



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:30 PM UTC

PDB ID : 2Z7X / pdb_00002z7x
Title : Crystal structure of the TLR1-TLR2 heterodimer induced by binding of a tri-acylated lipopeptide
Authors : Lee, J.O.; Jin, M.S.; Kim, S.E.; Heo, J.Y.
Deposited on : 2007-08-29
Resolution : 2.10 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

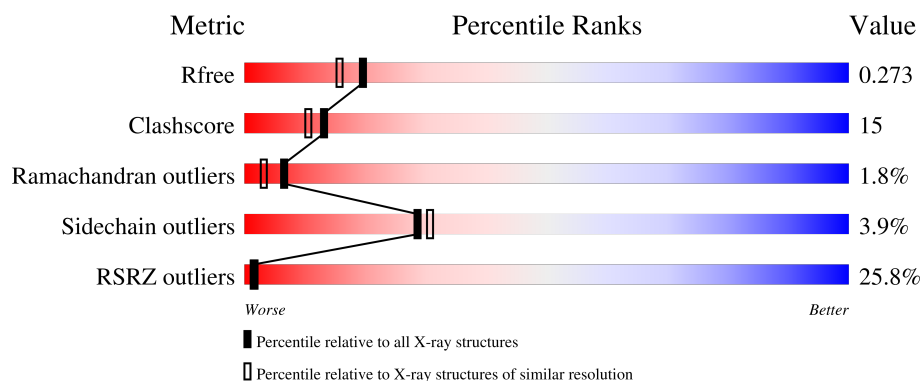
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	549	44% 58% 38% .
2	B	520	7% 74% 24% .
3	C	6	33% 67% 33%
4	D	3	33% 33% 33%
5	E	3	33% 67%

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Mol	Chain	Length	Quality of chain
6	F	3	 100%
7	G	2	 100%

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
8	NAG	A	901	X	-	-	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 9087 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 Toll-like receptor 2,Variable lymphocyte receptor B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	0	0	0
			4366	2766	735	844	21			

- Molecule 2 is a protein called Toll-like receptor 1,Variable lymphocyte receptor B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	520	Total	C	N	O	S	0	0	0
			4172	2671	697	784	20			

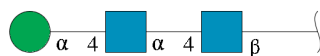
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	477	SER	-	linker	UNP Q15399

- Molecule 3 is a protein called Pam3CSK4.

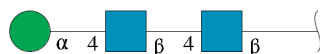
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	6	Total	C	N	O	S	0	0	0
			48	30	10	7	1			

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



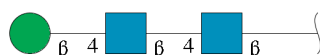
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	3	Total	C	N	O		0	0	0
			39	22	2	15				

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



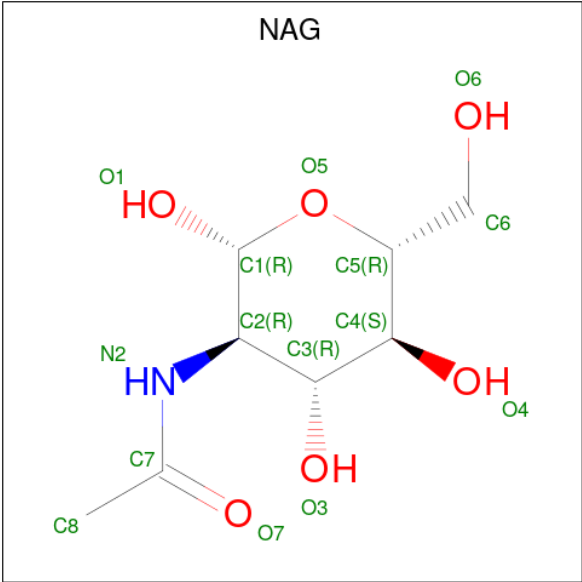
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	F	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



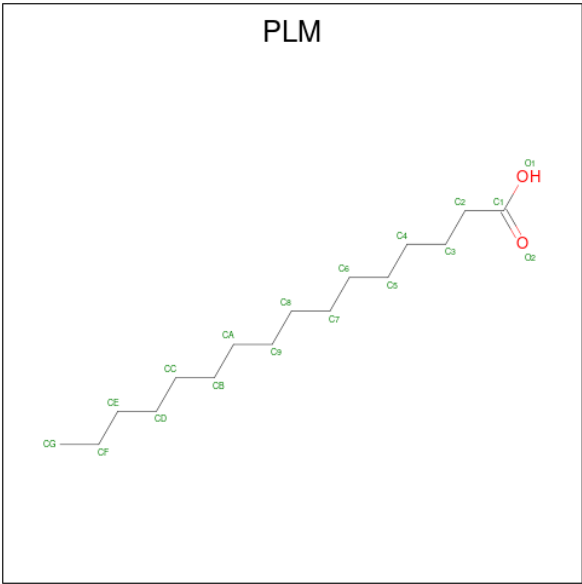
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	2	Total	C	N	O	0	0	0
			25	14	1	10			

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



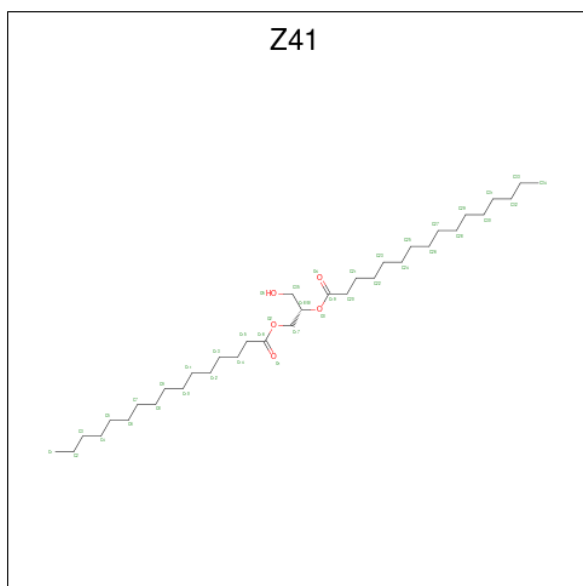
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 9 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			17	16	1		

- Molecule 10 is (2S)-3-hydroxypropane-1,2-diyl dihexadecanoate (CCD ID: Z41) (formula: $C_{35}H_{68}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	C	O	0	0
			39	35	4		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	67	Total	O	0	0
			67	67		
11	B	178	Total	O	0	0
			178	178		
11	C	2	Total	O	0	0
			2	2		

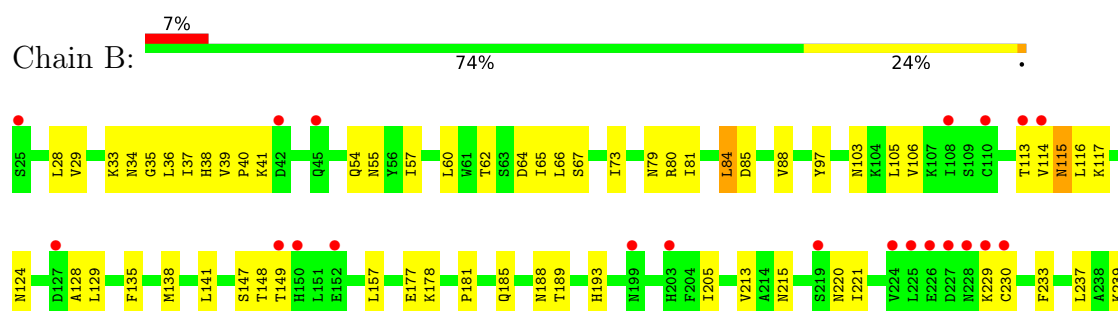
3 Residue-property plots

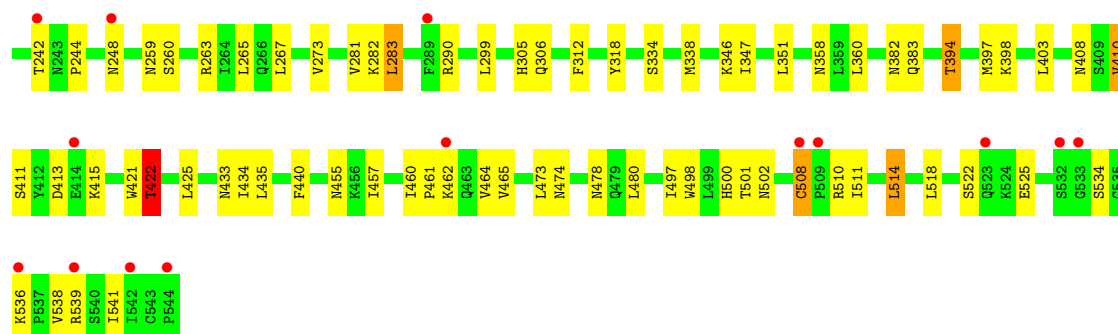
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Toll-like receptor 2, Variable lymphocyte receptor B

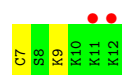


- Molecule 2: Toll-like receptor 1, Variable lymphocyte receptor B





• Molecule 3: Pam3CSK4



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



• Molecule 5: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	200.30Å 120.14Å 74.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.85 – 2.10 45.85 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.5 (45.85-2.10) 94.5 (45.85-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.08Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.244 , 0.270 0.250 , 0.273	Depositor DCC
R_{free} test set	5025 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	29.4	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9087	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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: PLM, NDG, BMA, DCY, Z41, MAN, 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	0.36	0/4442	0.90	14/6014 (0.2%)
2	B	0.44	0/4257	0.91	10/5766 (0.2%)
3	C	0.28	0/41	0.69	0/49
All	All	0.40	0/8740	0.90	24/11829 (0.2%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	351	VAL	N-CA-C	-10.85	97.41	108.15
1	A	425	PHE	N-CA-C	-8.60	95.51	109.96
2	B	508	CYS	N-CA-C	8.45	124.24	113.25
2	B	149	THR	N-CA-C	-8.01	102.99	114.12
1	A	235	ASP	N-CA-C	-7.44	100.00	110.50
2	B	185	GLN	N-CA-C	7.01	120.72	111.75
2	B	213	VAL	N-CA-C	6.57	118.26	108.54
2	B	117	LYS	N-CA-C	-6.53	105.85	113.88
1	A	374	GLU	N-CA-C	6.41	118.81	111.11
1	A	377	LEU	N-CA-C	-6.40	104.39	111.82
1	A	360	LYS	N-CA-C	6.21	120.32	112.87
2	B	410	VAL	N-CA-C	6.18	117.05	108.89
1	A	336	GLU	N-CA-C	6.16	118.79	111.71
2	B	65	ILE	N-CA-C	5.64	118.61	113.20
1	A	424	SER	N-CA-C	5.56	118.19	108.52
1	A	476	LEU	CA-C-N	5.43	125.77	119.47
1	A	476	LEU	C-N-CA	5.43	125.77	119.47
2	B	106	VAL	N-CA-C	-5.24	108.18	113.47
2	B	422	THR	N-CA-C	-5.22	103.14	110.50
1	A	97	SER	N-CA-C	-5.18	106.80	113.23
2	B	398	LYS	N-CA-C	5.15	118.66	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	437	LYS	N-CA-C	5.08	118.35	112.97
1	A	509	ASN	N-CA-C	5.04	121.15	113.19
1	A	520	ASP	N-CA-C	-5.04	107.14	113.28

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	4366	0	4418	160	0
2	B	4172	0	4221	100	0
3	C	48	0	60	1	0
4	D	39	0	33	4	0
5	E	39	0	34	0	0
6	F	39	0	34	0	0
7	G	25	0	22	2	0
8	A	42	0	39	1	0
8	B	14	0	13	0	0
9	C	17	0	31	2	0
10	C	39	0	0	0	0
11	A	67	0	0	3	0
11	B	178	0	0	3	0
11	C	2	0	0	0	0
All	All	9087	0	8905	264	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 15.

All (264) 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:511:LEU:H	1:A:533:ASN:HD22	1.01	0.95
2:B:229:LYS:HD2	2:B:263:ARG:HE	1.32	0.94
1:A:456:PRO:HG2	1:A:459:LEU:HD13	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:MET:H	1:A:397:ASN:HD22	1.25	0.84
2:B:81:ILE:H	2:B:103:ASN:HD22	1.27	0.81
1:A:170:PHE:HA	1:A:173:LEU:HD21	1.62	0.81
1:A:56:SER:HA	1:A:80:ALA:HB3	1.65	0.79
1:A:469:LEU:H	1:A:487:ASN:HD22	1.28	0.79
2:B:457:ILE:H	2:B:478:ASN:HD22	1.29	0.79
2:B:410:VAL:H	2:B:433:ASN:HD22	1.34	0.76
1:A:30:CYS:HA	1:A:36:CYS:HA	1.67	0.76
1:A:239:PHE:H	1:A:268:GLN:HE21	1.34	0.75
2:B:435:LEU:H	2:B:455:ASN:HD22	1.33	0.74
2:B:55:ASN:HB2	2:B:79:ASN:HD21	1.53	0.73
1:A:123:LEU:HD13	1:A:126:LEU:HD22	1.69	0.72
1:A:511:LEU:H	1:A:533:ASN:ND2	1.84	0.72
1:A:183:ALA:HB1	1:A:186:LEU:HB2	1.72	0.71
2:B:229:LYS:HD2	2:B:263:ARG:NE	2.04	0.71
2:B:54:GLN:HE22	4:D:2:NDG:H8C3	1.55	0.71
1:A:121:LYS:HB3	1:A:122:PRO:HD3	1.73	0.69
1:A:346:SER:H	1:A:370:ASN:HD21	1.38	0.69
2:B:103:ASN:HB2	2:B:124:ASN:HD21	1.57	0.69
2:B:410:VAL:H	2:B:433:ASN:ND2	1.89	0.69
1:A:571:SER:O	1:A:572:ILE:HG23	1.93	0.69
1:A:64:ILE:HB	1:A:86:ASN:HB3	1.74	0.69
1:A:166:GLN:HA	1:A:190:GLU:HB3	1.75	0.68
1:A:511:LEU:N	1:A:533:ASN:HD22	1.84	0.68
1:A:38:GLY:H	1:A:58:ASP:HB3	1.57	0.68
1:A:487:ASN:HB2	1:A:509:ASN:HD21	1.58	0.68
1:A:218:VAL:HG12	1:A:244:THR:HB	1.77	0.67
1:A:112:LEU:H	1:A:134:ASN:HD22	1.42	0.66
1:A:489:LEU:H	1:A:509:ASN:HD22	1.43	0.66
1:A:158:ASN:HD22	1:A:160:ASP:HB2	1.59	0.66
1:A:59:LEU:HD12	1:A:64:ILE:HD11	1.78	0.66
1:A:112:LEU:HD22	1:A:115:LEU:HD23	1.78	0.65
1:A:239:PHE:H	1:A:268:GLN:NE2	1.95	0.65
2:B:408:ASN:HB2	2:B:433:ASN:HD21	1.61	0.65
7:G:1:NAG:H62	7:G:2:BMA:O5	1.96	0.64
2:B:115:ASN:ND2	2:B:138:MET:HA	2.13	0.63
1:A:110:ASN:HB2	1:A:134:ASN:HD21	1.64	0.63
2:B:54:GLN:HE22	4:D:2:NDG:C8	2.12	0.63
1:A:310:GLU:HG3	1:A:311:THR:HG23	1.80	0.62
2:B:62:THR:HA	2:B:88:VAL:HG13	1.80	0.62
1:A:68:SER:HA	1:A:92:GLU:HB2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:LEU:H	1:A:43:LEU:HD12	1.62	0.62
1:A:158:ASN:ND2	1:A:160:ASP:HB2	2.13	0.62
1:A:489:LEU:HB2	1:A:509:ASN:HD22	1.64	0.62
2:B:397:MET:O	2:B:422:THR:HG21	2.01	0.61
2:B:281:VAL:HG12	2:B:283:LEU:HD13	1.82	0.61
2:B:360:LEU:H	2:B:382:ASN:HD22	1.48	0.61
1:A:489:LEU:HB2	1:A:509:ASN:ND2	2.15	0.61
2:B:239:LYS:O	2:B:242:THR:HG22	2.00	0.60
1:A:270:MET:HB3	1:A:304:ILE:HD12	1.83	0.60
2:B:57:ILE:H	2:B:79:ASN:HD22	1.49	0.60
1:A:395:ARG:O	1:A:421:SER:O	2.20	0.60
2:B:455:ASN:HB2	2:B:478:ASN:HD21	1.66	0.60
1:A:113:SER:HB3	1:A:135:PRO:HB2	1.84	0.60
2:B:433:ASN:HB2	2:B:455:ASN:HD21	1.67	0.60
1:A:73:GLN:HA	1:A:98:SER:HB2	1.82	0.59
2:B:460:ILE:HG23	2:B:464:VAL:HG21	1.83	0.59
1:A:522:LEU:HD22	1:A:522:LEU:H	1.68	0.58
1:A:569:VAL:HA	1:A:572:ILE:HD11	1.85	0.58
1:A:78:LEU:HD23	1:A:99:LEU:HD22	1.84	0.58
1:A:234:LEU:HB3	1:A:261:ILE:HD12	1.86	0.57
1:A:52:GLU:OE1	1:A:76:VAL:HG12	2.04	0.57
2:B:36:LEU:HD13	2:B:40:PRO:HD3	1.86	0.57
1:A:146:SER:HA	1:A:172:GLY:HA3	1.86	0.57
1:A:346:SER:H	1:A:370:ASN:ND2	2.02	0.57
2:B:338:MET:HE3	2:B:360:LEU:HD21	1.86	0.57
1:A:446:THR:CG2	1:A:448:ILE:HG23	2.35	0.56
2:B:242:THR:O	2:B:244:PRO:HD3	2.04	0.56
7:G:1:NAG:H4	7:G:2:BMA:O2	2.04	0.56
1:A:378:LYS:HA	1:A:408:THR:HG23	1.87	0.56
1:A:425:PHE:O	1:A:446:THR:O	2.23	0.56
1:A:537:CYS:HA	1:A:542:ILE:HG21	1.87	0.56
2:B:36:LEU:H	2:B:55:ASN:ND2	2.02	0.56
1:A:35:ILE:HG23	1:A:56:SER:HB2	1.87	0.56
1:A:481:GLU:HG2	1:A:503:VAL:HB	1.88	0.56
2:B:358:ASN:HB2	2:B:382:ASN:HD21	1.70	0.56
1:A:79:GLN:HA	1:A:102:LEU:HA	1.88	0.55
1:A:82:VAL:HA	1:A:106:ASP:HB3	1.89	0.55
1:A:85:SER:HA	1:A:109:TYR:O	2.07	0.55
1:A:167:ARG:C	1:A:169:ASP:H	2.15	0.55
1:A:335:THR:HB	1:A:359:LEU:HD23	1.89	0.55
2:B:80:ARG:HG2	2:B:80:ARG:HH11	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:230:CYS:HA	11:B:751:HOH:O	2.06	0.54
1:A:356:SER:HB3	1:A:385:ALA:HB1	1.89	0.54
1:A:506:ILE:HD12	1:A:511:LEU:HD11	1.88	0.54
1:A:540:PRO:O	1:A:541:ARG:HG3	2.07	0.54
2:B:282:LYS:HG2	11:B:807:HOH:O	2.06	0.54
2:B:538:VAL:HA	2:B:541:ILE:HD13	1.88	0.54
2:B:66:LEU:HD12	2:B:67:SER:N	2.23	0.54
2:B:273:VAL:HG23	2:B:299:LEU:HD21	1.90	0.54
1:A:535:TRP:CD1	1:A:560:ALA:HB1	2.42	0.53
2:B:193:HIS:HD2	11:B:823:HOH:O	1.91	0.53
2:B:522:SER:HA	2:B:539:ARG:HH21	1.72	0.53
1:A:212:LEU:HD22	1:A:215:GLU:OE1	2.09	0.53
1:A:469:LEU:H	1:A:487:ASN:ND2	2.02	0.53
1:A:36:CYS:HB2	1:A:57:LEU:HD23	1.89	0.53
1:A:506:ILE:HG23	1:A:506:ILE:O	2.08	0.53
1:A:129:LEU:HG	1:A:131:LEU:HD21	1.91	0.53
1:A:369:GLU:HA	1:A:396:GLN:O	2.10	0.52
2:B:147:SER:O	2:B:148:THR:HG23	2.08	0.52
1:A:121:LYS:H	1:A:122:PRO:CD	2.23	0.52
2:B:113:THR:HG23	2:B:114:VAL:O	2.10	0.52
1:A:573:ILE:HD12	1:A:573:ILE:N	2.24	0.52
1:A:377:LEU:HG	1:A:408:THR:HG21	1.91	0.51
1:A:138:THR:HG22	1:A:139:LEU:H	1.75	0.51
1:A:556:GLU:OE1	1:A:559:SER:HA	2.10	0.51
1:A:65:THR:HG23	1:A:89:ASN:OD1	2.10	0.51
1:A:124:SER:O	1:A:150:LYS:HD3	2.11	0.51
2:B:34:ASN:H	2:B:55:ASN:HD21	1.59	0.51
1:A:467:ASN:HB2	1:A:487:ASN:HD21	1.75	0.51
1:A:370:ASN:HB2	1:A:397:ASN:HD21	1.76	0.50
1:A:480:LYS:HE2	1:A:500:MET:HE2	1.93	0.50
1:A:418:ILE:HG13	1:A:438:MET:HE1	1.93	0.50
1:A:137:LYS:HA	1:A:162:PHE:HA	1.94	0.50
1:A:446:THR:HG22	1:A:448:ILE:HG23	1.93	0.50
1:A:443:LEU:O	1:A:446:THR:HB	2.11	0.50
1:A:510:GLN:NE2	1:A:534:PRO:HG2	2.27	0.50
2:B:215:ASN:HD22	2:B:248:ASN:HB2	1.75	0.50
1:A:548:TRP:HE3	1:A:549:LEU:HD12	1.76	0.50
1:A:385:ALA:O	1:A:386:TRP:C	2.55	0.49
1:A:270:MET:HE2	1:A:304:ILE:HG13	1.93	0.49
2:B:435:LEU:H	2:B:455:ASN:ND2	2.05	0.49
1:A:50:LEU:HD12	1:A:50:LEU:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:ILE:H	2:B:79:ASN:ND2	2.09	0.49
2:B:135:PHE:HA	2:B:138:MET:HE2	1.94	0.49
2:B:394:THR:CG2	2:B:422:THR:H	2.25	0.49
2:B:229:LYS:HB2	2:B:260:SER:OG	2.12	0.49
1:A:96:PHE:CE1	1:A:119:TRP:HB3	2.48	0.49
2:B:138:MET:HE3	2:B:141:LEU:HD22	1.94	0.49
2:B:312:PHE:O	9:C:101:PLM:H22	2.13	0.49
1:A:139:LEU:HB2	1:A:169:ASP:OD1	2.13	0.48
2:B:440:PHE:CD2	2:B:464:VAL:HG22	2.49	0.48
1:A:52:GLU:C	1:A:54:VAL:H	2.22	0.48
1:A:306:PRO:HG3	1:A:334:LEU:HA	1.96	0.48
1:A:218:VAL:HG13	1:A:242:LEU:HD22	1.95	0.48
1:A:142:THR:O	1:A:143:SER:C	2.56	0.48
1:A:198:GLN:HG2	1:A:199:ASN:OD1	2.13	0.48
2:B:480:LEU:H	2:B:502:ASN:HD22	1.62	0.48
2:B:500:HIS:HD2	2:B:501:THR:OG1	1.97	0.47
2:B:177:GLU:O	2:B:178:LYS:C	2.57	0.47
1:A:87:GLY:HA2	1:A:111:TYR:CD1	2.50	0.47
1:A:234:LEU:HD22	1:A:259:VAL:HG11	1.96	0.47
1:A:345:ASN:HA	1:A:369:GLU:O	2.15	0.47
1:A:512:LYS:HA	1:A:534:PRO:O	2.15	0.47
2:B:128:ALA:C	2:B:148:THR:HG22	2.40	0.47
2:B:273:VAL:HG23	2:B:299:LEU:CD2	2.44	0.47
2:B:33:LYS:HE3	4:D:1:NAG:C6	2.45	0.47
2:B:129:LEU:HA	2:B:148:THR:CG2	2.44	0.47
1:A:298:SER:HB3	1:A:303:VAL:HG12	1.97	0.46
1:A:118:SER:O	1:A:122:PRO:HD3	2.14	0.46
2:B:129:LEU:HA	2:B:148:THR:HG23	1.98	0.46
1:A:158:ASN:OD1	1:A:162:PHE:HB2	2.16	0.46
2:B:462:LYS:O	2:B:465:VAL:HG22	2.16	0.46
1:A:161:THR:O	1:A:163:THR:HG23	2.16	0.46
2:B:518:LEU:HG	2:B:525:GLU:OE2	2.16	0.46
2:B:115:ASN:HD21	2:B:138:MET:HA	1.77	0.45
2:B:508:CYS:C	2:B:510:ARG:H	2.23	0.45
2:B:474:ASN:HA	2:B:498:TRP:HB2	1.98	0.45
2:B:413:ASP:OD1	2:B:415:LYS:HG2	2.16	0.45
2:B:534:SER:OG	2:B:536:LYS:HG3	2.14	0.45
1:A:125:SER:HA	1:A:150:LYS:HD3	1.97	0.45
1:A:132:LEU:HD11	1:A:155:ARG:HB3	1.99	0.45
1:A:182:ASP:HA	1:A:206:HIS:HB2	1.97	0.45
1:A:469:LEU:N	1:A:487:ASN:HD22	2.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:LEU:N	1:A:173:LEU:HD23	2.31	0.45
1:A:328:LEU:HA	11:A:1027:HOH:O	2.17	0.45
1:A:475:ASN:HA	1:A:497:LEU:HB3	1.99	0.45
2:B:28:LEU:HD22	2:B:29:VAL:N	2.30	0.45
1:A:565:SER:C	1:A:567:LYS:H	2.24	0.45
2:B:37:ILE:HG13	2:B:38:HIS:CD2	2.52	0.45
1:A:398:HIS:ND1	2:B:383:GLN:NE2	2.64	0.44
2:B:188:ASN:C	2:B:188:ASN:HD22	2.25	0.44
2:B:305:HIS:CD2	2:B:334:SER:HB2	2.52	0.44
1:A:383:GLU:O	1:A:384:ASP:HB2	2.17	0.44
2:B:221:ILE:HD13	2:B:233:PHE:CZ	2.52	0.44
2:B:514:LEU:O	2:B:518:LEU:HB2	2.17	0.44
2:B:267:LEU:C	2:B:267:LEU:HD23	2.42	0.44
2:B:115:ASN:HD22	2:B:115:ASN:HA	1.58	0.44
2:B:541:ILE:HD12	2:B:541:ILE:N	2.33	0.44
1:A:28:LEU:HD13	1:A:36:CYS:HB3	2.00	0.44
2:B:181:PRO:HG3	2:B:205:ILE:HD12	2.00	0.44
8:A:902:NAG:C7	11:A:1021:HOH:O	2.66	0.44
1:A:138:THR:HG22	1:A:139:LEU:N	2.32	0.44
1:A:460:GLU:HG3	1:A:480:LYS:HG2	2.00	0.44
2:B:114:VAL:HG12	2:B:115:ASN:H	1.83	0.44
2:B:358:ASN:HB2	2:B:382:ASN:ND2	2.33	0.44
1:A:176:LEU:HD11	1:A:200:VAL:HG22	1.99	0.43
2:B:394:THR:HG21	2:B:421:TRP:HE3	1.83	0.43
1:A:67:ILE:HB	1:A:91:ILE:HG12	2.00	0.43
2:B:411:SER:HB3	2:B:434:ILE:HG13	1.99	0.43
1:A:115:LEU:HA	1:A:119:TRP:HZ3	1.84	0.43
1:A:132:LEU:HA	1:A:157:GLY:O	2.19	0.43
1:A:542:ILE:HD12	1:A:546:SER:OG	2.18	0.43
2:B:79:ASN:HB2	2:B:103:ASN:HD21	1.83	0.43
1:A:43:LEU:HD12	1:A:43:LEU:N	2.30	0.43
2:B:457:ILE:H	2:B:478:ASN:ND2	2.06	0.43
2:B:290:ARG:HD2	2:B:318:TYR:CE2	2.54	0.43
4:D:1:NAG:H61	4:D:2:NDG:H8C3	1.99	0.43
2:B:28:LEU:HD13	2:B:28:LEU:C	2.44	0.43
1:A:176:LEU:CD1	1:A:200:VAL:HG22	2.49	0.42
1:A:535:TRP:NE1	1:A:560:ALA:HB1	2.35	0.42
2:B:480:LEU:H	2:B:502:ASN:ND2	2.16	0.42
1:A:560:ALA:O	1:A:561:LYS:HD2	2.20	0.42
2:B:73:ILE:HG23	2:B:97:TYR:CD2	2.54	0.42
1:A:61:ASN:HA	1:A:85:SER:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:ILE:O	1:A:484:ILE:HG12	2.19	0.42
1:A:402:LEU:HD12	1:A:428:MET:HB3	2.02	0.42
1:A:519:PHE:HB2	1:A:544:TYR:OH	2.20	0.42
2:B:39:VAL:HG11	2:B:64:ASP:HB3	2.02	0.42
2:B:397:MET:C	2:B:422:THR:HG21	2.44	0.42
1:A:41:GLY:HA2	1:A:62:ASN:OD1	2.20	0.42
1:A:505:LYS:HA	1:A:529:TRP:HB2	2.01	0.42
1:A:195:LYS:HB2	1:A:219:ASP:HB3	2.02	0.42
2:B:229:LYS:HE2	2:B:259:ASN:HB2	2.02	0.42
2:B:511:ILE:HG13	2:B:511:ILE:O	2.20	0.42
1:A:134:ASN:HA	1:A:135:PRO:HD3	1.89	0.41
1:A:348:VAL:H	1:A:370:ASN:ND2	2.18	0.41
2:B:394:THR:O	2:B:422:THR:HG23	2.19	0.41
1:A:82:VAL:O	1:A:82:VAL:HG13	2.20	0.41
1:A:74:ARG:O	1:A:74:ARG:HG3	2.20	0.41
1:A:446:THR:HG22	1:A:448:ILE:HG12	2.02	0.41
1:A:451:VAL:HG21	1:A:472:PHE:CD1	2.55	0.41
2:B:84:LEU:HD22	2:B:85:ASP:N	2.35	0.41
1:A:131:LEU:N	1:A:131:LEU:HD22	2.34	0.41
2:B:28:LEU:HD22	2:B:29:VAL:H	1.85	0.41
2:B:105:LEU:H	2:B:124:ASN:HD22	1.69	0.41
1:A:78:LEU:HD23	1:A:99:LEU:CD2	2.50	0.41
1:A:158:ASN:HD21	1:A:161:THR:H	1.68	0.41
1:A:290:ASN:HB2	11:A:1034:HOH:O	2.19	0.41
2:B:73:ILE:HG12	2:B:97:TYR:HB3	2.03	0.41
1:A:64:ILE:HD12	1:A:86:ASN:CG	2.45	0.41
1:A:139:LEU:HD21	1:A:156:VAL:HG21	2.02	0.41
1:A:506:ILE:HG22	1:A:529:TRP:O	2.21	0.41
1:A:58:ASP:HA	1:A:82:VAL:CG1	2.50	0.41
1:A:141:GLU:HB3	1:A:168:LYS:HD2	2.03	0.41
1:A:418:ILE:HD12	1:A:438:MET:SD	2.61	0.41
1:A:515:PRO:HB2	1:A:518:ILE:HB	2.02	0.41
1:A:538:SER:O	1:A:542:ILE:HG12	2.20	0.41
2:B:35:GLY:N	2:B:55:ASN:ND2	2.69	0.41
2:B:360:LEU:H	2:B:382:ASN:ND2	2.16	0.41
1:A:224:VAL:HG12	1:A:225:GLU:N	2.36	0.41
1:A:560:ALA:C	1:A:561:LYS:HD2	2.45	0.41
2:B:440:PHE:CD1	2:B:461:PRO:HD2	2.56	0.41
3:C:7:DCY:HA	9:C:101:PLM:H21	1.84	0.41
1:A:50:LEU:HD12	1:A:50:LEU:N	2.36	0.41
1:A:121:LYS:HA	1:A:147:HIS:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:THR:OG1	2:B:114:VAL:N	2.52	0.41
2:B:346:LYS:O	2:B:347:ILE:C	2.64	0.41
1:A:112:LEU:H	1:A:134:ASN:ND2	2.15	0.40
1:A:573:ILE:HG22	1:A:574:CYS:N	2.36	0.40
2:B:188:ASN:C	2:B:188:ASN:ND2	2.78	0.40
1:A:155:ARG:HH11	1:A:155:ARG:HG2	1.87	0.40
1:A:234:LEU:HD22	1:A:259:VAL:CG1	2.51	0.40
2:B:473:LEU:O	2:B:497:ILE:HA	2.21	0.40
1:A:159:MET:H	1:A:159:MET:HG3	1.65	0.40
2:B:237:LEU:HB3	2:B:267:LEU:HD22	2.03	0.40
1:A:103:GLU:HA	1:A:126:LEU:HA	2.02	0.40
1:A:140:GLY:C	1:A:142:THR:H	2.30	0.40
1:A:145:PHE:HB3	1:A:148:LEU:HD11	2.02	0.40
1:A:230:ARG:HG2	1:A:257:ARG:HB3	2.03	0.40
1:A:84:THR:HG23	1:A:108:SER:HB2	2.02	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	547/549 (100%)	458 (84%)	72 (13%)	17 (3%)	3	1
2	B	518/520 (100%)	480 (93%)	36 (7%)	2 (0%)	30	28
3	C	4/6 (67%)	4 (100%)	0	0	100	100
All	All	1069/1075 (99%)	942 (88%)	108 (10%)	19 (2%)	6	3

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	SER
1	A	143	SER

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Mol	Chain	Res	Type
1	A	241	GLU
1	A	572	ILE
1	A	85	SER
1	A	395	ARG
1	A	494	ASP
1	A	40	SER
1	A	71	ASP
2	B	220	ASN
1	A	121	LYS
1	A	145	PHE
1	A	541	ARG
1	A	550	ASN
2	B	306	GLN
1	A	32	ARG
1	A	168	LYS
1	A	49	GLY
1	A	100	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	518/518 (100%)	494 (95%)	24 (5%)	24	25
2	B	494/494 (100%)	479 (97%)	15 (3%)	36	41
3	C	5/5 (100%)	4 (80%)	1 (20%)	1	0
All	All	1017/1017 (100%)	977 (96%)	40 (4%)	28	31

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	LEU
1	A	148	LEU
1	A	159	MET
1	A	173	LEU
1	A	176	LEU

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Mol	Chain	Res	Type
1	A	205	LEU
1	A	207	MET
1	A	227	LEU
1	A	229	LEU
1	A	234	LEU
1	A	242	LEU
1	A	270	MET
1	A	282	LEU
1	A	324	LEU
1	A	354	LEU
1	A	371	LEU
1	A	402	LEU
1	A	446	THR
1	A	459	LEU
1	A	470	ASN
1	A	490	MET
1	A	506	ILE
1	A	522	LEU
1	A	523	THR
2	B	41	LYS
2	B	60	LEU
2	B	84	LEU
2	B	115	ASN
2	B	116	LEU
2	B	157	LEU
2	B	189	THR
2	B	265	LEU
2	B	283	LEU
2	B	351	LEU
2	B	394	THR
2	B	403	LEU
2	B	422	THR
2	B	425	LEU
2	B	514	LEU
3	C	9	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	44	ASN
1	A	62	ASN

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Mol	Chain	Res	Type
1	A	73	GLN
1	A	134	ASN
1	A	147	HIS
1	A	158	ASN
1	A	202	HIS
1	A	258	ASN
1	A	268	GLN
1	A	290	ASN
1	A	318	HIS
1	A	370	ASN
1	A	379	ASN
1	A	397	ASN
1	A	417	ASN
1	A	423	ASN
1	A	426	HIS
1	A	470	ASN
1	A	475	ASN
1	A	478	GLN
1	A	487	ASN
1	A	509	ASN
1	A	510	GLN
1	A	526	GLN
1	A	531	HIS
1	A	533	ASN
1	A	557	GLN
2	B	38	HIS
2	B	54	GLN
2	B	55	ASN
2	B	78	HIS
2	B	79	ASN
2	B	82	GLN
2	B	92	ASN
2	B	102	HIS
2	B	103	ASN
2	B	115	ASN
2	B	118	HIS
2	B	124	ASN
2	B	140	GLN
2	B	188	ASN
2	B	193	HIS
2	B	199	ASN
2	B	215	ASN

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Mol	Chain	Res	Type
2	B	243	ASN
2	B	253	ASN
2	B	280	ASN
2	B	284	GLN
2	B	305	HIS
2	B	306	GLN
2	B	367	ASN
2	B	382	ASN
2	B	383	GLN
2	B	402	GLN
2	B	408	ASN
2	B	433	ASN
2	B	455	ASN
2	B	471	GLN
2	B	478	ASN
2	B	479	GLN
2	B	500	HIS
2	B	502	ASN
2	B	521	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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.

5.5 Carbohydrates ⓘ

11 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	D	1	4,2	14,14,15	0.79	0	17,19,21	0.74	1 (5%)
4	NDG	D	2	4	14,14,15	0.90	0	17,19,21	0.83	0
4	MAN	D	3	4	11,11,12	0.77	0	15,15,17	0.75	0
5	NAG	E	1	2,5	14,14,15	0.61	0	17,19,21	1.03	1 (5%)
5	NAG	E	2	5	14,14,15	0.70	0	17,19,21	0.76	1 (5%)
5	MAN	E	3	5	11,11,12	0.71	0	15,15,17	0.65	0
6	NAG	F	1	2,6	14,14,15	0.61	0	17,19,21	0.76	0
6	NAG	F	2	6	14,14,15	0.65	0	17,19,21	0.63	0
6	BMA	F	3	6	11,11,12	0.51	0	15,15,17	0.23	0
7	NAG	G	1	7	14,14,15	0.73	0	17,19,21	0.90	0
7	BMA	G	2	7	11,11,12	0.66	0	15,15,17	0.30	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
4	NAG	D	1	4,2	-	3/6/23/26	0/1/1/1
4	NDG	D	2	4	-	2/6/23/26	0/1/1/1
4	MAN	D	3	4	-	0/2/19/22	0/1/1/1
5	NAG	E	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	4/6/23/26	0/1/1/1
5	MAN	E	3	5	-	2/2/19/22	0/1/1/1
6	NAG	F	1	2,6	-	2/6/23/26	0/1/1/1
6	NAG	F	2	6	-	0/6/23/26	0/1/1/1
6	BMA	F	3	6	-	2/2/19/22	0/1/1/1
7	NAG	G	1	7	-	2/6/23/26	0/1/1/1
7	BMA	G	2	7	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1	NAG	C2-N2-C7	-2.78	119.17	122.90
5	E	2	NAG	C2-N2-C7	-2.16	120.00	122.90
4	D	1	NAG	C2-N2-C7	-2.08	120.11	122.90

There are no chirality outliers.

All (21) torsion outliers are listed below:

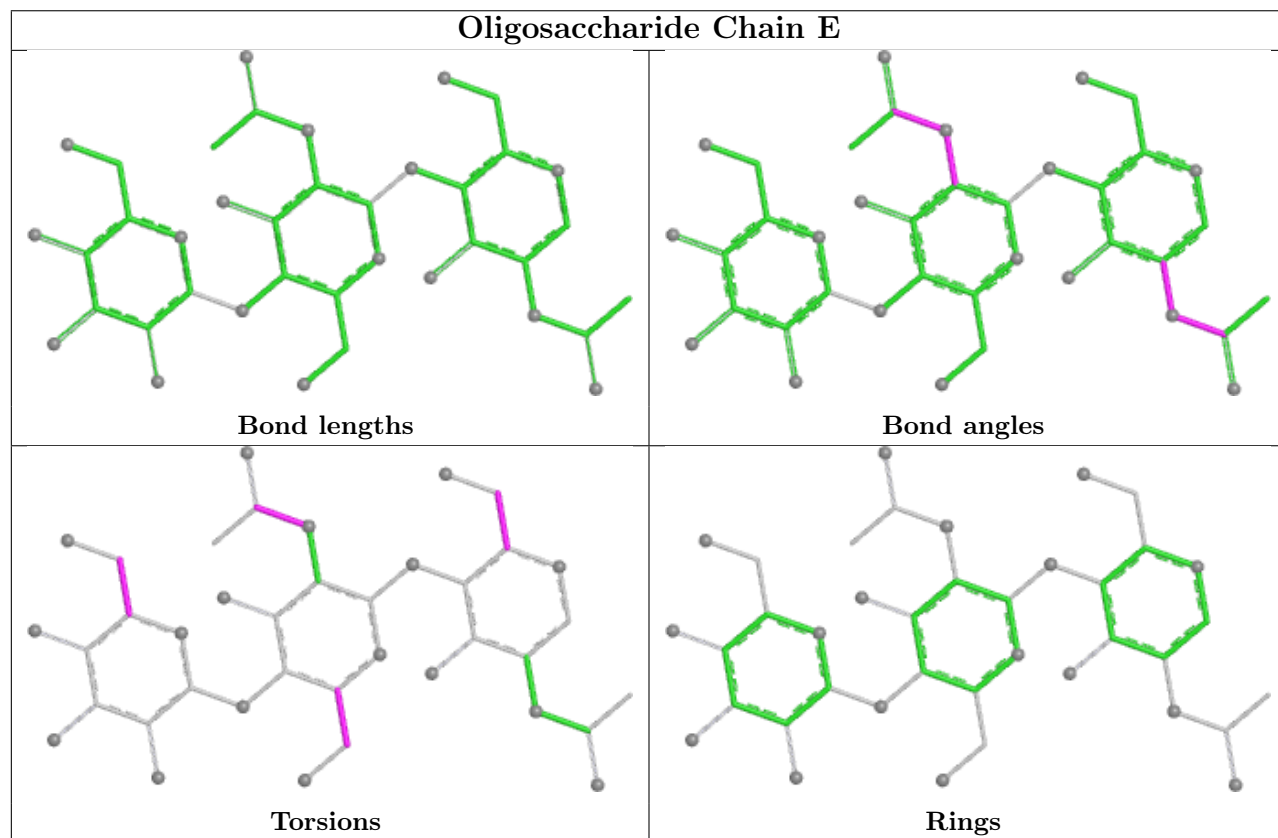
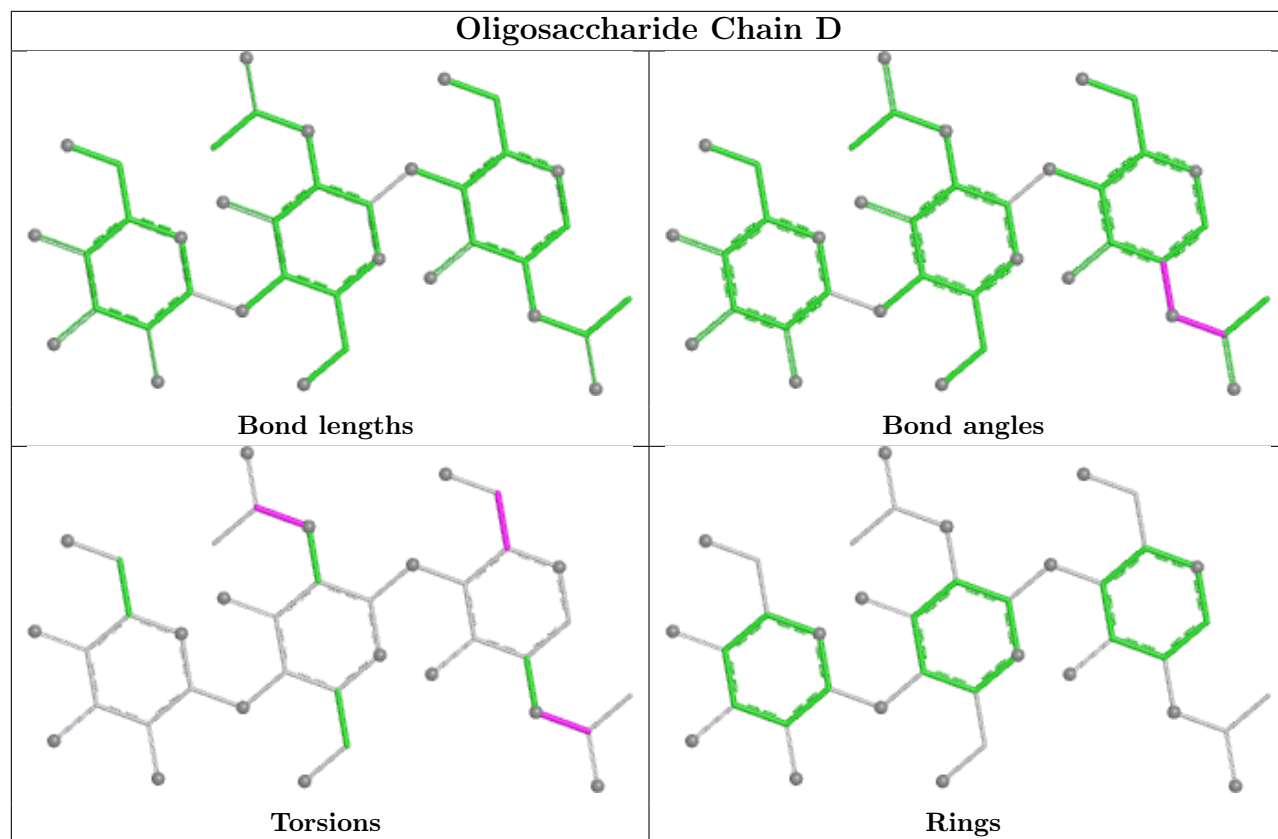
Mol	Chain	Res	Type	Atoms
4	D	2	NDG	C8-C7-N2-C2
4	D	2	NDG	O7-C7-N2-C2
7	G	1	NAG	C8-C7-N2-C2
7	G	1	NAG	O7-C7-N2-C2
5	E	3	MAN	O5-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
5	E	3	MAN	C4-C5-C6-O6
6	F	3	BMA	C4-C5-C6-O6
6	F	3	BMA	O5-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
4	D	1	NAG	C8-C7-N2-C2
5	E	2	NAG	C8-C7-N2-C2
7	G	2	BMA	C4-C5-C6-O6
5	E	2	NAG	O5-C5-C6-O6
6	F	1	NAG	C4-C5-C6-O6
4	D	1	NAG	O7-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2
7	G	2	BMA	O5-C5-C6-O6
6	F	1	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6

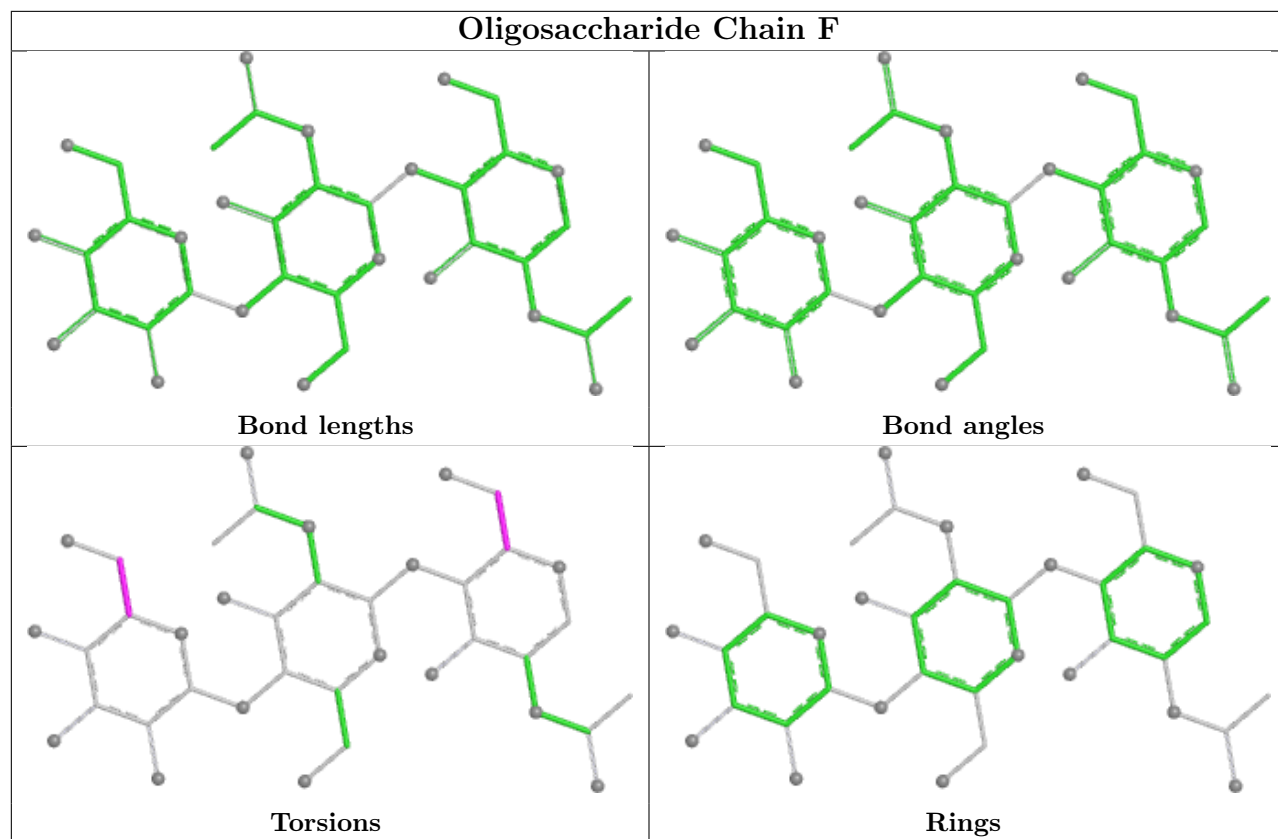
There are no ring outliers.

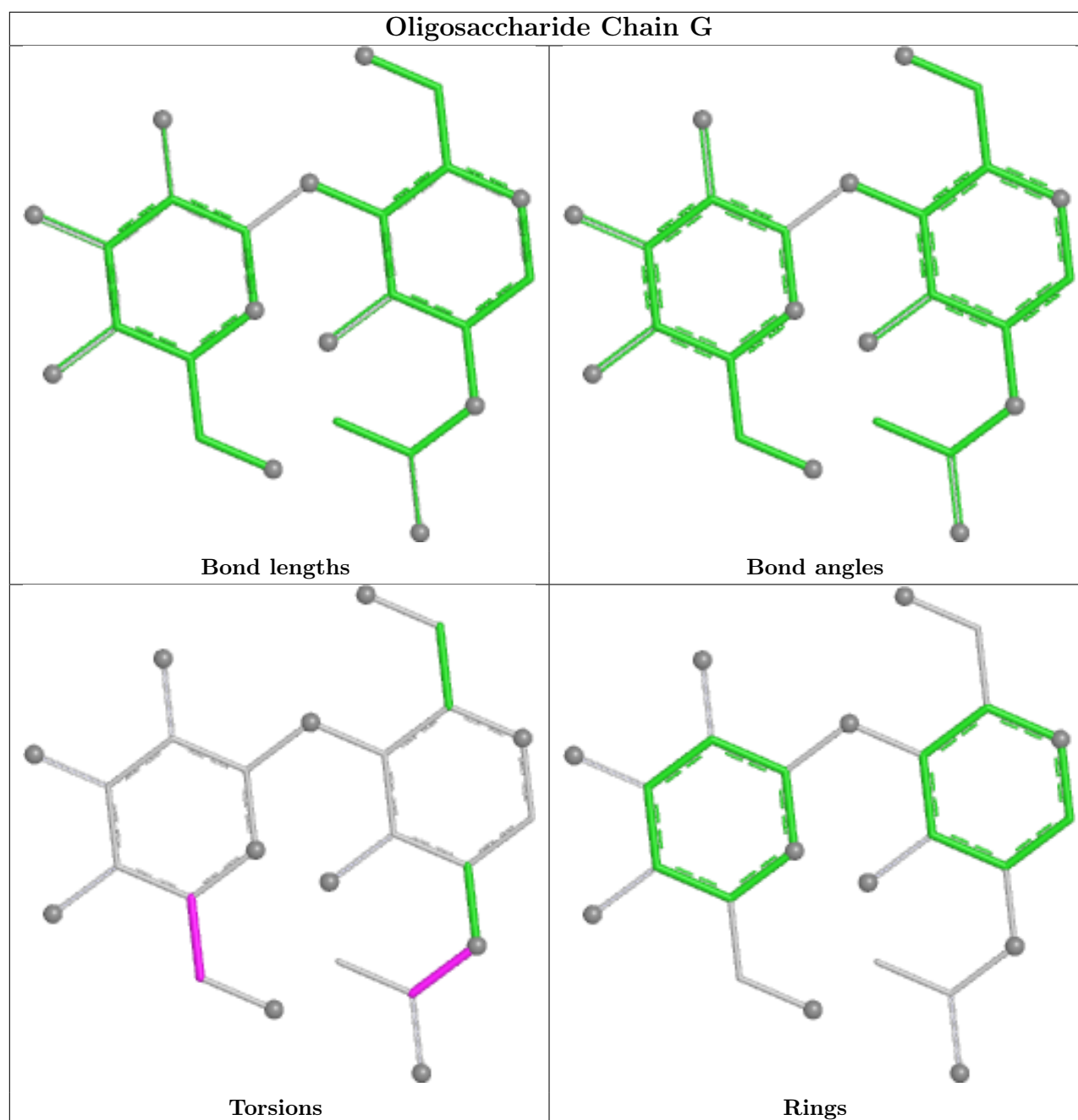
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	2	BMA	2	0
4	D	2	NDG	3	0
7	G	1	NAG	2	0
4	D	1	NAG	2	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](#)

6 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
10	Z41	C	102	3	38,38,39	0.61	1 (2%)	40,40,41	1.29	3 (7%)
9	PLM	C	101	3	15,16,17	0.22	0	14,15,17	0.62	0
8	NAG	A	901	1	14,14,15	0.61	0	17,19,21	0.64	0
8	NAG	A	902	1	14,14,15	0.67	0	17,19,21	0.59	0
8	NAG	B	601	2	14,14,15	0.58	0	17,19,21	0.70	1 (5%)
8	NAG	A	903	1	14,14,15	0.57	0	17,19,21	0.64	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	Z41	C	102	3	-	12/39/39/41	-
9	PLM	C	101	3	-	1/14/14/15	-
8	NAG	A	901	1	1/1/5/7	3/6/23/26	0/1/1/1
8	NAG	A	902	1	-	4/6/23/26	0/1/1/1
8	NAG	B	601	2	-	2/6/23/26	0/1/1/1
8	NAG	A	903	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	102	Z41	O3-C18	-2.83	1.42	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	102	Z41	C18-O3-C19	-4.77	110.91	117.78
10	C	102	Z41	O3-C19-C20	3.58	119.22	111.48
10	C	102	Z41	O2-C16-C15	2.67	119.97	111.83
8	B	601	NAG	C2-N2-C7	-2.28	119.84	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	901	NAG	C1

All (22) torsion outliers are listed below:

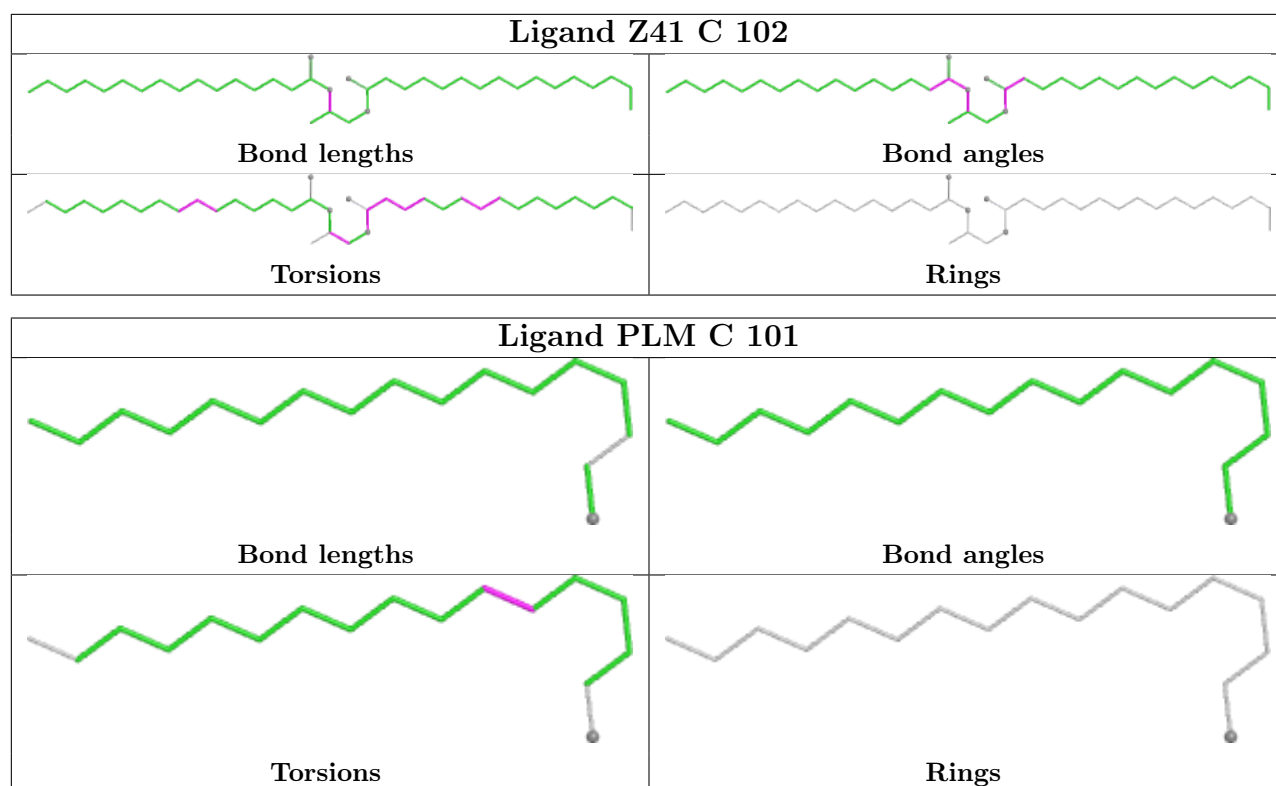
Mol	Chain	Res	Type	Atoms
8	A	901	NAG	C8-C7-N2-C2
8	A	901	NAG	O7-C7-N2-C2
8	A	902	NAG	C8-C7-N2-C2
8	A	902	NAG	O7-C7-N2-C2
8	B	601	NAG	C8-C7-N2-C2
8	B	601	NAG	O7-C7-N2-C2
10	C	102	Z41	O2-C17-C18-O3
8	A	902	NAG	O5-C5-C6-O6
8	A	902	NAG	C4-C5-C6-O6
10	C	102	Z41	C13-C14-C15-C16
10	C	102	Z41	C12-C13-C14-C15
10	C	102	Z41	C23-C24-C25-C26
10	C	102	Z41	C9-C10-C11-C12
8	A	901	NAG	O5-C5-C6-O6
10	C	102	Z41	O2-C17-C18-C35
10	C	102	Z41	C15-C16-O2-C17
10	C	102	Z41	C24-C25-C26-C27
10	C	102	Z41	O1-C16-O2-C17
9	C	101	PLM	C4-C5-C6-C7
10	C	102	Z41	C11-C10-C9-C8
10	C	102	Z41	C14-C15-C16-O2
10	C	102	Z41	C14-C15-C16-O1

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	101	PLM	2	0
8	A	902	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	549/549 (100%)	1.90	240 (43%) 0 1	22, 59, 130, 137	0
2	B	520/520 (100%)	0.39	35 (6%) 24 25	20, 35, 60, 83	0
3	C	5/6 (83%)	1.75	2 (40%) 1 1	41, 57, 74, 83	0
All	All	1074/1075 (99%)	1.16	277 (25%) 1 2	20, 43, 125, 137	0

All (277) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	96	PHE	8.3
1	A	148	LEU	7.4
1	A	244	THR	7.3
1	A	120	PHE	7.2
1	A	123	LEU	7.1
1	A	145	PHE	7.0
1	A	144	LEU	7.0
1	A	126	LEU	6.8
1	A	242	LEU	6.7
1	A	50	LEU	6.7
1	A	99	LEU	6.6
1	A	35	ILE	6.6
1	A	572	ILE	6.6
1	A	573	ILE	6.5
2	B	508	CYS	6.3
1	A	46	ILE	6.3
2	B	509	PRO	6.2
1	A	100	GLY	6.2
1	A	67	ILE	5.6
2	B	229	LYS	5.6
1	A	139	LEU	5.5
2	B	225	LEU	5.5
1	A	175	PHE	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	127	THR	5.5
1	A	51	THR	5.4
1	A	542	ILE	5.4
1	A	170	PHE	5.4
1	A	119	TRP	5.3
1	A	540	PRO	5.3
1	A	76	VAL	5.2
1	A	47	PRO	5.2
1	A	176	LEU	5.2
1	A	140	GLY	5.1
1	A	30	CYS	5.1
1	A	54	VAL	5.0
1	A	57	LEU	5.0
1	A	59	LEU	5.0
1	A	172	GLY	4.9
1	A	53	ALA	4.9
1	A	154	LEU	4.8
1	A	138	THR	4.8
1	A	571	SER	4.8
1	A	88	ILE	4.7
1	A	97	SER	4.7
1	A	105	LEU	4.6
1	A	91	ILE	4.6
1	A	171	ALA	4.6
1	A	43	LEU	4.6
1	A	107	LEU	4.6
1	A	522	LEU	4.5
1	A	156	VAL	4.5
1	A	143	SER	4.4
1	A	102	LEU	4.4
1	A	112	LEU	4.4
1	A	298	SER	4.4
1	A	165	ILE	4.4
1	A	510	GLN	4.3
1	A	81	LEU	4.3
1	A	157	GLY	4.3
1	A	83	LEU	4.3
1	A	129	LEU	4.3
1	A	64	ILE	4.2
2	B	242	THR	4.2
1	A	29	SER	4.2
1	A	28	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	77	ASN	4.2
2	B	228	ASN	4.2
1	A	247	THR	4.2
1	A	151	LEU	4.2
1	A	149	THR	4.2
1	A	111	TYR	4.2
1	A	78	LEU	4.2
1	A	86	ASN	4.1
1	A	128	PHE	4.1
1	A	27	SER	4.1
1	A	36	CYS	4.1
1	A	141	GLU	4.1
1	A	300	ASN	4.1
1	A	136	TYR	4.1
1	A	40	SER	4.1
1	A	72	LEU	4.0
1	A	545	LEU	4.0
1	A	142	THR	4.0
1	A	549	LEU	4.0
1	A	153	ILE	4.0
2	B	219	SER	3.9
2	B	114	VAL	3.9
1	A	539	CYS	3.9
1	A	117	SER	3.9
1	A	514	VAL	3.9
1	A	37	LYS	3.9
1	A	174	THR	3.9
1	A	87	GLY	3.9
2	B	230	CYS	3.9
1	A	55	LYS	3.9
1	A	52	GLU	3.9
1	A	568	PRO	3.9
1	A	135	PRO	3.8
1	A	124	SER	3.8
1	A	75	CYS	3.8
1	A	173	LEU	3.7
1	A	63	ARG	3.7
1	A	245	GLY	3.7
2	B	25	SER	3.7
1	A	162	PHE	3.7
1	A	519	PHE	3.7
1	A	574	CYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	49	GLY	3.7
1	A	509	ASN	3.7
1	A	570	ARG	3.6
1	A	297	ALA	3.6
1	A	115	LEU	3.6
1	A	168	LYS	3.6
1	A	48	SER	3.6
1	A	146	SER	3.6
1	A	198	GLN	3.6
1	A	243	SER	3.6
1	A	548	TRP	3.5
1	A	547	ARG	3.5
2	B	226	GLU	3.5
1	A	544	TYR	3.5
1	A	569	VAL	3.5
1	A	302	ARG	3.5
1	A	189	TYR	3.4
1	A	575	PRO	3.4
1	A	541	ARG	3.4
1	A	103	GLU	3.4
1	A	502	LEU	3.4
1	A	69	ASN	3.4
1	A	109	TYR	3.4
1	A	118	SER	3.4
1	A	125	SER	3.4
2	B	532	SER	3.4
1	A	38	GLY	3.3
1	A	113	SER	3.3
1	A	167	ARG	3.3
1	A	137	LYS	3.3
2	B	224	VAL	3.3
1	A	150	LYS	3.3
1	A	523	THR	3.3
1	A	74	ARG	3.2
1	A	80	ALA	3.2
1	A	95	SER	3.2
1	A	147	HIS	3.2
1	A	65	THR	3.2
1	A	122	PRO	3.2
1	A	104	HIS	3.2
1	A	158	ASN	3.2
2	B	227	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	215	GLU	3.1
1	A	159	MET	3.1
1	A	94	ASP	3.1
1	A	535	TRP	3.1
1	A	82	VAL	3.1
1	A	179	LEU	3.1
1	A	116	SER	3.1
1	A	90	THR	3.1
1	A	45	SER	3.1
1	A	131	LEU	3.0
1	A	68	SER	3.0
1	A	101	SER	3.0
1	A	538	SER	3.0
1	A	565	SER	3.0
1	A	61	ASN	3.0
1	A	44	ASN	3.0
1	A	199	ASN	3.0
2	B	544	PRO	3.0
3	C	12	LYS	3.0
2	B	113	THR	3.0
1	A	164	LYS	3.0
2	B	42	ASP	3.0
2	B	127	ASP	3.0
1	A	188	SER	2.9
1	A	194	LEU	2.9
1	A	299	ASP	2.9
1	A	152	GLN	2.9
2	B	533	GLY	2.9
1	A	160	ASP	2.9
1	A	79	GLN	2.9
1	A	191	PRO	2.9
1	A	490	MET	2.9
1	A	93	GLU	2.9
1	A	236	THR	2.9
1	A	177	GLU	2.9
1	A	39	SER	2.9
1	A	85	SER	2.9
1	A	432	CYS	2.8
1	A	537	CYS	2.8
1	A	555	LYS	2.8
1	A	564	GLY	2.8
2	B	108	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	201	SER	2.8
1	A	200	VAL	2.8
1	A	546	SER	2.8
1	A	132	LEU	2.8
1	A	525	LEU	2.8
1	A	121	LYS	2.8
1	A	449	HIS	2.7
1	A	560	ALA	2.7
1	A	491	THR	2.7
1	A	89	ASN	2.7
2	B	203	HIS	2.7
1	A	169	ASP	2.7
1	A	192	LYS	2.7
2	B	289	PHE	2.7
1	A	489	LEU	2.7
1	A	56	SER	2.7
1	A	303	VAL	2.7
1	A	518	ILE	2.7
1	A	161	THR	2.6
1	A	470	ASN	2.6
1	A	195	LYS	2.6
1	A	543	ASP	2.6
1	A	163	THR	2.6
1	A	66	TYR	2.6
1	A	84	THR	2.6
1	A	250	LEU	2.6
1	A	261	ILE	2.5
1	A	551	LYS	2.5
2	B	539	ARG	2.5
1	A	34	GLY	2.5
1	A	506	ILE	2.5
1	A	520	ASP	2.5
1	A	73	GLN	2.5
1	A	524	SER	2.5
1	A	471	LEU	2.5
1	A	501	LEU	2.5
2	B	248	ASN	2.5
1	A	70	SER	2.4
1	A	211	ILE	2.4
1	A	557	GLN	2.4
1	A	492	LEU	2.4
1	A	511	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	150	HIS	2.4
1	A	31	ASP	2.4
3	C	11	LYS	2.4
1	A	186	LEU	2.3
1	A	512	LYS	2.3
1	A	92	GLU	2.3
1	A	114	ASN	2.3
1	A	32	ARG	2.3
1	A	473	SER	2.3
1	A	33	ASN	2.3
1	A	225	GLU	2.3
2	B	110	CYS	2.2
1	A	550	ASN	2.2
1	A	301	ASP	2.2
2	B	523	GLN	2.2
1	A	296	ARG	2.2
1	A	521	ARG	2.2
1	A	556	GLU	2.2
2	B	536	LYS	2.2
2	B	152	GLU	2.1
1	A	155	ARG	2.1
2	B	462	LYS	2.1
2	B	199	ASN	2.1
1	A	106	ASP	2.1
2	B	414	GLU	2.1
1	A	202	HIS	2.1
1	A	531	HIS	2.1
1	A	495	ALA	2.1
1	A	62	ASN	2.1
1	A	414	ASN	2.1
2	B	542	ILE	2.1
1	A	513	SER	2.1
2	B	45	GLN	2.1
1	A	515	PRO	2.1
1	A	532	THR	2.1
2	B	149	THR	2.1
1	A	566	GLY	2.1
1	A	218	VAL	2.1
1	A	526	GLN	2.0
1	A	190	GLU	2.0
1	A	42	SER	2.0
1	A	214	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	534	PRO	2.0
1	A	41	GLY	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	DCY	C	7	6/7	0.96	0.09	31,35,37,38	0

6.3 Carbohydrates [i](#)

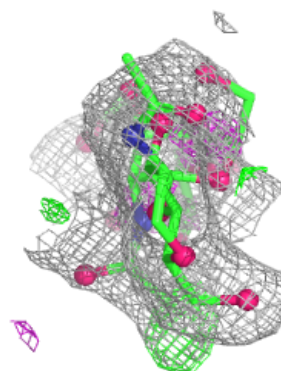
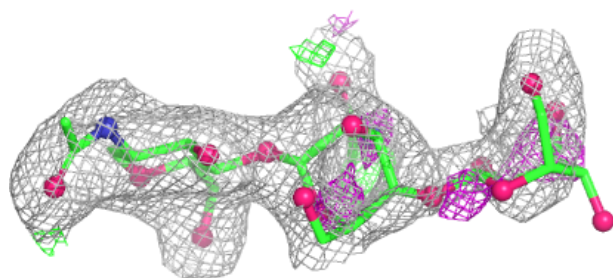
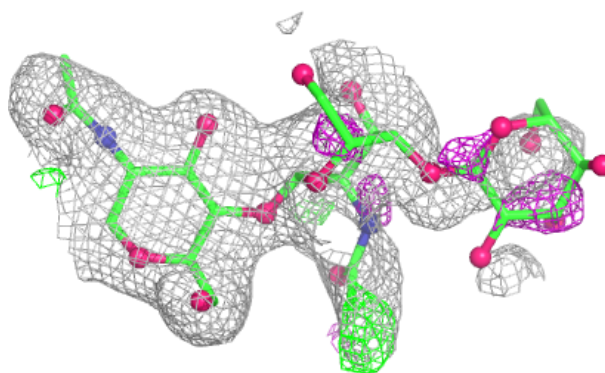
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MAN	D	3	11/12	0.34	0.18	98,100,102,102	0
7	BMA	G	2	11/12	0.38	0.20	96,98,99,99	0
4	NDG	D	2	14/15	0.39	0.19	80,85,89,94	0
5	MAN	E	3	11/12	0.44	0.17	81,84,86,88	0
6	BMA	F	3	11/12	0.58	0.15	68,72,74,77	0
7	NAG	G	1	14/15	0.61	0.24	90,93,96,96	0
5	NAG	E	2	14/15	0.84	0.12	55,65,71,75	0
5	NAG	E	1	14/15	0.89	0.10	41,46,52,56	0
4	NAG	D	1	14/15	0.91	0.12	53,58,62,72	0
6	NAG	F	2	14/15	0.92	0.09	35,48,54,62	0
6	NAG	F	1	14/15	0.95	0.07	24,30,33,40	0

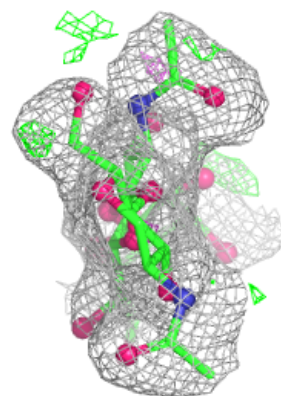
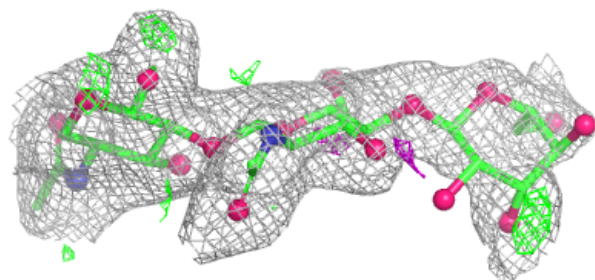
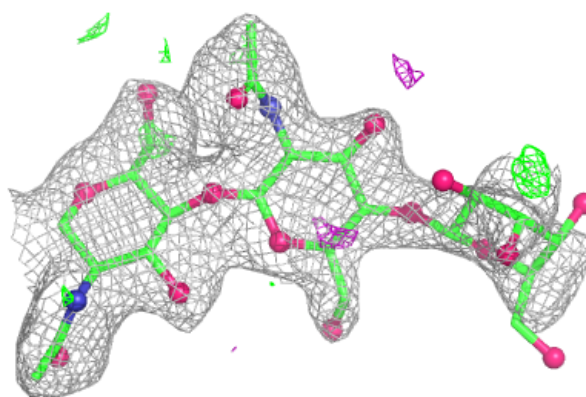
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain D:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

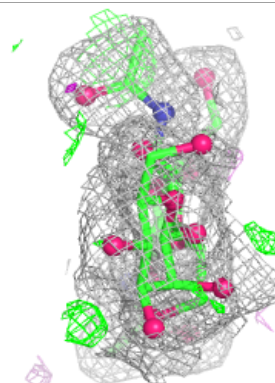
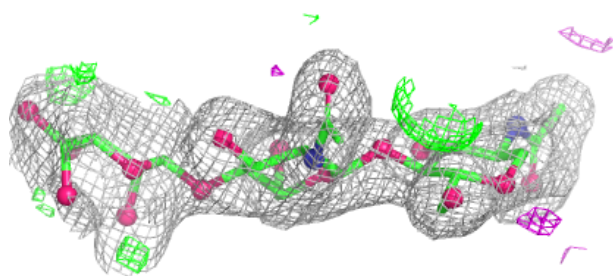
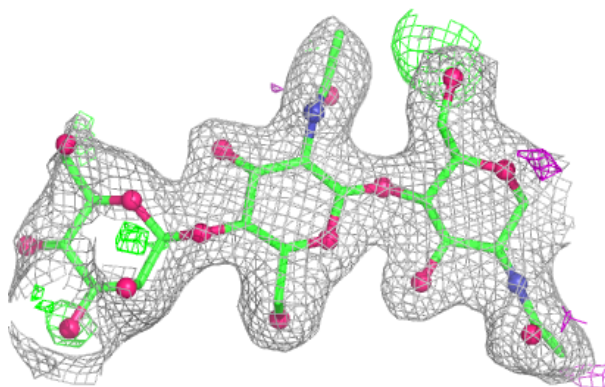
**Electron density around Chain E:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

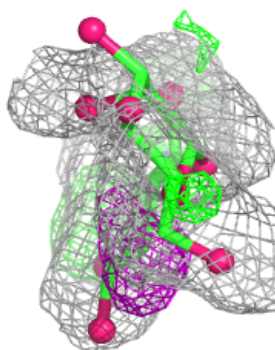
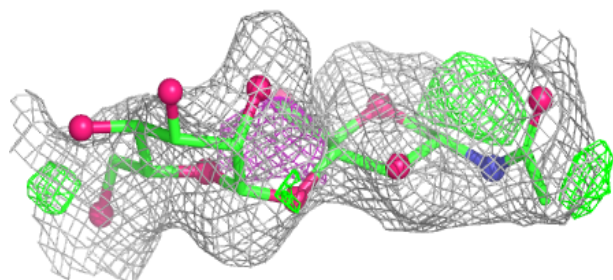
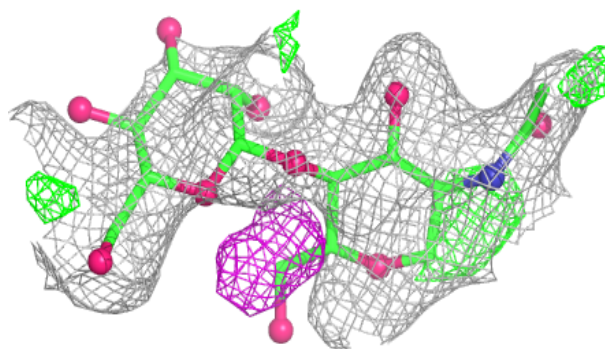


Electron density around Chain F:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain G:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

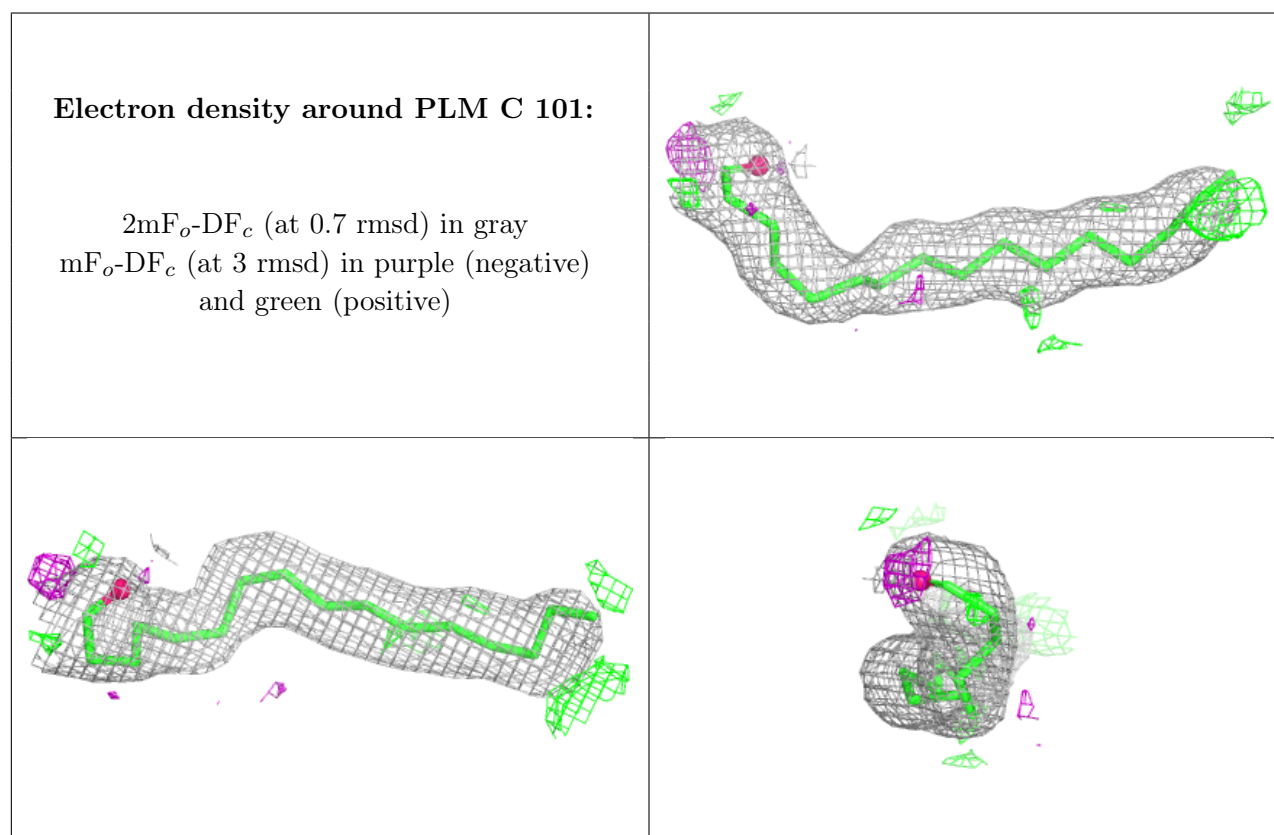


6.4 Ligands ⓘ

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.

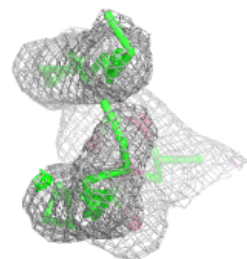
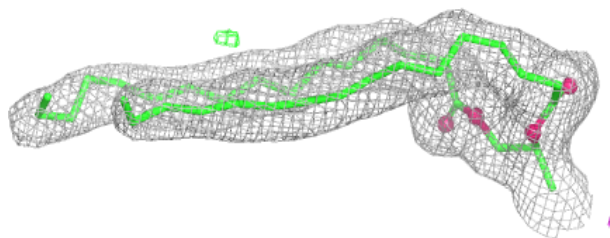
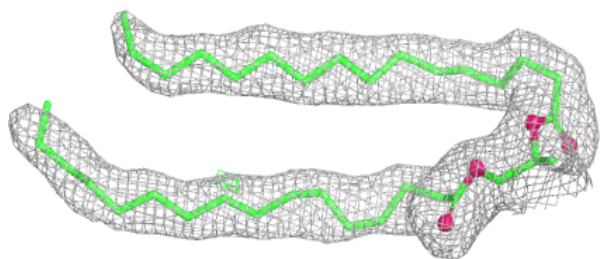
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	NAG	A	902	14/15	0.44	0.23	71,74,77,78	0
8	NAG	A	901	14/15	0.46	0.20	104,106,107,107	0
8	NAG	B	601	14/15	0.70	0.16	74,78,80,81	0
9	PLM	C	101	17/18	0.90	0.14	28,35,39,41	0
8	NAG	A	903	14/15	0.94	0.08	31,34,37,37	0
10	Z41	C	102	39/40	0.95	0.11	28,40,54,56	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Z41 C 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.