



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 15, 2026 – 02:09 PM JST

PDB ID : 24MR / pdb_000024mr
Title : Structure of the GH136 lacto-N-biosidase LnbX D418S glycosynthase mutant
Authors : Yamada, C.; Fujio, N.; Fushinobu, S.
Deposited on : 2026-03-11
Resolution : 2.47 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

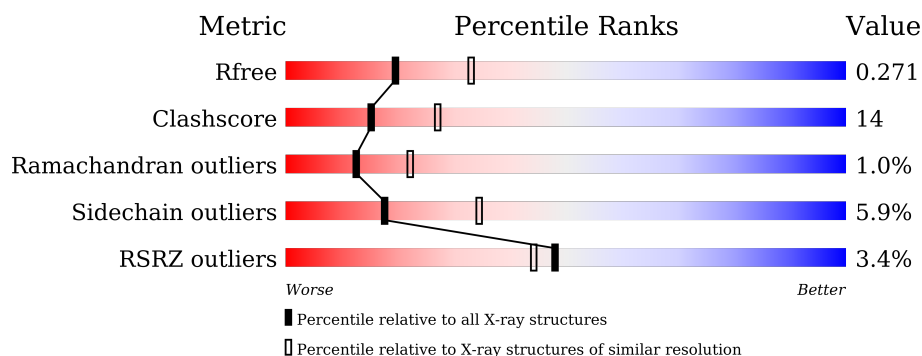
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.47 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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	589	4% 65% 30% ..
1	B	589	2% 71% 26% .
2	C	2	100%
2	D	2	50% 50%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9128 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 Lacto-N-biosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	582	Total	C	N	O	S	0	0	0
			4466	2759	772	923	12			
1	B	589	Total	C	N	O	S	0	0	0
			4528	2797	787	932	12			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	418	SER	ASP	engineered mutation	UNP A0A024QYS6
A	626	ALA	-	expression tag	UNP A0A024QYS6
A	627	ALA	-	expression tag	UNP A0A024QYS6
A	628	ALA	-	expression tag	UNP A0A024QYS6
A	629	LEU	-	expression tag	UNP A0A024QYS6
A	630	GLU	-	expression tag	UNP A0A024QYS6
A	631	HIS	-	expression tag	UNP A0A024QYS6
A	632	HIS	-	expression tag	UNP A0A024QYS6
A	633	HIS	-	expression tag	UNP A0A024QYS6
A	634	HIS	-	expression tag	UNP A0A024QYS6
B	418	SER	ASP	engineered mutation	UNP A0A024QYS6
B	626	ALA	-	expression tag	UNP A0A024QYS6
B	627	ALA	-	expression tag	UNP A0A024QYS6
B	628	ALA	-	expression tag	UNP A0A024QYS6
B	629	LEU	-	expression tag	UNP A0A024QYS6
B	630	GLU	-	expression tag	UNP A0A024QYS6
B	631	HIS	-	expression tag	UNP A0A024QYS6
B	632	HIS	-	expression tag	UNP A0A024QYS6
B	633	HIS	-	expression tag	UNP A0A024QYS6
B	634	HIS	-	expression tag	UNP A0A024QYS6

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			26	14	1	11			
2	D	2	Total	C	N	O	0	0	0
			26	14	1	11			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		
3	B	2	Total	Ca	0	0
			2	2		

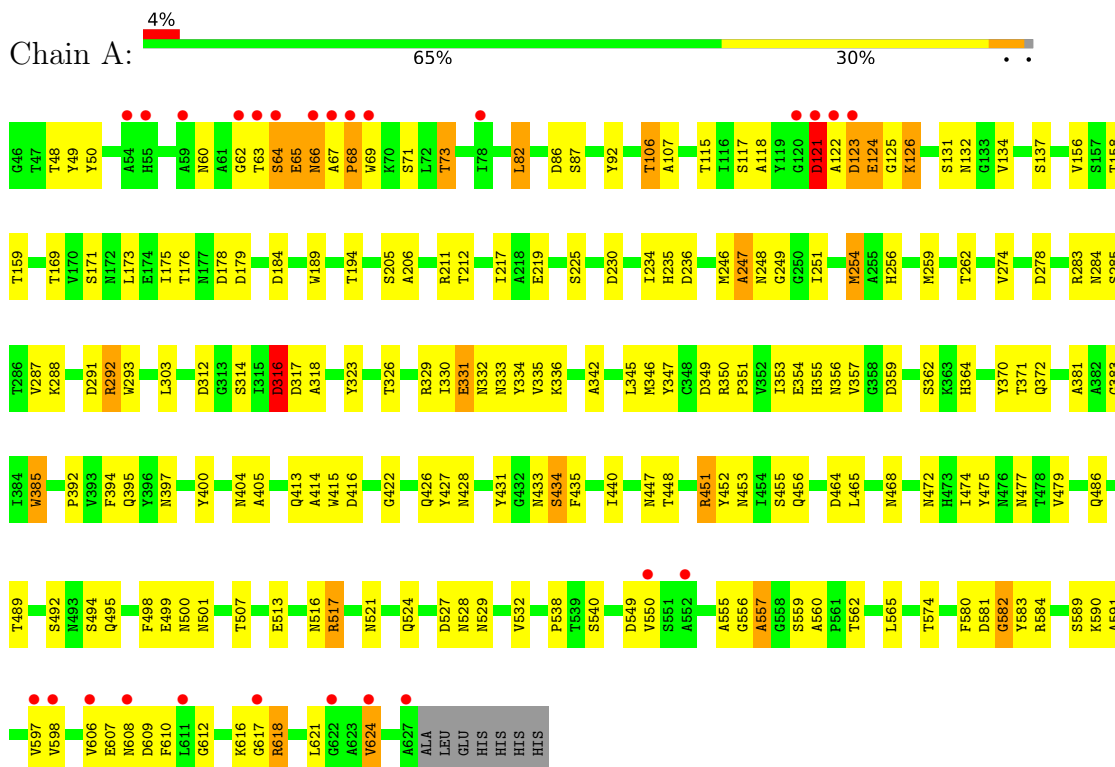
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	37	Total	O	0	0
			37	37		
4	B	41	Total	O	0	0
			41	41		

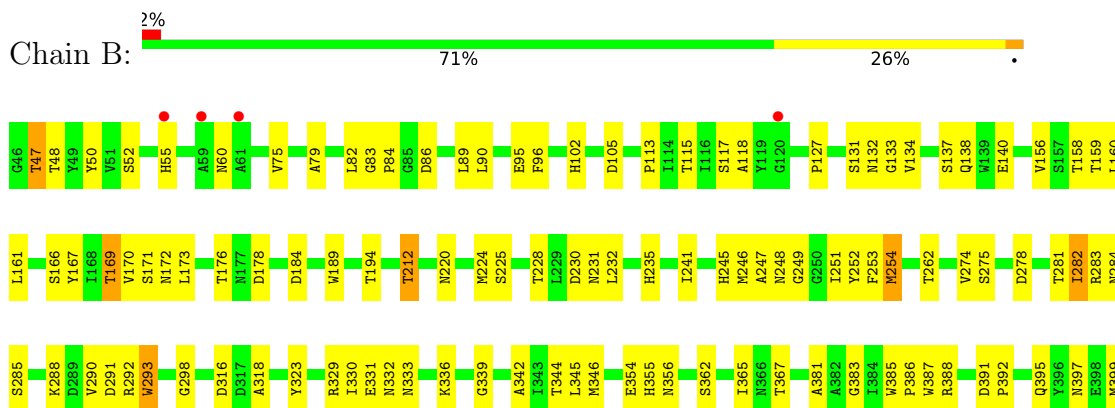
3 Residue-property plots

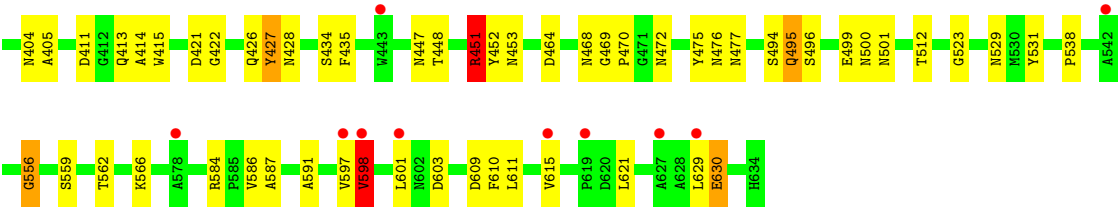
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



- Molecule 1: Lacto-N-biosidase





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

Chain C: 100%



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

Chain D: 50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.56Å 141.93Å 144.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.72 – 2.47 47.72 – 2.47	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.72-2.47) 99.9 (47.72-2.47)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0431	Depositor
R, R_{free}	0.217 , 0.271 0.222 , 0.271	Depositor DCC
R_{free} test set	2401 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	46.4	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.009 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9128	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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: GAL, CA, NDG

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	0.55	0/4565	1.10	15/6221 (0.2%)
1	B	0.54	0/4631	1.07	14/6311 (0.2%)
All	All	0.54	0/9196	1.09	29/12532 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	3
All	All	0	4

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	THR	CA-CB-OG1	-7.50	98.35	109.60
1	B	262	THR	CA-CB-OG1	-6.46	99.91	109.60
1	A	123	ASP	N-CA-C	-6.42	106.07	114.04
1	B	47	THR	CA-CB-OG1	-6.33	100.10	109.60
1	A	371	THR	CA-CB-OG1	-6.23	100.26	109.60
1	A	574	THR	CA-CB-OG1	-6.09	100.46	109.60
1	A	179	ASP	CA-CB-CG	5.99	118.59	112.60
1	A	597	VAL	N-CA-CB	5.95	118.10	110.13
1	B	464	ASP	CA-CB-CG	5.94	118.54	112.60
1	A	513	GLU	CB-CA-C	-5.90	98.01	109.76
1	A	316	ASP	CA-CB-CG	5.88	118.48	112.60
1	B	86	ASP	CA-CB-CG	5.80	118.40	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	140	GLU	CB-CA-C	5.76	120.17	110.79
1	B	598	VAL	N-CA-CB	5.71	118.34	111.31
1	A	331	GLU	CB-CA-C	-5.66	100.18	109.80
1	A	385	TRP	N-CA-C	5.58	113.24	108.22
1	B	421	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	370	TYR	N-CA-CB	-5.52	104.17	110.35
1	A	464	ASP	CB-CA-C	5.52	118.96	110.62
1	B	245	HIS	CA-CB-CG	-5.48	108.32	113.80
1	B	184	ASP	CA-CB-CG	5.46	118.06	112.60
1	B	169	THR	CA-CB-OG1	-5.40	101.50	109.60
1	A	549	ASP	CA-CB-CG	5.13	117.73	112.60
1	B	291	ASP	CA-CB-CG	5.11	117.71	112.60
1	B	562	THR	CA-CB-OG1	-5.08	101.98	109.60
1	A	121	ASP	CA-CB-CG	5.06	117.66	112.60
1	B	367	THR	CA-CB-OG1	-5.04	102.03	109.60
1	B	584	ARG	CB-CA-C	-5.01	101.55	109.82
1	A	464	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	292	ARG	Sidechain
1	B	224	MET	Peptide
1	B	451	ARG	Sidechain
1	B	630	GLU	Peptide

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	4466	0	4136	138	0
1	B	4528	0	4186	98	0
2	C	26	0	21	0	0
2	D	26	0	21	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	37	0	0	0	0
4	B	41	0	0	0	0
All	All	9128	0	8364	236	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 14.

All (236) 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:448:THR:HB	1:A:472:ASN:HD22	1.47	0.79
1:B:470:PRO:HA	1:B:495:GLN:HG2	1.65	0.79
1:A:317:ASP:OD2	1:A:350:ARG:NH2	2.24	0.71
1:A:589:SER:C	1:A:591:ALA:H	2.00	0.69
1:A:171:SER:O	1:A:173:LEU:HD13	1.93	0.69
1:A:617:GLY:O	1:A:618:ARG:C	2.35	0.69
1:A:82:LEU:O	1:A:106:THR:CG2	2.41	0.68
1:A:283:ARG:HA	1:A:331:GLU:O	1.94	0.67
1:A:217:ILE:CD1	1:A:254:MET:HE3	2.25	0.66
1:A:486:GLN:HE22	1:A:517:ARG:NH2	1.95	0.65
1:A:217:ILE:HD11	1:A:254:MET:HE3	1.79	0.65
1:A:477:ASN:H	1:A:501:ASN:HD22	1.42	0.64
1:A:246:MET:O	1:A:248:ASN:N	2.31	0.64
1:A:486:GLN:HE22	1:A:517:ARG:HH21	1.44	0.63
1:B:48:THR:HG22	1:B:50:TYR:CE2	2.33	0.63
1:B:422:GLY:HA2	1:B:447:ASN:O	1.99	0.62
1:A:342:ALA:HB3	1:A:383:GLY:O	1.98	0.62
1:B:501:ASN:H	1:B:529:ASN:HD22	1.48	0.62
1:A:499:GLU:HA	1:A:527:ASP:O	1.99	0.61
1:A:556:GLY:H	1:A:582:GLY:HA2	1.64	0.61
1:A:134:VAL:O	1:A:137:SER:OG	2.18	0.60
1:B:75:VAL:O	1:B:79:ALA:HB2	2.00	0.60
1:A:397:ASN:H	1:A:428:ASN:HD22	1.48	0.60
1:A:468:ASN:ND2	1:A:494:SER:HB3	2.16	0.59
1:A:225:SER:HA	1:A:278:ASP:O	2.02	0.59
1:A:609:ASP:O	1:A:612:GLY:N	2.35	0.59
1:B:395:GLN:HA	1:B:426:GLN:O	2.02	0.58
1:A:82:LEU:O	1:A:106:THR:HG21	2.02	0.58
1:A:345:LEU:HD13	1:A:353:ILE:HG12	1.85	0.58
1:B:189:TRP:HH2	1:B:404:ASN:HD21	1.52	0.58
1:B:495:GLN:HA	1:B:523:GLY:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:THR:OG1	1:B:212:THR:HG23	2.03	0.58
1:B:172:ASN:HD22	1:B:231:ASN:HD22	1.51	0.58
1:B:451:ARG:HA	1:B:475:TYR:O	2.04	0.58
1:A:235:HIS:HD2	1:A:236:ASP:OD2	1.87	0.57
1:A:278:ASP:OD1	1:A:326:THR:OG1	2.20	0.57
1:B:331:GLU:HA	1:B:354:GLU:O	2.05	0.57
1:A:189:TRP:HH2	1:A:404:ASN:HD21	1.52	0.56
1:A:556:GLY:O	1:A:557:ALA:CB	2.52	0.56
1:A:465:LEU:HB3	1:A:468:ASN:HD21	1.71	0.56
1:A:397:ASN:H	1:A:428:ASN:ND2	2.03	0.56
1:A:354:GLU:HA	1:A:395:GLN:O	2.06	0.56
1:B:354:GLU:HA	1:B:395:GLN:O	2.05	0.56
1:A:131:SER:OG	1:A:159:THR:HA	2.06	0.56
1:B:253:PHE:C	1:B:254:MET:HE2	2.31	0.56
1:B:90:LEU:O	1:B:118:ALA:HA	2.06	0.55
1:A:283:ARG:HG3	1:A:284:ASN:HD22	1.70	0.55
1:B:252:TYR:HB3	1:B:254:MET:HE1	1.87	0.55
1:A:212:THR:HA	1:A:249:GLY:O	2.06	0.55
1:A:125:GLY:O	1:A:126:LYS:C	2.49	0.55
1:A:474:ILE:O	1:A:498:PHE:HA	2.06	0.55
1:B:212:THR:HB	1:B:247:ALA:O	2.07	0.55
1:A:395:GLN:HA	1:A:426:GLN:O	2.07	0.55
1:B:283:ARG:HA	1:B:331:GLU:O	2.07	0.55
1:A:312:ASP:OD1	1:A:314:SER:OG	2.24	0.54
1:A:501:ASN:H	1:A:529:ASN:HD22	1.53	0.54
1:B:428:ASN:H	1:B:453:ASN:HD22	1.55	0.54
1:A:477:ASN:H	1:A:501:ASN:ND2	2.04	0.54
1:A:455:SER:HB3	1:A:479:VAL:HG12	1.90	0.54
1:A:440:ILE:O	1:A:468:ASN:HB3	2.08	0.54
1:B:171:SER:HA	1:B:230:ASP:O	2.07	0.53
1:B:102:HIS:CD2	1:B:161:LEU:HB3	2.43	0.53
1:B:235:HIS:HA	1:B:288:LYS:O	2.07	0.53
1:A:556:GLY:O	1:A:557:ALA:HB2	2.08	0.53
1:B:138:GLN:HA	1:B:156:VAL:O	2.08	0.53
1:B:477:ASN:H	1:B:501:ASN:HD22	1.55	0.53
1:A:131:SER:HG	1:A:159:THR:CB	2.22	0.52
1:A:48:THR:HG22	1:A:50:TYR:CE1	2.44	0.52
1:A:397:ASN:HB2	1:A:428:ASN:ND2	2.24	0.52
1:B:134:VAL:O	1:B:137:SER:OG	2.28	0.52
1:B:298:GLY:HA3	1:B:346:MET:O	2.10	0.52
1:A:589:SER:C	1:A:591:ALA:N	2.67	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:LYS:HA	1:B:336:LYS:O	2.11	0.51
1:A:171:SER:HA	1:A:230:ASP:O	2.09	0.51
1:A:235:HIS:HA	1:A:288:LYS:O	2.09	0.51
1:A:426:GLN:HA	1:A:451:ARG:O	2.10	0.51
1:A:332:ASN:HA	1:A:355:HIS:O	2.11	0.51
1:B:274:VAL:HG11	1:B:323:TYR:HA	1.93	0.51
1:A:426:GLN:HG3	1:A:427:TYR:CD2	2.46	0.51
1:B:426:GLN:HA	1:B:451:ARG:O	2.11	0.50
1:A:330:ILE:HG13	1:A:345:LEU:HD11	1.93	0.50
1:A:486:GLN:NE2	1:A:517:ARG:HH21	2.09	0.50
1:A:500:ASN:HA	1:A:621:LEU:HD12	1.93	0.50
1:A:121:ASP:O	1:A:122:ALA:HB3	2.12	0.50
1:A:303:LEU:HD12	1:A:303:LEU:C	2.37	0.50
1:A:584:ARG:HG2	1:A:584:ARG:HH11	1.76	0.50
1:A:589:SER:O	1:A:591:ALA:N	2.43	0.50
1:A:49:TYR:HA	1:A:62:GLY:O	2.12	0.50
1:B:89:LEU:C	1:B:90:LEU:HD12	2.36	0.50
1:B:249:GLY:HA3	1:B:293:TRP:O	2.11	0.50
1:B:475:TYR:HA	1:B:499:GLU:O	2.12	0.50
1:A:353:ILE:O	1:A:394:PHE:HA	2.12	0.50
1:B:117:SER:OG	1:B:118:ALA:N	2.38	0.49
1:A:288:LYS:HA	1:A:336:LYS:O	2.13	0.49
1:A:532:VAL:HG11	1:A:550:VAL:HG22	1.95	0.49
1:B:391:ASP:N	1:B:392:PRO:CD	2.76	0.49
1:A:274:VAL:HG11	1:A:323:TYR:HA	1.95	0.49
1:A:316:ASP:OD1	1:A:318:ALA:N	2.45	0.49
1:A:49:TYR:CD2	1:A:69:TRP:CH2	3.01	0.49
1:A:499:GLU:O	1:A:500:ASN:HB2	2.12	0.49
1:A:538:PRO:C	1:A:540:SER:H	2.21	0.49
1:B:332:ASN:HA	1:B:355:HIS:O	2.13	0.49
1:B:477:ASN:H	1:B:501:ASN:ND2	2.11	0.49
1:A:71:SER:HB3	1:A:73:THR:HG22	1.95	0.49
1:A:158:THR:OG1	1:A:212:THR:CG2	2.60	0.49
1:B:397:ASN:H	1:B:428:ASN:HD22	1.61	0.49
1:B:90:LEU:HD23	1:B:96:PHE:CE2	2.48	0.48
1:A:212:THR:HB	1:A:247:ALA:O	2.13	0.48
1:B:105:ASP:OD1	1:B:220:ASN:ND2	2.41	0.48
1:B:586:VAL:O	1:B:587:ALA:C	2.56	0.48
1:A:234:ILE:O	1:A:287:VAL:HA	2.13	0.48
1:A:82:LEU:O	1:A:106:THR:HG22	2.12	0.48
1:A:132:ASN:HA	1:A:178:ASP:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:GLN:NE2	1:A:560:ALA:HB3	2.29	0.48
1:B:83:GLY:O	1:B:84:PRO:C	2.57	0.48
1:B:531:TYR:CE1	1:B:538:PRO:HD3	2.48	0.48
1:A:495:GLN:HB2	1:A:521:ASN:O	2.15	0.47
1:B:339:GLY:O	1:B:365:ILE:HG12	2.15	0.47
1:A:489:THR:O	1:A:492:SER:HB3	2.15	0.47
1:B:411:ASP:HB3	1:B:413:GLN:OE1	2.15	0.47
1:B:342:ALA:HB3	1:B:383:GLY:O	2.14	0.47
1:B:469:GLY:O	1:B:472:ASN:OD1	2.31	0.47
1:B:472:ASN:H	1:B:495:GLN:HE21	1.62	0.47
1:A:66:ASN:OD1	1:A:67:ALA:N	2.47	0.47
1:A:117:SER:OG	1:A:118:ALA:N	2.46	0.47
1:A:121:ASP:HB2	1:A:124:GLU:H	1.80	0.47
1:A:159:THR:CG2	1:A:175:ILE:HG23	2.45	0.47
1:A:413:GLN:HG3	1:A:435:PHE:O	2.15	0.47
1:B:405:ALA:HB3	1:B:434:SER:HB2	1.97	0.47
1:A:499:GLU:OE1	1:A:598:VAL:HG23	2.15	0.46
1:B:448:THR:HB	1:B:472:ASN:HD22	1.80	0.46
1:A:331:GLU:HA	1:A:354:GLU:O	2.15	0.46
1:A:451:ARG:O	1:A:451:ARG:HG3	2.14	0.46
1:A:583:TYR:O	1:A:624:VAL:HG13	2.16	0.46
1:B:512:THR:HG23	1:B:512:THR:O	2.16	0.46
1:A:329:ARG:HD3	1:A:331:GLU:OE2	2.16	0.46
1:A:351:PRO:HD2	1:A:392:PRO:HA	1.97	0.46
1:A:356:ASN:H	1:A:397:ASN:HD22	1.63	0.46
1:A:415:TRP:CZ2	1:A:428:ASN:HB3	2.50	0.46
1:B:391:ASP:N	1:B:392:PRO:HD3	2.31	0.46
1:A:451:ARG:HA	1:A:475:TYR:O	2.16	0.46
1:B:281:THR:HA	1:B:329:ARG:O	2.16	0.46
1:A:448:THR:HB	1:A:472:ASN:ND2	2.23	0.46
1:A:159:THR:HG21	1:A:175:ILE:HG23	1.97	0.46
1:A:336:LYS:HA	1:A:359:ASP:O	2.16	0.45
1:B:556:GLY:O	1:B:559:SER:OG	2.18	0.45
1:B:131:SER:OG	1:B:159:THR:HA	2.16	0.45
1:A:452:TYR:CD2	1:A:609:ASP:HA	2.51	0.45
1:A:291:ASP:HA	1:A:292:ARG:HA	1.69	0.45
1:A:453:ASN:H	1:A:477:ASN:HD22	1.64	0.45
1:B:231:ASN:HA	1:B:284:ASN:O	2.17	0.45
1:A:501:ASN:H	1:A:529:ASN:ND2	2.15	0.45
1:A:158:THR:HG23	1:A:212:THR:HG23	1.99	0.45
1:B:476:ASN:CG	1:B:500:ASN:HB3	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:GLU:HG3	1:A:256:HIS:HB2	1.99	0.45
1:A:475:TYR:HA	1:A:499:GLU:O	2.17	0.44
1:B:127:PRO:HD2	1:B:172:ASN:O	2.17	0.44
1:B:169:THR:HA	1:B:228:THR:O	2.17	0.44
1:B:330:ILE:CD1	1:B:345:LEU:HD11	2.48	0.44
1:B:212:THR:HG21	1:B:247:ALA:HB1	1.99	0.44
1:A:121:ASP:CG	1:A:124:GLU:HB2	2.42	0.44
1:B:285:SER:H	1:B:333:ASN:ND2	2.15	0.44
1:B:333:ASN:H	1:B:356:ASN:HD22	1.65	0.44
1:B:413:GLN:HG3	1:B:435:PHE:O	2.16	0.44
1:B:609:ASP:O	1:B:610:PHE:C	2.61	0.44
1:A:121:ASP:HB2	1:A:123:ASP:H	1.82	0.44
1:A:516:ASN:HA	1:A:524:GLN:OE1	2.17	0.44
1:A:584:ARG:HG2	1:A:584:ARG:NH1	2.32	0.44
1:B:132:ASN:HA	1:B:178:ASP:O	2.18	0.44
1:B:356:ASN:H	1:B:397:ASN:HD22	1.66	0.43
1:B:427:TYR:CD1	1:B:427:TYR:N	2.85	0.43
1:B:451:ARG:HD2	1:B:452:TYR:HD2	1.83	0.43
1:B:131:SER:C	1:B:133:GLY:H	2.25	0.43
1:B:468:ASN:ND2	1:B:494:SER:HB3	2.34	0.43
1:A:87:SER:HA	1:A:115:THR:O	2.18	0.43
1:B:176:THR:HA	1:B:235:HIS:O	2.19	0.43
1:A:125:GLY:O	1:A:126:LYS:O	2.37	0.43
1:A:156:VAL:HG11	1:A:247:ALA:HB3	2.01	0.43
1:B:158:THR:OG1	1:B:212:THR:CG2	2.67	0.43
1:B:285:SER:H	1:B:333:ASN:HD22	1.65	0.43
1:B:160:LEU:HD21	1:B:170:VAL:HG11	2.01	0.43
1:A:500:ASN:HA	1:A:621:LEU:CD1	2.49	0.42
1:A:334:TYR:HA	1:A:357:VAL:O	2.19	0.42
1:B:246:MET:O	1:B:248:ASN:N	2.53	0.42
1:B:475:TYR:HD1	1:B:476:ASN:HD22	1.67	0.42
1:A:285:SER:H	1:A:333:ASN:HD22	1.66	0.42
1:A:346:MET:O	1:A:347:TYR:C	2.62	0.42
1:A:422:GLY:HA2	1:A:447:ASN:O	2.20	0.42
1:B:131:SER:C	1:B:133:GLY:N	2.75	0.42
1:A:65:GLU:O	1:A:66:ASN:C	2.61	0.42
1:B:225:SER:HA	1:B:278:ASP:O	2.19	0.42
1:B:362:SER:OG	1:B:381:ALA:HB3	2.20	0.42
1:A:581:ASP:O	1:A:583:TYR:N	2.52	0.42
1:B:391:ASP:HA	1:B:422:GLY:O	2.19	0.42
1:A:211:ARG:HH11	1:A:211:ARG:HD3	1.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:ILE:HD13	1:B:345:LEU:HD21	2.02	0.42
1:B:399:MET:HG2	1:B:414:ALA:HA	2.01	0.42
1:A:234:ILE:HD13	1:A:251:ILE:CG1	2.50	0.41
1:A:385:TRP:HB2	1:A:416:ASP:O	2.20	0.41
1:B:316:ASP:OD1	1:B:318:ALA:HB3	2.20	0.41
1:B:475:TYR:CD1	1:B:598:VAL:HG11	2.55	0.41
1:A:50:TYR:HE1	1:A:64:SER:HA	1.85	0.41
1:A:349:ASP:O	1:A:350:ARG:C	2.62	0.41
1:B:156:VAL:HG11	1:B:247:ALA:HB3	2.02	0.41
1:B:173:LEU:H	1:B:232:LEU:HD23	1.84	0.41
1:A:413:GLN:H	1:A:413:GLN:CD	2.28	0.41
1:A:456:GLN:HE22	1:A:560:ALA:H	1.68	0.41
1:B:356:ASN:H	1:B:397:ASN:ND2	2.18	0.41
1:B:426:GLN:HG3	1:B:427:TYR:CD2	2.55	0.41
1:A:362:SER:OG	1:A:381:ALA:HB3	2.21	0.41
1:B:241:ILE:O	1:B:292:ARG:HD2	2.21	0.41
1:B:251:ILE:HG21	1:B:282:ILE:HD13	2.02	0.41
1:A:106:THR:HG22	1:A:107:ALA:H	1.85	0.41
1:A:405:ALA:HB3	1:A:434:SER:HB3	2.01	0.41
1:A:583:TYR:O	1:A:624:VAL:CG1	2.68	0.41
1:A:400:TYR:CD1	1:A:431:TYR:HB3	2.56	0.41
1:B:288:LYS:O	1:B:290:VAL:HG13	2.21	0.41
1:A:397:ASN:HB2	1:A:428:ASN:HD22	1.85	0.41
1:A:414:ALA:HB2	1:A:433:ASN:ND2	2.36	0.41
1:A:609:ASP:OD1	1:A:609:ASP:C	2.64	0.41
1:B:166:SER:O	1:B:167:TYR:C	2.64	0.41
1:B:397:ASN:H	1:B:428:ASN:ND2	2.19	0.41
1:A:206:ALA:H	1:A:372:GLN:NE2	2.18	0.41
1:A:285:SER:H	1:A:333:ASN:ND2	2.19	0.41
1:A:335:VAL:HG11	1:A:342:ALA:HA	2.03	0.40
1:B:344:THR:HA	1:B:385:TRP:O	2.20	0.40
1:A:184:ASP:OD2	1:A:364:HIS:NE2	2.55	0.40
1:B:591:ALA:HA	1:B:621:LEU:HD12	2.04	0.40
1:A:353:ILE:HD13	1:A:394:PHE:CE1	2.55	0.40
1:B:415:TRP:CZ2	1:B:428:ASN:HB3	2.57	0.40
1:A:63:THR:C	1:A:65:GLU:N	2.80	0.40
1:A:353:ILE:HD13	1:A:394:PHE:CZ	2.56	0.40
1:A:580:PHE:CD1	1:A:580:PHE:N	2.89	0.40
1:A:609:ASP:O	1:A:610:PHE:C	2.65	0.40
1:B:52:SER:HB3	1:B:55:HIS:O	2.20	0.40
1:B:387:TRP:O	1:B:388:ARG:C	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	580/589 (98%)	506 (87%)	65 (11%)	9 (2%)	7	13
1	B	587/589 (100%)	534 (91%)	50 (8%)	3 (0%)	24	40
All	All	1167/1178 (99%)	1040 (89%)	115 (10%)	12 (1%)	12	22

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	247	ALA
1	A	557	ALA
1	A	590	LYS
1	A	555	ALA
1	B	60	ASN
1	B	556	GLY
1	A	92	TYR
1	A	68	PRO
1	A	126	LYS
1	A	582	GLY
1	A	618	ARG
1	B	386	PRO

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	470/476 (99%)	438 (93%)	32 (7%)	14	28
1	B	476/476 (100%)	452 (95%)	24 (5%)	22	41
All	All	946/952 (99%)	890 (94%)	56 (6%)	18	34

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	64	SER
1	A	65	GLU
1	A	66	ASN
1	A	68	PRO
1	A	73	THR
1	A	82	LEU
1	A	86	ASP
1	A	106	THR
1	A	121	ASP
1	A	124	GLU
1	A	169	THR
1	A	176	THR
1	A	205	SER
1	A	254	MET
1	A	259	MET
1	A	262	THR
1	A	293	TRP
1	A	316	ASP
1	A	434	SER
1	A	451	ARG
1	A	507	THR
1	A	517	ARG
1	A	528	ASN
1	A	559	SER
1	A	562	THR
1	A	565	LEU
1	A	606	VAL
1	A	607	GLU
1	A	608	ASN
1	A	616	LYS
1	A	624	VAL
1	B	47	THR
1	B	82	LEU
1	B	95	GLU

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Mol	Chain	Res	Type
1	B	113	PRO
1	B	115	THR
1	B	194	THR
1	B	212	THR
1	B	254	MET
1	B	275	SER
1	B	282	ILE
1	B	293	TRP
1	B	427	TYR
1	B	451	ARG
1	B	495	GLN
1	B	496	SER
1	B	566	LYS
1	B	597	VAL
1	B	598	VAL
1	B	601	LEU
1	B	603	ASP
1	B	611	LEU
1	B	615	VAL
1	B	629	LEU
1	B	630	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	138	GLN
1	A	235	HIS
1	A	284	ASN
1	A	333	ASN
1	A	368	GLN
1	A	372	GLN
1	A	397	ASN
1	A	404	ASN
1	A	428	ASN
1	A	447	ASN
1	A	456	GLN
1	A	457	ASN
1	A	460	GLN
1	A	468	ASN
1	A	472	ASN
1	A	476	ASN

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Mol	Chain	Res	Type
1	A	477	ASN
1	A	486	GLN
1	A	501	ASN
1	A	528	ASN
1	A	529	ASN
1	A	593	ASN
1	A	602	ASN
1	B	66	ASN
1	B	102	HIS
1	B	138	GLN
1	B	226	ASN
1	B	231	ASN
1	B	243	ASN
1	B	279	HIS
1	B	284	ASN
1	B	333	ASN
1	B	356	ASN
1	B	368	GLN
1	B	397	ASN
1	B	404	ASN
1	B	428	ASN
1	B	447	ASN
1	B	453	ASN
1	B	457	ASN
1	B	468	ASN
1	B	472	ASN
1	B	473	HIS
1	B	495	GLN
1	B	501	ASN
1	B	520	GLN
1	B	528	ASN
1	B	529	ASN
1	B	533	ASN
1	B	608	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	NDG	C	1	2	15,15,15	0.36	0	21,21,21	1.50	3 (14%)
2	GAL	C	2	2	11,11,12	0.52	0	15,15,17	1.13	2 (13%)
2	NDG	D	1	2	15,15,15	0.44	0	21,21,21	1.31	1 (4%)
2	GAL	D	2	2	11,11,12	0.57	0	15,15,17	0.81	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	NDG	C	1	2	-	3/6/26/26	0/1/1/1
2	GAL	C	2	2	-	1/2/19/22	0/1/1/1
2	NDG	D	1	2	-	4/6/26/26	0/1/1/1
2	GAL	D	2	2	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NDG	O5-C1-C2	5.47	115.02	109.52
2	D	1	NDG	O5-C1-C2	5.15	114.70	109.52
2	C	2	GAL	C1-C2-C3	2.91	113.24	109.67
2	C	2	GAL	C1-O5-C5	2.53	115.62	112.19
2	C	1	NDG	C3-C2-N2	2.35	115.06	110.62
2	C	1	NDG	C1-C2-N2	-2.22	108.16	110.73

There are no chirality outliers.

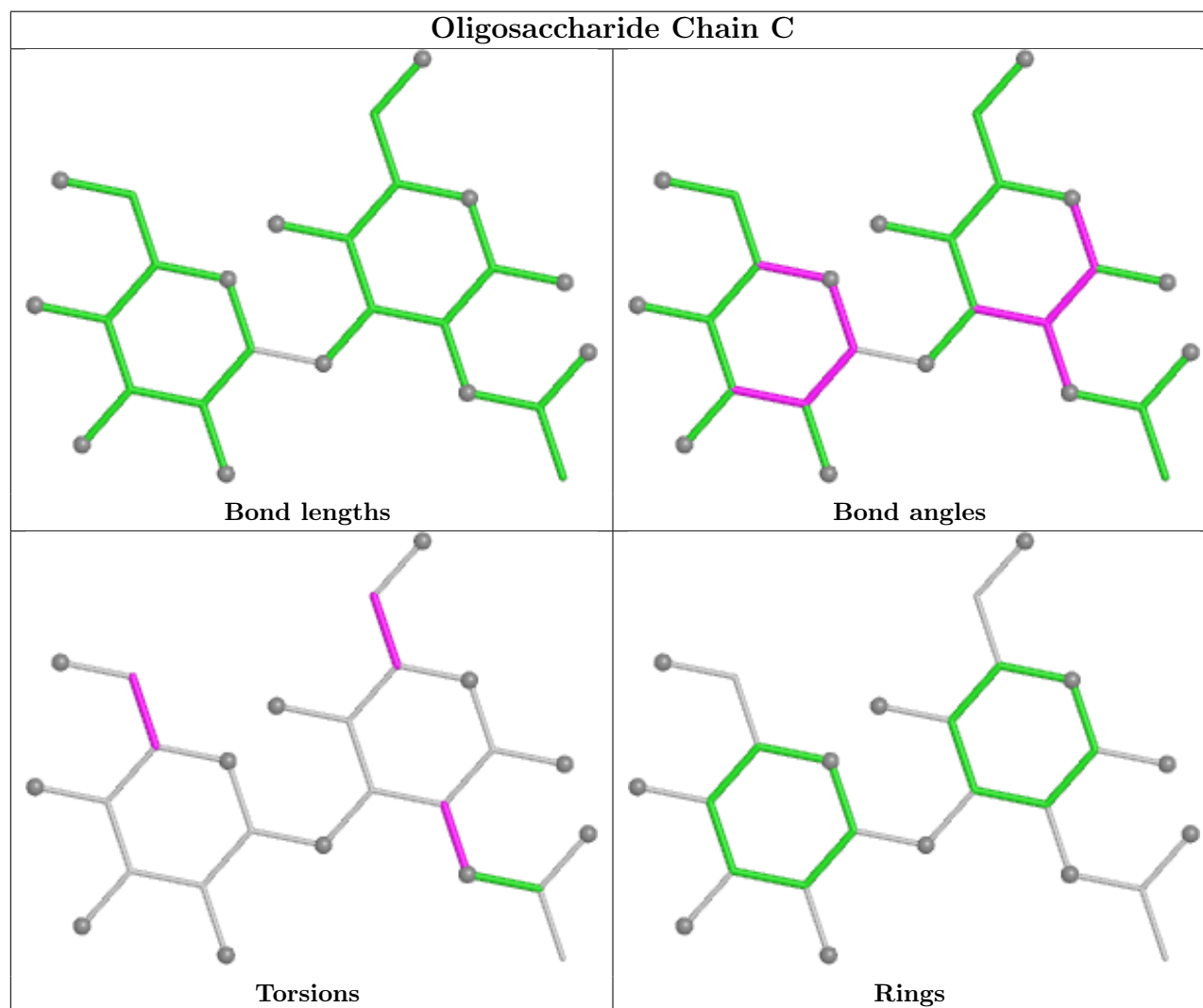
All (9) torsion outliers are listed below:

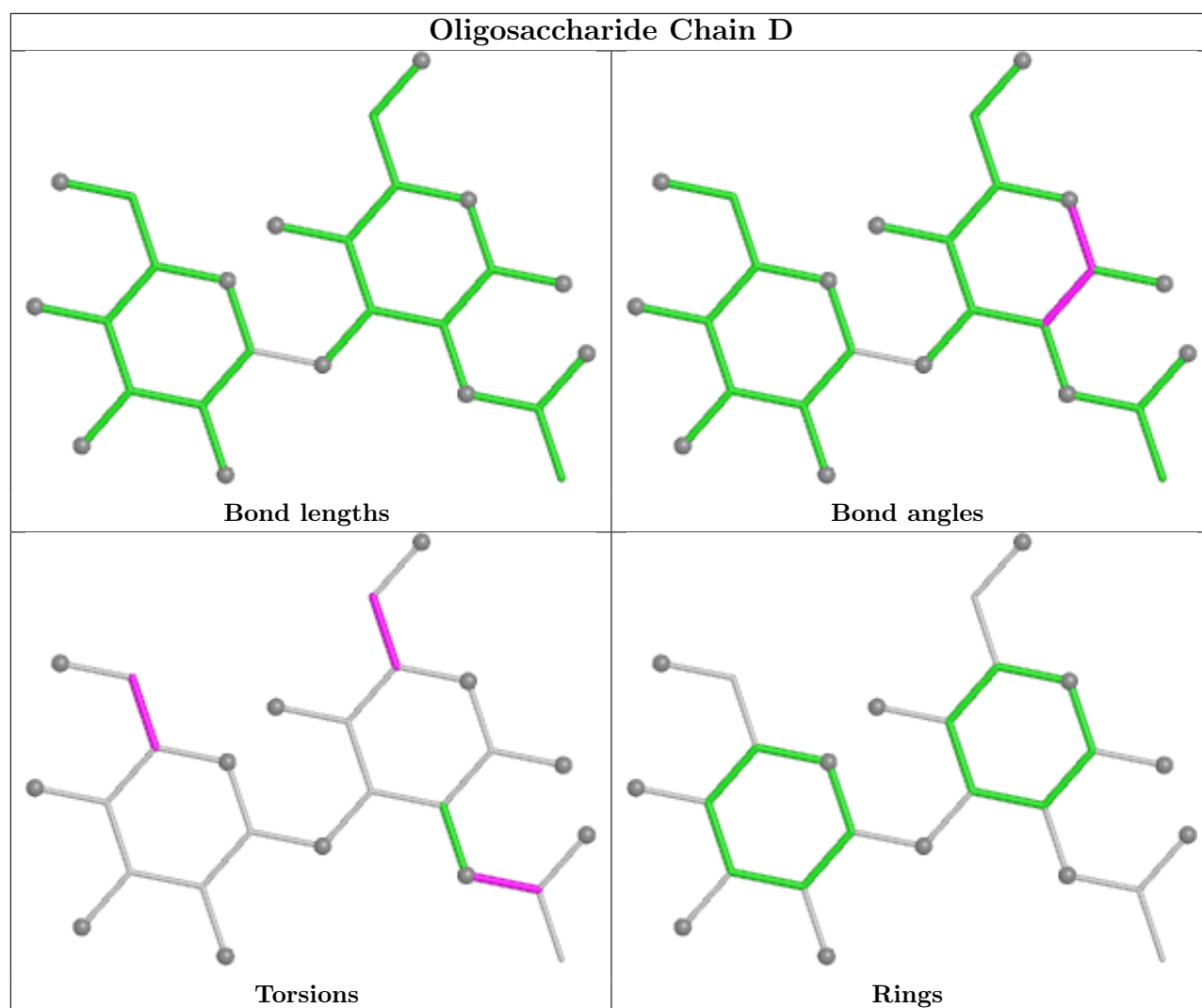
Mol	Chain	Res	Type	Atoms
2	D	1	NDG	O5-C5-C6-O6
2	D	1	NDG	C4-C5-C6-O6
2	D	1	NDG	C8-C7-N2-C2
2	C	1	NDG	O5-C5-C6-O6
2	D	2	GAL	O5-C5-C6-O6
2	C	1	NDG	C4-C5-C6-O6
2	D	1	NDG	O7-C7-N2-C2
2	C	2	GAL	O5-C5-C6-O6
2	C	1	NDG	C1-C2-N2-C7

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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	582/589 (98%)	0.36	26 (4%) 38 34	28, 51, 78, 127	0
1	B	589/589 (100%)	0.30	14 (2%) 59 56	23, 52, 83, 116	0
All	All	1171/1178 (99%)	0.33	40 (3%) 48 44	23, 51, 80, 127	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	627	ALA	3.9
1	A	66	ASN	3.6
1	A	63	THR	3.6
1	B	61	ALA	3.5
1	A	121	ASP	3.5
1	A	67	ALA	3.4
1	B	443	TRP	3.2
1	B	629	LEU	3.2
1	B	598	VAL	3.1
1	A	62	GLY	2.9
1	A	64	SER	2.9
1	B	59	ALA	2.9
1	B	601	LEU	2.7
1	A	606	VAL	2.7
1	A	598	VAL	2.6
1	A	550	VAL	2.6
1	A	120	GLY	2.5
1	A	55	HIS	2.5
1	A	68	PRO	2.5
1	A	617	GLY	2.5
1	B	55	HIS	2.5
1	B	597	VAL	2.4
1	B	615	VAL	2.4
1	B	542	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	578	ALA	2.4
1	A	611	LEU	2.4
1	B	627	ALA	2.4
1	A	122	ALA	2.4
1	A	69	TRP	2.3
1	B	619	PRO	2.3
1	B	120	GLY	2.2
1	A	597	VAL	2.2
1	A	608	ASN	2.2
1	A	622	GLY	2.2
1	A	123	ASP	2.2
1	A	59	ALA	2.1
1	A	552	ALA	2.1
1	A	54	ALA	2.1
1	A	78	ILE	2.1
1	A	624	VAL	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](#)

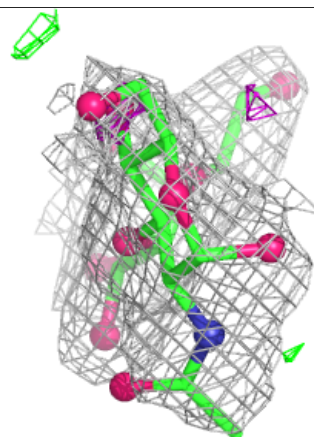
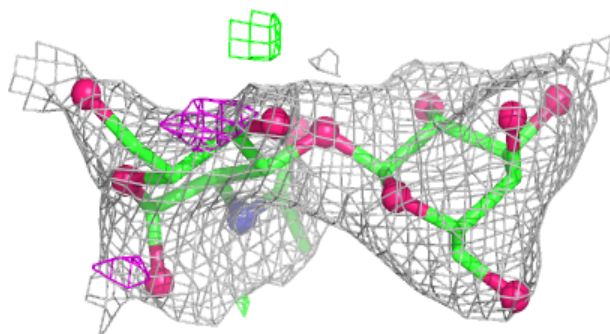
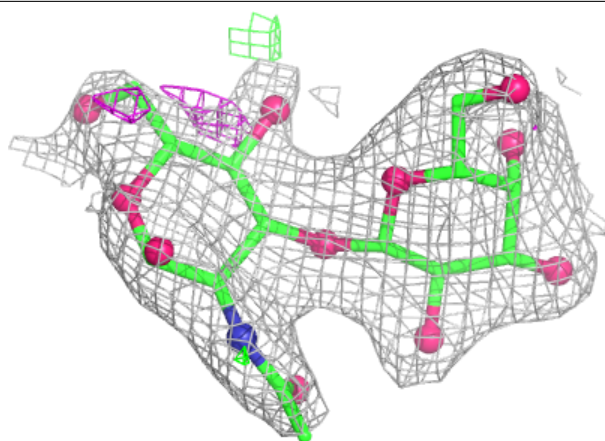
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

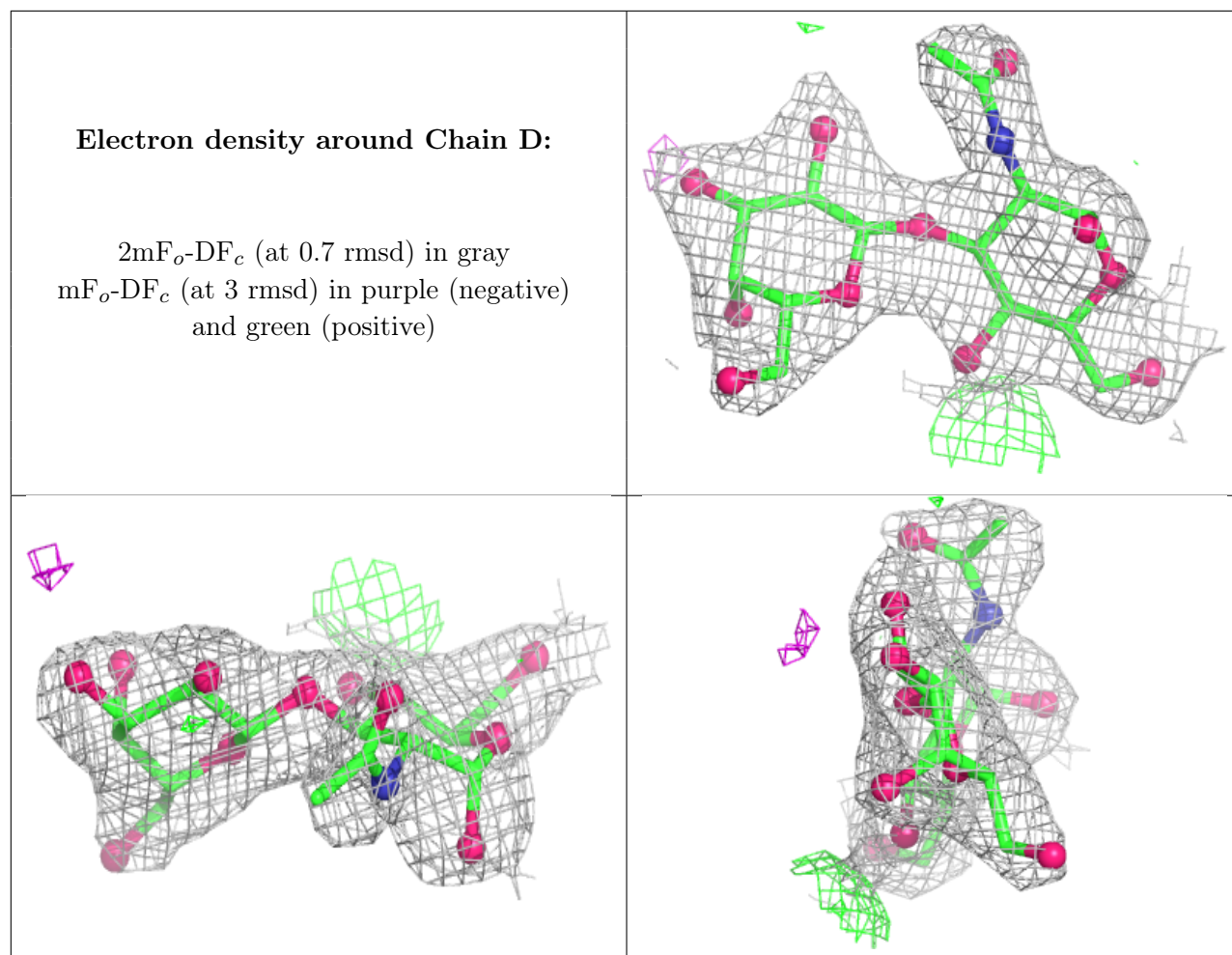
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NDG	C	1	15/15	0.90	0.12	34,46,69,73	0
2	NDG	D	1	15/15	0.92	0.09	51,58,68,75	0
2	GAL	C	2	11/12	0.93	0.09	34,41,44,47	0
2	GAL	D	2	11/12	0.95	0.08	44,49,56,57	0

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 [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	A	701	1/1	0.97	0.05	73,73,73,73	0
3	CA	A	702	1/1	0.98	0.04	57,57,57,57	0
3	CA	B	701	1/1	0.98	0.03	64,64,64,64	0
3	CA	B	702	1/1	0.98	0.04	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.