



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:12 AM UTC

PDB ID : 2Z64 / pdb_00002z64
Title : Crystal structure of mouse TLR4 and mouse MD-2 complex
Authors : Lee, J.-O.; Kim, H.M.; Park, B.S.
Deposited on : 2007-07-22
Resolution : 2.84 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

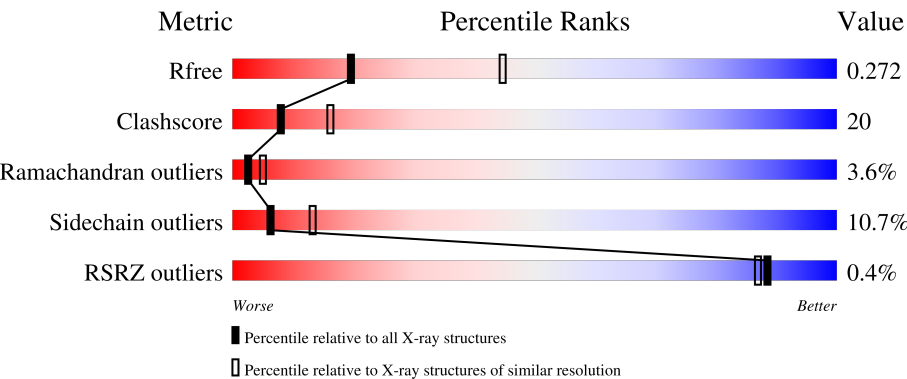
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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	599	54%38%8%
2	C	135	% 63%31%5%
3	B	2	50%50%
4	D	3	33%33%33%
4	E	3	33%67%

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Mol	Chain	Length	Quality of chain
5	F	4	

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
6	NAG	A	1441	X	-	-	-
6	NAG	A	1451	X	-	-	-
6	NAG	A	1471	X	-	-	-
6	NAG	A	1481	X	-	-	-
6	NAG	C	1511	X	-	-	-
6	NAG	C	1521	X	-	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6302 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 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	599	Total	C	N	O	S	0	0	0
			4774	3055	785	906	28			

- Molecule 2 is a protein called Lymphocyte antigen 96.

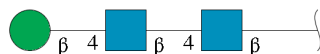
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	135	Total	C	N	O	S	0	0	0
			1093	706	182	198	7			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 4 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.



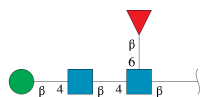
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

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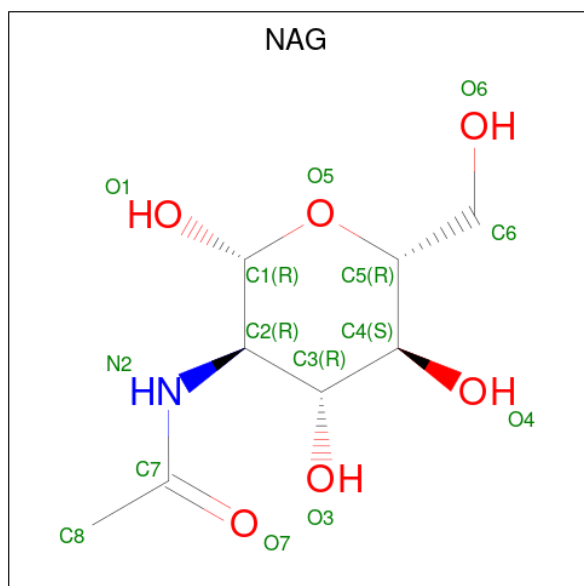
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 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
5	F	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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

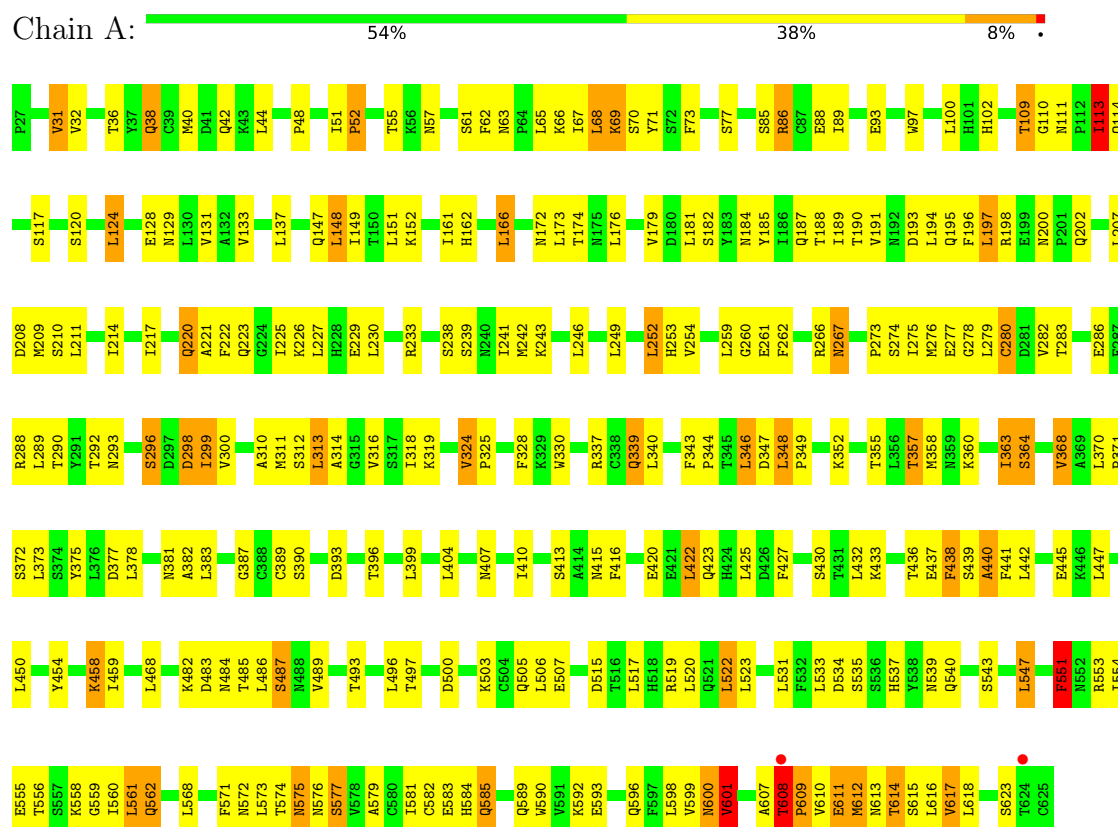
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	124	Total	O	0	0
			124	124		
7	C	30	Total	O	0	0
			30	30		

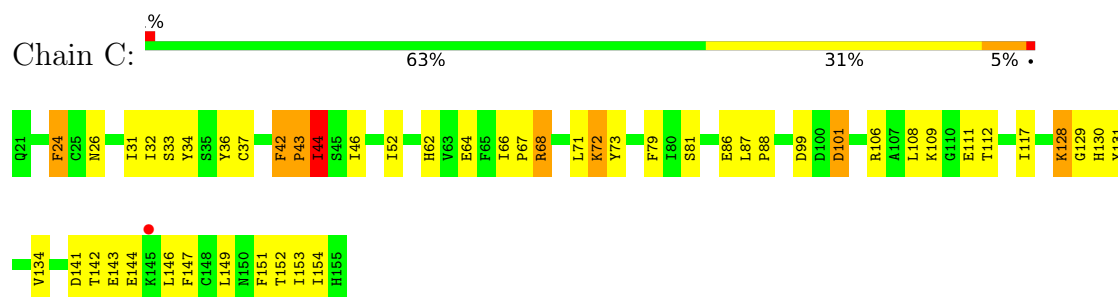
3 Residue-property plots

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 4



• Molecule 2: Lymphocyte antigen 96



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:  50% 50%



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

Chain D:  33% 33% 33%



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

Chain E:  33% 67%



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-D-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  25% 25% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.16Å 101.88Å 126.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.84 20.00 – 2.84	Depositor EDS
% Data completeness (in resolution range)	90.1 (20.00-2.84) 89.8 (20.00-2.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.46 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.242 , 0.290 0.229 , 0.272	Depositor DCC
R_{free} test set	1188 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å ²)	64.0	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6302	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, FUL, BMA

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	0.59	0/4874	0.92	6/6604 (0.1%)
2	C	0.68	0/1124	0.98	8/1519 (0.5%)
All	All	0.61	0/5998	0.93	14/8123 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	C	42	PHE	CA-C-N	7.97	128.02	119.89
2	C	42	PHE	C-N-CA	7.97	128.02	119.89
2	C	24	PHE	N-CA-C	6.58	118.94	109.14
1	A	348	LEU	CA-C-N	6.03	126.20	119.32
1	A	348	LEU	C-N-CA	6.03	126.20	119.32
2	C	117	ILE	CA-C-N	5.75	126.20	119.99
2	C	117	ILE	C-N-CA	5.75	126.20	119.99
1	A	166	LEU	CA-C-N	5.54	125.54	119.89
1	A	166	LEU	C-N-CA	5.54	125.54	119.89
2	C	130	HIS	N-CA-C	5.50	117.38	108.41
1	A	440	ALA	N-CA-C	5.40	122.31	110.80
1	A	601	VAL	CB-CA-C	-5.30	105.10	112.04
2	C	43	PRO	N-CA-C	5.05	119.14	111.11
2	C	44	ILE	CB-CA-C	-5.02	103.06	111.29

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	608	THR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4774	0	4729	206	0
2	C	1093	0	1048	33	0
3	B	28	0	25	1	0
4	D	39	0	34	1	0
4	E	39	0	34	2	0
5	F	49	0	43	2	0
6	A	84	0	78	0	0
6	C	42	0	39	1	0
7	A	124	0	0	7	0
7	C	30	0	0	2	0
All	All	6302	0	6030	239	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 20.

All (239) 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:383:LEU:HB3	1:A:407:ASN:HD22	1.00	1.16
1:A:608:THR:HB	1:A:609:PRO:HD3	1.21	1.12
1:A:109:THR:HG23	1:A:133:VAL:HB	1.25	1.10
1:A:383:LEU:HB3	1:A:407:ASN:ND2	1.68	1.06
1:A:608:THR:HB	1:A:609:PRO:CD	2.01	0.91
1:A:381:ASN:C	1:A:383:LEU:H	1.85	0.85
1:A:404:LEU:HD12	1:A:427:PHE:HE2	1.44	0.82
1:A:166:LEU:HD22	1:A:197:LEU:HD21	1.61	0.80
1:A:97:TRP:HB3	1:A:124:LEU:HD13	1.65	0.79
1:A:582:CYS:O	1:A:585:GLN:HG3	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ARG:HG3	7:A:1604:HOH:O	1.84	0.77
1:A:259:LEU:HD12	1:A:260:GLY:H	1.51	0.76
1:A:337:ARG:HA	1:A:358:MET:O	1.87	0.75
1:A:593:GLU:HB2	5:F:2:NAG:H81	1.70	0.73
1:A:36:THR:HG23	1:A:57:ASN:HB2	1.71	0.72
1:A:598:LEU:HB2	1:A:601:VAL:HG22	1.72	0.70
1:A:222:PHE:HD2	1:A:225:ILE:HD11	1.57	0.69
1:A:296:SER:O	1:A:299:ILE:HG22	1.94	0.67
2:C:32:ILE:HG12	2:C:153:ILE:HG13	1.75	0.67
1:A:189:ILE:HG22	1:A:194:LEU:HD11	1.75	0.67
1:A:381:ASN:O	1:A:383:LEU:N	2.27	0.66
1:A:423:GLN:HA	1:A:447:LEU:HA	1.76	0.66
2:C:44:ILE:HD12	2:C:149:LEU:HD11	1.78	0.66
2:C:87:LEU:HB3	2:C:88:PRO:HD2	1.78	0.66
1:A:387:GLY:HA2	1:A:413:SER:HB3	1.77	0.65
1:A:589:GLN:HG3	5:F:1:NAG:H5	1.78	0.65
3:B:1:NAG:H83	4:D:1:NAG:H3	1.79	0.64
1:A:89:ILE:H	1:A:111:ASN:HD22	1.45	0.63
1:A:346:LEU:O	1:A:368:VAL:HG23	1.99	0.63
1:A:612:MET:C	1:A:614:THR:H	2.06	0.63
1:A:319:LYS:HA	1:A:339:GLN:O	1.98	0.63
1:A:249:LEU:HB3	1:A:282:VAL:HG11	1.81	0.63
1:A:404:LEU:HD12	1:A:427:PHE:CE2	2.30	0.62
1:A:531:LEU:HA	1:A:553:ARG:O	1.98	0.62
1:A:556:THR:HG21	1:A:584:HIS:CG	2.34	0.62
2:C:67:PRO:HD2	2:C:111:GLU:O	1.99	0.62
4:E:1:NAG:H61	4:E:2:NAG:HN2	1.65	0.61
1:A:288:ARG:HD3	2:C:99:ASP:OD1	1.99	0.61
1:A:533:LEU:HD11	1:A:554:ILE:HD13	1.82	0.61
1:A:575:ASN:N	1:A:575:ASN:HD22	1.99	0.61
1:A:86:ARG:HH11	1:A:86:ARG:HB2	1.66	0.61
1:A:493:THR:HB	1:A:496:LEU:HD13	1.83	0.60
2:C:106:ARG:HB2	7:C:1540:HOH:O	2.01	0.60
1:A:581:ILE:HG22	1:A:583:GLU:H	1.66	0.60
1:A:137:LEU:HD12	1:A:161:ILE:HD11	1.83	0.60
1:A:222:PHE:CD2	1:A:225:ILE:HD11	2.38	0.59
1:A:355:THR:HA	1:A:377:ASP:HB3	1.85	0.58
1:A:226:LYS:HD2	7:A:1592:HOH:O	2.03	0.58
1:A:579:ALA:HA	1:A:608:THR:OG1	2.04	0.58
1:A:445:GLU:HB2	7:A:1550:HOH:O	2.03	0.57
2:C:72:LYS:O	2:C:73:TYR:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:LEU:HD13	1:A:506:LEU:HD11	1.87	0.57
1:A:458:LYS:O	1:A:458:LYS:HD3	2.05	0.57
1:A:290:THR:HA	1:A:314:ALA:O	2.04	0.56
2:C:68:ARG:O	2:C:109:LYS:HD3	2.06	0.56
1:A:276:MET:O	1:A:279:LEU:HB2	2.06	0.56
1:A:522:LEU:HD13	1:A:522:LEU:C	2.30	0.56
1:A:373:LEU:HB3	1:A:396:THR:HG21	1.87	0.56
1:A:387:GLY:HA2	1:A:413:SER:CB	2.35	0.56
1:A:381:ASN:C	1:A:383:LEU:N	2.57	0.56
1:A:363:ILE:HG13	1:A:383:LEU:HD23	1.88	0.55
1:A:117:SER:O	1:A:120:SER:OG	2.22	0.55
1:A:166:LEU:HD22	1:A:197:LEU:CD2	2.35	0.55
1:A:349:PRO:HA	1:A:371:PRO:HG2	1.88	0.55
1:A:279:LEU:HA	1:A:282:VAL:HG22	1.89	0.54
1:A:422:LEU:HD11	1:A:425:LEU:HD13	1.89	0.54
1:A:589:GLN:HE22	1:A:592:LYS:HD2	1.72	0.54
1:A:97:TRP:CB	1:A:124:LEU:HD13	2.38	0.54
1:A:311:MET:HE3	1:A:330:TRP:CZ2	2.43	0.54
1:A:166:LEU:CD2	1:A:197:LEU:HD21	2.35	0.54
1:A:615:SER:HB3	1:A:618:LEU:HD23	1.90	0.54
2:C:131:TYR:HB2	2:C:153:ILE:HB	1.90	0.54
1:A:276:MET:HG3	1:A:279:LEU:HD22	1.90	0.53
1:A:296:SER:C	1:A:298:ASP:H	2.17	0.53
1:A:459:ILE:HG21	1:A:489:VAL:HG11	1.91	0.53
1:A:42:GLN:HB2	1:A:44:LEU:HG	1.91	0.53
1:A:608:THR:CB	1:A:609:PRO:HD3	2.14	0.53
1:A:162:HIS:HA	1:A:185:TYR:O	2.08	0.53
1:A:577:SER:HA	1:A:607:ALA:HB2	1.90	0.53
1:A:195:GLN:HA	1:A:198:ARG:HG3	1.91	0.52
1:A:278:GLY:C	1:A:280:CYS:H	2.16	0.52
1:A:555:GLU:O	1:A:556:THR:HG23	2.10	0.52
1:A:574:THR:CG2	1:A:600:ASN:HD22	2.23	0.52
1:A:189:ILE:CG2	1:A:194:LEU:HD11	2.39	0.52
1:A:484:ASN:HB2	1:A:507:GLU:OE1	2.09	0.52
1:A:97:TRP:HB3	1:A:124:LEU:CD1	2.38	0.52
1:A:198:ARG:HG3	1:A:198:ARG:HH11	1.75	0.52
1:A:447:LEU:HD21	1:A:450:LEU:HB2	1.92	0.51
1:A:246:LEU:HD22	1:A:279:LEU:HD11	1.93	0.51
1:A:454:TYR:HH	1:A:503:LYS:HD2	1.75	0.51
1:A:179:VAL:HG12	1:A:181:LEU:HD11	1.93	0.51
1:A:497:THR:HA	1:A:520:LEU:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:GLN:HE22	1:A:40:MET:HE3	1.75	0.51
1:A:66:LYS:HE3	1:A:88:GLU:OE2	2.10	0.50
1:A:610:VAL:HG22	1:A:610:VAL:O	2.12	0.50
1:A:191:VAL:HG12	1:A:221:ALA:HA	1.93	0.50
1:A:226:LYS:O	1:A:227:LEU:HD23	2.11	0.50
1:A:220:GLN:HE21	1:A:223:GLN:HG2	1.76	0.50
1:A:238:SER:HB3	1:A:241:ILE:HG13	1.92	0.50
1:A:300:VAL:HG11	1:A:313:LEU:HD11	1.94	0.50
1:A:612:MET:C	1:A:614:THR:N	2.70	0.50
1:A:572:ASN:HA	1:A:599:VAL:HG12	1.94	0.50
1:A:278:GLY:C	1:A:280:CYS:N	2.71	0.49
1:A:577:SER:C	1:A:607:ALA:HB2	2.37	0.49
2:C:128:LYS:HD3	2:C:129:GLY:H	1.75	0.49
1:A:200:ASN:HA	1:A:202:GLN:OE1	2.13	0.49
1:A:551:PHE:N	1:A:551:PHE:CD1	2.80	0.49
1:A:69:LYS:HD3	1:A:93:GLU:OE1	2.12	0.49
1:A:194:LEU:C	1:A:196:PHE:H	2.21	0.49
1:A:572:ASN:ND2	1:A:599:VAL:HG11	2.28	0.49
4:E:1:NAG:H61	4:E:2:NAG:N2	2.28	0.49
1:A:517:LEU:HA	7:A:1505:HOH:O	2.12	0.49
1:A:577:SER:CA	1:A:607:ALA:HB2	2.43	0.49
2:C:87:LEU:HB3	2:C:88:PRO:CD	2.43	0.49
1:A:441:PHE:HB3	1:A:468:LEU:HD21	1.94	0.49
1:A:535:SER:HB2	1:A:559:GLY:O	2.13	0.49
1:A:583:GLU:OE1	1:A:583:GLU:HA	2.13	0.49
1:A:427:PHE:CG	1:A:432:LEU:HD21	2.48	0.48
1:A:220:GLN:HG2	1:A:223:GLN:HB2	1.94	0.48
1:A:313:LEU:HB3	1:A:316:VAL:HG21	1.96	0.48
1:A:571:PHE:HB3	1:A:598:LEU:HD23	1.95	0.48
1:A:267:ASN:OD1	1:A:293:ASN:HB2	2.13	0.48
1:A:343:PHE:HB2	1:A:364:SER:O	2.14	0.48
1:A:551:PHE:N	1:A:551:PHE:HD1	2.12	0.48
1:A:616:LEU:C	1:A:618:LEU:H	2.22	0.48
1:A:68:LEU:HD22	1:A:89:ILE:HD13	1.96	0.48
1:A:547:LEU:HB2	1:A:568:LEU:HD11	1.95	0.48
1:A:340:LEU:HD23	1:A:344:PRO:HD3	1.96	0.48
2:C:62:HIS:NE2	2:C:64:GLU:OE1	2.47	0.48
1:A:207:LEU:O	1:A:230:LEU:HA	2.14	0.47
1:A:172:ASN:O	1:A:174:THR:N	2.46	0.47
1:A:211:LEU:HD21	1:A:262:PHE:CE1	2.48	0.47
2:C:72:LYS:HD3	2:C:73:TYR:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LEU:O	1:A:67:ILE:N	2.47	0.47
1:A:52:PRO:HB2	1:A:55:THR:HG23	1.97	0.47
1:A:249:LEU:O	1:A:282:VAL:HG12	2.15	0.47
1:A:574:THR:HG21	1:A:600:ASN:ND2	2.30	0.47
1:A:575:ASN:HD22	1:A:575:ASN:H	1.62	0.47
2:C:24:PHE:HB3	2:C:33:SER:CB	2.44	0.47
1:A:482:LYS:HE3	1:A:487:SER:HB3	1.97	0.47
1:A:500:ASP:C	1:A:500:ASP:OD1	2.58	0.47
1:A:226:LYS:HG2	1:A:253:HIS:HB2	1.96	0.47
1:A:611:GLU:OE2	1:A:614:THR:HG21	2.15	0.47
1:A:73:PHE:HB3	1:A:100:LEU:HD21	1.96	0.47
1:A:420:GLU:CD	1:A:420:GLU:H	2.23	0.47
2:C:34:TYR:HB3	2:C:151:PHE:CD2	2.50	0.47
2:C:24:PHE:HE2	7:C:1543:HOH:O	1.98	0.46
2:C:79:PHE:HB2	2:C:134:VAL:CG2	2.45	0.46
1:A:238:SER:H	1:A:241:ILE:HD12	1.80	0.46
1:A:89:ILE:HG22	1:A:113:ILE:CG2	2.46	0.46
1:A:445:GLU:HG2	1:A:445:GLU:O	2.16	0.46
1:A:561:LEU:HB3	1:A:590:TRP:CD1	2.51	0.46
1:A:69:LYS:HG3	1:A:70:SER:H	1.81	0.46
1:A:581:ILE:HG22	1:A:582:CYS:N	2.30	0.46
1:A:352:LYS:HA	1:A:372:SER:O	2.16	0.46
1:A:195:GLN:NE2	7:A:1562:HOH:O	2.48	0.45
1:A:522:LEU:HD13	1:A:523:LEU:N	2.31	0.45
1:A:534:ASP:HB3	1:A:537:HIS:CD2	2.51	0.45
1:A:71:TYR:HA	7:A:1517:HOH:O	2.15	0.45
1:A:522:LEU:C	1:A:522:LEU:CD1	2.89	0.45
1:A:533:LEU:CD1	1:A:554:ILE:HD13	2.46	0.45
2:C:31:ILE:HG13	2:C:154:ILE:HB	1.98	0.45
2:C:142:THR:O	2:C:144:GLU:N	2.49	0.45
1:A:437:GLU:HB3	1:A:438:PHE:HD2	1.81	0.45
2:C:79:PHE:HB2	2:C:134:VAL:HG23	1.99	0.45
1:A:399:LEU:O	1:A:422:LEU:HA	2.17	0.45
1:A:454:TYR:OH	1:A:503:LYS:HD2	2.17	0.45
1:A:128:GLU:HA	1:A:151:LEU:HA	1.98	0.45
1:A:517:LEU:C	1:A:519:ARG:H	2.24	0.45
1:A:198:ARG:HG3	1:A:198:ARG:NH1	2.33	0.44
1:A:259:LEU:HD12	1:A:260:GLY:N	2.27	0.44
1:A:608:THR:CB	1:A:609:PRO:CD	2.84	0.44
1:A:496:LEU:HB3	1:A:520:LEU:HD13	1.99	0.44
2:C:101:ASP:OD1	2:C:101:ASP:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:GLN:NE2	1:A:223:GLN:HG2	2.32	0.44
1:A:220:GLN:HG2	1:A:223:GLN:CB	2.48	0.44
1:A:438:PHE:HD2	1:A:438:PHE:N	2.15	0.44
1:A:161:ILE:HB	1:A:184:ASN:OD1	2.17	0.44
1:A:288:ARG:HG3	1:A:312:SER:HB2	1.99	0.44
2:C:43:PRO:C	2:C:44:ILE:HG12	2.42	0.44
1:A:189:ILE:HB	1:A:217:ILE:HG23	1.99	0.44
1:A:241:ILE:HG13	1:A:241:ILE:H	1.68	0.44
1:A:415:ASN:O	1:A:416:PHE:HB2	2.18	0.44
1:A:77:SER:O	1:A:102:HIS:HD2	2.00	0.44
1:A:133:VAL:HG21	2:C:108:LEU:HD12	2.00	0.43
1:A:438:PHE:N	1:A:438:PHE:CD2	2.85	0.43
1:A:555:GLU:O	1:A:556:THR:CG2	2.66	0.43
1:A:68:LEU:HD12	1:A:68:LEU:HA	1.92	0.43
2:C:24:PHE:HB3	2:C:33:SER:HA	2.00	0.43
2:C:72:LYS:O	2:C:73:TYR:CB	2.66	0.43
2:C:147:PHE:C	2:C:147:PHE:CD2	2.96	0.43
1:A:599:VAL:HG22	1:A:600:ASN:ND2	2.34	0.43
1:A:194:LEU:HD12	1:A:194:LEU:H	1.83	0.43
1:A:239:SER:HB2	1:A:275:ILE:HD11	2.00	0.43
1:A:410:ILE:HD12	1:A:430:SER:HB3	2.00	0.43
2:C:36:TYR:OH	2:C:43:PRO:HA	2.19	0.43
2:C:66:ILE:HG12	2:C:112:THR:HA	2.01	0.43
1:A:390:SER:O	1:A:393:ASP:HB2	2.18	0.43
1:A:89:ILE:O	1:A:113:ILE:HG23	2.19	0.42
1:A:182:SER:HA	1:A:210:SER:O	2.19	0.42
1:A:293:ASN:ND2	7:A:1566:HOH:O	2.52	0.42
1:A:48:PRO:HB2	1:A:51:ILE:HG13	2.01	0.42
1:A:539:ASN:O	1:A:540:GLN:HB2	2.18	0.42
1:A:31:VAL:HG23	1:A:32:VAL:HG23	2.00	0.42
1:A:152:LYS:O	1:A:176:LEU:HD12	2.20	0.42
1:A:252:LEU:HG	1:A:254:VAL:HG23	2.01	0.42
1:A:296:SER:C	1:A:298:ASP:N	2.78	0.42
1:A:375:TYR:CE2	1:A:377:ASP:HB2	2.55	0.42
1:A:190:THR:O	1:A:193:ASP:N	2.51	0.42
1:A:61:SER:HB3	1:A:85:SER:HB2	2.01	0.42
1:A:316:VAL:HG12	1:A:318:ILE:H	1.85	0.42
1:A:274:SER:O	1:A:277:GLU:HB2	2.19	0.42
1:A:148:LEU:HD12	1:A:148:LEU:HA	1.88	0.42
1:A:324:VAL:HG12	1:A:348:LEU:HD21	2.01	0.42
1:A:44:LEU:N	1:A:63:ASN:OD1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:26:ASN:OD1	6:C:1501:NAG:N2	2.53	0.41
1:A:370:LEU:HA	1:A:371:PRO:HD2	1.75	0.41
1:A:242:MET:O	1:A:243:LYS:C	2.63	0.41
2:C:24:PHE:HB3	2:C:33:SER:HB3	2.02	0.41
1:A:131:VAL:HG13	1:A:133:VAL:HG23	2.02	0.41
1:A:531:LEU:HD23	1:A:553:ARG:HB2	2.02	0.41
1:A:222:PHE:HB3	1:A:252:LEU:HB2	2.03	0.41
1:A:286:GLU:HG3	1:A:310:ALA:CB	2.50	0.41
1:A:325:PRO:HG2	1:A:328:PHE:CD2	2.56	0.41
2:C:42:PHE:N	2:C:42:PHE:CD2	2.89	0.41
1:A:196:PHE:HD2	1:A:197:LEU:HD22	1.86	0.41
1:A:62:PHE:HE1	2:C:68:ARG:HA	1.86	0.41
1:A:249:LEU:HB3	1:A:282:VAL:CG1	2.50	0.41
1:A:261:GLU:OE2	1:A:267:ASN:HA	2.20	0.41
1:A:355:THR:HG22	1:A:357:THR:HG22	2.01	0.41
1:A:86:ARG:HH12	1:A:110:GLY:HA3	1.86	0.41
1:A:187:GLN:HA	1:A:214:ILE:HA	2.03	0.41
1:A:208:ASP:OD1	1:A:208:ASP:C	2.64	0.41
1:A:562:GLN:H	1:A:562:GLN:CD	2.29	0.41
1:A:113:ILE:H	1:A:113:ILE:HG12	1.75	0.40
1:A:573:LEU:O	1:A:576:ASN:ND2	2.54	0.40
2:C:31:ILE:HG13	2:C:31:ILE:O	2.21	0.40
1:A:137:LEU:HD13	1:A:137:LEU:C	2.46	0.40
1:A:179:VAL:HB	1:A:207:LEU:HD12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	597/599 (100%)	495 (83%)	79 (13%)	23 (4%)	2 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	133/135 (98%)	115 (86%)	15 (11%)	3 (2%)	5	10
All	All	730/734 (100%)	610 (84%)	94 (13%)	26 (4%)	2	5

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	382	ALA
1	A	440	ALA
1	A	608	THR
2	C	143	GLU
1	A	347	ASP
1	A	609	PRO
2	C	37	CYS
1	A	266	ARG
1	A	442	LEU
1	A	505	GLN
2	C	44	ILE
1	A	360	LYS
1	A	577	SER
1	A	613	ASN
1	A	623	SER
1	A	114	GLN
1	A	483	ASP
1	A	487	SER
1	A	551	PHE
1	A	560	ILE
1	A	612	MET
1	A	52	PRO
1	A	113	ILE
1	A	363	ILE
1	A	273	PRO
1	A	617	VAL

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	558/558 (100%)	498 (89%)	60 (11%)	6	13
2	C	122/122 (100%)	109 (89%)	13 (11%)	6	13
All	All	680/680 (100%)	607 (89%)	73 (11%)	6	13

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	VAL
1	A	38	GLN
1	A	68	LEU
1	A	69	LYS
1	A	86	ARG
1	A	109	THR
1	A	113	ILE
1	A	124	LEU
1	A	129	ASN
1	A	147	GLN
1	A	148	LEU
1	A	149	ILE
1	A	173	LEU
1	A	188	THR
1	A	197	LEU
1	A	209	MET
1	A	220	GLN
1	A	229	GLU
1	A	252	LEU
1	A	267	ASN
1	A	280	CYS
1	A	283	THR
1	A	289	LEU
1	A	292	THR
1	A	296	SER
1	A	298	ASP
1	A	299	ILE
1	A	313	LEU
1	A	324	VAL
1	A	339	GLN
1	A	346	LEU
1	A	357	THR
1	A	364	SER
1	A	368	VAL
1	A	378	LEU

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Mol	Chain	Res	Type
1	A	389	CYS
1	A	422	LEU
1	A	433	LYS
1	A	436	THR
1	A	438	PHE
1	A	439	SER
1	A	458	LYS
1	A	485	THR
1	A	515	ASP
1	A	522	LEU
1	A	543	SER
1	A	547	LEU
1	A	551	PHE
1	A	558	LYS
1	A	561	LEU
1	A	562	GLN
1	A	575	ASN
1	A	585	GLN
1	A	596	GLN
1	A	600	ASN
1	A	601	VAL
1	A	608	THR
1	A	611	GLU
1	A	614	THR
1	A	617	VAL
2	C	44	ILE
2	C	46	ILE
2	C	52	ILE
2	C	68	ARG
2	C	71	LEU
2	C	72	LYS
2	C	81	SER
2	C	86	GLU
2	C	101	ASP
2	C	128	LYS
2	C	141	ASP
2	C	146	LEU
2	C	152	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	102	HIS
1	A	111	ASN
1	A	114	GLN
1	A	147	GLN
1	A	155	ASN
1	A	195	GLN
1	A	220	GLN
1	A	223	GLN
1	A	228	HIS
1	A	235	ASN
1	A	240	ASN
1	A	247	GLN
1	A	248	ASN
1	A	255	HIS
1	A	293	ASN
1	A	339	GLN
1	A	401	HIS
1	A	407	ASN
1	A	428	GLN
1	A	484	ASN
1	A	521	GLN
1	A	527	HIS
1	A	537	HIS
1	A	539	ASN
1	A	575	ASN
1	A	584	HIS
1	A	589	GLN
1	A	594	GLN
1	A	596	GLN
1	A	600	ASN
2	C	83	ASN
2	C	98	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

12 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$
3	NAG	B	1	3,1	14,14,15	0.58	0	17,19,21	1.68	5 (29%)
3	NAG	B	2	3	14,14,15	0.58	0	17,19,21	2.56	3 (17%)
4	NAG	D	1	4,1	14,14,15	0.54	0	17,19,21	1.48	2 (11%)
4	NAG	D	2	4	14,14,15	0.45	0	17,19,21	0.80	0
4	BMA	D	3	4	11,11,12	0.62	0	15,15,17	1.01	2 (13%)
4	NAG	E	1	4,1	14,14,15	0.63	0	17,19,21	1.56	4 (23%)
4	NAG	E	2	4	14,14,15	0.42	0	17,19,21	1.34	3 (17%)
4	BMA	E	3	4	11,11,12	0.62	0	15,15,17	0.48	0
5	NAG	F	1	5	14,14,15	0.54	0	17,19,21	1.15	1 (5%)
5	NAG	F	2	5	14,14,15	0.59	0	17,19,21	1.48	3 (17%)
5	BMA	F	3	5	11,11,12	0.59	0	15,15,17	0.83	0
5	FUL	F	4	5	10,10,11	0.68	0	14,14,16	1.30	2 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	B	2	3	-	2/6/23/26	0/1/1/1
4	NAG	D	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	4/6/23/26	0/1/1/1
4	BMA	D	3	4	-	1/2/19/22	0/1/1/1
4	NAG	E	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	BMA	E	3	4	-	2/2/19/22	0/1/1/1
5	NAG	F	1	5	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	F	2	5	-	2/6/23/26	0/1/1/1
5	BMA	F	3	5	-	2/2/19/22	0/1/1/1
5	FUL	F	4	5	-	-	0/1/1/1

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2	NAG	C1-O5-C5	8.62	123.73	112.19
3	B	2	NAG	O5-C1-C2	4.61	118.42	111.29
4	D	1	NAG	O5-C1-C2	-4.37	104.53	111.29
4	E	1	NAG	C4-C3-C2	4.36	117.41	111.02
3	B	1	NAG	C1-O5-C5	4.17	117.78	112.19
5	F	4	FUL	C1-C2-C3	3.56	114.82	109.64
5	F	2	NAG	C1-C2-N2	3.16	115.41	110.43
4	E	2	NAG	C1-O5-C5	3.02	116.23	112.19
3	B	1	NAG	O5-C1-C2	-3.00	106.65	111.29
4	E	2	NAG	C4-C3-C2	-2.73	107.02	111.02
5	F	2	NAG	O5-C1-C2	-2.54	107.36	111.29
4	D	1	NAG	C2-N2-C7	-2.46	119.61	122.90
5	F	1	NAG	O5-C1-C2	-2.44	107.52	111.29
4	E	1	NAG	C1-C2-N2	-2.43	106.60	110.43
3	B	1	NAG	C2-N2-C7	-2.40	119.68	122.90
4	E	1	NAG	O4-C4-C3	-2.34	104.86	110.38
3	B	1	NAG	C4-C3-C2	2.32	114.42	111.02
4	D	3	BMA	C3-C4-C5	2.29	114.39	110.23
4	E	1	NAG	C1-O5-C5	2.26	115.21	112.19
3	B	1	NAG	O4-C4-C3	-2.25	105.06	110.38
5	F	2	NAG	C4-C3-C2	-2.24	107.73	111.02
5	F	4	FUL	C2-C3-C4	2.20	114.74	110.86
3	B	2	NAG	O5-C5-C4	2.10	115.94	110.83
4	D	3	BMA	C2-C3-C4	2.09	114.54	110.86
4	E	2	NAG	O5-C1-C2	-2.02	108.17	111.29

There are no chirality outliers.

All (24) torsion outliers are listed below:

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

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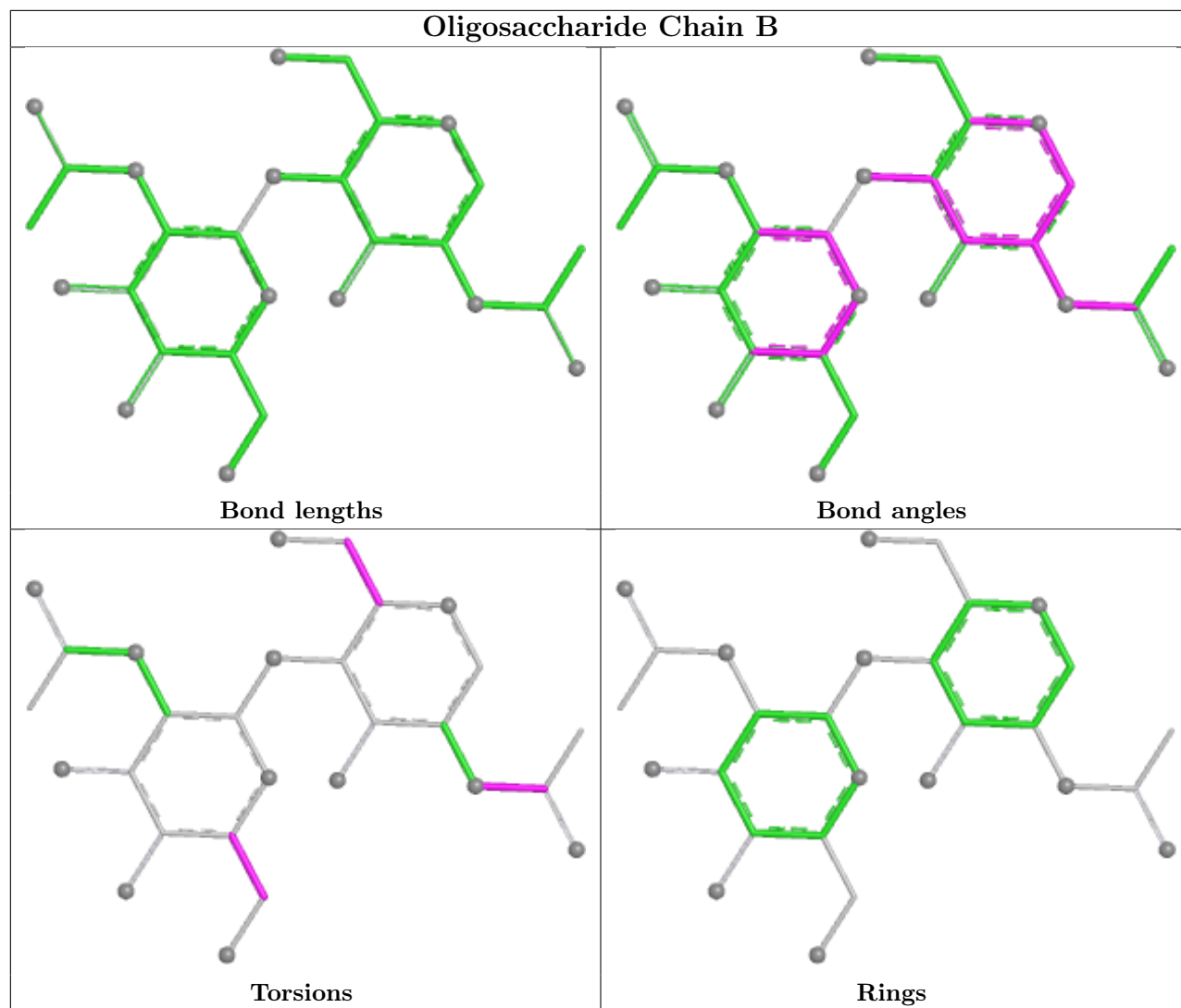
Mol	Chain	Res	Type	Atoms
5	F	1	NAG	C8-C7-N2-C2
5	F	1	NAG	O7-C7-N2-C2
5	F	2	NAG	C8-C7-N2-C2
5	F	2	NAG	O7-C7-N2-C2
4	D	2	NAG	C8-C7-N2-C2
5	F	3	BMA	O5-C5-C6-O6
3	B	1	NAG	C8-C7-N2-C2
3	B	1	NAG	O7-C7-N2-C2
4	E	3	BMA	O5-C5-C6-O6
3	B	1	NAG	O5-C5-C6-O6
3	B	1	NAG	C4-C5-C6-O6
4	E	3	BMA	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6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

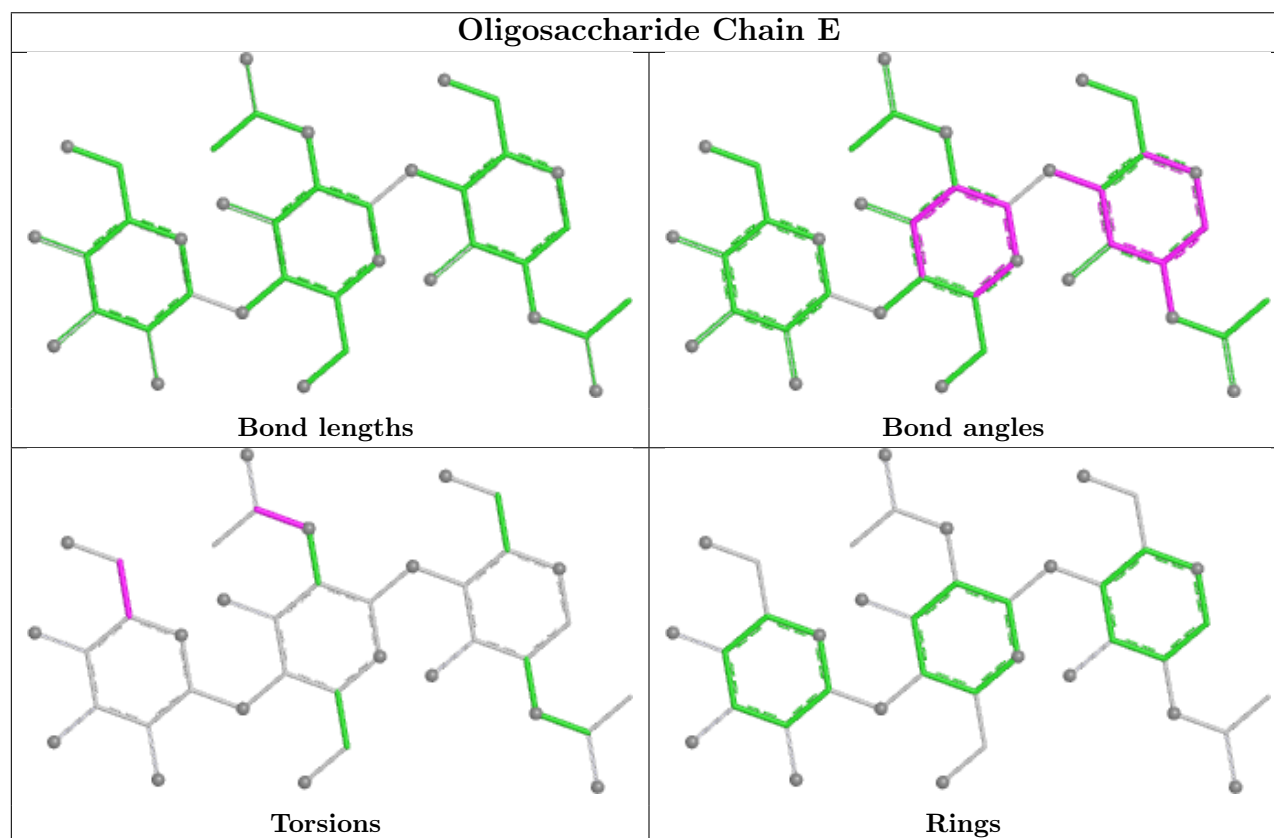
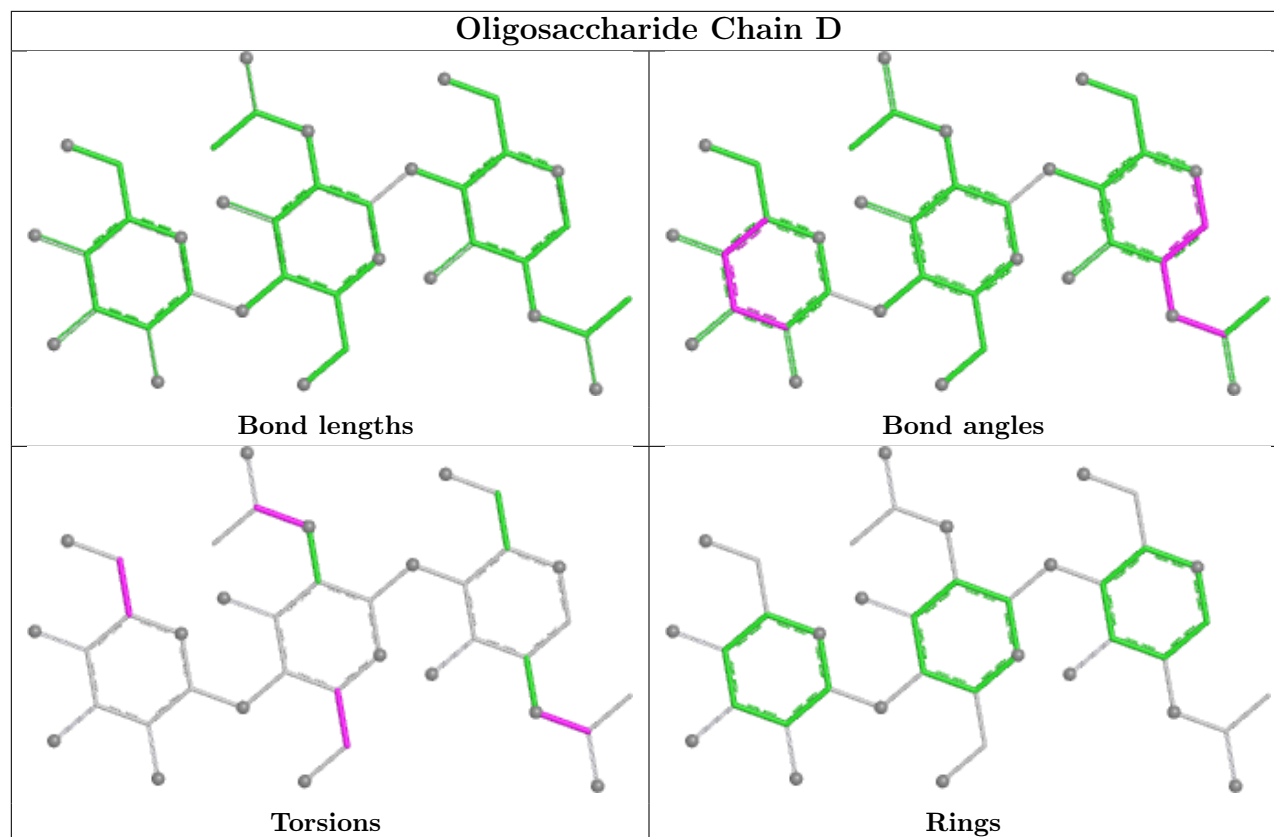
There are no ring outliers.

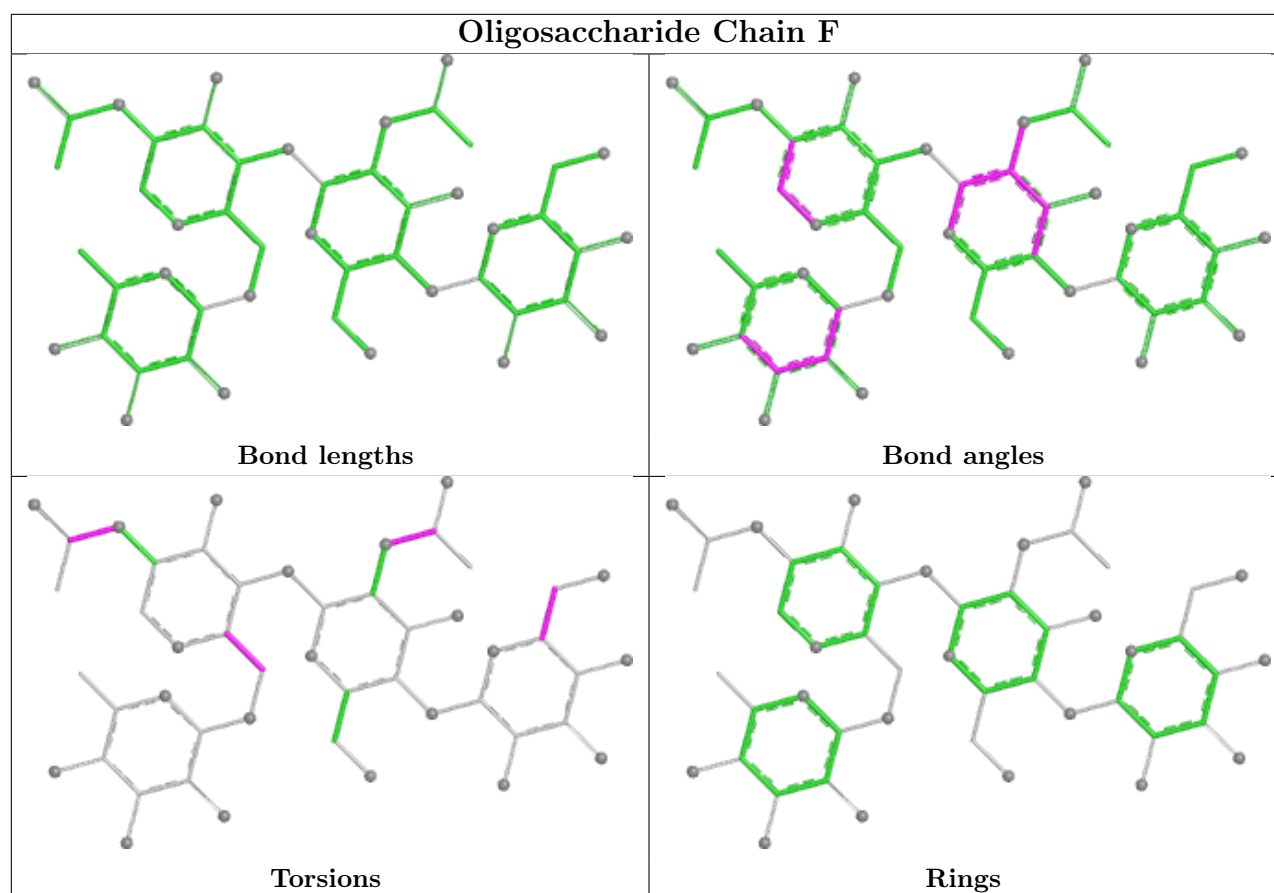
6 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	1	0
5	F	1	NAG	1	0
4	E	1	NAG	2	0
5	F	2	NAG	1	0
4	E	2	NAG	2	0
3	B	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.







5.6 Ligand geometry [i](#)

9 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	$\# Z > 2$
6	NAG	A	1451	1	14,14,15	0.49	0	17,19,21	1.38	2 (11%)
6	NAG	C	1521	2	14,14,15	0.76	0	17,19,21	1.16	1 (5%)
6	NAG	A	1471	1	14,14,15	0.52	0	17,19,21	1.15	1 (5%)
6	NAG	C	1501	2	14,14,15	0.78	1 (7%)	17,19,21	1.28	1 (5%)
6	NAG	C	1511	2	14,14,15	0.51	0	17,19,21	0.89	1 (5%)
6	NAG	A	1481	1	14,14,15	0.70	0	17,19,21	0.87	0
6	NAG	A	1491	1	14,14,15	0.63	0	17,19,21	1.16	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	1431	1	14,14,15	0.61	0	17,19,21	0.96	1 (5%)
6	NAG	A	1441	1	14,14,15	0.52	0	17,19,21	1.33	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	1451	1	1/1/5/7	3/6/23/26	0/1/1/1
6	NAG	C	1521	2	1/1/5/7	4/6/23/26	0/1/1/1
6	NAG	A	1471	1	1/1/5/7	2/6/23/26	0/1/1/1
6	NAG	C	1501	2	-	3/6/23/26	0/1/1/1
6	NAG	C	1511	2	1/1/5/7	2/6/23/26	0/1/1/1
6	NAG	A	1481	1	1/1/5/7	4/6/23/26	0/1/1/1
6	NAG	A	1491	1	-	4/6/23/26	0/1/1/1
6	NAG	A	1431	1	-	4/6/23/26	0/1/1/1
6	NAG	A	1441	1	1/1/5/7	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1501	NAG	C1-C2	2.40	1.55	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1501	NAG	C1-O5-C5	3.81	117.30	112.19
6	A	1451	NAG	O5-C1-C2	-3.56	105.78	111.29
6	A	1471	NAG	O5-C1-C2	-3.36	106.10	111.29
6	A	1491	NAG	C2-N2-C7	3.14	127.11	122.90
6	A	1431	NAG	C1-O5-C5	3.11	116.35	112.19
6	A	1451	NAG	C1-O5-C5	2.93	116.12	112.19
6	A	1441	NAG	O5-C1-C2	-2.78	106.98	111.29
6	C	1521	NAG	C4-C3-C2	2.69	114.96	111.02
6	A	1441	NAG	C3-C4-C5	2.49	114.75	110.23
6	C	1511	NAG	C1-O5-C5	2.44	115.45	112.19
6	A	1491	NAG	C1-O5-C5	2.43	115.44	112.19
6	A	1441	NAG	C4-C3-C2	2.15	114.17	111.02

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	1441	NAG	C1
6	A	1451	NAG	C1
6	A	1471	NAG	C1
6	A	1481	NAG	C1
6	C	1511	NAG	C1
6	C	1521	NAG	C1

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1431	NAG	C8-C7-N2-C2
6	A	1431	NAG	O7-C7-N2-C2
6	A	1441	NAG	C8-C7-N2-C2
6	A	1441	NAG	O7-C7-N2-C2
6	A	1451	NAG	C8-C7-N2-C2
6	A	1451	NAG	O7-C7-N2-C2
6	A	1471	NAG	C8-C7-N2-C2
6	A	1471	NAG	O7-C7-N2-C2
6	A	1481	NAG	C8-C7-N2-C2
6	A	1481	NAG	O7-C7-N2-C2
6	A	1491	NAG	C3-C2-N2-C7
6	A	1491	NAG	C8-C7-N2-C2
6	A	1491	NAG	O7-C7-N2-C2
6	C	1501	NAG	C8-C7-N2-C2
6	C	1501	NAG	O7-C7-N2-C2
6	C	1511	NAG	C8-C7-N2-C2
6	C	1511	NAG	O7-C7-N2-C2
6	C	1521	NAG	C8-C7-N2-C2
6	C	1521	NAG	O7-C7-N2-C2
6	A	1481	NAG	C4-C5-C6-O6
6	A	1481	NAG	O5-C5-C6-O6
6	C	1521	NAG	C4-C5-C6-O6
6	C	1521	NAG	O5-C5-C6-O6
6	A	1491	NAG	O5-C5-C6-O6
6	A	1431	NAG	C4-C5-C6-O6
6	C	1501	NAG	O5-C5-C6-O6
6	A	1431	NAG	O5-C5-C6-O6
6	A	1451	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1501	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	599/599 (100%)	-0.52	2 (0%) 90 89	8, 28, 46, 66	0
2	C	135/135 (100%)	-0.35	1 (0%) 84 80	3, 30, 44, 69	2 (1%)
All	All	734/734 (100%)	-0.49	3 (0%) 88 87	3, 28, 45, 69	2 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	145	LYS	5.3
1	A	608	THR	3.1
1	A	624	THR	2.1

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.

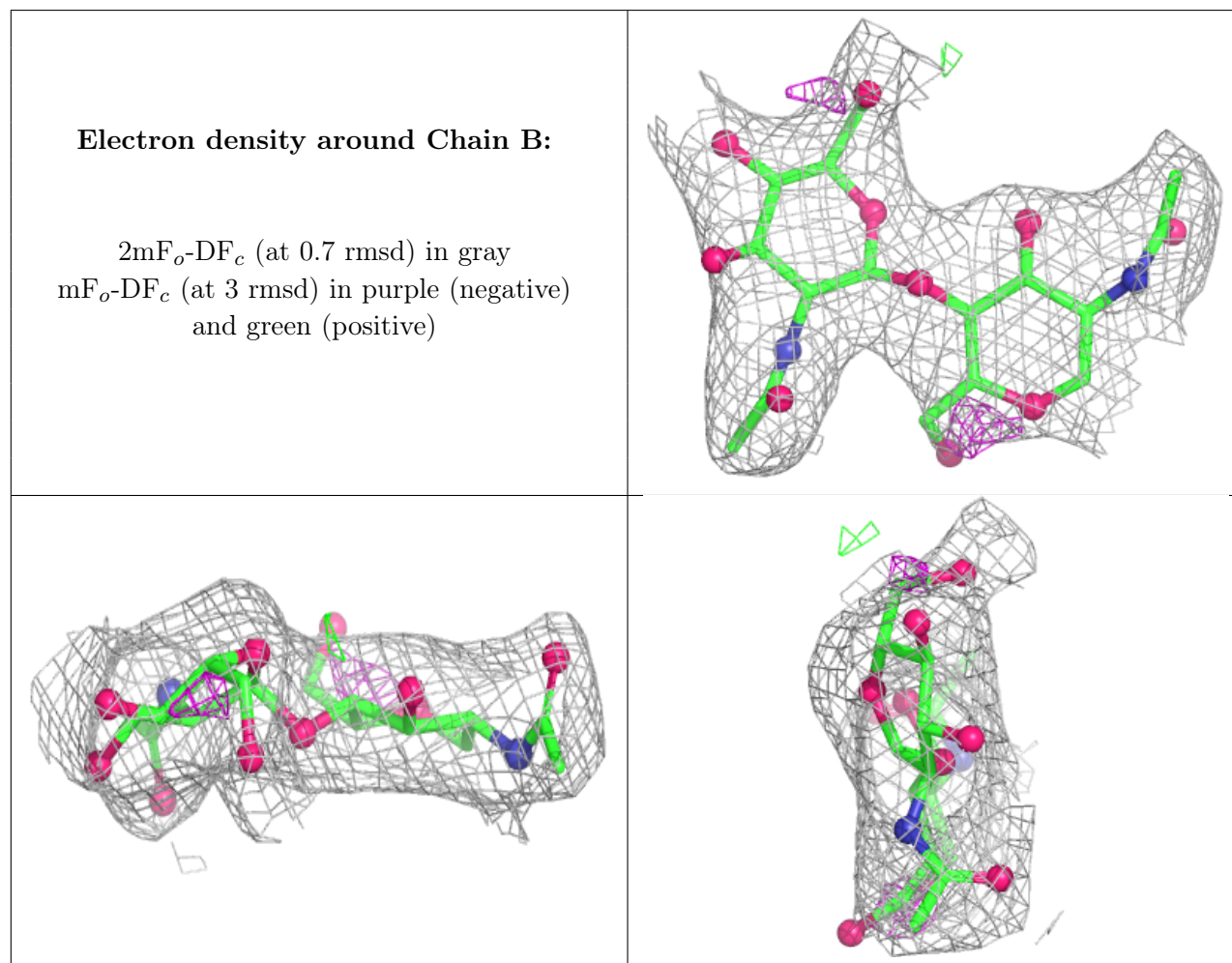
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	B	1	14/15	-	-	28,38,47,54	0
3	NAG	B	2	14/15	-	-	41,47,54,61	0
4	BMA	D	3	11/12	0.29	0.14	90,95,96,97	0
4	BMA	E	3	11/12	0.53	0.12	94,97,101,102	0
5	BMA	F	3	11/12	0.53	0.12	87,92,94,95	0
5	NAG	F	2	14/15	0.62	0.12	74,78,80,87	0

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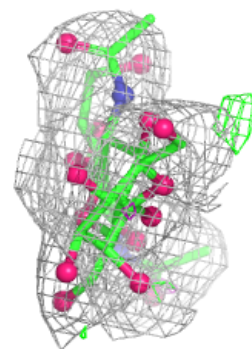
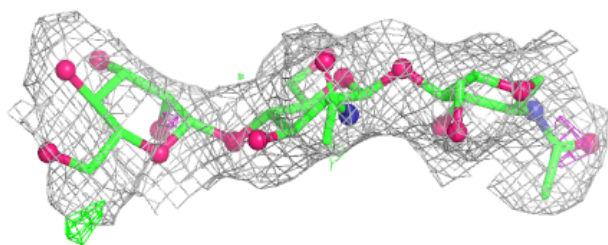
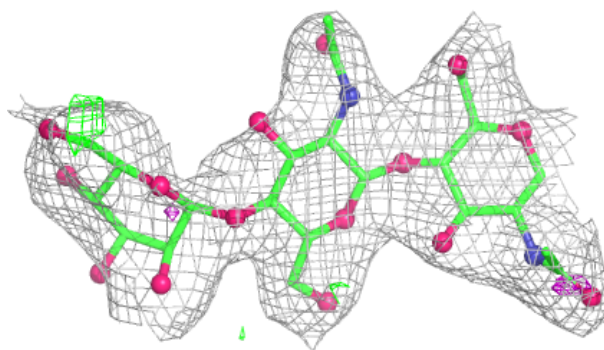
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	FUL	F	4	10/11	0.74	0.14	87,92,94,96	0
4	NAG	E	2	14/15	0.80	0.11	72,82,86,93	0
5	NAG	F	1	14/15	0.81	0.10	67,72,77,82	0
4	NAG	E	1	14/15	0.86	0.11	39,45,63,67	0
4	NAG	D	2	14/15	0.89	0.07	51,56,68,81	0
4	NAG	D	1	14/15	0.92	0.07	18,28,33,43	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.

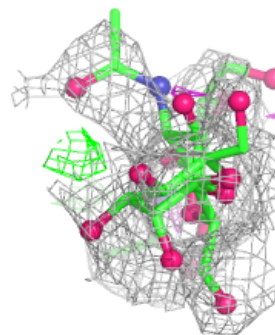
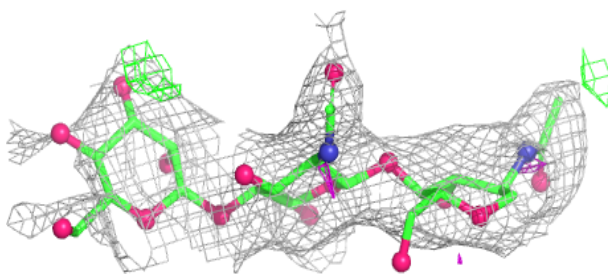
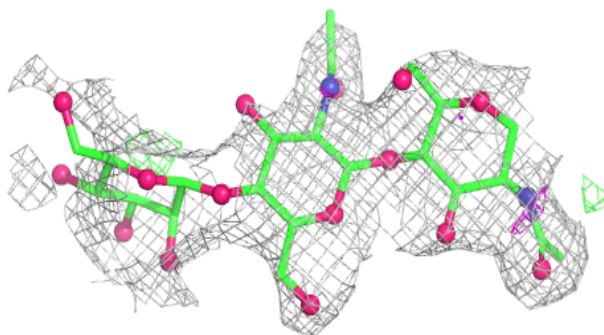


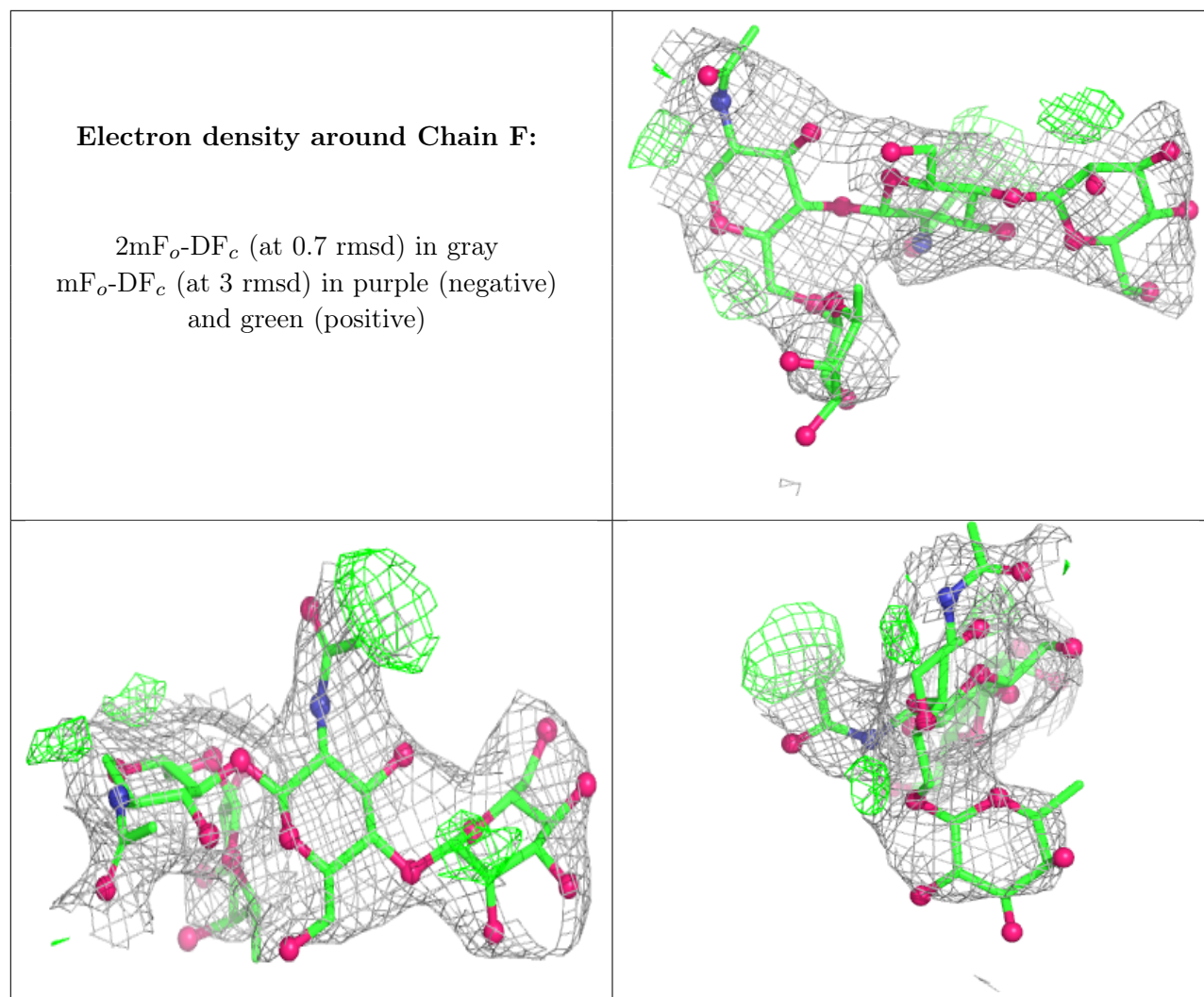
Electron density around Chain D:

$2mF_o-DF_c$ (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)





6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	A	1491	14/15	0.32	0.15	80,88,94,96	0
6	NAG	A	1431	14/15	0.43	0.13	82,91,94,95	0
6	NAG	A	1451	14/15	0.60	0.14	79,85,88,89	0
6	NAG	A	1441	14/15	0.64	0.12	48,59,65,66	0
6	NAG	A	1471	14/15	0.72	0.10	54,63,72,75	0
6	NAG	A	1481	14/15	0.79	0.11	57,65,69,70	0
6	NAG	C	1521	14/15	0.82	0.12	22,49,73,76	0
6	NAG	C	1501	14/15	0.85	0.08	65,71,85,86	0
6	NAG	C	1511	14/15	0.88	0.12	38,42,44,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.