



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:50 PM UTC

PDB ID : 3S94 / pdb_00003s94
Title : Crystal structure of LRP6-E1E2
Authors : Cheng, Z.; Xu, W.
Deposited on : 2011-05-31
Resolution : 2.80 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

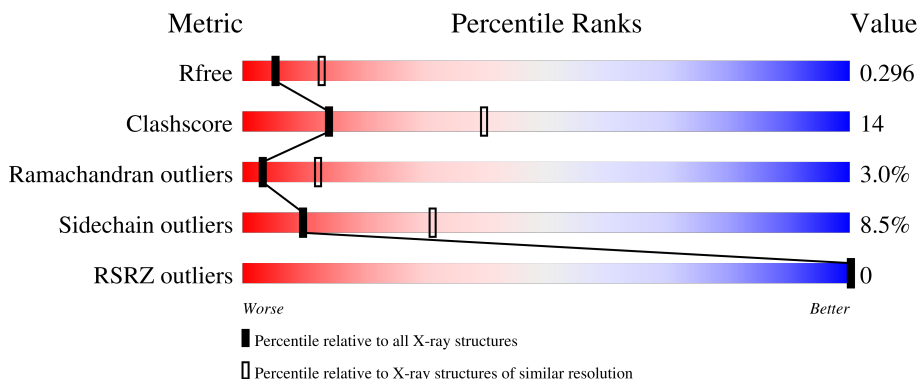
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

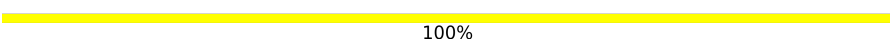
The reported resolution of this entry is 2.80 Å.

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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	619	 62% 29% 5% 5%
1	B	619	 60% 29% 5% 6%
2	C	2	 100%
2	D	2	 50% 50%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9406 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 Low-density lipoprotein receptor-related protein 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	587	Total	C	N	O	S	0	0	0
			4684	2973	799	888	24			
1	B	583	Total	C	N	O	S	0	0	0
			4652	2949	796	883	24			

There are 16 discrepancies between the modelled and reference sequences:

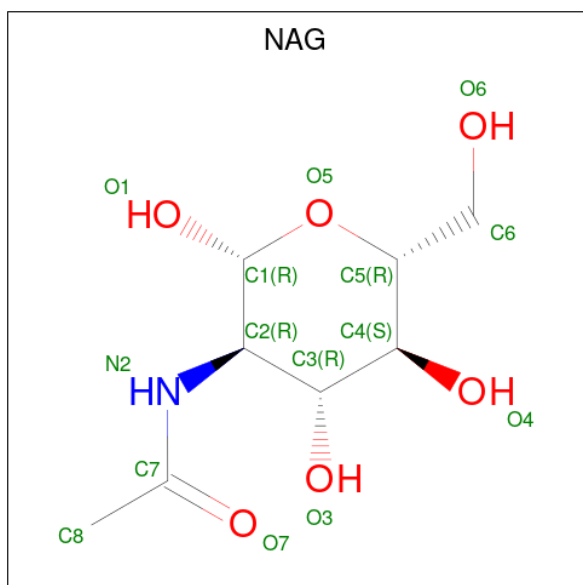
Chain	Residue	Modelled	Actual	Comment	Reference
A	12	HIS	-	expression tag	UNP O75581
A	13	HIS	-	expression tag	UNP O75581
A	14	HIS	-	expression tag	UNP O75581
A	15	HIS	-	expression tag	UNP O75581
A	16	HIS	-	expression tag	UNP O75581
A	17	HIS	-	expression tag	UNP O75581
A	18	HIS	-	expression tag	UNP O75581
A	19	HIS	-	expression tag	UNP O75581
B	12	HIS	-	expression tag	UNP O75581
B	13	HIS	-	expression tag	UNP O75581
B	14	HIS	-	expression tag	UNP O75581
B	15	HIS	-	expression tag	UNP O75581
B	16	HIS	-	expression tag	UNP O75581
B	17	HIS	-	expression tag	UNP O75581
B	18	HIS	-	expression tag	UNP O75581
B	19	HIS	-	expression tag	UNP O75581

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

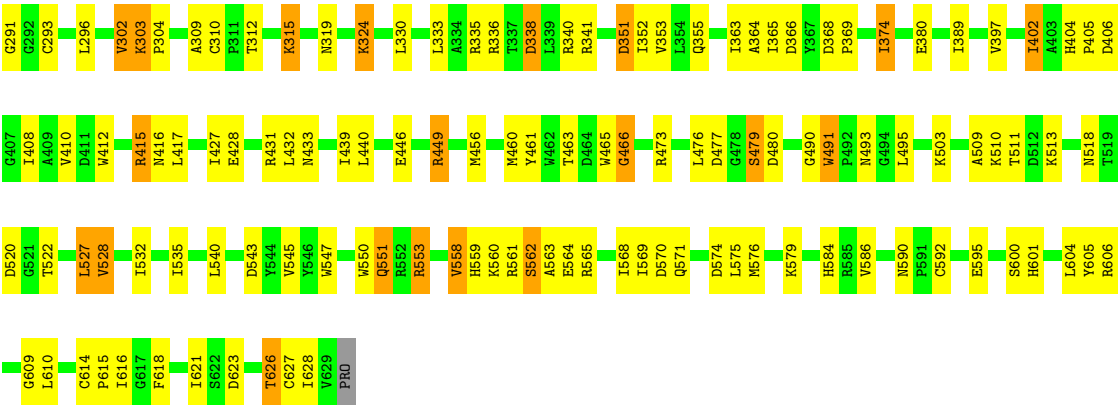


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.54Å 144.51Å 70.76Å 90.00° 96.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-2.80) 99.1 (30.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.62Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.237 , 0.296 0.237 , 0.296	Depositor DCC
R_{free} test set	2179 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 22.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.287 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9406	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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

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	0.68	0/4795	0.86	4/6519 (0.1%)
1	B	0.68	1/4758 (0.0%)	0.84	1/6466 (0.0%)
All	All	0.68	1/9553 (0.0%)	0.85	5/12985 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	404	HIS	CG-CD2	5.77	1.42	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	532	ILE	N-CA-C	5.43	116.28	107.71
1	B	219	VAL	N-CA-C	-5.25	105.28	111.00
1	A	146	ASP	CA-C-N	5.05	124.22	118.97
1	A	146	ASP	C-N-CA	5.05	124.22	118.97
1	A	470	LYS	N-CA-C	5.04	116.50	108.79

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4684	0	4536	130	0
1	B	4652	0	4506	131	0
2	C	28	0	25	0	0
2	D	28	0	25	1	0
3	A	14	0	13	0	0
All	All	9406	0	9105	262	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 (262) 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:555:ILE:HD12	1:A:569:ILE:HD12	1.37	1.07
1:B:303:LYS:HB3	1:B:304:PRO:HD3	1.48	0.95
1:B:553:ARG:HG3	1:B:553:ARG:HH11	1.30	0.95
1:B:302:VAL:HG13	1:B:303:LYS:H	1.31	0.94
1:A:303:LYS:CB	1:A:304:PRO:HD2	1.99	0.92
1:A:210:ASN:O	1:A:211:LEU:HD13	1.72	0.91
1:B:364:ALA:HB2	1:B:406:ASP:O	1.72	0.90
1:B:231:THR:HG21	1:B:273:ALA:H	1.36	0.89
1:A:303:LYS:HB3	1:A:304:PRO:CD	2.05	0.87
1:A:621:ILE:HG12	1:A:622:SER:H	1.39	0.85
1:A:303:LYS:CB	1:A:304:PRO:CD	2.55	0.85
1:B:162:LYS:HD2	1:B:175:ILE:HD12	1.56	0.84
1:B:188:THR:HG21	1:B:231:THR:HA	1.58	0.84
1:A:303:LYS:HB2	1:A:304:PRO:HD2	1.60	0.82
1:A:568:ILE:HG22	1:A:569:ILE:HG13	1.62	0.82
1:B:333:LEU:HD11	1:B:575:LEU:HD22	1.61	0.81
1:A:601:HIS:HD2	1:A:627:CYS:HB2	1.46	0.79
1:A:555:ILE:HD12	1:A:569:ILE:CD1	2.13	0.79
1:A:28:ARG:HG2	1:A:52:ASP:HA	1.66	0.77
1:B:553:ARG:HH11	1:B:553:ARG:CG	1.97	0.76
1:A:379:ASP:OD1	1:A:404:HIS:HD2	1.69	0.76
1:A:310:CYS:HB3	1:A:314:VAL:CG2	2.17	0.74
1:A:333:LEU:HD23	1:A:340:ARG:HB2	1.69	0.74
1:B:550:TRP:O	1:B:551:GLN:HB2	1.86	0.74
1:A:518:ASN:HB2	1:A:521:GLY:O	1.88	0.73
1:B:417:LEU:HB2	1:B:432:LEU:HD23	1.73	0.71
1:B:237:LEU:HD23	1:B:252:LYS:HA	1.73	0.71
1:B:364:ALA:CB	1:B:406:ASP:O	2.39	0.70
1:B:601:HIS:CD2	1:B:627:CYS:HB2	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:ALA:HB3	1:B:271:ILE:HG22	1.72	0.69
1:A:145:LEU:HB3	1:A:168:MET:CE	2.22	0.69
1:B:330:LEU:HD22	1:B:341:ARG:HG3	1.76	0.67
1:B:231:THR:HG21	1:B:273:ALA:N	2.09	0.67
1:B:249:ALA:HB2	1:B:261:ILE:HD11	1.76	0.66
1:A:303:LYS:HB3	1:A:304:PRO:HD2	1.66	0.66
1:B:547:TRP:CH2	1:B:558:VAL:HG11	2.30	0.66
1:A:386:ARG:HD3	1:A:397:VAL:HG22	1.78	0.66
1:A:342:ILE:HD11	1:A:351:ASP:HB3	1.78	0.65
1:B:232:LEU:HD23	1:B:237:LEU:HB3	1.79	0.65
1:A:145:LEU:HB3	1:A:168:MET:HE2	1.78	0.64
1:B:412:TRP:CZ2	1:B:456:MET:HE1	2.32	0.64
1:B:181:ILE:HD11	1:B:184:PRO:HB3	1.80	0.64
1:B:365:ILE:HD11	1:B:374:ILE:HD11	1.80	0.64
1:A:601:HIS:CD2	1:A:627:CYS:HB2	2.31	0.63
1:B:590:ASN:OD1	1:B:592:CYS:HB2	1.98	0.63
1:B:27:ASN:O	1:B:28:ARG:HB2	1.97	0.63
1:A:495:LEU:HD22	1:A:504:ILE:HD11	1.80	0.62
1:B:302:VAL:HG13	1:B:303:LYS:N	2.10	0.62
1:A:463:THR:HB	1:A:492:PRO:HB2	1.82	0.62
1:B:303:LYS:CB	1:B:304:PRO:HD3	2.28	0.61
1:B:568:ILE:HG13	1:B:569:ILE:H	1.66	0.61
1:B:101:ALA:HB2	1:B:143:ILE:HG23	1.83	0.61
1:A:494:GLY:O	1:A:506:TRP:HA	1.99	0.60
1:A:621:ILE:HG12	1:A:622:SER:N	2.14	0.60
1:B:415:ARG:HB3	1:B:431:ARG:HH21	1.67	0.60
1:A:231:THR:HG22	1:A:232:LEU:H	1.66	0.60
1:B:251:ASN:HB3	1:B:255:GLY:H	1.67	0.60
1:A:614:CYS:HB3	1:A:618:PHE:HB3	1.83	0.59
1:A:208:LYS:HZ2	1:A:215:ASN:HD22	1.51	0.59
1:B:219:VAL:O	1:B:220:VAL:HB	2.02	0.59
1:B:550:TRP:O	1:B:551:GLN:CB	2.51	0.58
1:B:235:ASP:HA	1:B:252:LYS:CE	2.34	0.58
1:B:229:ALA:CB	1:B:271:ILE:HG22	2.34	0.57
1:A:310:CYS:HB3	1:A:314:VAL:HG22	1.87	0.57
1:B:558:VAL:HA	1:B:564:GLU:O	2.04	0.57
1:A:132:LEU:CD1	1:A:152:MET:HE1	2.34	0.57
1:B:315:LYS:HB3	1:B:324:LYS:HE2	1.87	0.57
1:B:52:ASP:HB3	1:B:70:VAL:HG23	1.87	0.57
1:B:167:GLY:C	1:B:169:ASP:H	2.14	0.56
1:B:333:LEU:HD23	1:B:340:ARG:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ASN:HD22	1:A:254:THR:H	1.52	0.56
1:B:427:ILE:HG21	1:B:460:MET:HE1	1.87	0.55
1:A:233:PHE:CD2	1:A:234:GLU:HG2	2.41	0.55
1:A:199:ALA:HB2	1:A:230:LEU:HD23	1.88	0.55
1:A:89:VAL:HG12	1:A:90:VAL:HG23	1.89	0.55
1:A:95:LEU:HB3	1:A:115:GLU:HG2	1.89	0.54
1:B:553:ARG:HG3	1:B:553:ARG:NH1	2.11	0.54
1:B:275:SER:O	1:B:278:ARG:HB3	2.07	0.54
1:A:447:GLU:HB2	1:A:465:TRP:HB2	1.90	0.54
1:B:397:VAL:HG13	1:B:433:ASN:O	2.07	0.54
1:B:476:LEU:HD12	1:B:605:TYR:HB3	1.88	0.54
1:B:78:THR:HG22	1:B:86:VAL:HG22	1.89	0.54
1:A:416:ASN:HA	1:A:431:ARG:HA	1.90	0.54
1:A:302:VAL:HG22	1:A:303:LYS:H	1.73	0.53
1:B:152:MET:HG2	1:B:166:ALA:O	2.09	0.53
1:A:379:ASP:OD1	1:A:404:HIS:CD2	2.56	0.53
1:B:198:TRP:HZ3	1:B:209:SER:HB2	1.71	0.53
1:B:335:ARG:HB2	1:B:338:ASP:HB3	1.91	0.53
1:B:198:TRP:CZ3	1:B:209:SER:HB2	2.44	0.53
1:A:545:VAL:O	1:A:557:ARG:HA	2.08	0.53
1:A:556:GLU:HG2	1:A:567:VAL:HG22	1.89	0.53
1:A:377:THR:HG22	1:A:384:ILE:HG12	1.91	0.53
1:A:557:ARG:HD3	1:A:568:ILE:HD11	1.91	0.53
1:B:402:ILE:HD11	1:B:405:PRO:HG3	1.90	0.53
1:B:235:ASP:HA	1:B:252:LYS:HE3	1.90	0.53
1:B:621:ILE:HG13	1:B:623:ASP:OD1	2.09	0.52
1:A:303:LYS:HB3	1:A:304:PRO:HD3	1.90	0.52
1:B:559:HIS:CE1	1:B:561:ARG:HB3	2.45	0.52
1:A:145:LEU:HB3	1:A:168:MET:HE1	1.91	0.52
1:A:333:LEU:HD11	1:A:575:LEU:HD22	1.92	0.52
1:B:57:ASP:OD2	1:B:101:ALA:HA	2.09	0.52
1:B:490:GLY:HA3	1:B:510:LYS:HB3	1.92	0.52
1:B:503:LYS:NZ	1:B:518:ASN:OD1	2.34	0.52
1:A:382:ARG:HD2	1:A:402:ILE:O	2.10	0.52
1:B:449:ARG:NE	1:B:491:TRP:CH2	2.77	0.52
1:B:181:ILE:HG13	1:B:184:PRO:HD3	1.92	0.51
1:A:302:VAL:HG13	1:A:303:LYS:HG3	1.92	0.51
1:A:375:TYR:OH	1:A:432:LEU:HB3	2.09	0.51
1:A:491:TRP:HB2	1:A:509:ALA:HB3	1.93	0.51
1:A:568:ILE:HG22	1:A:569:ILE:CG1	2.37	0.51
1:A:229:ALA:CB	1:A:271:ILE:HG22	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LEU:HD13	1:A:152:MET:HE1	1.92	0.51
1:A:511:THR:HB	1:A:513:LYS:HE2	1.93	0.51
1:B:70:VAL:HG12	1:B:96:SER:HA	1.93	0.50
1:B:446:GLU:HB3	1:B:466:GLY:HA2	1.93	0.50
1:A:152:MET:HE2	1:A:168:MET:HA	1.93	0.50
1:A:183:TRP:HB2	1:A:202:LYS:HB2	1.93	0.50
1:B:351:ASP:OD1	1:B:351:ASP:N	2.44	0.50
1:B:527:LEU:HG	1:B:528:VAL:HG23	1.93	0.50
1:B:553:ARG:CG	1:B:553:ARG:NH1	2.63	0.50
1:B:302:VAL:CG1	1:B:303:LYS:H	2.15	0.50
1:B:92:SER:HB2	1:B:353:VAL:HB	1.92	0.50
1:A:614:CYS:HB3	1:A:618:PHE:CB	2.42	0.50
1:B:615:PRO:O	1:B:618:PHE:HB2	2.11	0.50
1:B:100:LEU:HD22	1:B:109:LEU:HD11	1.92	0.50
1:A:459:TYR:CD1	1:A:473:ARG:HD2	2.47	0.49
1:B:545:VAL:CG1	1:B:558:VAL:HG13	2.43	0.49
1:B:427:ILE:O	1:B:440:LEU:HB3	2.12	0.49
1:B:477:ASP:OD1	1:B:479:SER:HB2	2.13	0.49
1:A:69:ASP:HB3	1:A:72:GLU:HB2	1.95	0.49
1:A:121:VAL:HG22	1:A:122:SER:N	2.28	0.49
1:A:310:CYS:HB3	1:A:314:VAL:HG23	1.93	0.48
1:B:570:ASP:OD1	1:B:571:GLN:N	2.46	0.48
1:B:477:ASP:HA	1:B:604:LEU:HD13	1.95	0.48
1:A:131:VAL:O	1:A:131:VAL:HG13	2.12	0.48
1:A:152:MET:HE3	1:A:167:GLY:O	2.13	0.48
1:A:498:ASP:HB3	1:A:503:LYS:HB2	1.95	0.48
1:A:511:THR:O	1:A:513:LYS:HG3	2.13	0.48
1:A:547:TRP:HZ3	1:A:558:VAL:HB	1.78	0.48
1:A:446:GLU:CG	1:A:466:GLY:HA3	2.43	0.48
1:B:241:ASP:HB2	1:B:244:THR:OG1	2.13	0.48
1:B:415:ARG:HB3	1:B:431:ARG:NH2	2.27	0.48
1:B:251:ASN:HD22	1:B:254:THR:H	1.60	0.48
1:A:66:TYR:OH	1:A:77:ARG:NH1	2.48	0.47
1:A:515:GLU:HG2	1:A:526:VAL:HG22	1.95	0.47
1:A:208:LYS:NZ	1:A:215:ASN:HD22	2.11	0.47
1:B:89:VAL:HG12	1:B:90:VAL:HG23	1.96	0.47
1:B:198:TRP:HZ3	1:B:209:SER:CB	2.27	0.47
1:B:296:LEU:HB2	1:B:309:ALA:HB3	1.95	0.47
1:A:29:ARG:HA	1:A:50:LEU:O	2.15	0.47
1:B:330:LEU:CD2	1:B:341:ARG:HG3	2.41	0.47
1:B:363:ILE:HG21	1:B:406:ASP:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1:NAG:O3	2:D:2:NAG:C1	2.63	0.47
1:A:111:TRP:HZ3	1:A:122:SER:HB3	1.80	0.47
1:A:231:THR:HG21	1:A:273:ALA:N	2.30	0.47
1:A:237:LEU:HD23	1:A:252:LYS:HA	1.97	0.47
1:B:51:GLU:O	1:B:52:ASP:HB2	2.14	0.47
1:B:606:ARG:HB2	1:B:609:GLY:O	2.15	0.46
1:B:57:ASP:OD1	1:B:58:PHE:N	2.38	0.46
1:A:55:ALA:HB2	1:A:98:ASP:O	2.16	0.46
1:A:509:ALA:HA	1:A:532:ILE:HB	1.97	0.45
1:A:400:ALA:O	1:A:402:ILE:N	2.49	0.45
1:B:75:ILE:O	1:B:89:VAL:O	2.33	0.45
1:B:184:PRO:HA	1:B:199:ALA:O	2.16	0.45
1:B:289:ASP:C	1:B:291:GLY:H	2.25	0.45
1:A:456:MET:SD	1:A:456:MET:N	2.81	0.45
1:B:237:LEU:CD2	1:B:252:LYS:HA	2.43	0.45
1:A:156:ASP:HB2	1:A:162:LYS:HG2	1.98	0.45
1:A:233:PHE:HE1	1:A:275:SER:CB	2.30	0.45
1:B:290:ASN:HB3	1:B:293:CYS:HB2	1.98	0.45
1:A:555:ILE:CD1	1:A:569:ILE:HD12	2.26	0.45
1:B:415:ARG:HA	1:B:415:ARG:HD2	1.69	0.45
1:A:153:TYR:CD1	1:A:165:ARG:HB3	2.52	0.45
1:B:130:LYS:HG3	1:B:310:CYS:O	2.17	0.45
1:B:428:GLU:OE2	1:B:439:ILE:HG12	2.17	0.45
1:A:459:TYR:CG	1:A:473:ARG:HD2	2.51	0.45
1:B:439:ILE:H	1:B:616:ILE:HD11	1.81	0.45
1:B:543:ASP:HA	1:B:560:LYS:HD3	1.98	0.45
1:B:416:ASN:HD22	1:B:431:ARG:HA	1.81	0.45
1:A:91:VAL:C	1:A:93:GLY:H	2.25	0.44
1:A:200:ASP:C	1:A:202:LYS:H	2.25	0.44
1:A:207:HIS:NE2	1:A:216:ARG:HG3	2.32	0.44
1:A:302:VAL:HG22	1:A:303:LYS:N	2.32	0.44
1:B:235:ASP:HA	1:B:252:LYS:HE2	1.98	0.44
1:B:476:LEU:HB2	1:B:605:TYR:O	2.17	0.44
1:A:164:GLU:HB3	1:A:175:ILE:HA	1.97	0.44
1:A:231:THR:HG21	1:A:273:ALA:H	1.82	0.44
1:B:105:LEU:HB3	1:B:147:PRO:HB3	1.98	0.44
1:B:114:SER:HA	1:B:140:PRO:HD2	1.98	0.44
1:B:623:ASP:OD2	1:B:626:THR:HG23	2.18	0.44
1:A:241:ASP:HB2	1:A:248:LEU:HD12	2.00	0.44
1:B:138:ASP:CG	1:B:158:GLY:HA3	2.43	0.44
1:A:241:ASP:HB3	1:A:244:THR:OG1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:PHE:CD2	1:B:276:GLN:HB2	2.53	0.44
1:A:251:ASN:ND2	1:A:254:THR:H	2.13	0.44
1:A:465:TRP:CD1	1:A:492:PRO:HD2	2.53	0.44
1:B:509:ALA:HA	1:B:532:ILE:HB	2.00	0.44
1:A:34:VAL:HG12	1:A:35:ASP:H	1.83	0.44
1:A:117:ASN:ND2	1:A:138:ASP:O	2.51	0.44
1:A:183:TRP:N	1:A:184:PRO:HD3	2.33	0.44
1:B:324:LYS:H	1:B:324:LYS:HG2	1.56	0.44
1:A:475:ALA:HB1	1:A:606:ARG:HG2	2.00	0.44
1:A:451:ILE:HD11	1:A:460:MET:HG3	2.00	0.43
1:A:207:HIS:CD2	1:A:216:ARG:HG3	2.53	0.43
1:A:513:LYS:HD2	1:A:526:VAL:HG21	1.99	0.43
1:B:366:ASP:OD1	1:B:579:LYS:HE3	2.18	0.43
1:A:250:CYS:HB2	1:A:255:GLY:O	2.19	0.43
1:B:239:TRP:HZ3	1:B:250:CYS:HG	1.64	0.43
1:A:403:ALA:HB3	1:A:423:GLY:HA3	2.01	0.43
1:B:23:LEU:HD22	1:B:271:ILE:HD11	2.00	0.43
1:A:155:THR:HG23	1:A:187:LEU:HD13	1.99	0.43
1:B:203:LEU:HB3	1:B:205:PHE:CD2	2.54	0.43
1:B:119:ILE:HG21	1:B:152:MET:HE1	2.01	0.43
1:B:520:ASP:HB2	1:B:522:THR:HG22	2.00	0.43
1:A:91:VAL:O	1:A:93:GLY:N	2.52	0.43
1:B:336:ARG:NH1	1:B:574:ASP:OD1	2.52	0.43
1:A:247:ILE:HG13	1:A:265:ILE:HG12	2.00	0.42
1:A:461:TYR:CE1	1:A:473:ARG:HD3	2.54	0.42
1:B:576:MET:HE3	1:B:576:MET:HB3	1.89	0.42
1:A:146:ASP:H	1:A:168:MET:CE	2.32	0.42
1:A:266:PHE:O	1:A:268:PRO:HD3	2.19	0.42
1:A:376:TRP:CE2	1:A:385:ARG:HB2	2.55	0.42
1:B:600:SER:OG	1:B:601:HIS:HD2	2.01	0.42
1:B:545:VAL:HG13	1:B:558:VAL:HG13	2.00	0.42
1:A:411:ASP:OD1	1:A:411:ASP:C	2.63	0.42
1:A:496:ALA:HB1	1:A:540:LEU:HB3	2.00	0.42
1:B:239:TRP:HZ3	1:B:250:CYS:SG	2.42	0.42
1:A:57:ASP:OD2	1:A:58:PHE:N	2.40	0.42
1:A:621:ILE:CG1	1:A:622:SER:H	2.21	0.42
1:B:95:LEU:HB2	1:B:115:GLU:HB3	2.01	0.42
1:A:440:LEU:HD23	1:A:441:ILE:HG13	2.02	0.42
1:B:207:HIS:CD2	1:B:218:ALA:HA	2.55	0.42
1:A:445:LEU:HB2	1:A:481:ARG:NH2	2.36	0.41
1:A:544:TYR:CD1	1:A:557:ARG:HD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:559:HIS:HB3	1:B:562:SER:HB2	2.01	0.41
1:B:610:LEU:H	1:B:610:LEU:HD23	1.85	0.41
1:B:249:ALA:CB	1:B:261:ILE:HD11	2.47	0.41
1:A:65:ILE:O	1:A:77:ARG:HA	2.21	0.41
1:A:210:ASN:OD1	1:A:210:ASN:N	2.52	0.41
1:A:400:ALA:HB3	1:A:437:ARG:HH12	1.85	0.41
1:A:346:THR:HB	1:A:348:ASP:OD1	2.21	0.41
1:A:495:LEU:HA	1:A:505:TYR:O	2.19	0.41
1:A:229:ALA:HB3	1:A:271:ILE:HG22	2.02	0.41
1:A:446:GLU:HG3	1:A:466:GLY:HA3	2.03	0.41
1:B:408:ILE:O	1:B:408:ILE:HG23	2.20	0.41
1:B:463:THR:HG23	1:B:495:LEU:HG	2.01	0.41
1:B:511:THR:HB	1:B:513:LYS:HE2	2.03	0.41
1:A:278:ARG:HA	1:A:278:ARG:HH11	1.86	0.41
1:A:477:ASP:OD1	1:A:479:SER:HB2	2.20	0.41
1:B:185:ASN:OD1	1:B:186:GLY:N	2.52	0.41
1:A:149:SER:HB3	1:A:151:PHE:CD2	2.56	0.40
1:A:285:PRO:CD	1:A:299:MET:HE1	2.51	0.40
1:A:518:ASN:CB	1:A:521:GLY:O	2.65	0.40
1:B:95:LEU:HD12	1:B:116:THR:HG23	2.02	0.40
1:B:528:VAL:HG11	1:B:565:ARG:HD2	2.03	0.40
1:B:614:CYS:HB3	1:B:618:PHE:CB	2.51	0.40
1:A:125:ASP:OD1	1:A:125:ASP:N	2.54	0.40
1:B:368:ASP:HA	1:B:369:PRO:HD2	1.96	0.40
1:B:465:TRP:O	1:B:465:TRP:CG	2.74	0.40
1:B:461:TYR:CD1	1:B:473:ARG:HB2	2.55	0.40
1:A:476:LEU:HB2	1:A:605:TYR:O	2.22	0.40
1:B:231:THR:HG21	1:B:272:HIS:HA	2.04	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	579/619 (94%)	504 (87%)	61 (10%)	14 (2%)	4	17
1	B	573/619 (93%)	499 (87%)	53 (9%)	21 (4%)	2	9
All	All	1152/1238 (93%)	1003 (87%)	114 (10%)	35 (3%)	3	12

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	268	PRO
1	A	303	LYS
1	A	562	SER
1	B	28	ARG
1	B	479	SER
1	B	562	SER
1	B	563	ALA
1	A	28	ARG
1	A	201	ALA
1	A	521	GLY
1	B	290	ASN
1	B	302	VAL
1	B	352	ILE
1	B	480	ASP
1	B	551	GLN
1	A	92	SER
1	A	400	ALA
1	A	401	GLN
1	A	520	ASP
1	B	52	ASP
1	B	338	ASP
1	B	527	LEU
1	A	27	ASN
1	A	211	LEU
1	A	290	ASN
1	B	90	VAL
1	B	168	MET
1	B	210	ASN
1	A	134	TRP
1	B	257	GLY
1	B	586	VAL
1	B	243	SER
1	B	303	LYS
1	B	535	ILE
1	B	466	GLY

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	508/535 (95%)	464 (91%)	44 (9%)	9	30
1	B	504/535 (94%)	462 (92%)	42 (8%)	10	32
All	All	1012/1070 (95%)	926 (92%)	86 (8%)	10	31

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LEU
1	A	24	LEU
1	A	32	ARG
1	A	37	THR
1	A	47	VAL
1	A	50	LEU
1	A	69	ASP
1	A	71	SER
1	A	77	ARG
1	A	86	VAL
1	A	94	LEU
1	A	96	SER
1	A	100	LEU
1	A	135	GLN
1	A	160	VAL
1	A	181	ILE
1	A	210	ASN
1	A	231	THR
1	A	232	LEU
1	A	237	LEU
1	A	242	TRP
1	A	314	VAL
1	A	328	THR
1	A	329	GLU
1	A	337	THR
1	A	339	LEU
1	A	386	ARG

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Mol	Chain	Res	Type
1	A	387	SER
1	A	395	GLN
1	A	425	ASP
1	A	446	GLU
1	A	447	GLU
1	A	451	ILE
1	A	452	VAL
1	A	453	LEU
1	A	456	MET
1	A	479	SER
1	A	527	LEU
1	A	528	VAL
1	A	569	ILE
1	A	574	ASP
1	A	579	LYS
1	A	610	LEU
1	A	621	ILE
1	B	47	VAL
1	B	50	LEU
1	B	76	LYS
1	B	78	THR
1	B	79	GLU
1	B	100	LEU
1	B	128	LEU
1	B	129	ARG
1	B	180	GLU
1	B	188	THR
1	B	189	LEU
1	B	203	LEU
1	B	231	THR
1	B	235	ASP
1	B	236	ILE
1	B	237	LEU
1	B	242	TRP
1	B	243	SER
1	B	258	LEU
1	B	312	THR
1	B	315	LYS
1	B	319	ASN
1	B	324	LYS
1	B	351	ASP
1	B	355	GLN

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Mol	Chain	Res	Type
1	B	374	ILE
1	B	380	GLU
1	B	389	ILE
1	B	402	ILE
1	B	410	VAL
1	B	415	ARG
1	B	449	ARG
1	B	491	TRP
1	B	493	ASN
1	B	528	VAL
1	B	540	LEU
1	B	553	ARG
1	B	558	VAL
1	B	584	HIS
1	B	595	GLU
1	B	626	THR
1	B	628	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	135	GLN
1	A	139	GLN
1	A	215	ASN
1	A	251	ASN
1	A	290	ASN
1	A	319	ASN
1	A	404	HIS
1	A	493	ASN
1	B	117	ASN
1	B	204	ASN
1	B	207	HIS
1	B	215	ASN
1	B	251	ASN
1	B	272	HIS
1	B	276	GLN
1	B	295	HIS
1	B	416	ASN
1	B	493	ASN
1	B	582	ASN
1	B	601	HIS

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	0.69	0	17,19,21	1.55	3 (17%)
2	NAG	C	2	2	14,14,15	0.52	0	17,19,21	1.77	2 (11%)
2	NAG	D	1	1,2	14,14,15	0.66	1 (7%)	17,19,21	1.75	5 (29%)
2	NAG	D	2	2	14,14,15	0.63	0	17,19,21	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	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	NAG	C1-C2	2.13	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C1-O5-C5	6.32	120.65	112.19
2	C	1	NAG	C1-O5-C5	3.58	116.99	112.19
2	D	1	NAG	C3-C4-C5	-3.47	103.95	110.23
2	C	1	NAG	C4-C3-C2	3.19	115.69	111.02
2	D	1	NAG	C1-O5-C5	2.96	116.16	112.19
2	D	1	NAG	O4-C4-C3	2.56	116.41	110.38
2	C	1	NAG	O5-C1-C2	2.54	115.22	111.29
2	D	1	NAG	O5-C5-C6	2.32	112.18	107.66
2	D	1	NAG	C4-C3-C2	-2.26	107.70	111.02
2	C	2	NAG	O5-C1-C2	2.20	114.69	111.29

There are no chirality outliers.

All (3) torsion outliers are listed below:

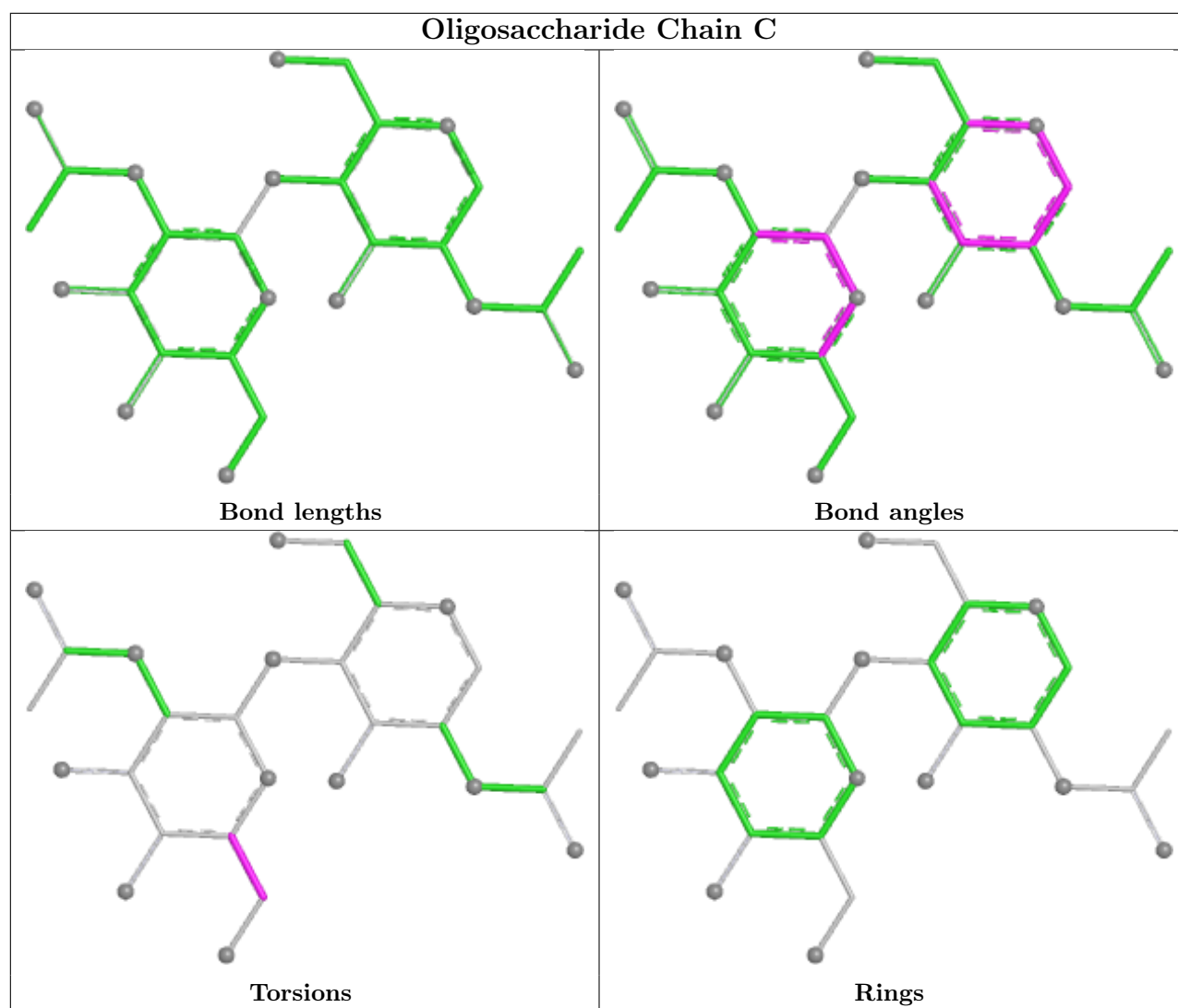
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6

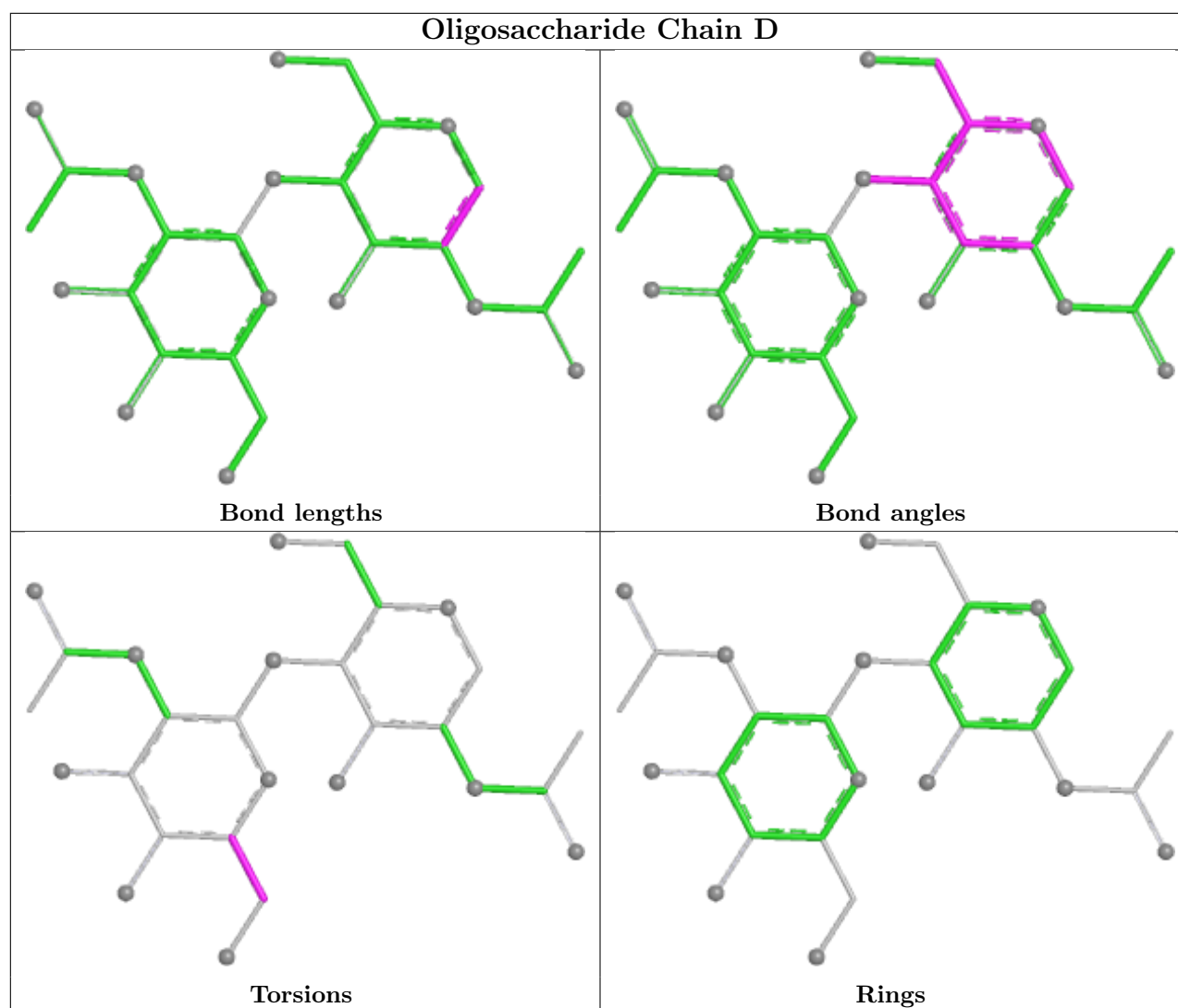
There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	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](#)

1 ligand is 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	635	1	14,14,15	0.57	0	17,19,21	0.91	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	NAG	A	635	1	-	0/6/23/26	0/1/1/1

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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	587/619 (94%)	-0.94	0 100 100	33, 69, 107, 140	0
1	B	583/619 (94%)	-1.01	0 100 100	33, 65, 101, 122	0
All	All	1170/1238 (94%)	-0.97	0 100 100	33, 67, 105, 140	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

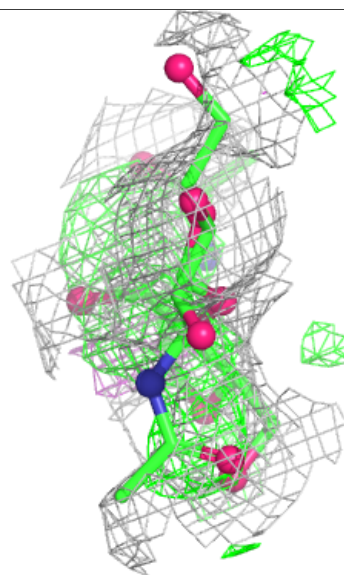
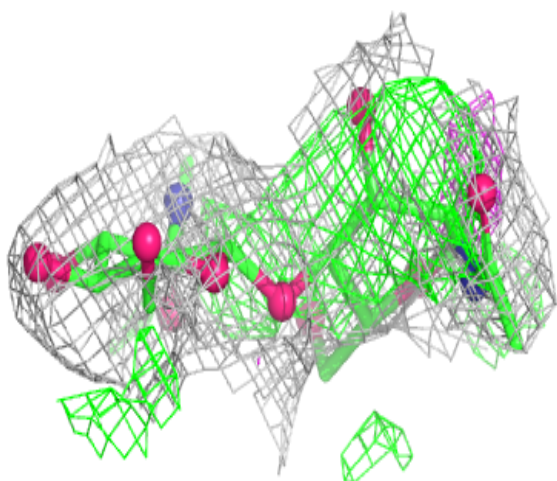
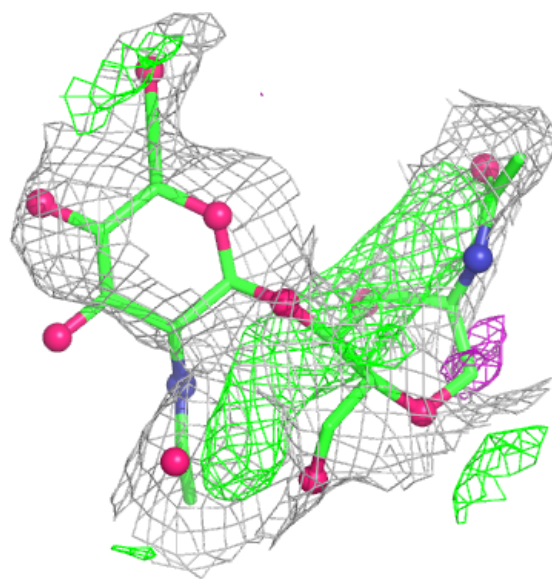
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

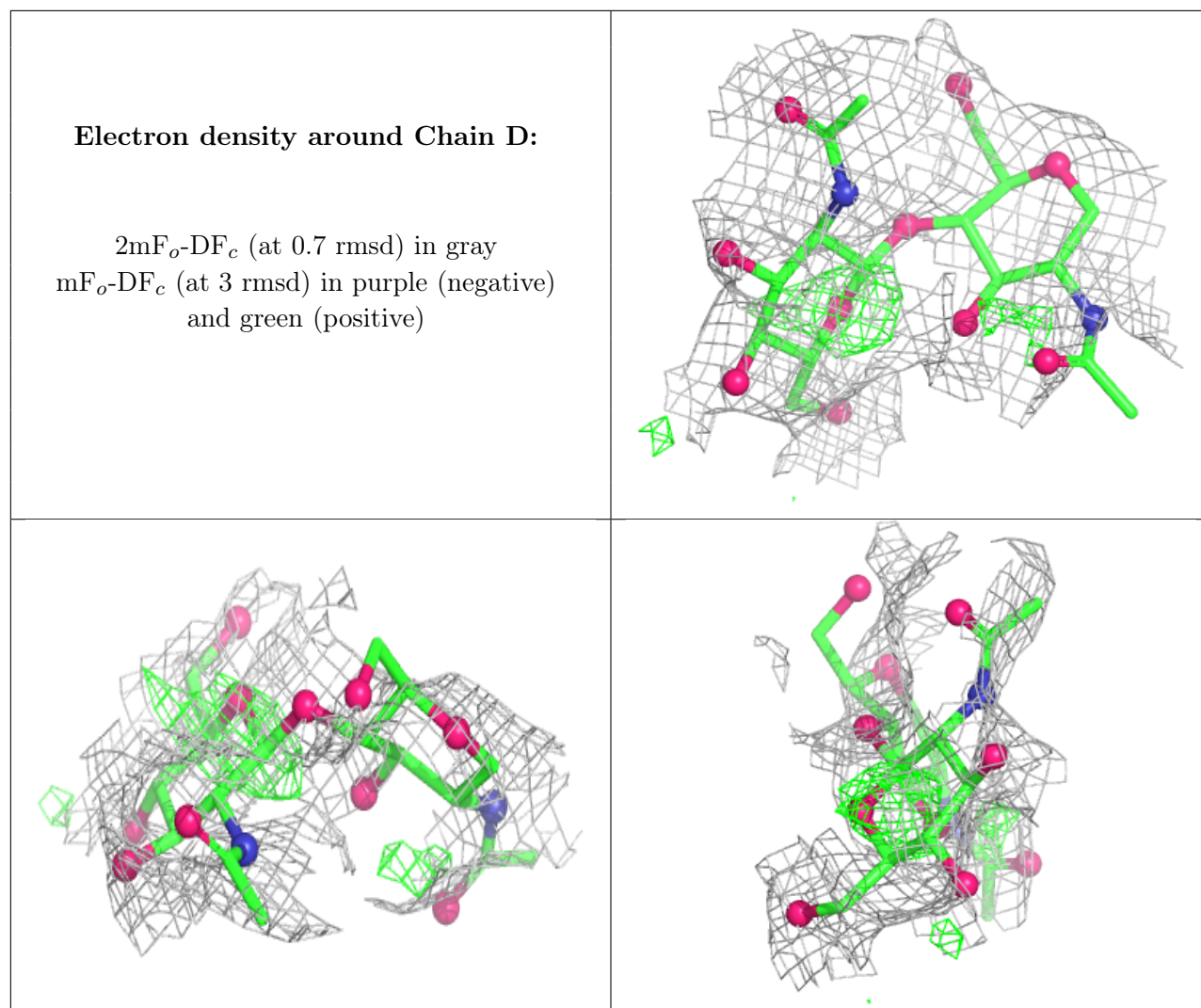
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	D	1	14/15	0.94	0.11	130,130,130,130	0
2	NAG	D	2	14/15	0.94	0.07	130,130,130,130	0
2	NAG	C	1	14/15	0.95	0.15	136,136,136,136	0
2	NAG	C	2	14/15	0.96	0.10	136,136,136,136	0

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(Å ²)	Q<0.9
3	NAG	A	635	14/15	0.93	0.08	130,130,130,130	0

6.5 Other polymers [i](#)

There are no such residues in this entry.