	B	327	SER	2.2
1	B	123	ILE	2.2
1	B	531	PHE	2.1
1	A	304	CYS	2.1
1	A	554	CYS	2.1
1	B	546	CYS	2.1
1	A	559	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	272	PRO	2.1
1	B	322	GLN	2.1
1	A	289	ASP	2.1
1	B	163	SER	2.1
1	A	402	ARG	2.1
1	B	106	THR	2.1
1	B	550	GLY	2.1
1	B	566	CYS	2.1
1	B	204	PRO	2.0
1	B	585	PRO	2.0
1	B	107	ASN	2.0
1	B	533	CYS	2.0
1	B	528	ALA	2.0
1	B	66	GLY	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](#)

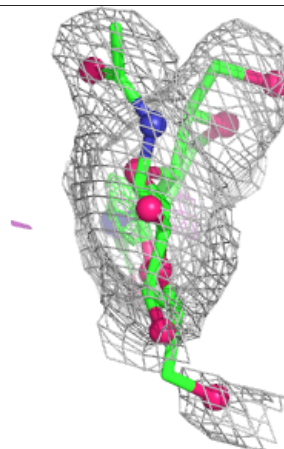
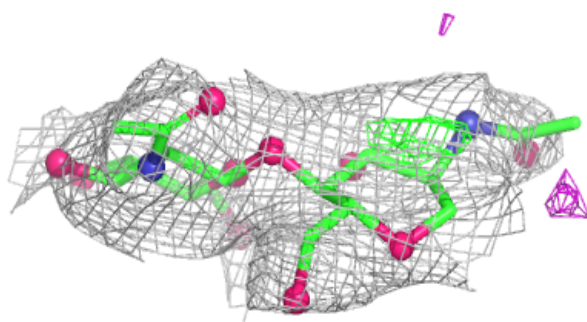
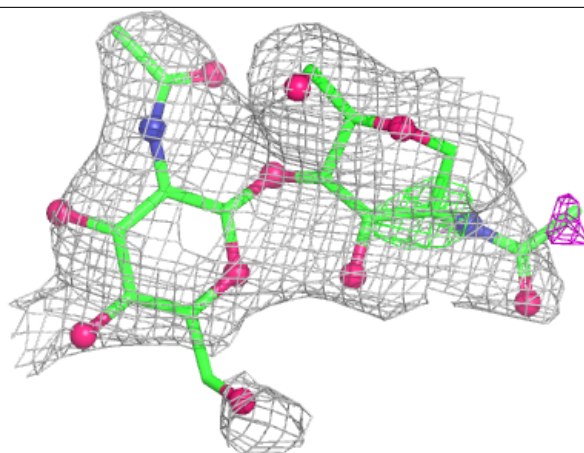
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

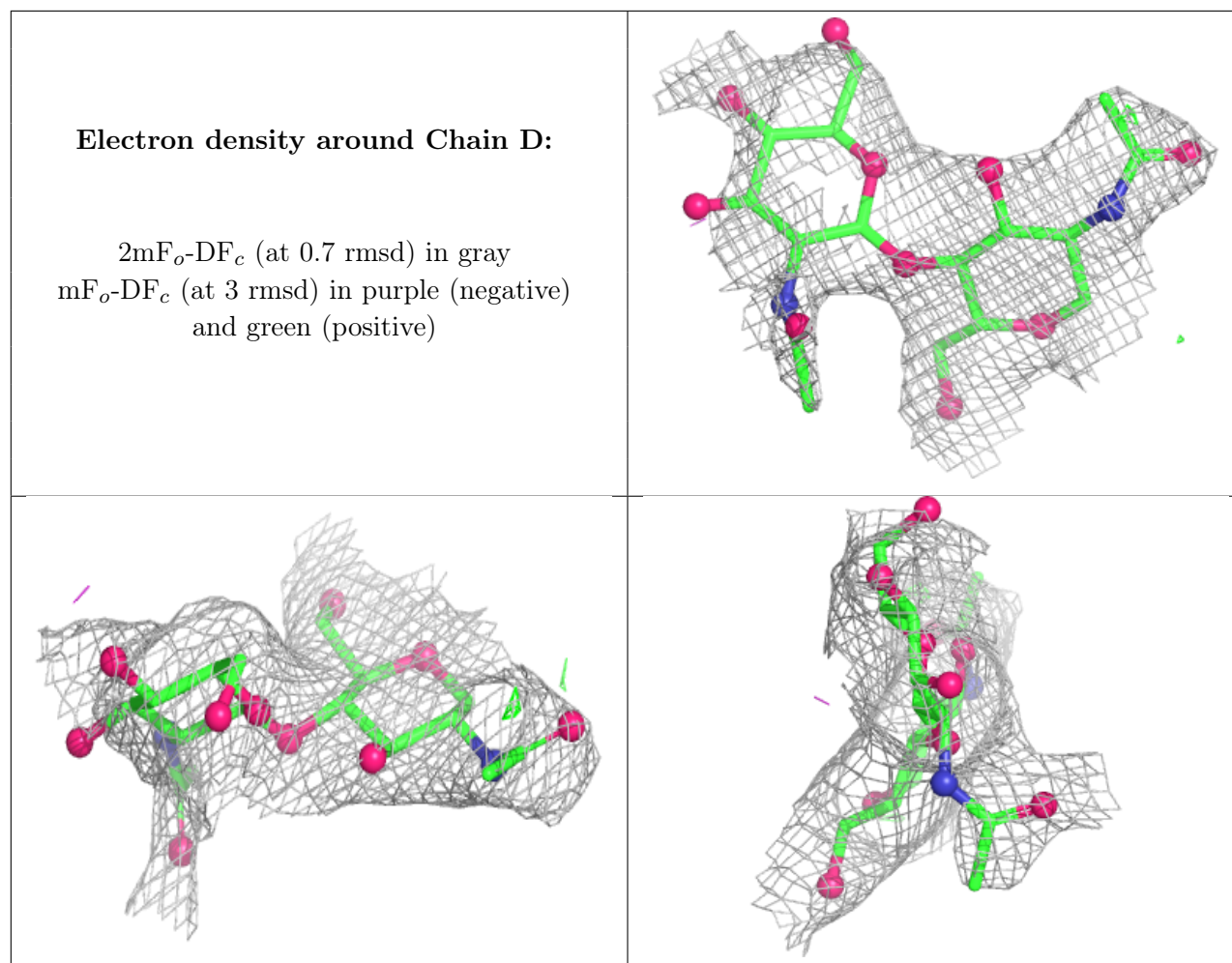
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	C	2	14/15	0.63	0.21	73,78,80,81	0
2	NAG	D	2	14/15	0.71	0.19	82,87,89,90	0
2	NAG	D	1	14/15	0.76	0.18	53,65,68,75	0
2	NAG	C	1	14/15	0.87	0.21	44,55,62,66	0

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)





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
3	NAG	A	623	14/15	0.62	0.17	65,75,77,79	0
3	NAG	B	623	14/15	0.65	0.18	65,76,78,79	0
3	NAG	A	630	14/15	0.66	0.17	67,76,79,80	0
3	NAG	A	626	14/15	0.69	0.13	62,74,79,81	0
3	NAG	B	626	14/15	0.69	0.16	64,73,80,81	0
3	NAG	B	622	14/15	0.71	0.24	46,59,64,64	0
3	NAG	B	629	14/15	0.71	0.18	63,72,75,77	0
3	NAG	A	629	14/15	0.72	0.16	58,70,74,74	0
3	NAG	B	627	14/15	0.74	0.18	59,69,73,74	0
3	NAG	A	622	14/15	0.79	0.16	42,49,52,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	A	628	14/15	0.80	0.15	63,71,75,76	0
3	NAG	A	627	14/15	0.82	0.19	58,68,70,72	0
4	SO4	B	5001	5/5	0.82	0.19	86,87,88,89	0
3	NAG	B	628	14/15	0.87	0.20	53,62,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.