



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:00 AM UTC

PDB ID : 1OKE / pdb_00001oke
Title : Crystal structure of the dengue 2 virus envelope protein in complex with n-oc
tyl-beta-D-glucoside
Authors : Modis, Y.; Harrison, S.C.
Deposited on : 2003-07-22
Resolution : 2.40 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

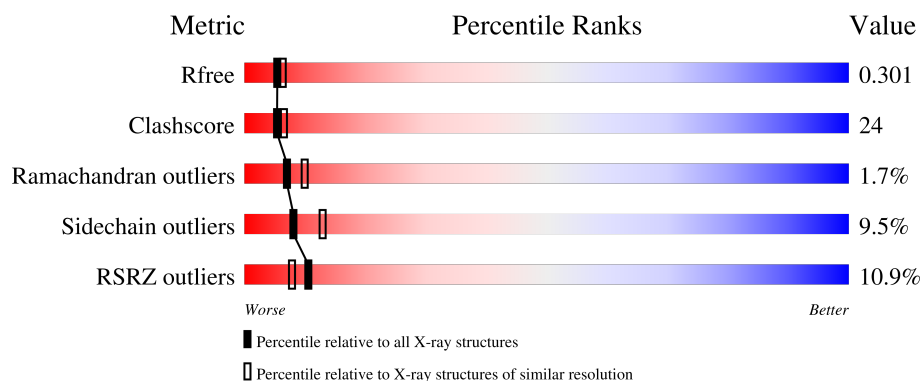
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	394	19% 57% 35% 6%
1	B	394	3% 60% 32% 7%
2	C	4	25% 25% 50%
2	D	4	25% 25% 50%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6426 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.

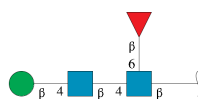
- Molecule 1 is a protein called MAJOR ENVELOPE PROTEIN E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	0	0
			3062	1931	526	579	26			
1	B	394	Total	C	N	O	S	0	0	0
			3062	1931	526	579	26			

There are 4 discrepancies between the modelled and reference sequences:

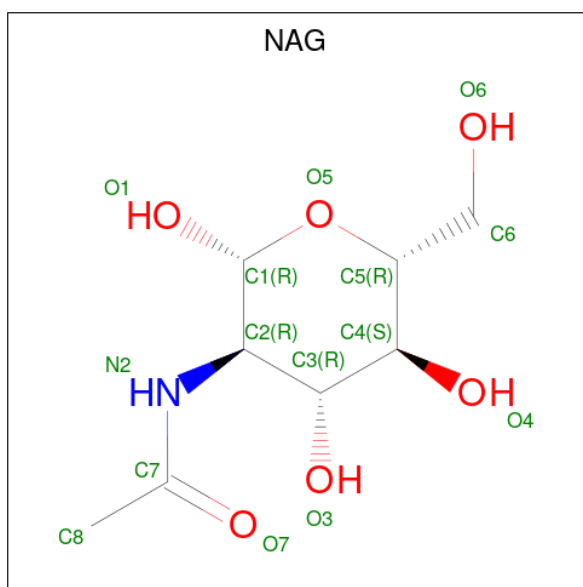
Chain	Residue	Modelled	Actual	Comment	Reference
A	71	GLU	ASP	conflict	UNP P12823
A	390	ASN	ASP	conflict	UNP P12823
B	71	GLU	ASP	conflict	UNP P12823
B	390	ASN	ASP	conflict	UNP P12823

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



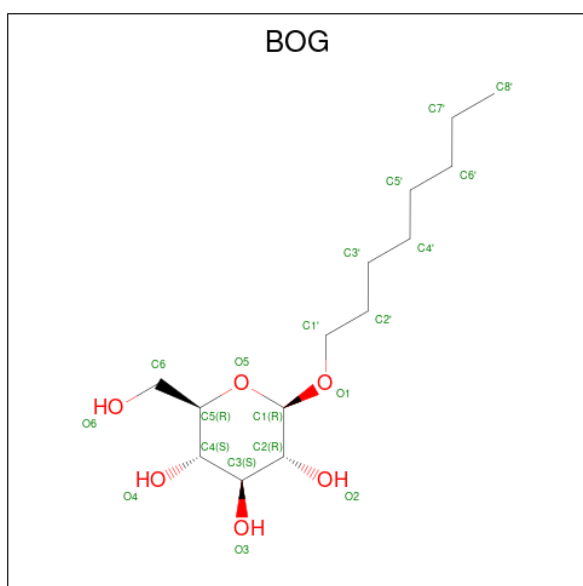
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	0	0	0
			49	28	2	19			
2	D	4	Total	C	N	O	0	0	0
			49	28	2	19			

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



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

- Molecule 4 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	14	6		
4	B	1	Total	C	O	0	0
			20	14	6		

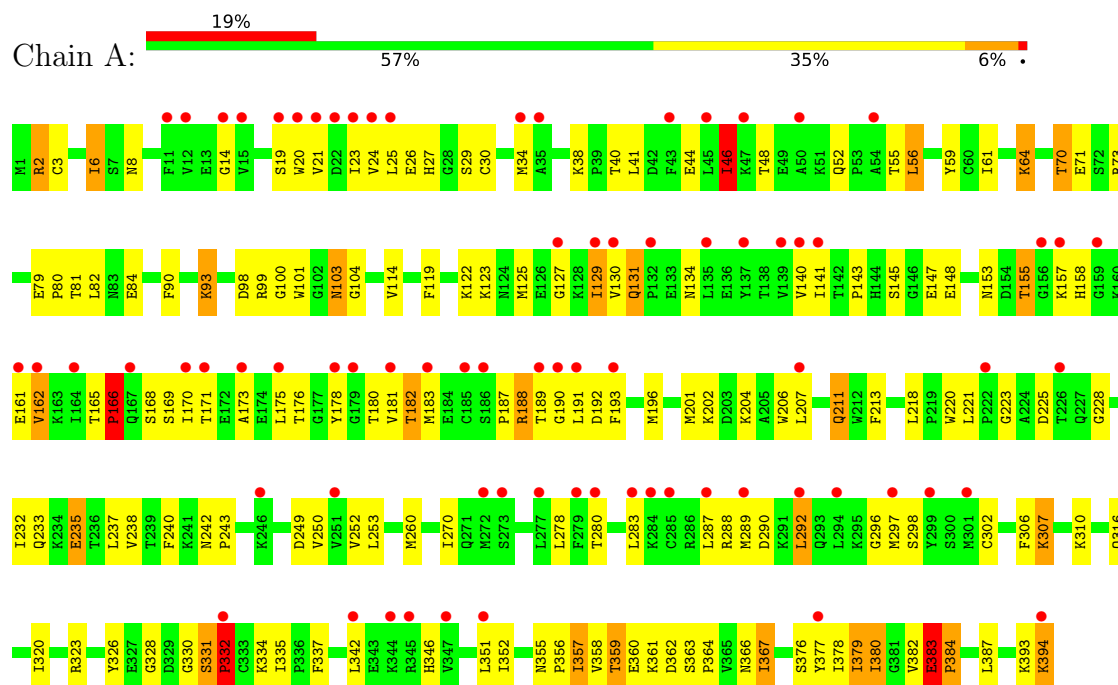
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	49	Total 49	O 49	0	0
5	B	87	Total 87	O 87	0	0

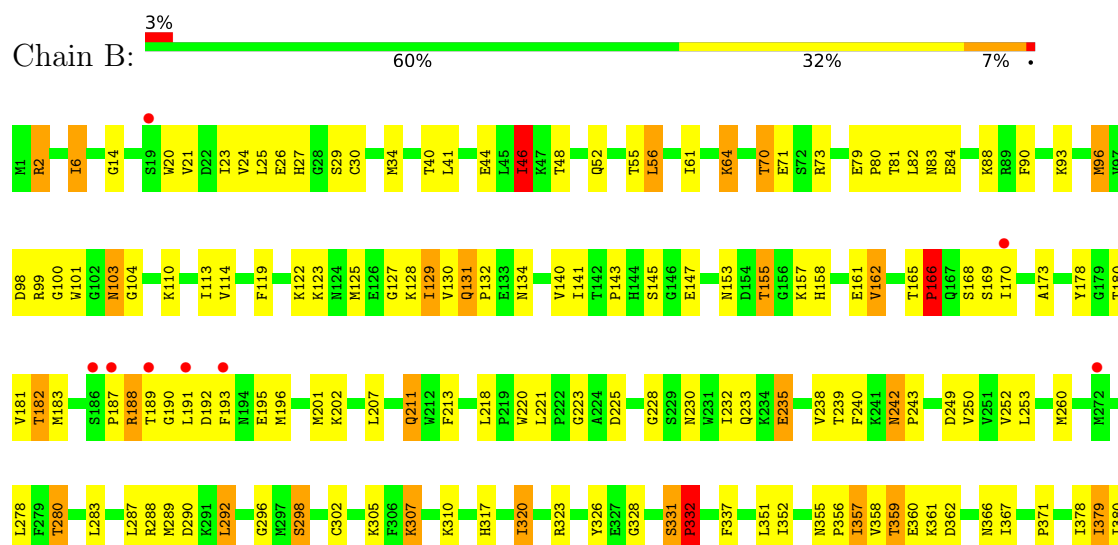
3 Residue-property plots

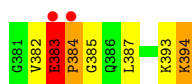
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

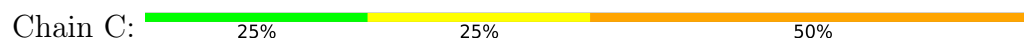


• Molecule 1: MAJOR ENVELOPE PROTEIN E

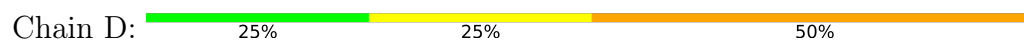




- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta a-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta a-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	81.60Å 81.60Å 287.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.00 – 2.40 45.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.7 (45.00-2.40) 94.7 (45.00-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.16Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.263 , 0.294 0.271 , 0.301	Depositor DCC
R_{free} test set	2469 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	55.3	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6426	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.20% 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: FUL, BOG, BMA, 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	0.62	1/3124 (0.0%)	1.15	22/4219 (0.5%)
1	B	0.70	2/3124 (0.1%)	1.16	19/4219 (0.5%)
All	All	0.66	3/6248 (0.0%)	1.15	41/8438 (0.5%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	380	ILE	CG1-CD1	-5.76	1.29	1.51
1	A	380	ILE	CG1-CD1	-5.35	1.30	1.51
1	B	96	MET	SD-CE	-5.19	1.66	1.79

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	352	ILE	N-CA-C	-13.23	100.43	111.81
1	A	352	ILE	N-CA-C	-13.19	100.47	111.81
1	B	158	HIS	N-CA-C	-10.57	101.43	114.75
1	A	158	HIS	N-CA-C	-10.21	101.88	114.75
1	A	165	THR	CA-C-N	9.95	132.28	119.84
1	A	165	THR	C-N-CA	9.95	132.28	119.84
1	B	165	THR	CA-C-N	9.74	132.02	119.84
1	B	165	THR	C-N-CA	9.74	132.02	119.84
1	B	190	GLY	N-CA-C	-9.66	90.29	113.18
1	A	190	GLY	N-CA-C	-9.53	90.61	113.18
1	A	383	GLU	CA-CB-CG	-9.20	95.70	114.10
1	A	242	ASN	CA-C-N	8.68	128.39	119.19
1	A	242	ASN	C-N-CA	8.68	128.39	119.19
1	A	104	GLY	N-CA-C	8.57	126.07	114.92
1	B	189	THR	N-CA-C	7.69	127.19	110.80
1	A	189	THR	N-CA-C	7.59	126.97	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	242	ASN	CA-C-N	7.45	126.97	118.85
1	B	242	ASN	C-N-CA	7.45	126.97	118.85
1	A	383	GLU	N-CA-C	7.03	125.35	109.81
1	B	104	GLY	N-CA-C	6.77	124.81	115.27
1	A	131	GLN	CA-C-N	6.63	128.13	119.84
1	A	131	GLN	C-N-CA	6.63	128.13	119.84
1	B	220	TRP	N-CA-C	6.24	117.66	108.86
1	A	358	VAL	N-CA-C	-6.23	103.26	110.05
1	B	225	ASP	N-CA-C	6.18	118.95	110.24
1	B	383	GLU	CB-CG-CD	6.09	122.96	112.60
1	B	383	GLU	CA-CB-CG	5.98	126.05	114.10
1	A	383	GLU	CB-CG-CD	5.97	122.75	112.60
1	B	358	VAL	N-CA-C	-5.88	103.64	110.05
1	A	362	ASP	N-CA-C	5.82	119.36	112.72
1	A	367	ILE	CB-CA-C	-5.82	102.57	110.42
1	B	113	ILE	N-CA-C	-5.72	100.24	108.42
1	A	134	ASN	N-CA-C	5.64	117.12	109.11
1	B	362	ASP	N-CA-C	5.61	119.12	112.72
1	A	220	TRP	N-CA-C	5.61	117.49	109.14
1	A	225	ASP	N-CA-C	5.58	118.10	110.24
1	B	134	ASN	N-CA-C	5.53	116.97	109.11
1	A	46	ILE	CB-CA-C	-5.36	104.10	111.65
1	A	3	CYS	N-CA-C	5.25	118.95	112.54
1	B	46	ILE	CB-CA-C	-5.15	104.39	111.65
1	B	298	SER	N-CA-C	-5.04	107.17	113.72

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	3062	0	3065	154	0
1	B	3062	0	3065	148	0
2	C	49	0	43	3	0
2	D	49	0	43	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	14	0	13	0	0
3	B	14	0	13	1	0
4	A	20	0	28	1	0
4	B	20	0	28	1	0
5	A	49	0	0	15	0
5	B	87	0	0	11	0
All	All	6426	0	6298	302	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 24.

All (302) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:PRO:HB3	1:B:187:PRO:CG	1.52	1.37
1:A:166:PRO:HB3	1:A:187:PRO:CG	1.52	1.36
1:A:166:PRO:CB	1:A:187:PRO:HG3	1.73	1.16
1:B:166:PRO:CB	1:B:187:PRO:HG3	1.74	1.16
1:A:289:MET:HA	5:A:2023:HOH:O	1.57	1.04
1:A:323:ARG:HE	1:A:366:ASN:HD21	1.04	1.01
1:B:166:PRO:HB3	1:B:187:PRO:HG3	1.02	1.01
1:A:166:PRO:HB3	1:A:187:PRO:HG3	1.02	0.99
1:B:323:ARG:HE	1:B:366:ASN:HD21	1.13	0.94
1:B:383:GLU:HB3	1:B:384:PRO:HD3	1.51	0.91
1:B:337:PHE:CD1	1:B:351:LEU:HD21	2.10	0.86
1:B:46:ILE:HG12	1:B:140:VAL:HG23	1.57	0.86
1:A:377:TYR:HD1	5:A:2043:HOH:O	1.58	0.86
1:A:201:MET:HB2	5:A:2015:HOH:O	1.76	0.85
1:A:383:GLU:HB3	1:A:384:PRO:HD3	1.58	0.83
1:B:359:THR:HG22	1:B:360:GLU:HG3	1.60	0.82
1:A:140:VAL:HG22	1:A:161:GLU:HG2	1.61	0.81
1:B:289:MET:HE1	5:B:2007:HOH:O	1.78	0.81
1:A:166:PRO:HB3	1:A:187:PRO:CD	2.11	0.80
1:B:140:VAL:HG22	1:B:161:GLU:HG2	1.62	0.80
1:A:323:ARG:HE	1:A:366:ASN:ND2	1.79	0.80
1:A:46:ILE:HG12	1:A:140:VAL:HG23	1.64	0.79
1:B:166:PRO:HB3	1:B:187:PRO:CD	2.12	0.79
1:A:178:TYR:HA	5:A:2012:HOH:O	1.83	0.79
1:A:323:ARG:NE	1:A:366:ASN:HD21	1.82	0.78
1:A:56:LEU:HG	1:A:129:ILE:HD11	1.66	0.78
1:A:61:ILE:HD11	1:A:123:LYS:HG2	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:PHE:CD1	1:A:351:LEU:HD21	2.19	0.77
1:A:359:THR:HG22	1:A:360:GLU:HG3	1.64	0.77
1:B:61:ILE:HD11	1:B:123:LYS:HG2	1.67	0.76
1:A:162:VAL:HG21	1:A:183:MET:HE1	1.66	0.75
1:B:155:THR:HG22	1:B:157:LYS:H	1.52	0.74
1:B:191:LEU:HD12	1:B:192:ASP:H	1.50	0.74
1:B:323:ARG:HE	1:B:366:ASN:ND2	1.86	0.73
1:A:38:LYS:HE3	5:A:2003:HOH:O	1.89	0.73
1:A:331:SER:HB2	1:A:332:PRO:HD2	1.71	0.72
1:A:19:SER:HB2	5:A:2003:HOH:O	1.90	0.72
1:A:101:TRP:CE2	1:B:310:LYS:HE3	2.24	0.71
1:A:191:LEU:HD12	1:A:192:ASP:H	1.53	0.71
1:B:323:ARG:NE	1:B:366:ASN:HD21	1.89	0.71
1:A:48:THR:OG1	1:A:280:THR:HG21	1.90	0.71
1:A:166:PRO:HB3	1:A:187:PRO:HG2	1.68	0.70
1:A:155:THR:HG22	1:A:157:LYS:H	1.56	0.70
1:B:166:PRO:HB3	1:B:187:PRO:HG2	1.69	0.70
1:B:48:THR:OG1	1:B:280:THR:HG21	1.91	0.69
1:B:56:LEU:HG	1:B:129:ILE:HD11	1.73	0.69
1:A:14:GLY:HA3	1:A:21:VAL:HG12	1.74	0.68
1:B:14:GLY:HA3	1:B:21:VAL:HG12	1.76	0.68
1:A:166:PRO:CG	1:A:187:PRO:HG3	2.25	0.67
1:B:331:SER:HB2	1:B:332:PRO:HD2	1.77	0.67
1:B:162:VAL:HG21	1:B:183:MET:HE1	1.75	0.67
1:A:243:PRO:HG3	1:B:278:LEU:HD22	1.75	0.66
1:B:166:PRO:CG	1:B:187:PRO:HG3	2.25	0.66
1:B:239:THR:HA	5:B:2056:HOH:O	1.93	0.66
1:A:55:THR:O	1:A:223:GLY:HA3	1.97	0.65
1:A:64:LYS:HB2	1:A:122:LYS:HD2	1.79	0.65
1:B:357:ILE:HG12	1:B:357:ILE:O	1.94	0.64
1:B:64:LYS:HB2	1:B:122:LYS:HD2	1.78	0.64
1:B:207:LEU:HD22	4:B:1400:BOG:H8'3	1.79	0.64
1:A:71:GLU:HG2	1:A:81:THR:H	1.63	0.64
1:B:141:ILE:N	1:B:141:ILE:HD12	2.13	0.64
1:A:141:ILE:HD12	1:A:141:ILE:N	2.13	0.64
2:C:2:NAG:H4	2:C:3:BMA:O2	1.98	0.63
1:A:331:SER:HB2	1:A:332:PRO:CD	2.28	0.63
1:A:166:PRO:CB	1:A:187:PRO:CG	2.45	0.63
1:B:240:PHE:CD2	1:B:250:VAL:HG22	2.33	0.63
1:B:320:ILE:HD13	1:B:371:PRO:HD3	1.80	0.63
1:A:206:TRP:HZ3	5:A:2015:HOH:O	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:THR:HG22	1:B:280:THR:O	1.99	0.62
1:B:331:SER:HB2	1:B:332:PRO:CD	2.29	0.62
1:A:125:MET:HE1	1:A:260:MET:SD	2.40	0.62
1:B:166:PRO:CB	1:B:187:PRO:CG	2.45	0.62
1:A:14:GLY:CA	1:A:21:VAL:HG12	2.30	0.62
1:B:178:TYR:O	1:B:292:LEU:HD23	1.99	0.62
1:B:235:GLU:CD	1:B:235:GLU:H	2.08	0.62
2:C:1:NAG:H62	2:C:2:NAG:H82	1.81	0.62
2:D:2:NAG:H4	2:D:3:BMA:O2	1.99	0.62
1:A:288:ARG:HH11	1:A:288:ARG:HG2	1.64	0.62
1:A:130:VAL:O	1:A:193:PHE:HB3	1.99	0.61
1:A:178:TYR:O	1:A:292:LEU:HD23	2.00	0.61
1:B:52:GLN:HA	1:B:52:GLN:NE2	2.14	0.61
1:A:100:GLY:H	1:A:103:ASN:HD21	1.48	0.61
2:D:1:NAG:H62	2:D:2:NAG:H82	1.83	0.60
1:A:204:LYS:HB2	5:A:2015:HOH:O	2.01	0.60
1:A:162:VAL:HG21	1:A:183:MET:CE	2.30	0.60
1:A:337:PHE:CD2	1:A:380:ILE:HD12	2.37	0.60
1:A:235:GLU:H	1:A:235:GLU:CD	2.09	0.60
1:A:328:GLY:O	1:A:361:LYS:HE3	2.02	0.60
1:A:310:LYS:HE3	1:B:101:TRP:CE2	2.37	0.59
1:B:23:ILE:HD12	1:B:25:LEU:HD21	1.82	0.59
1:A:48:THR:HG21	1:A:280:THR:CG2	2.32	0.59
1:B:14:GLY:CA	1:B:21:VAL:HG12	2.32	0.59
1:B:317:HIS:ND1	5:B:2070:HOH:O	2.32	0.59
1:A:307:LYS:HB3	1:A:307:LYS:NZ	2.18	0.59
1:B:100:GLY:H	1:B:103:ASN:HD21	1.50	0.59
1:A:280:THR:HG22	1:A:280:THR:O	2.03	0.59
1:B:288:ARG:HG2	1:B:288:ARG:HH11	1.66	0.59
1:A:316:GLN:HE22	1:B:110:LYS:HE2	1.67	0.58
1:A:240:PHE:CD2	1:A:250:VAL:HG22	2.38	0.58
3:B:1395:NAG:O6	5:B:2084:HOH:O	2.17	0.58
1:A:170:ILE:H	1:A:170:ILE:HD12	1.69	0.58
1:B:328:GLY:O	1:B:361:LYS:HE3	2.03	0.58
1:B:356:PRO:HB3	1:B:367:ILE:HD12	1.86	0.58
1:A:23:ILE:HD12	1:A:25:LEU:HD21	1.85	0.57
1:B:71:GLU:OE2	1:B:73:ARG:NH1	2.37	0.57
1:A:307:LYS:HB3	1:A:307:LYS:HZ3	1.70	0.57
1:A:232:ILE:HG22	1:A:233:GLN:HG3	1.87	0.57
1:B:394:LYS:HD2	5:B:2082:HOH:O	2.04	0.57
1:B:128:LYS:NZ	5:B:2041:HOH:O	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ILE:HD12	1:B:170:ILE:H	1.70	0.56
1:A:41:LEU:HD23	1:A:143:PRO:HB3	1.87	0.56
1:B:130:VAL:O	1:B:193:PHE:HB3	2.05	0.56
1:B:162:VAL:HG21	1:B:183:MET:CE	2.35	0.56
1:B:305:LYS:HG2	5:B:2067:HOH:O	2.06	0.56
1:B:55:THR:O	1:B:223:GLY:HA3	2.05	0.56
1:A:24:VAL:C	1:A:25:LEU:HD23	2.31	0.55
1:A:71:GLU:HG3	1:A:80:PRO:HB3	1.88	0.55
1:A:101:TRP:CD2	1:B:310:LYS:HE3	2.41	0.55
1:B:48:THR:HG21	1:B:280:THR:CG2	2.36	0.55
1:A:41:LEU:CD2	1:A:143:PRO:HB3	2.37	0.55
1:B:71:GLU:HG2	1:B:81:THR:H	1.70	0.55
1:A:288:ARG:HG2	1:A:288:ARG:NH1	2.22	0.54
1:B:307:LYS:NZ	1:B:307:LYS:HB3	2.22	0.54
1:B:331:SER:CB	1:B:332:PRO:CD	2.85	0.54
1:B:240:PHE:CE2	1:B:250:VAL:HG22	2.42	0.54
1:A:20:TRP:HA	1:A:287:LEU:O	2.07	0.54
1:B:41:LEU:HD23	1:B:143:PRO:HB3	1.89	0.54
1:B:307:LYS:HB3	1:B:307:LYS:HZ3	1.72	0.54
1:A:71:GLU:OE2	1:A:73:ARG:NH1	2.41	0.54
1:B:337:PHE:CE1	1:B:351:LEU:HD21	2.43	0.54
1:B:232:ILE:HG22	1:B:233:GLN:HG3	1.87	0.54
1:B:355:ASN:N	1:B:356:PRO:HD3	2.22	0.54
1:A:170:ILE:HD12	1:A:170:ILE:N	2.22	0.54
1:B:383:GLU:HB3	1:B:384:PRO:CD	2.32	0.54
1:A:127:GLY:HA3	1:A:213:PHE:CZ	2.43	0.54
1:A:331:SER:CB	1:A:332:PRO:HD2	2.38	0.54
1:A:356:PRO:HB3	1:A:367:ILE:HD12	1.90	0.54
1:A:183:MET:HG2	1:A:287:LEU:HD23	1.89	0.53
1:A:357:ILE:CG1	1:A:357:ILE:O	2.54	0.53
1:A:331:SER:CB	1:A:332:PRO:CD	2.85	0.53
1:B:20:TRP:HA	1:B:287:LEU:O	2.09	0.53
1:B:41:LEU:CD2	1:B:143:PRO:HB3	2.39	0.53
1:B:125:MET:HE1	1:B:260:MET:HE2	1.90	0.53
1:B:288:ARG:HG2	1:B:288:ARG:NH1	2.24	0.53
1:A:183:MET:HG2	1:A:287:LEU:CD2	2.37	0.53
1:A:330:GLY:N	5:A:2034:HOH:O	2.41	0.53
1:A:2:ARG:CZ	1:A:6:ILE:HD11	2.38	0.53
1:B:383:GLU:CB	1:B:384:PRO:HD3	2.31	0.53
1:B:170:ILE:HD12	1:B:170:ILE:N	2.24	0.52
1:B:24:VAL:C	1:B:25:LEU:HD23	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:ILE:O	1:B:320:ILE:HG12	2.08	0.52
1:A:71:GLU:HG3	1:A:80:PRO:CB	2.38	0.52
1:B:356:PRO:HB3	1:B:367:ILE:CD1	2.40	0.52
1:A:355:ASN:N	1:A:356:PRO:HD3	2.24	0.52
1:B:393:LYS:HG3	5:B:2068:HOH:O	2.09	0.52
1:A:196:MET:HB2	5:A:2014:HOH:O	2.09	0.51
1:B:183:MET:HG2	1:B:287:LEU:HD23	1.91	0.51
1:A:383:GLU:HB3	1:A:384:PRO:CD	2.37	0.51
1:B:27:HIS:HD2	1:B:280:THR:HB	1.74	0.51
1:B:360:GLU:O	1:B:361:LYS:C	2.54	0.51
1:A:378:ILE:CG2	1:A:380:ILE:HD11	2.41	0.51
1:B:127:GLY:HA3	1:B:213:PHE:CZ	2.45	0.51
1:B:331:SER:CB	1:B:332:PRO:HD2	2.40	0.51
1:B:182:THR:HG22	1:B:288:ARG:HG3	1.93	0.50
1:B:191:LEU:HD12	1:B:192:ASP:N	2.24	0.50
1:A:191:LEU:CD1	1:A:192:ASP:H	2.23	0.50
1:A:173:ALA:O	1:A:180:THR:HG23	2.10	0.50
1:A:173:ALA:HB3	1:A:181:VAL:HG12	1.94	0.50
1:A:182:THR:HG22	1:A:288:ARG:HG3	1.94	0.50
1:B:83:ASN:HB2	5:B:2016:HOH:O	2.11	0.50
1:A:27:HIS:HD2	1:A:280:THR:HB	1.76	0.50
1:A:181:VAL:HA	5:A:2023:HOH:O	2.10	0.50
1:A:61:ILE:CD1	1:A:123:LYS:HG2	2.39	0.50
1:A:240:PHE:CE2	1:A:250:VAL:HG22	2.47	0.50
1:B:183:MET:HG2	1:B:287:LEU:CD2	2.41	0.50
1:B:173:ALA:O	1:B:180:THR:HG23	2.11	0.50
1:B:125:MET:HE1	1:B:260:MET:SD	2.51	0.50
1:A:80:PRO:HB2	1:A:114:VAL:HG12	1.92	0.49
1:B:191:LEU:HD21	1:B:196:MET:HE2	1.94	0.49
1:A:191:LEU:HD12	1:A:192:ASP:N	2.26	0.49
1:B:296:GLY:C	1:B:298:SER:H	2.18	0.49
1:A:48:THR:CB	1:A:280:THR:HG21	2.42	0.49
1:A:357:ILE:O	1:A:357:ILE:HG12	2.12	0.49
1:A:360:GLU:O	1:A:361:LYS:C	2.56	0.49
1:B:2:ARG:CZ	1:B:6:ILE:HD11	2.43	0.49
1:A:302:CYS:HB3	1:A:326:TYR:CZ	2.48	0.49
1:A:296:GLY:C	1:A:298:SER:H	2.21	0.48
1:A:346:HIS:HA	5:A:2036:HOH:O	2.12	0.48
1:B:125:MET:HB3	1:B:201:MET:HG2	1.94	0.48
1:A:100:GLY:H	1:A:103:ASN:ND2	2.12	0.48
1:B:191:LEU:CD1	1:B:192:ASP:H	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:THR:HA	1:A:82:LEU:HD11	1.94	0.48
1:A:393:LYS:HG2	1:A:394:LYS:N	2.28	0.48
1:B:24:VAL:O	1:B:25:LEU:HD23	2.13	0.48
1:B:191:LEU:CD2	1:B:196:MET:HE2	2.44	0.48
1:A:323:ARG:HB2	1:A:366:ASN:ND2	2.29	0.48
1:A:153:ASN:OD1	1:A:155:THR:HB	2.14	0.48
1:B:100:GLY:H	1:B:103:ASN:ND2	2.12	0.48
1:B:173:ALA:HB3	1:B:181:VAL:HG12	1.96	0.48
1:A:48:THR:HG21	1:A:280:THR:HG23	1.95	0.47
1:A:26:GLU:O	1:A:29:SER:HB3	2.14	0.47
1:A:383:GLU:CB	1:A:384:PRO:HD3	2.35	0.47
1:B:2:ARG:HD2	1:B:44:GLU:OE1	2.14	0.47
1:B:71:GLU:HG3	1:B:80:PRO:HB3	1.96	0.47
1:B:80:PRO:HB2	1:B:114:VAL:HG12	1.95	0.47
1:B:46:ILE:HG12	1:B:140:VAL:CG2	2.37	0.47
1:B:202:LYS:HE2	1:B:202:LYS:HA	1.97	0.47
1:A:221:LEU:CD1	1:A:228:GLY:HA2	2.44	0.47
1:A:46:ILE:HG12	1:A:140:VAL:CG2	2.41	0.47
1:B:153:ASN:OD1	1:B:155:THR:HB	2.15	0.47
1:B:280:THR:O	1:B:280:THR:CG2	2.61	0.47
1:A:61:ILE:HD11	1:A:123:LYS:CG	2.40	0.47
1:A:337:PHE:CE1	1:A:351:LEU:HD21	2.50	0.47
1:B:48:THR:CB	1:B:280:THR:HG21	2.45	0.46
1:A:202:LYS:HE2	1:A:202:LYS:HA	1.97	0.46
1:A:8:ASN:HD22	1:A:29:SER:HA	1.79	0.46
1:B:310:LYS:HB3	1:B:323:ARG:HB3	1.96	0.46
1:B:71:GLU:HG3	1:B:80:PRO:CB	2.46	0.46
1:B:98:ASP:O	1:B:99:ARG:HD2	2.15	0.46
1:A:382:VAL:HG12	1:A:383:GLU:N	2.30	0.46
1:B:26:GLU:O	1:B:29:SER:HB3	2.15	0.46
1:B:145:SER:OG	1:B:147:GLU:HB2	2.16	0.46
1:B:188:ARG:HA	1:B:188:ARG:HD2	1.78	0.46
1:B:103:ASN:C	1:B:103:ASN:HD22	2.23	0.46
1:B:211:GLN:CA	1:B:211:GLN:HE21	2.28	0.46
1:A:103:ASN:HD22	1:A:103:ASN:C	2.24	0.45
1:A:24:VAL:O	1:A:25:LEU:HD23	2.16	0.45
1:A:2:ARG:HD2	1:A:44:GLU:OE1	2.17	0.45
1:A:48:THR:HG21	1:A:280:THR:HG21	1.98	0.45
1:A:125:MET:HB3	1:A:201:MET:HG2	1.98	0.45
1:A:188:ARG:HA	1:A:188:ARG:HD2	1.81	0.45
1:A:207:LEU:HD12	1:A:207:LEU:HA	1.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:PHE:CD1	1:A:119:PHE:C	2.95	0.45
1:A:376:SER:C	5:A:2043:HOH:O	2.59	0.45
1:B:70:THR:HA	1:B:82:LEU:HD11	1.98	0.45
2:C:1:NAG:H61	2:C:2:NAG:N2	2.32	0.45
1:B:61:ILE:CD1	1:B:123:LYS:HG2	2.43	0.45
1:B:305:LYS:HA	5:B:2066:HOH:O	2.16	0.45
1:A:98:ASP:O	1:A:99:ARG:HD2	2.16	0.44
1:B:393:LYS:HG2	1:B:394:LYS:N	2.32	0.44
1:A:211:GLN:CA	1:A:211:GLN:HE21	2.29	0.44
1:A:306:PHE:CZ	1:A:335:ILE:HG12	2.52	0.44
1:A:377:TYR:HB3	1:A:379:ILE:CD1	2.47	0.44
1:B:73:ARG:HD3	5:B:2010:HOH:O	2.17	0.44
1:A:145:SER:OG	1:A:147:GLU:HB2	2.18	0.44
1:B:71:GLU:CG	1:B:81:THR:H	2.31	0.44
1:A:378:ILE:HG22	1:A:380:ILE:HD11	1.99	0.44
1:B:240:PHE:CE2	1:B:250:VAL:CG2	3.00	0.44
1:A:337:PHE:CE2	1:A:380:ILE:HD12	2.52	0.43
1:B:71:GLU:HG2	1:B:81:THR:O	2.18	0.43
1:A:8:ASN:ND2	1:A:29:SER:HA	2.33	0.43
1:B:323:ARG:HB2	1:B:366:ASN:ND2	2.33	0.43
1:B:302:CYS:HB3	1:B:326:TYR:CZ	2.53	0.43
1:A:148:GLU:CD	1:A:364:PRO:HD2	2.44	0.43
1:A:280:THR:CG2	1:A:280:THR:O	2.64	0.43
1:B:101:TRP:CD1	1:B:101:TRP:N	2.86	0.43
1:B:119:PHE:CD1	1:B:119:PHE:C	2.95	0.43
1:B:48:THR:HG21	1:B:280:THR:HG23	1.99	0.43
1:A:52:GLN:HA	1:A:52:GLN:NE2	2.34	0.43
1:B:48:THR:HG21	1:B:280:THR:HG21	2.01	0.43
1:B:96:MET:O	1:B:242:ASN:ND2	2.48	0.43
1:A:34:MET:HG2	1:A:40:THR:OG1	2.20	0.42
1:B:379:ILE:HD13	1:B:379:ILE:N	2.33	0.42
1:A:155:THR:HG22	1:A:157:LYS:HB2	2.01	0.42
1:A:278:LEU:HD22	1:B:243:PRO:HG3	2.01	0.42
1:A:46:ILE:O	1:A:46:ILE:HG22	2.19	0.42
1:A:71:GLU:CG	1:A:81:THR:H	2.31	0.42
1:B:52:GLN:HA	1:B:52:GLN:HE21	1.80	0.42
1:A:168:SER:O	1:A:169:SER:OG	2.33	0.42
1:B:155:THR:HG22	1:B:157:LYS:HB2	2.02	0.42
1:A:21:VAL:HG22	1:A:287:LEU:HB2	2.02	0.42
1:A:84:GLU:HG2	1:A:90:PHE:CE2	2.55	0.42
1:A:93:LYS:HB3	1:A:240:PHE:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:SER:HA	5:A:2039:HOH:O	2.19	0.42
1:B:34:MET:HG2	1:B:40:THR:OG1	2.20	0.42
1:B:41:LEU:HD11	1:B:292:LEU:HD11	2.01	0.42
1:B:195:GLU:OE1	1:B:195:GLU:HA	2.20	0.42
1:A:100:GLY:N	1:A:103:ASN:HD21	2.16	0.42
1:B:305:LYS:HE2	1:B:385:GLY:HA3	2.02	0.41
1:A:59:TYR:CD1	1:A:218:LEU:HB2	2.54	0.41
1:A:270:ILE:HD12	4:A:1400:BOG:H7'1	2.01	0.41
1:A:342:LEU:HA	5:A:2043:HOH:O	2.20	0.41
1:A:79:GLU:HA	1:A:80:PRO:HD3	1.87	0.41
1:B:125:MET:HE1	1:B:260:MET:CE	2.50	0.41
1:A:170:ILE:HG22	1:A:171:THR:N	2.35	0.41
1:A:155:THR:CG2	1:A:157:LYS:HB2	2.51	0.41
1:B:155:THR:CG2	1:B:157:LYS:HB2	2.50	0.41
1:B:79:GLU:HA	1:B:80:PRO:HD3	1.85	0.41
1:A:297:MET:HA	1:A:334:LYS:NZ	2.34	0.41
1:A:237:LEU:HD23	1:A:237:LEU:HA	1.88	0.41
1:B:168:SER:O	1:B:169:SER:OG	2.35	0.41
1:B:84:GLU:HG2	1:B:90:PHE:CE2	2.56	0.41
1:B:88:LYS:HB2	1:B:230:ASN:ND2	2.36	0.41
1:B:131:GLN:O	1:B:132:PRO:C	2.64	0.41
1:A:155:THR:HG22	1:A:157:LYS:N	2.32	0.41
1:B:221:LEU:CD1	1:B:228:GLY:HA2	2.50	0.41
1:B:21:VAL:HG22	1:B:287:LEU:HB2	2.03	0.40
1:B:382:VAL:HG12	1:B:383:GLU:N	2.36	0.40
1:B:125:MET:HE2	1:B:218:LEU:CD1	2.52	0.40
1:A:175:LEU:O	1:A:176:THR:C	2.64	0.40
1:A:307:LYS:NZ	1:A:307:LYS:CB	2.85	0.40
1:B:207:LEU:HA	1:B:207:LEU:HD12	1.82	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	392/394 (100%)	354 (90%)	32 (8%)	6 (2%)	8	12
1	B	392/394 (100%)	352 (90%)	33 (8%)	7 (2%)	6	9
All	All	784/788 (100%)	706 (90%)	65 (8%)	13 (2%)	7	10

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	383	GLU
1	B	383	GLU
1	A	331	SER
1	B	331	SER
1	A	166	PRO
1	A	188	ARG
1	B	166	PRO
1	B	188	ARG
1	A	332	PRO
1	B	332	PRO
1	B	280	THR
1	A	384	PRO
1	B	384	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	342/342 (100%)	310 (91%)	32 (9%)	8	13
1	B	342/342 (100%)	309 (90%)	33 (10%)	8	12
All	All	684/684 (100%)	619 (90%)	65 (10%)	8	13

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	6	ILE
1	A	30	CYS

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Mol	Chain	Res	Type
1	A	46	ILE
1	A	56	LEU
1	A	64	LYS
1	A	70	THR
1	A	93	LYS
1	A	103	ASN
1	A	129	ILE
1	A	131	GLN
1	A	155	THR
1	A	162	VAL
1	A	166	PRO
1	A	182	THR
1	A	211	GLN
1	A	235	GLU
1	A	238	VAL
1	A	249	ASP
1	A	252	VAL
1	A	253	LEU
1	A	283	LEU
1	A	290	ASP
1	A	292	LEU
1	A	307	LYS
1	A	320	ILE
1	A	332	PRO
1	A	357	ILE
1	A	359	THR
1	A	379	ILE
1	A	387	LEU
1	A	394	LYS
1	B	2	ARG
1	B	6	ILE
1	B	30	CYS
1	B	46	ILE
1	B	56	LEU
1	B	64	LYS
1	B	70	THR
1	B	93	LYS
1	B	103	ASN
1	B	129	ILE
1	B	131	GLN
1	B	155	THR
1	B	162	VAL

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Mol	Chain	Res	Type
1	B	166	PRO
1	B	182	THR
1	B	211	GLN
1	B	235	GLU
1	B	238	VAL
1	B	249	ASP
1	B	252	VAL
1	B	253	LEU
1	B	283	LEU
1	B	290	ASP
1	B	292	LEU
1	B	307	LYS
1	B	320	ILE
1	B	332	PRO
1	B	357	ILE
1	B	359	THR
1	B	378	ILE
1	B	379	ILE
1	B	387	LEU
1	B	394	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	37	ASN
1	A	52	GLN
1	A	103	ASN
1	A	131	GLN
1	A	200	GLN
1	A	211	GLN
1	A	256	GLN
1	A	316	GLN
1	A	325	GLN
1	A	346	HIS
1	A	366	ASN
1	A	390	ASN
1	B	8	ASN
1	B	37	ASN
1	B	52	GLN
1	B	86	GLN
1	B	103	ASN

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Mol	Chain	Res	Type
1	B	131	GLN
1	B	144	HIS
1	B	200	GLN
1	B	211	GLN
1	B	248	GLN
1	B	256	GLN
1	B	276	ASN
1	B	316	GLN
1	B	317	HIS
1	B	325	GLN
1	B	346	HIS
1	B	366	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 ⓘ

8 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	2,1	14,14,15	0.68	0	17,19,21	0.88	1 (5%)
2	NAG	C	2	2	14,14,15	0.75	0	17,19,21	1.02	2 (11%)
2	BMA	C	3	2	11,11,12	0.58	0	15,15,17	0.57	0
2	FUL	C	4	2	10,10,11	0.42	0	14,14,16	0.72	0
2	NAG	D	1	2,1	14,14,15	0.72	0	17,19,21	0.94	1 (5%)
2	NAG	D	2	2	14,14,15	0.87	1 (7%)	17,19,21	1.01	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BMA	D	3	2	11,11,12	0.51	0	15,15,17	0.55	0
2	FUL	D	4	2	10,10,11	0.58	0	14,14,16	0.72	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	2,1	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
2	FUL	C	4	2	-	-	0/1/1/1
2	NAG	D	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1
2	FUL	D	4	2	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	NAG	C1-C2	2.02	1.55	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	C2-N2-C7	-2.64	119.36	122.90
2	C	2	NAG	C4-C3-C2	2.15	114.17	111.02
2	D	2	NAG	C2-N2-C7	-2.13	120.05	122.90
2	C	1	NAG	C2-N2-C7	-2.09	120.09	122.90
2	D	2	NAG	C4-C3-C2	2.09	114.08	111.02
2	C	2	NAG	C2-N2-C7	-2.04	120.17	122.90

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6

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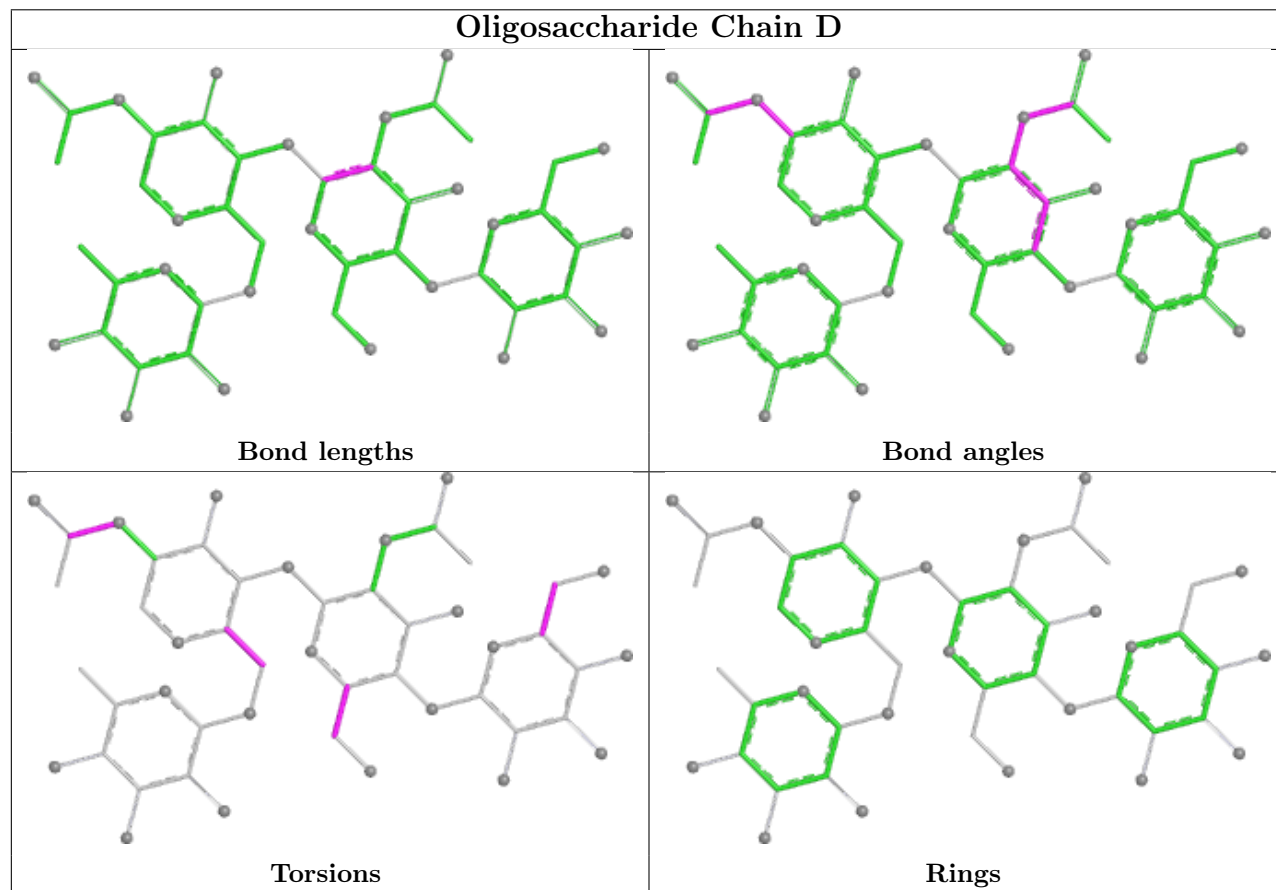
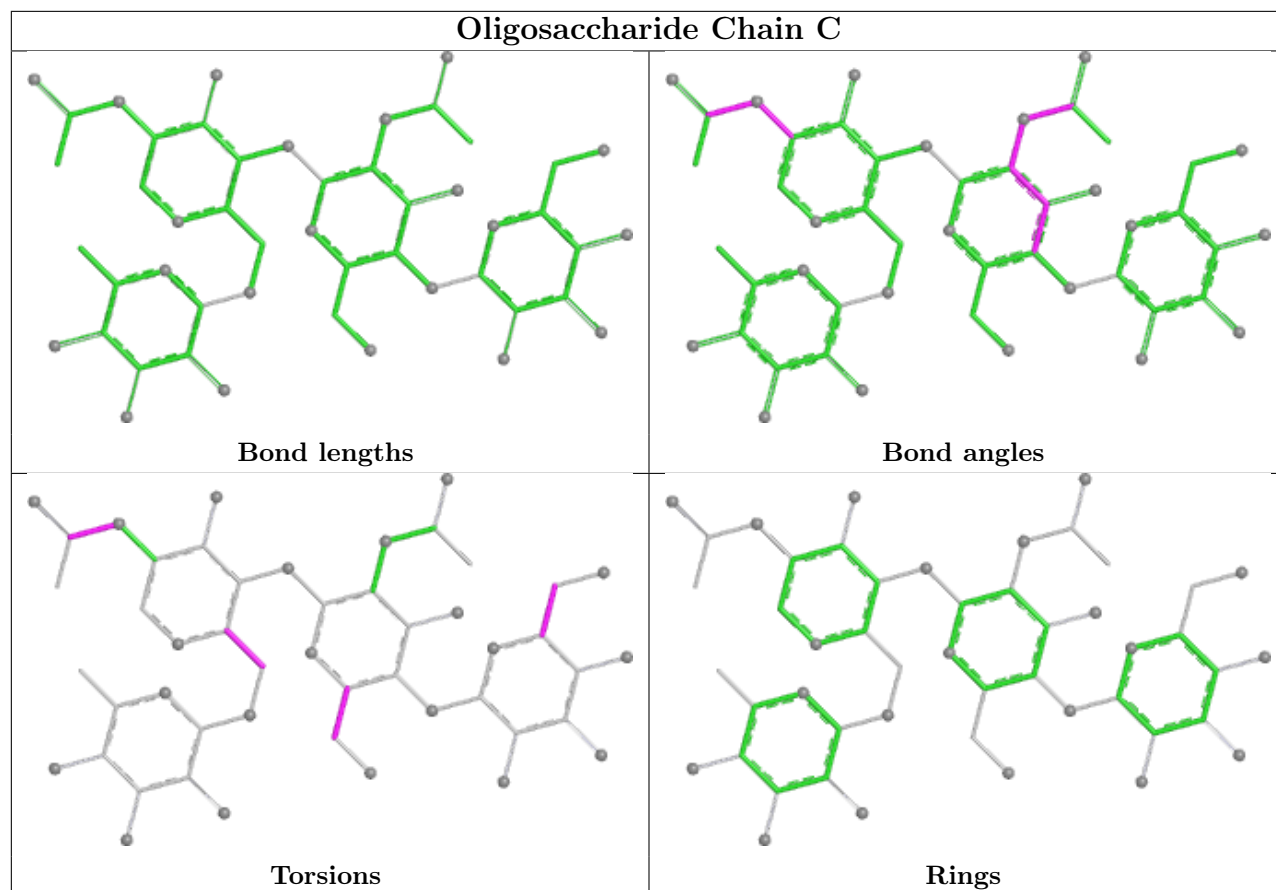
Mol	Chain	Res	Type	Atoms
2	D	3	BMA	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	D	3	BMA	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2

There are no ring outliers.

6 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3	BMA	1	0
2	C	3	BMA	1	0
2	D	1	NAG	1	0
2	C	2	NAG	3	0
2	D	2	NAG	2	0
2	C	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

4 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
4	BOG	A	1400	-	20,20,20	1.80	1 (5%)	25,25,25	1.06	2 (8%)
4	BOG	B	1400	-	20,20,20	1.65	1 (5%)	25,25,25	1.61	4 (16%)
3	NAG	B	1395	1	14,14,15	0.58	0	17,19,21	0.77	0
3	NAG	A	1395	1	14,14,15	0.75	1 (7%)	17,19,21	0.66	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	BOG	A	1400	-	-	8/11/31/31	0/1/1/1
4	BOG	B	1400	-	-	7/11/31/31	0/1/1/1
3	NAG	B	1395	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1395	1	-	4/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1400	BOG	O1-C1'	6.90	1.61	1.43
4	B	1400	BOG	O1-C1'	6.62	1.61	1.43
3	A	1395	NAG	C1-C2	2.07	1.55	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1400	BOG	O1-C1-C2	-5.47	99.97	108.27
4	B	1400	BOG	O5-C1-O1	3.66	118.69	110.04
4	A	1400	BOG	C1'-O1-C1	-3.31	108.03	113.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1400	BOG	O1-C1'-C2'	-2.87	99.63	109.37
4	A	1400	BOG	O1-C1-C2	-2.57	104.37	108.27
4	B	1400	BOG	C1'-O1-C1	-2.43	109.53	113.68

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1400	BOG	C2'-C1'-O1-C1
4	B	1400	BOG	O5-C1-O1-C1'
4	B	1400	BOG	C2'-C1'-O1-C1
4	A	1400	BOG	O5-C1-O1-C1'
3	B	1395	NAG	O5-C5-C6-O6
3	B	1395	NAG	C4-C5-C6-O6
3	B	1395	NAG	C8-C7-N2-C2
3	A	1395	NAG	C8-C7-N2-C2
4	A	1400	BOG	O5-C5-C6-O6
4	B	1400	BOG	O5-C5-C6-O6
3	A	1395	NAG	O5-C5-C6-O6
3	A	1395	NAG	C4-C5-C6-O6
3	B	1395	NAG	O7-C7-N2-C2
4	A	1400	BOG	C1'-C2'-C3'-C4'
4	B	1400	BOG	C1'-C2'-C3'-C4'
4	A	1400	BOG	C2'-C3'-C4'-C5'
4	B	1400	BOG	C2'-C3'-C4'-C5'
3	A	1395	NAG	O7-C7-N2-C2
4	A	1400	BOG	C3'-C4'-C5'-C6'
4	B	1400	BOG	C3'-C4'-C5'-C6'
4	A	1400	BOG	C5'-C6'-C7'-C8'
4	B	1400	BOG	C5'-C6'-C7'-C8'
4	A	1400	BOG	O1-C1'-C2'-C3'

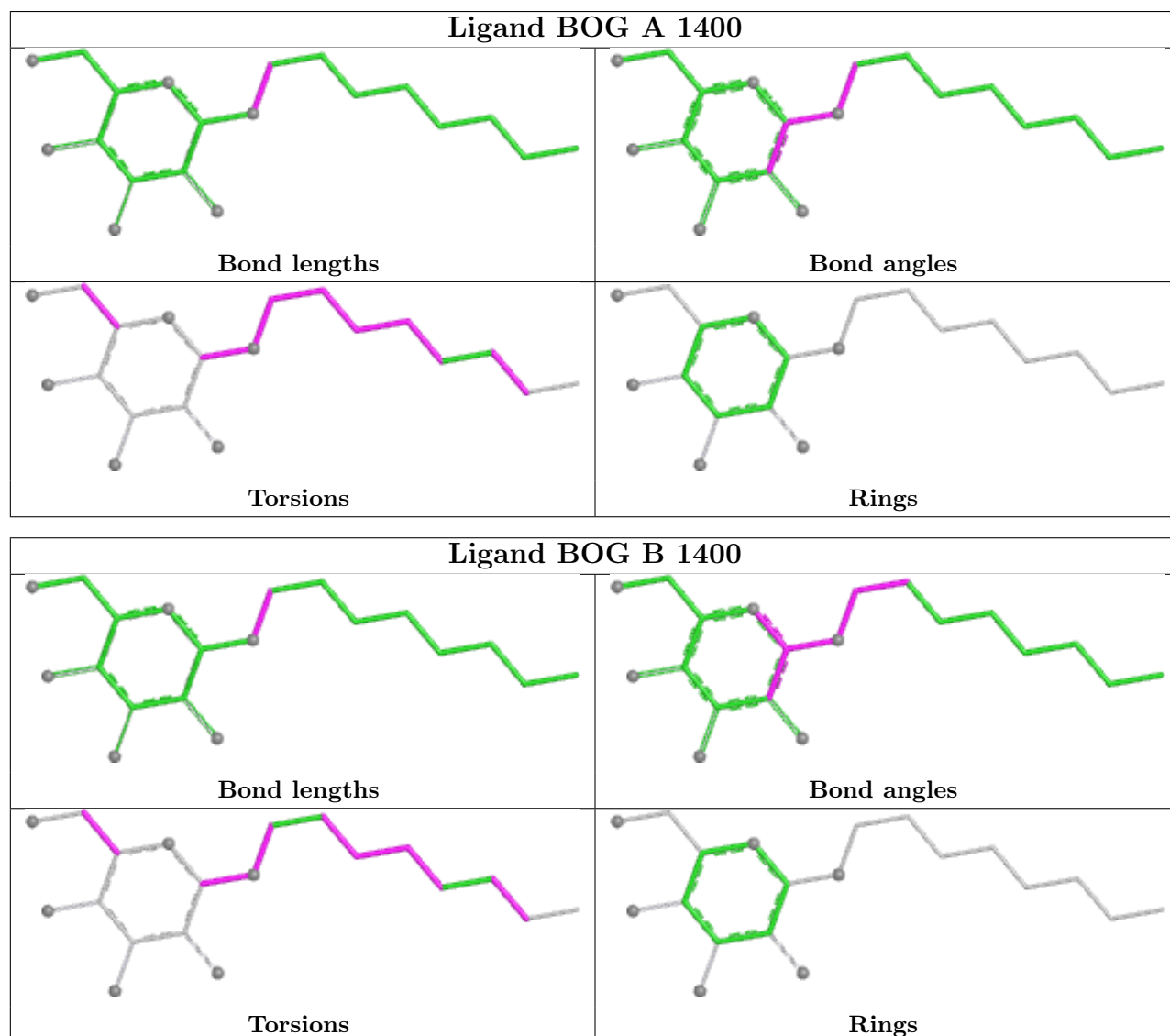
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1400	BOG	1	0
4	B	1400	BOG	1	0
3	B	1395	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 ⓘ

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	394/394 (100%)	1.13	76 (19%) 3 2	37, 80, 140, 164	0
1	B	394/394 (100%)	0.23	10 (2%) 58 54	25, 60, 102, 150	0
All	All	788/788 (100%)	0.68	86 (10%) 10 8	25, 70, 133, 164	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	25	LEU	4.8
1	A	162	VAL	4.8
1	A	277	LEU	4.2
1	A	342	LEU	4.1
1	A	23	ILE	3.9
1	A	347	VAL	3.9
1	A	181	VAL	3.6
1	A	178	TYR	3.6
1	A	287	LEU	3.5
1	A	183	MET	3.4
1	A	130	VAL	3.3
1	A	191	LEU	3.3
1	A	207	LEU	3.3
1	B	189	THR	3.3
1	A	292	LEU	3.2
1	A	170	ILE	3.2
1	A	50	ALA	3.2
1	A	137	TYR	3.2
1	A	173	ALA	3.1
1	A	283	LEU	3.0
1	A	12	VAL	3.0
1	A	15	VAL	3.0
1	A	193	PHE	3.0
1	A	285	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	189	THR	3.0
1	B	383	GLU	2.9
1	A	35	ALA	2.9
1	A	129	ILE	2.9
1	B	191	LEU	2.9
1	A	289	MET	2.9
1	A	45	LEU	2.9
1	A	132	PRO	2.9
1	B	193	PHE	2.9
1	A	127	GLY	2.9
1	A	344	LYS	2.8
1	A	171	THR	2.8
1	A	141	ILE	2.8
1	A	297	MET	2.8
1	A	24	VAL	2.7
1	A	272	MET	2.7
1	A	280	THR	2.6
1	A	20	TRP	2.5
1	B	272	MET	2.5
1	A	164	ILE	2.5
1	A	43	PHE	2.5
1	A	251	VAL	2.5
1	A	135	LEU	2.5
1	A	279	PHE	2.5
1	A	156	GLY	2.5
1	A	11	PHE	2.4
1	A	21	VAL	2.4
1	B	384	PRO	2.4
1	A	175	LEU	2.4
1	A	139	VAL	2.3
1	B	187	PRO	2.3
1	A	351	LEU	2.3
1	B	170	ILE	2.3
1	A	332	PRO	2.3
1	A	226	THR	2.2
1	A	273	SER	2.2
1	B	186	SER	2.2
1	A	179	GLY	2.2
1	A	284	LYS	2.2
1	A	294	LEU	2.2
1	B	19	SER	2.2
1	A	54	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	22	ASP	2.2
1	A	394	LYS	2.2
1	A	47	LYS	2.2
1	A	34	MET	2.1
1	A	14	GLY	2.1
1	A	190	GLY	2.1
1	A	299	TYR	2.1
1	A	185	CYS	2.1
1	A	161	GLU	2.1
1	A	345	ARG	2.1
1	A	167	GLN	2.1
1	A	377	TYR	2.1
1	A	157	LYS	2.1
1	A	159	GLY	2.1
1	A	301	MET	2.1
1	A	140	VAL	2.0
1	A	246	LYS	2.0
1	A	222	PRO	2.0
1	A	19	SER	2.0
1	A	186	SER	2.0

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

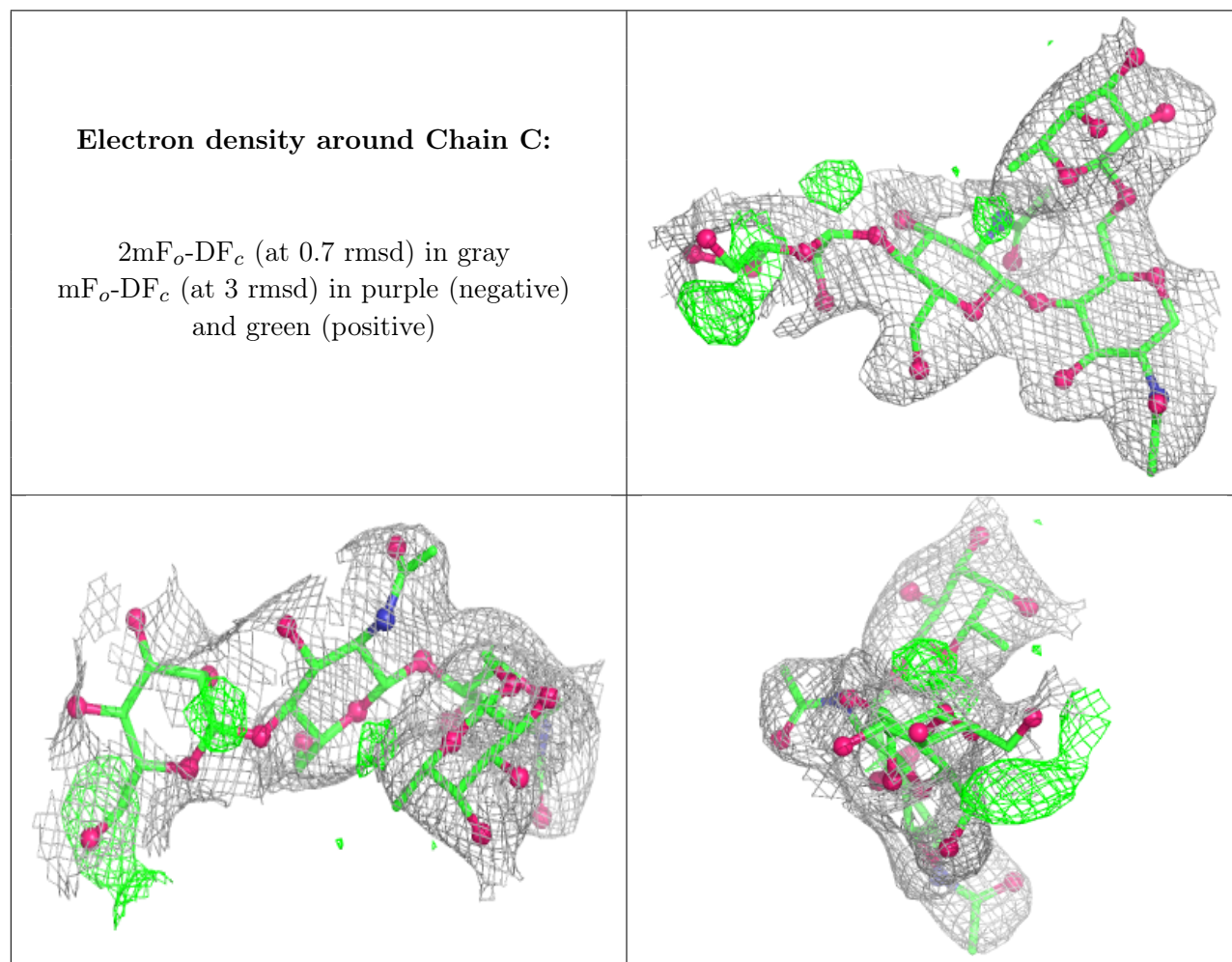
There are no non-standard protein/DNA/RNA residues in this entry.

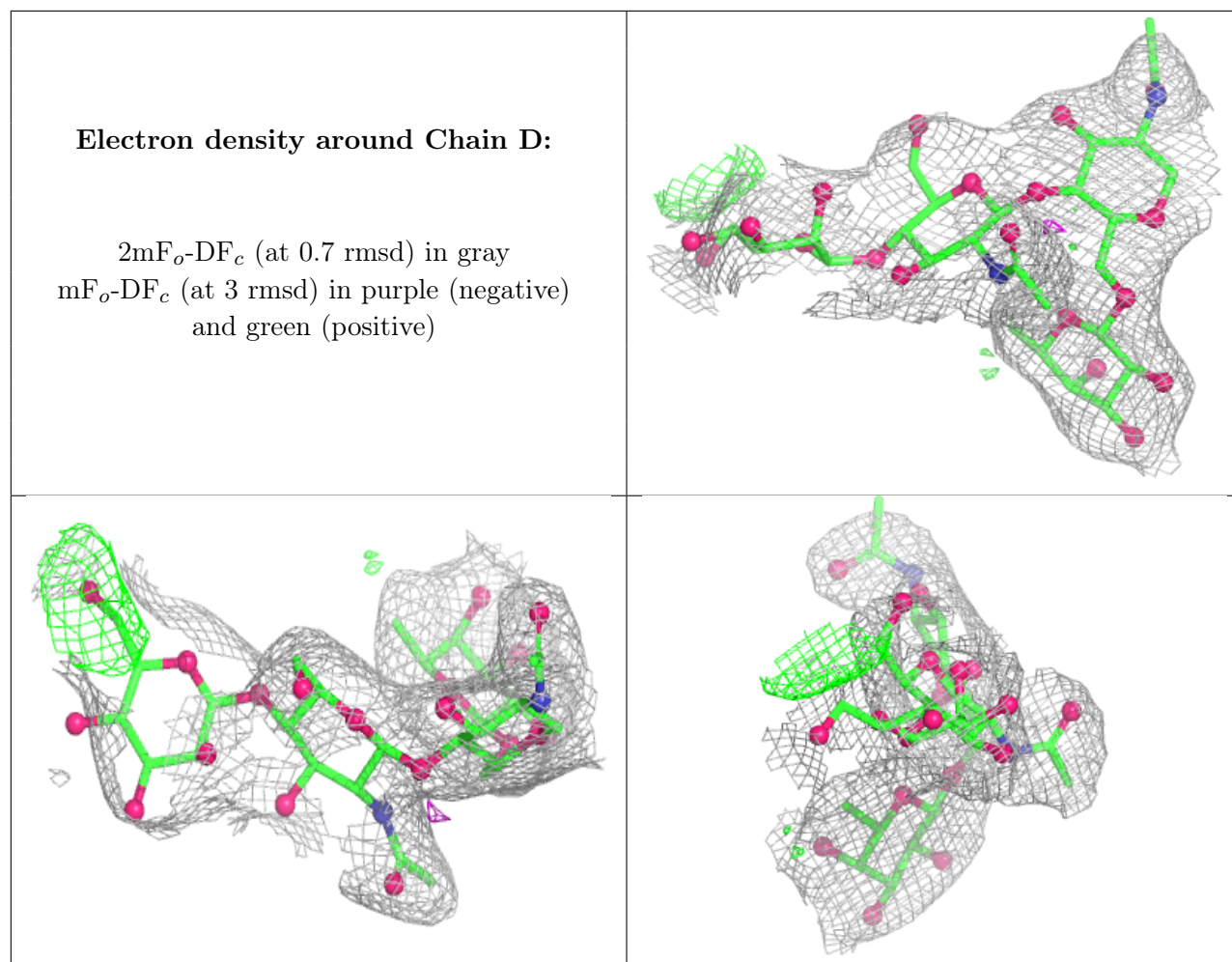
6.3 Carbohydrates [i](#)

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(Å ²)	Q<0.9
2	BMA	C	3	11/12	0.14	0.16	120,127,131,132	0
2	BMA	D	3	11/12	0.14	0.14	121,129,132,134	0
2	NAG	D	2	14/15	0.75	0.12	73,100,111,120	0
2	FUL	C	4	10/11	0.81	0.13	75,81,89,94	0
2	NAG	C	2	14/15	0.82	0.11	85,103,109,116	0
2	FUL	D	4	10/11	0.84	0.11	64,73,76,80	0
2	NAG	C	1	14/15	0.91	0.12	75,78,90,92	0
2	NAG	D	1	14/15	0.93	0.11	63,70,78,90	0

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





6.4 Ligands [i](#)

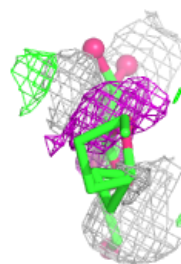
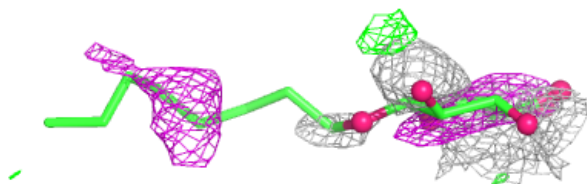
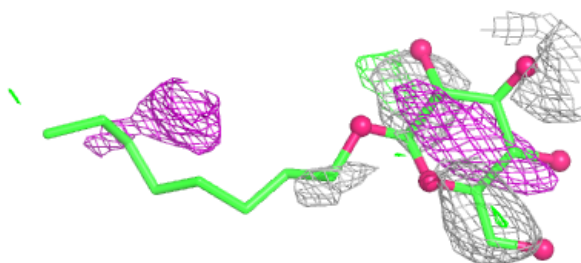
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	BOG	A	1400	20/20	0.74	0.28	119,124,153,153	0
3	NAG	A	1395	14/15	0.78	0.16	96,108,115,117	0
3	NAG	B	1395	14/15	0.79	0.13	57,81,87,91	0
4	BOG	B	1400	20/20	0.89	0.21	89,119,122,124	0

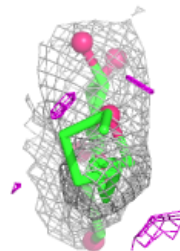
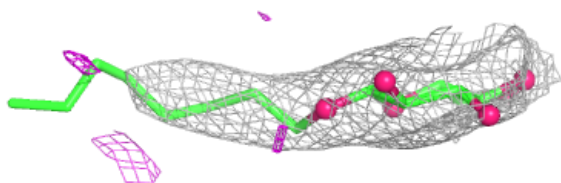
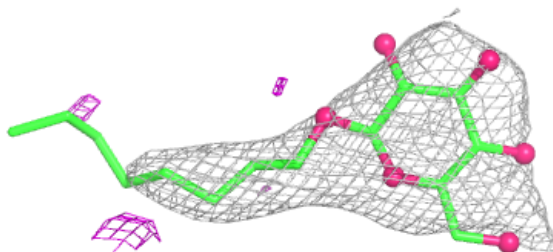
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BOG A 1400:

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

**Electron density around BOG B 1400:**

$2mF_o-DF_c$ (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.